X-RAY DIFFRACTION ANALYSIS OF ORGANOMETALLIC COMPOUNDS WITH CATALYTIC PROPERTIES

VOLUME I

Submitted to the University of Glasgow in partial fulfilment of the requirements for the degree of Doctor of Philosophy in the Faculty of Science

by

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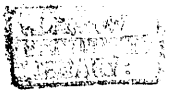

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SECTION III: MISCELLANEOUS STRUCTURES

PREFACE

The study, by use of X-ray diffraction analysis, of the structures of organometallic complexes with catalytic properties has proved to be of great importance in understanding the chemistry of catalytic processes. It is this technique that has been vital in determining the structures of the complexes reported in this thesis.

The thesis is divided into three sections. Section 1 discusses the structural features of new dppm-stabilised triplatinum complexes derived from the parent cluster $[Pt_3(CO)(dppm)_3]^{2+}$ (dppm = $Ph_2PCH_2PPh_2$). The structural work was carried out to determine how closely Pt_3 clusters could model the behaviour of similar Pt_3 species which occur on platinum surfaces. The new complexes are derived by chemical modification of the $M_3(dppm)_3$ nucleus which is unusually stable to fragmentation into species containing one or two metal atoms. The structure analyses reported here have been of critical importance in the development of this new field of cluster chemistry.

Brief reviews on binuclear dppm complexes and on platinum cluster chemistry have been carried out and earlier work on $M_3(dppm)_3$ species is also reported. A brief analysis on the conformations of the dppm ligand has also been carried out.

The work reported in Section 2 relates to the addition of an alkyne to the complex $[CpM(SR)(hfb)_2]$, where M = Mo or W, Cp = η^5-C_5H_5, R = an alkyl or aryl group and hfb = $F_3CC{\equiv}CCF_3$. The products of this reaction can adopt at least twelve different structural forms. The form isolated

depends on several factors including the natures of the thiolato substituent R, of the metal atom and of the incoming ligand. This work is directed to enhancing our in understanding of transition metal catalysed oligomerisation and polymerisation reactions of alkynes.

The structures of other related products are also reported including those of the thermolysis reaction of a $[CpM(SR)(hfb)_2]$ complex and those of the addition of ligands other than alkynes to the starting complex.

Reported in Section 3 are three unrelated structure analyses. The sulphimide complex of palladium is of interest because of its similarity to *cis*-$[PtCl_2(NH_3)_2]$, a chemotherapeutic but toxic compound.

$[Ru(SC(NH_2)_2)_6][CF_3SO_3]_2$ is the first characterised thiourea complex of ruthenium(II). Its structure was determined because the mode of attachement of thiourea to the ruthenium was unclear.

A pilot study of electron deformation density analysis is also reported. Two data sets were collected for $C_4Cl_4O_2S$, one at 295K the other at 150K using profile analysis of the Bragg reflections. Although the data did not lead to a satisfactory deformation density the analysis gave a clearer picture of the experimental and computational requirements for such work.

A brief summary of the experimental techniques and equations used is given in Appendix 1.

Appendix 2, bound in a separate volume, contains the calculated and observed structure factors of all the non-published structures reported in this thesis.

SECTION I: STRUCTURAL STUDIES OF PLATINUM CLUSTERS CONTAINING DIPHOSPHINOMETHANE LIGANDS

CHAPTER 1: INTRODUCTION

Although phosphine ligands have been used to stabilise complexes of transition metals for many years it was only in the 1970s that the unusual properties of diphosphinomethanes, $R_2PCH_2PR_2$, began to be systematically exploited. During the last fifteen years $R_2PCH_2PR_2$-stabilised complexes of many transition metals have been synthesized and several hundred structural studies, almost exclusively on binuclear species, have been reported.

A new departure in this field was the synthesis in 1983 of the trinuclear dicationic cluster $[Pd_3(CO)(dppm)_3]^{2+}$, where dppm is $Ph_2PCH_2PPh_2$, the most commonly-used diphosphinomethane ligand, by Professor Puddephatt's group at the University of Western Ontario.[1] This synthesis and that of the platinum analogue has allowed Puddephatt's group to develop a new chemistry of tripalladium and triplatinum species. The nine structure analyses described below have been an integral part of this development. The strategic objectives of the structural work have been (i) characterisation of key new derivatives, (ii) provision of the experimental basis for the assessment of structure and bonding and (iii) clarification of the parallels between the behaviour of M_3 species (M = Pd, Pt) and those of the corresponding metal surfaces.

These topics are discussed and the new structures, together with the experimental details of their structure determinations, are described in Chapters 5-8. Before this, brief reviews, with the emphasis on structural features, are first given of binuclear complexes containing dppm and

related ligands (Chapter 2), of platinum cluster chemistry (Chapter 3) and of the earlier work on $M_3(dppm)_3$, M = Pd and Pt, species (Chapter 4).

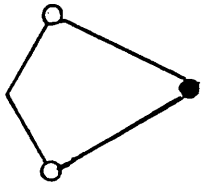
A number of papers on the new structures reported here have already been published.[2-6]

CHAPTER 2: DINUCLEAR BIS(DIPHENYLPHOSPHINO)METHANE COMPLEXES OF PALLADIUM AND PLATINUM

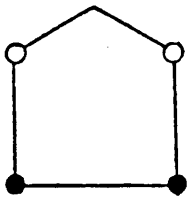
Tertiary phosphine ligands have been widely used to stabilise the lower oxidation states of transition metals.[7] These ligands can be easily synthesized with a variety of substituents on phosphorus and are thus capable of displaying a wide range of electronic and steric properties.[8] With diphosphines, $R_2P(CH_2)_nPR_2$, the length of the carbon chain connecting the phosphorus atoms is a further factor in determining ligand behaviour.

As noted above a substantial structural literature is now available on diphosphinomethane complexes, especially for dppm (R = Ph) but increasingly for other members of the family, notably for dmpm (R = Me), and four modes of ligation are known: (a) incorporation in a four-membered chelate ring, 2(i), as in *trans*-$[RhHCl(dppm)_2]^+$,[9] (b) bridging a metal-metal bond, 2(ii), as in $[Pt_2Cl_2(\mu\text{-}dppm)_2]$,[10] (c) bridging two metal atoms which are not directly bonded to one another, 2(iii), as in $[Rh(CO)_4(CN)_2(\mu\text{-}dppm)_2]$ [11] and (d) coordination through only one phosphorus atom, 2(iv), as in *trans*-$[Pd(Bu^tNC)_2(dppm)_2]^{2+}$ [12] (see Figure 2(a)). Similar ligation modes are of course available to diphosphines with two or more methylene groups between the phosphorus atoms but such ligands tend to prefer the chelate arrangement 2(i) to the bridging structures 2(ii) and 2(iii) for steric reasons whereas the reverse is true of diphosphinomethanes.

In consequence, dppm and its relatives show a strong tendency to stabilise dinuclear complexes, as may be seen



2(i)



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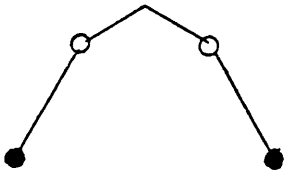

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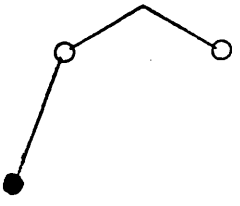
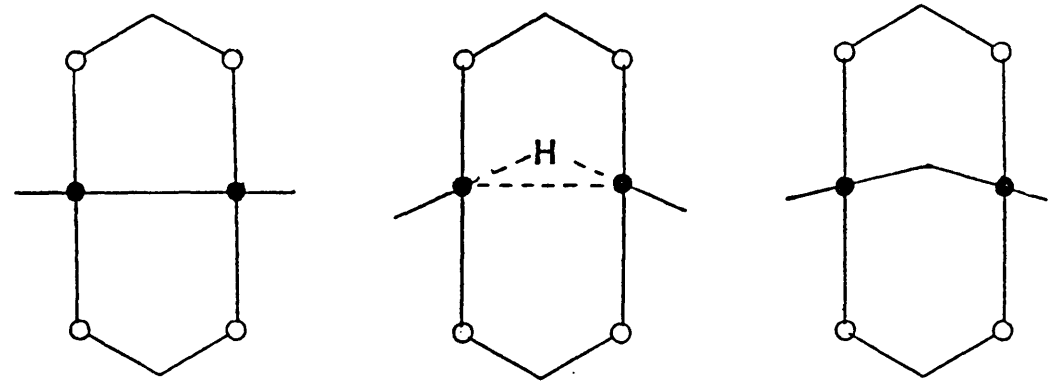


2(iv)

Figure 2(a). Modes of bonding of diphosphinomethane to a metal atom. M = ● P = O .

from a recent review by Puddephatt.[13] Such complexes are particularly diverse for platinum and palladium and so far nine distinct structural arrangements of the nucleus M_2L_n, M = Pt or Pd, L = dppm or dmpm and n = 2 or 3 have been described (see 2(v)-2(xiii) in Figure 2(b)).

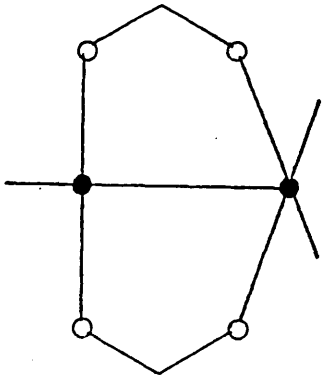
In 2(v) two metals with square-planar coordination are directly bonded to one another and are also linked by a pair of bridging diphosphine ligands, an arrangement typified by $[Pt_2Cl_2(dppm)_2]$.[10] The cation $[Pt_2Me_2(\mu\text{-}H)(\mu\text{-}dppm)_2]^+$,[14] type 2(vi), formally arises from protonation and consequent weakening of the Pt-Pt bond of 2(v). In 2(vii) μ-H is replaced by a larger bridging group such as CH_2^{2+}, μ-methylene, and the M-M distance is now much longer and clearly non-bonding, e.g. in $[Pt_2I_2(CH_2)(dppm)_2]$ [15] the



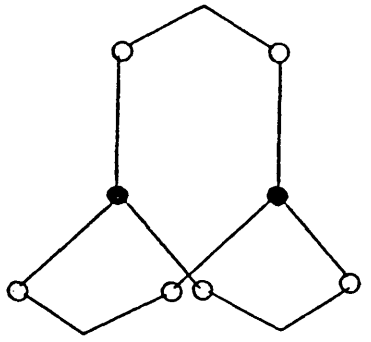
2(v)

2(vi)

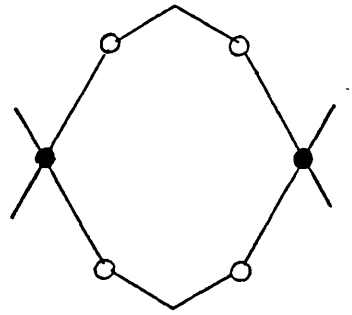
2(vii)



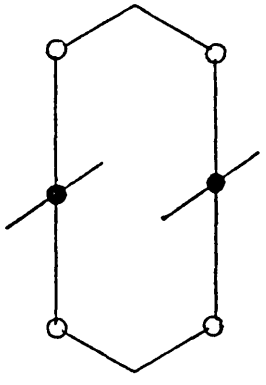
2(viii)



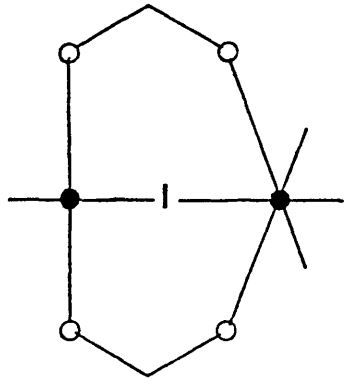
2(ix)



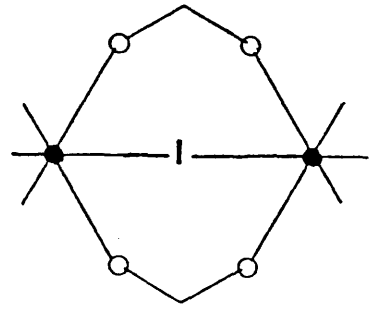
2(x)



2(xi)



2(xii)



2(xiii)

Figure 2(b). Structural arrangements of the nucleus M_2L_n, M = Pt or Pd, L = dppm or dmpm and n = 2 or 3.

Pt...Pt distance is 3.35 Å, compared with 2.77 Å and 2.65 Å for species of types 2(vi) and 2(v) respectively. Typical Pt-Pt bonding distances are in the range 2.6-2.8 Å.[16] Both terminal ligands lie on the opposite side of the Pt_2P_4 plane from the bridging group in 2(vi) and 2(vii) which have therefore come to be known as A-frame complexes.

Bridging dppm ligands can also stabilise donor-acceptor metal-metal bonds: in $[Pt_2Me_3(\mu\text{-dppm})_2]^+$ [17] which has skeleton 2(viii) the electron-rich $PtMe_2$ centre donates an electron-pair to the PtMe centre. 2(ix) is the only type of binuclear complex with three μ-dppm ligands and is exemplified by $[Pd_2(\mu\text{-dppm})_3]$.[18] Such compounds have a rich chemistry with addition possible at one or both metal centres.[13]

Binuclear complexes, $[X_2M(\mu\text{-dppm})_2MX_2]$, in which a pair of μ-dppm ligands is the link between the metal atoms can have *cis* 2(x) or *trans* 2(xi) coordination at the metal atoms: $[Pt_2Me_4(\mu\text{-dppm})_2]$ has the *cis* stereochemistry [19] whereas in $[Pt_2(C{\equiv}CR)_4(\mu\text{-dppm})_2]$ [20] there is a *trans* coordination of the metal atoms.

Reaction of *cis*-$[Pt_2(dmpm)_2Me_4]$ [21] with diiodine forms the mixed-valence Pt(II)-Pt(IV) complex $[Pt_2I(dmpm)_2Me_4]^+$ of type 2(xii) [22] while reaction with methyl iodide gives $[Pt_2IMe_6(dmpm)_2]^+$,[23] a Pt(IV)-Pt(IV) complex of type 2(xiii). Steric factors preclude similar reactions with the analogous dppm complexes.

Much of the interest in the $M_2(dppm)_2$ system arises from its stability both with and without direct M-M bonding since reactions involving M-M bond formation and scission

can occur without fragmentation into mononuclear fragments. Poilblanc [24] has emphasized that such reactions are relevant to homogeneous catalysis by bimetallic systems and may also serve as simple models for catalysis at metal surfaces. The ability of the system to accommodate bridging groups is also significant. Indeed $[Pd_2Cl_2(\mu\text{-dppm})_2]$ catalyses the cyclotrimerisation of alkynes [25] while $[Pt_2H_2(\mu\text{-H})(\mu\text{-dppm})_2]^+$ is a short-lived catalyst for the reduction of CO to CH_4.[13]

CHAPTER 3: THE STRUCTURES OF PLATINUM CLUSTER COMPLEXES STABILISED BY $Ph_2PCH_2PPh_2$

3.1 Introduction

As we have seen, although dinuclear transition metal complexes stabilised by dppm have been extensively studied, very little was known about corresponding trinuclear $M_3(dppm)_3$ species prior to 1983.[1] Since then the chemistry and structural characterisation of such complexes, particularly with M = Pd or Pt, has become an active area of research. Partly, this has been prompted by the consideration that the behaviour of these trinuclear complexes offers a model for that of metal surfaces. Additionally, there has been a continuing theoretical debate about the nature of the bonding in palladium and platinum cluster compounds. The structural results described below provide insights into both of these topics.

3.2 Some Comments on the Chemistry of Metal Surfaces

The chemisorption of small molecules, such as alkenes, alkynes and H_2S, on metal surfaces has been widely investigated because of its relevance to the catalytic properties of such surfaces. Techniques used to characterize the surface species include temperature-programmed desorption (TDS), low energy electron diffraction (LEED), and Auger electron spectroscopy (AES).[26-28]

The results for Pt(111) surfaces are particularly relevant to the structural studies discussed below. Many species are thought to bind in a μ_3-fashion to the Pt_3 triangular units present on such surfaces. Acetylene, for example, is adsorbed to give $Pt_3(\mu_3\text{-}\eta^2\text{-HCCH})$ species at low temperatures. On heating $Pt_3(\mu_3\text{-}\eta^2\text{-C=CH}_2)$ units are found and these appear to react with surface-bound hydrogen so that $Pt_3(\mu_3\text{-CCH}_3)$ units are ultimately observed.[26] Likewise, hydrogen sulphide is adsorbed on the Pt(111) surface to form a layer of sulphur with emission of hydrogen gas.[27,28] LEED analysis suggests that the surface layer consists of $Pt_3(\mu_3\text{-S})$ species.[28] The involvement of Pt_3 triangular units in the attachment of small molecules on the Pt(111) surface makes the study of triangulo-Pt_3 clusters of particular interest. An ability to mimic reactions happening on these surfaces could lead to a better understanding of the catalytic processes which occur.

3.3 Current Views on Bonding in Platinum Clusters

For most transition metal cluster complexes it has long been known that the geometry of the cluster is related to the number of skeletal electron pairs required to fill all the bonding metal-metal molecular orbitals.[30] This has become known as the polyhedral skeletal electron pair theory.[31] This theory succesfully explained the geometry of many metal clusters, particularly those containing conical $M(CO)_3$ and $M(\eta^5\text{-}C_5H_5)$ fragments, because of their isolobal relationship[32] to main group fragments such as BH and

CH_2.[33] In its initial form the theory was not usually applicable to platinum and palladium clusters, and this has triggered a theoretical discussion which still continues.

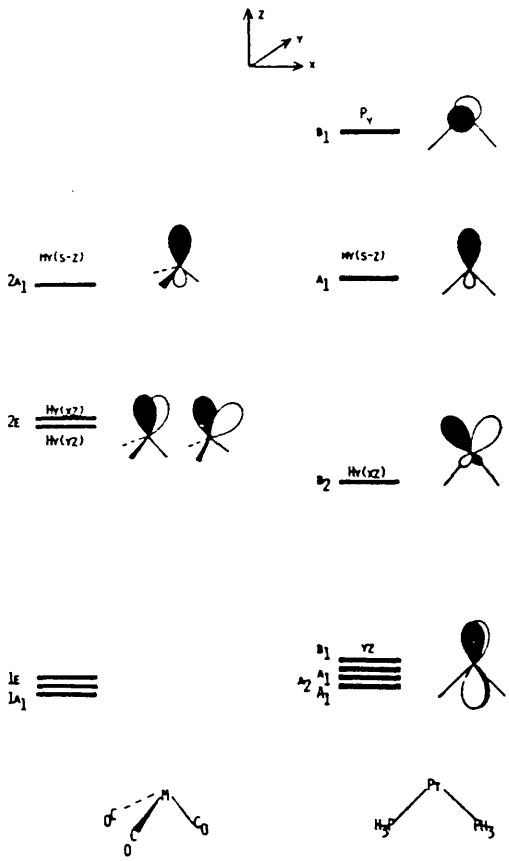


Figure 3(a). A comparison of the frontier molecular orbitals of $Pt(PH_3)_2$ and $M(CO)_3$.[34]

In 1982 Evans and Mingos[34] extended the polyhedral skeletal electron pair theory to cover the non-conical ML_2 fragments which are found in many platinum and palladium clusters. They compared the frontier molecular orbitals of $M(CO)_3$ and $Pt(PH_3)_2$ fragments (see Figure 3(a)),[34] and concluded that the Hy(s-z), Hy(xz) and p_y orbitals of the $Pt(PH_3)_2$ fragment had the potential to form radial and tangential molecular orbitals equivalent to those formed by

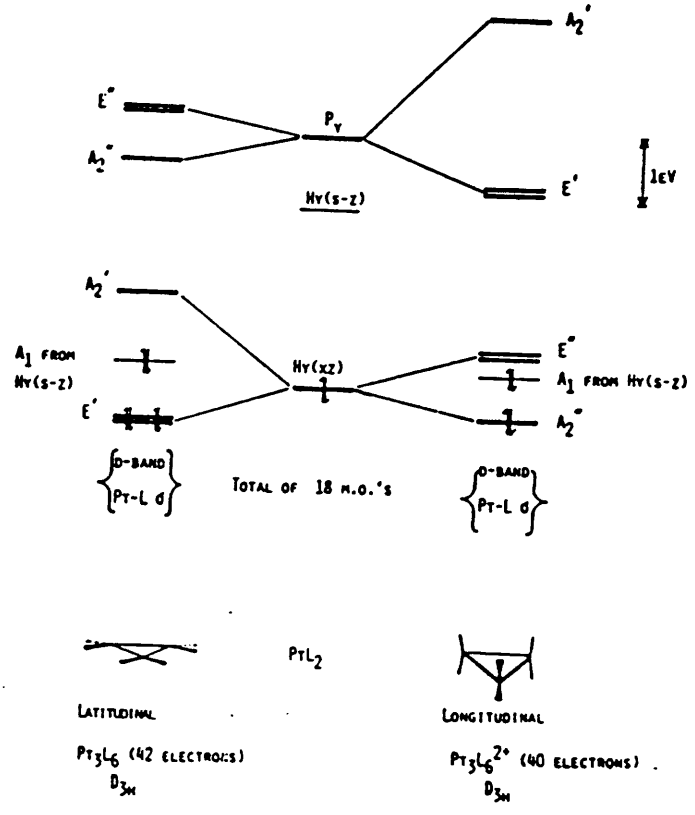


Figure 3(b). A comparison of the bonding molecular orbital diagrams for latitudinal and longitudinal geometries of $P_3(PH_3)_6$.[34]

$M(CO)_3$ fragments in a similar polyhedral cluster. However, those bonding molecular orbitals derived from p_y orbitals were not sufficiently stable for electron occupation. this meant the bonding would be dominated by the molecular orbitals formed from the Hy(s-z) and Hy(xz) orbitals which depend heavily on the conformation of the PtL_2 fragments relative to the principle axis of the polyhedron. Figure 3(b)[34] shows that for a triangular $Pt_3(PH_3)_6$ species the latitudinal geometry needs 42 valence electrons and the

longitudinal geometry 40 valence electrons to fill the bonding molecular orbitals. Evans and Mingos showed that the more stable geometry is that with more filled bonding molecular orbitals derived from Hy(xz), hence $Pt_3(PH_3)_6$ is expected to adopt a latitudinal geometry.

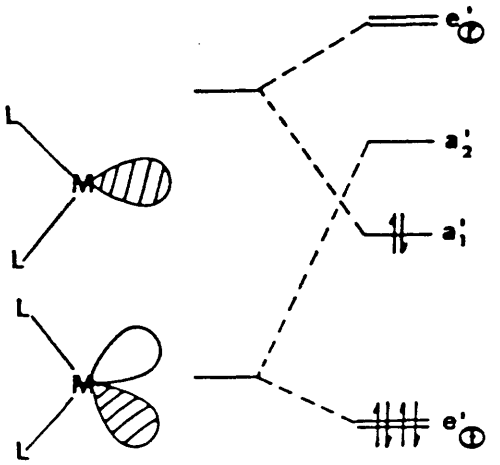


Figure 3(c). The molecular orbital diagram for a ML_2 fragment.[35]

Mealli[35] used qualitative pertubation theory arguments to study the M_3L_6 species by comparing it to the isolobally equivalent cyclopropane.[32] Each metal atom of the Pt_3 triangle contributes one σ and one π orbital, to produce two tangential and one radial bonding, and one tangential and two radial antibonding molecular orbital combinations. The resulting molecular orbital diagram (see Figure 3(c))[35] is similar to that found by Evans and Mingos.[34] The cluster is stable when the a_1' orbital is of lower energy than a_2'. For the L_6Pt_3 model with all ligands terminal (see Figure 3(d))[35] this ordering does not occur, unless there are additional ligands present to stabilize the cluster. This is because the σ orbitals from each L_2Pt

fragment are destabilized and hence the radial bonding orbital, a_1', is higher in energy than the tangential antibonding combination, a_2', of the π orbitals.

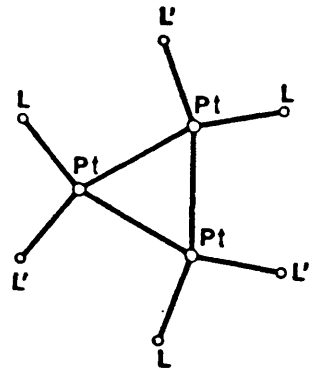


Figure 3(d). Latitudinal Pt_3L_6 with all ligands terminal.

When the $[Pt_3L_6]$ cluster is μ_3-capped by CO^{2+} Mealli showed that the bonding molecular orbitals are stabilized by added sp-orbital character. This reduces direct metal-metal overlap slightly, but there is a much larger gain in stability due to metal-carbon bonding. A similar effect is noted due to the bridging hydrogen ligands in $[Pt_3(CO)_6(\mu\text{-}H)_3]$.[35]

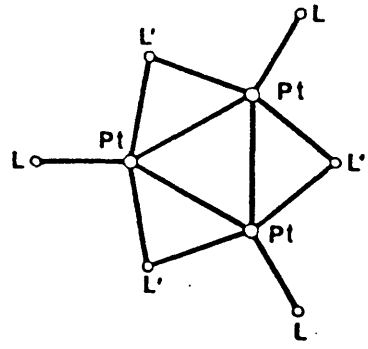


Figure 3(e). Latitudinal Pt_3L_6 with three bridging ligands.

Mealli also showed that an alternative geometry for the 42-electron Pt_3L_6 cluster, with three of the six ligands

acting as bridges between metals (see Figure 3(e))[35] is stable, without requiring the presence of additional ligands. This geometry has been observed experimentally in $[Pt_3(\mu\text{-}CO)_3(CO)_3]_n^{2-}$ for example.[36]

3.4 Structural Types of M_3 Clusters (M = Pd, Pt)

In 1985 Mingos and Wardle published a comprehensive review of platinum cluster chemistry.[29] This, together with a survey using the Cambridge Structural Database to identify structurally characterised triangulo-M_3 (M = Pd, Pt) clusters reveals that the great majority of tripalladium and triplatinum complexes are 42-electron, planar species of the $[M_3L_3(\mu\text{-}L')_3]$ bridged type discussed by Mealli. In general, either the terminal L ligands or the bridging L' ligands, or in some cases both, are fairly bulky. Pt-Pt distances lie in the range 2.618-2.816 Å.[37,38] The longer bonds tend to be associated with bulkier μ-P and μ-S bridging ligands, e.g. as in $[Pt_3(PPh_3)_3(\mu\text{-}SO_2)(\mu\text{-}Ph)(\mu\text{-}PPh_2)]$.[38]

Sometimes an additional ligand has added to the basic $[M_3L_3(\mu\text{-}L')_3]$ skeleton to give a 44-electron cluster. Examples include $AuPR_3^+$, R=C_6H_{11},[39] and Tl^+,[40] acting as μ_3-capping groups to the M_3 triangle. Alternatively, an extra terminal ligand, e.g. $P(C_6H_{11})_3$ in $[Pt_3(P(C_6H_{11})_3)_4(\mu\text{-}CO)_3]$,[41] is found attached to a single metal atom. A few examples are also known of 46-electron species with two additional ligands, e.g. the bis-capped $[Pt_3(Au(P(p\text{-}C_6H_4F)_3))(\mu\text{-}Cl)(\mu\text{-}SO_2)_2(P(C_6H_{11})_3)_3]^+$ [42] or $[Pt_3(Au(PPh_3)\text{-}(PPh_3)_4(\mu\text{-}CO)_3]^+$ [43] which contains additional μ_3-capping

and terminal ligands. The addition of extra ligands to the basic 42-electron $M_3L_3(\mu\text{-}L')_3$ species results in electrons occupying non-bonding and anti-bonding orbitals. This generally is associated with a lengthening of Pt-Pt bonds e.g. compare $[Pt_3(P(C_6H_{11})_3(\mu\text{-}CO)_3]$ [44] (42e) with $[Pt_3(\mu_3\text{-}Au(P(C_6H_{11})_3))(P(C_6H_{11})_3)_3(\mu\text{-}CO)_3]$ [39] (44e) and $[Pt_3\text{-}(P(C_6H_{11})_3)_4(\mu\text{-}CO)_3]$ [41] (44e) where average Pt-Pt bond lengths are 2.654, 2.696 and 2.708 Å respectively.

In some cases complete Pt-Pt bond rupture has occurred, e.g. in the two isomers of the 44-electron species $[Pt_3(PPh_3)_2(Ph)(\mu\text{-}PPh_2)_3]$.[45]

Other structures not falling into the above categories include the 42-electron $M_3L_6(\mu\text{-}L')_3$ species $[Pt_3H_3(PBu^t_3)_3(\mu\text{-}H)_3]$,[46] and the 44-electron $[Pt_3(cod)_3(\mu_3\text{-}SnCl_3)_2]$,[47] (cod = cyclo-octadiene).

Attempts to develop the chemistry of clusters based on the $M_3L_3(\mu\text{-}L')_3$ skeleton have been greatly hampered by their tendency to fragment into mononuclear species. The $M_3(dppm)_3$ species discussed in subsequent chapters do not have this disadvantage.

CHAPTER 4: SALTS OF THE 42-ELECTRON DICATIONIC CLUSTER $[M_3(CO)(DPPM)_3]^{2+}$, M = Pd, Pt

The exploration of this new area of platinum metal cluster chemistry began in 1983 with the synthesis from palladium acetate, the diphosphine ligand and carbon monoxide of $[Pd_3(CO)(dppm)_3][CF_3CO_2]_2.3Me_2CO$ (1) and its subsequent X-ray characterisation.[1] Since 1983 X-ray analyses have been completed on $[M_3(CO)(dppm)_3]^{2+}$, M = Pd, chloride (2) and iodide (3) salts [48,49] and M = Pt, PF_6^- (4) and thiocyanate (5) salts.[50,51]

All these complexes contain an equilateral triangle of metal atoms with each M-M bond bridged by a dppm ligand so that the M_3P_6 core is roughly planar, corresponding to the latitudinal geometry for such species, as defined by Mingos.[34] The single carbonyl ligand triply bridges one face of the M_3 triangle.

Mingos pointed out that for a 42-electron M_3P_6 cluster the expected geometry is latitudinal, since such a skeleton permits filling of all the bonding cluster orbitals. This view seems to imply that the dicationic cluster is chemically saturated. However, salts of the dication behave as 1:1 rather than 1:2 electrolytes and softer anions displace harder ones, with the anion affinity order $SCN^- \simeq I^- > Br^- > Cl^- > CF_3CO_2^- >> PF_6^-$. Furthermore, X-ray studies of (1)-(5) reveal that the anion is attached to the cluster in every case, except that of the PF_6^- salt (4), suggesting an electron count of 44 rather than 42.

Pertinent structural details in (1)-(5) are summarised in Table 4.1. In (4), where the PF_6^- anions do not interact

with the M_3 triangle, the Pt-CO distances are experimentally equal [2.08(1)-2.10(1) Å]. In (5) the SCN^- anion lies above the face of the M_3 triangle opposite to CO and is attached weakly to one platinum atom only [Pt-S 2.656(4) Å]. The Pt-CO bond lengths [2.04(1), 2.17(1) and 2.18(1) Å] indicate that the triply bridging CO is more strongly bound to the SCN^--substituted metal atom. In contrast, in the Pd/I^- complex (3), although the Pd-I distances show some variation [2.951(1)-3.083(1) Å], the iodo ligand is triply-bridging, as is the carbonyl ligand [Pd-C 2.14(1)-2.19(1) Å]. The Pd/Cl^- complex (2) appears to have a similar bis-μ_3-Cl/CO structure but Cl/CO disorder obscures the details. In (1) both oxygen atoms of a $CF_3CO_2^-$ anion are involved in weak Pd-O interactions [Pd-O 2.77(2)-3.24(2) Å] and the Pd-CO distances are irregular [2.08(1)-2.18(1) Å].

Individual M-M bond lengths (Table 4.1) do not appear to reflect the differences in anion coordination: for example, contrast the regularity of the Pt-Pt distances in the unsymmetrical SCN^- complex (5) with their variation in the PF_6^- complex (4). The only trend apparent in the mean M-M distances can be ascribed to the difference in the Pauling single bond metallic radii for Pd and Pt, respectively 1.283 and 1.295 Å.[52] Likewise, the slightly greater mean M-P distances in the palladium complexes is expected and can be ascribed, according to Ibers,[53] to the greater hard acid character of palladium relative to platinum.

These results leave unanswered several important questions. Is the interaction of the anion with the

dication mainly ionic, i.e. a kind of ion pairing, or is there a significant covalent component? If the latter, how are the extra electrons accommodated without occupation of anti-bonding molecular orbitals and disruption of the cluster skeleton? How significant is the difference between the μ_3-iodo and mono-hapto SCN^- interactions (and its effect on the μ-CO bonding)? These problems were the starting point for structural studies described in the following sections of this thesis.

Of chemical interest were the questions: how well do reactions involving the Pt_3 clusters mimic those on platinum surfaces and how are the differences, if any, explained?

Table 4.1. Comparison of geometries of $[M_3X(CO)(dppm)_3]^{n+}$ structures with different anions X^-. Distances are in Å, angles in degrees.

M	Pt [30]	Pt [31]	Pd [1]	*Pd [48]	Pd [49]
X	-	SCN^-	$CF_3CO_2^-$	Cl^-	I^-
n	2	1	1	1	1
	42	44	44	44	44
Pt(1)-Pt(2)	2.638(1)	2.620(1)	2.576(1)	2.604(1)	2.599(1)
Pt(1)-Pt(3)	2.650(1)	2.625(1)	2.607(2)	2.583(1)	2.599(1)
Pt(2)-Pt(3)	2.613(1)	2.623(1)	2.610(2)	2.586(1)	2.591(1)
Pt(1)-P(1)	2.284(2)	2.313(4)	2.304(4)	2.300(2)	2.320(2)
Pt(1)-P(6)	2.304(2)	2.306(4)	2.303(3)	2.321(2)	2.316(2)
Pt(2)-P(2)	2.277(2)	2.294(4)	2.296(3)	2.314(2)	2.317(2)
Pt(2)-P(3)	2.271(2)	2.271(4)	2.324(3)	2.309(2)	2.309(2)
Pt(3)-P(4)	2.294(2)	2.280(4)	2.336(3)	2.303(2)	2.301(2)
Pt(3)-P(5)	2.262(2)	2.280(4)	2.340(3)	2.310(2)	2.325(2)
mean Pt-Pt	2.634(19)	2.623(3)	2.598(19)	2.591(11)	2.596(5)
mean Pt-P	2.282(15)	2.291(16)	2.317(19)	2.310(8)	2.315(9)
Pt(1)-C	2.095(9)	2.042(13)	2.175(11)	2.14 2.14	2.137(8)
Pt(2)-C	2.089(8)	2.165(13)	2.141(12)	2.25 2.21	2.192(8)
Pt(3)-C	2.080(9)	2.175(13)	2.080(10)	2.17 2.14	2.160(8)
Pt(1)-C-O	131.8(6)	143.8(11)	130.3(9)	-	143.4(6)
Pt(2)-C-O	133.1(7)	129.8(10)	133.2(10)	-	131.9(6)
Pt(3)-C-O	134.9(7)	128.9(10)	141.6(12)	-	132.3(6)
C=O	1.154(9)	1.165(14)	1.105(14)	-	1.114(9)
Pt(1)-X	-	2.656(4)	- 2.83(2)	2.74 2.94	2.951(1)
Pt(2)-X	-	3.380(4)	2.77(2) -	3.17 2.76	3.083(1)
Pt(3)-X	-	3.243(4)	2.92(2) 3.24(2)	2.79 2.83	3.031(1)
CH_2 to CO[b]	uud	ddu	ddu	(ddu)	ddu
mean P-CH_2	1.840(11)	1.842(18)	1.833(12)	1.839(4)	1.836(8)
mean P-C(Ph)	1.806(8)	1.820(6)	1.821(13)	1.829(9)	1.819(6)
MMP	91.0(1)- 97.3(1)	93.6(1)- 95.8(1)	92.9(1)- 97.7(1)	93.7- 95.8	93.5(1)- 96.3(1)
MPC	107.6(3)-111.6(3)	106.4(5)-110.9(5)	107.9(4)-111.6(4)	108.2-110.8	107.7(3)-110.1(3)
PCP	109.0(4)-112.8(4)	111.0(7)-112.0(7)	108.7(6)-113.2(6)	109.5-111.9	110.1(4)-111.7(4)
MPCP		52.2(6) -41.9(5)	-45.2(5) 49.7(5)	-48.2 45.5	-46.9(3) 47.1(3)
		-44.7(6) 46.2(6)	42.9(5) -47.9(5)	-52.1 42.1	50.3(4) -48.7(4)
		39.8(6) -51.8(6)	41.8(5) -48.4(5)	45.7 -48.7	-39.3(3) 49.5(4)
mean Pt-C	2.088(7)	2.127(74)	2.132(48)	2.18	2.163(28)

*Cl and CO are disordered.
[b]See Chapter 8.

CHAPTER 5: $[Pt_3(\mu_3\text{-}CO)(\mu\text{-}DPPM)_3L]^{2+}$ COMPLEXES

The 44-electron cations $[Pt_3(\mu_3\text{-}CO)(\mu\text{-}dppm)_3L]^{2+}$, L = phosphine or phosphite, have recently been synthesised by Professor Puddephatt by ligand addition to the parent cation $[Pt_3(\mu_3\text{-}CO)(\mu\text{-}dppm)_3]^{2+}$,(1).[50] This reaction can be regarded as a model for non-dissociative chemisorption of such species as PH_3 and PF_3 on platinum surfaces.[54]

When L is a less sterically demanding ligand, e.g. phosphite or PMe_2Ph, the new complexes are thermally stable, whereas with more bulky phosphines, such as $PMePh_2$ or PPh_3, dissociation occurs in solution at room temperature. Detailed N.M.R. studies suggest that at low temperatures the additional L ligand is terminally bonded but, on heating, a novel fluxional process, involving rapid migration of L around the Pt_3 triangle, gives a time-averaged $\mu_3\text{-}PR_3$ spectrum.

Accordingly, the structure of a typical member of the group of new 44-electron complexes, namely that with $L = P(OPh)_3$, (2), has been determined in order to establish the nature of the attachment of the $P(OPh)_3$ ligand to the cluster and how this affects the cluster bonding (see Tables 5.1-5.3). Also described briefly here is the structure of a related species with $L = CNC_6H_{11}$, (3), although in this case severe disorder obscures important structural details (see Tables 5.1, 5.4 and 5.5). The structures of these 44-electron dicationic species afford an interesting comparison with that of the anionic adducts $[M(\mu_3\text{-}CO)(X)(\mu\text{-}dppm)_3]^+$, (4), ($X = CF_3CO_2^-$, Cl^-, SCN^-, I^-, and M = Pd or Pt), where the weak cluster-anion bonding

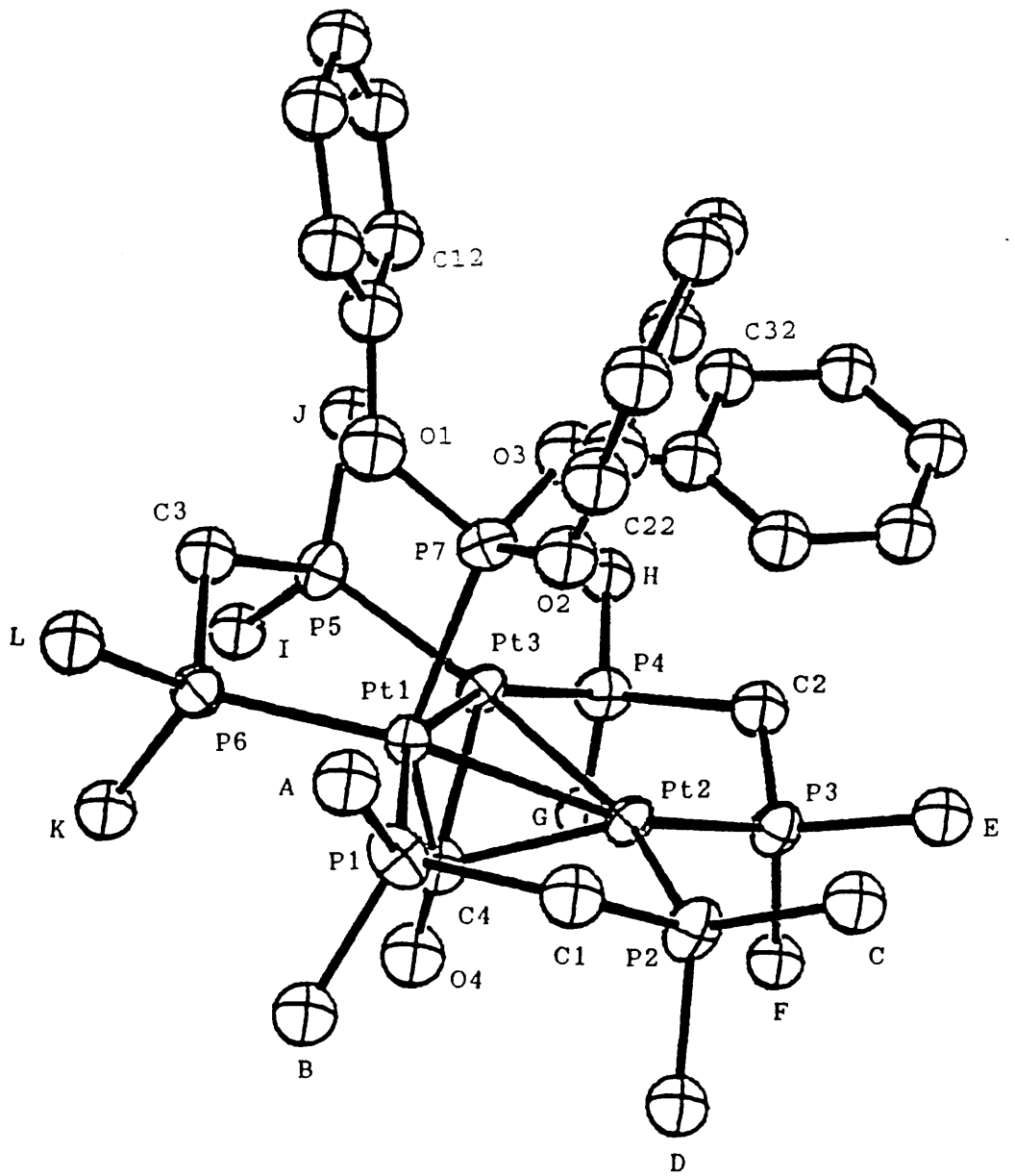
appears to be partially ionic (see Table 4.1).[1,48,49,51]

The structure of (2) is shown in Figure 5(a). X-ray diffraction analysis of a crystal of the PF_6^- salt of (2), showed it to consist of two PF_6^- anions for every one cation (2). Two regions of diffuse electron density were also present in the asymmetric unit. These were tentatively ascribed to disorderd solvent molecules (see Experimental). All non-bonded contacts between the various species present in the crystal were consistent with normal van der Waals radii.[52]

The incoming $P(OPh)_3$ ligand is attached only to Pt(1), with the Pt(1)-P(7) bond vector at an angle of 85.4° to the Pt_3 plane. The Pt(1)-P(7) bond length of 2.293(8) Å is in the range considered typical for platinum-phosphite complexes.[55,56] The phosphite conformation appears to be dictated by the need to reduce steric congestion with the $Pt_3(\mu\text{-dppm})_3$ nucleus. Thus, two of the phosphite phenyl groups point away from the cluster centre [Pt(1)-P(7)-C-O torsion angles respectively -163.2(23) and 166.1(24)° for C(11) and C(21)]. The third ring lies across the face of the Pt_3 triangle [Pt(1)-P(7)-O(3)-C(31)= -76.2(21)°] and the shortest interligand contact involving this ring is the C(35)...C(E2) distance of 3.28 Å. The conformation of the $Pt_3(\mu\text{-dppm})_3$ nucleus also shows evidence of steric congestion. The envelope-shaped Pt_2P_2C rings all have their methylene flaps lying on the same side of the Pt_3 triangle as the $P(OPh)_3$ ligand (see Figure 5(a)). This arrangement is the more favourable one for attachment of a bulky terminal ligand normal to the Pt_3 face (see Chapter 8).

The mean Pt-Pt bond length in (2) is comparable to that

Figure 5(a). A view of the $[Pt_3(\mu_3\text{-}CO)(P(OPh)_3)(dppm)_3]^{2+}$ cation. For clarity only the ipso carbons of phenyl rings A-L and no hydrogen atoms are displayed. Carbon atoms are shown as spheres of arbitrary size. Probability ellipsoids(50%) are shown for all other atoms.

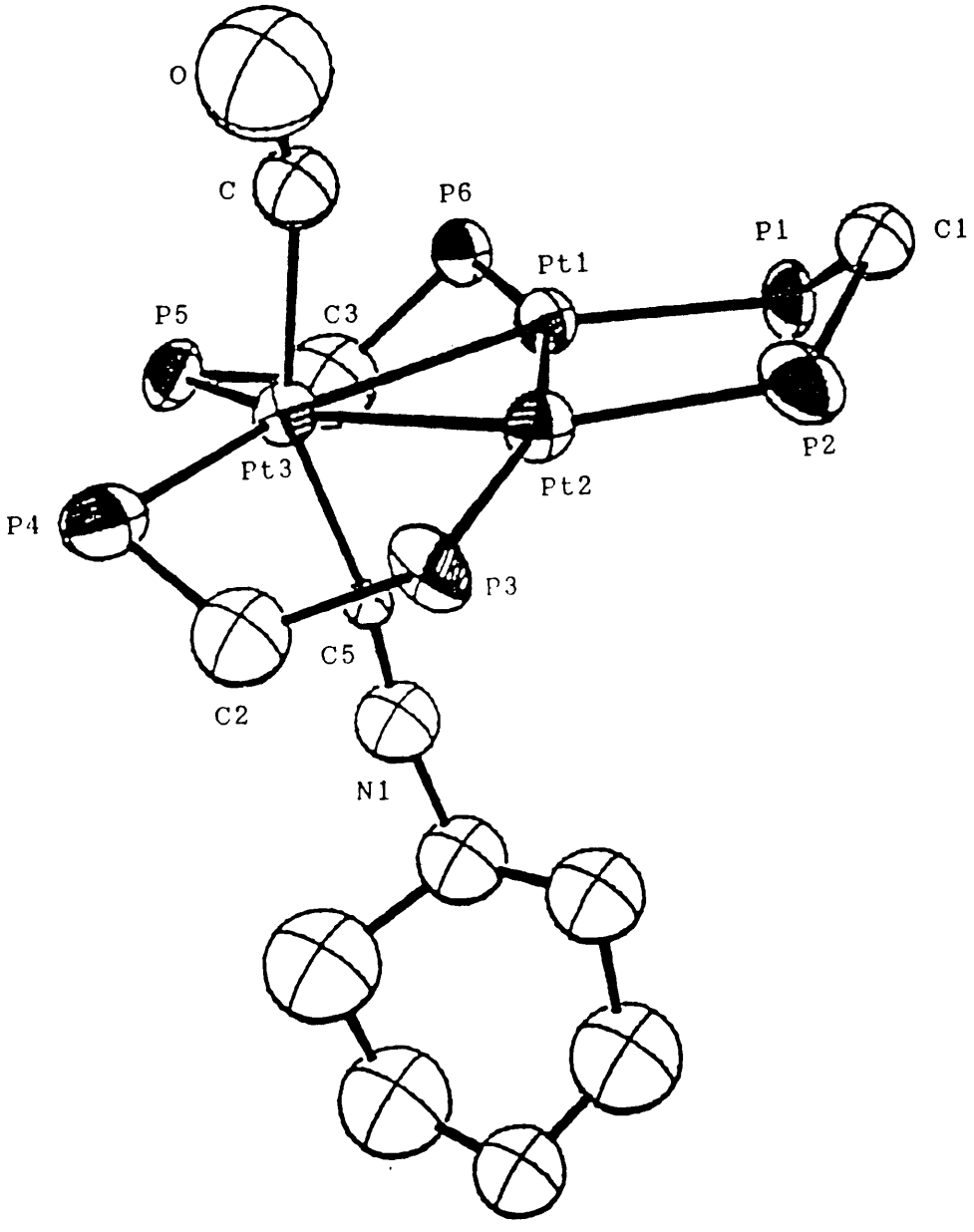


in (1) and in the 44-electron anion adducts of (1) and its palladium analogue (see Tables 4.1 and 5.1). The individual Pt-Pt distances show slight irregularities [2.626(2)-2.656(2) Å] but these do not seem to be attributable to the addition of an extra ligand to Pt(1). However, the greater coordination number of Pt(1) may explain the slight lengthening of the Pt(1)-P(dppm) distances [2.341(8) and 2.335(8) Å] compared with those involving Pt(2) and Pt(3) of 2.288(8)-2.323(8) Å.

The most dramatic effect of the addition of the $P(OPh)_3$ ligand to the $Pt_3(\mu_3\text{-}CO)(\mu\text{-}dppm)_3$ nucleus is shown by the carbonyl bonding. In (1) the CO carbon atom is equidistant from the three metal atoms (see Table 4.1), whereas in (2) the Pt(1)-CO bond length of 1.93(3) Å is 0.23(4) and 0.36(4) Å shorter than the corresponding distances involving Pt(2) and Pt(3) (see Table 5.1). Likewise, the Pt(1)-C-O angle of 155(2)° is some 30° closer to linearity than the corresponding Pt(2) and Pt(3) angles. A similar, but less marked, asymmetry in the $\mu_3\text{-}CO\text{-}Pt_3$ bonding is found in the thiocyanate adduct (see Table 4.1). The bonding implications of this result are considered below.

The finer details of the structure of the cluster $[Pt_3(CO)(CNC_6H_{11})(\mu\text{-}dppm)_3]^{2+}$ (3) are obscured by problems with disorder of occluded solvent and one PF_6^- anion but also by CO/CNC_6H_{11} disorder. The model used in the final refinement included the $Pt_3dppm_3(CNC_6H_{11})^{2+}$ fragment of the cation as well as one PF_6^- anion and the phosphorus atom of the other PF_6^- anion. In the final difference synthesis the two highest peaks had positions consistent with those of a terminal carbonyl group attached to the same platinum atom

Figure 5(b). A view of the proposed structure of complex (3). For clarity all phenyl rings have been removed.



as the isonitrile substituent (see Figure 5(b)). However, these positions are also consistent with those of the CN part of another isonitrile group and there were also peaks, though much less pronounced, consistent with five of the six carbon atoms of an attached cyclohexane ring. This is clearly due to CO/CNC_6H_{11} disorder with the model shown in Figure 5(b) likely to be the major isomer. However, no model could be found which refined satisfactorily.

Although the mean Pt-Pt distance is comparable with those for related 44-electron triangulo-$Pt_3(dppm)_3$ systems (Tables 4.1 and 5.1) the bond between the two metal atoms not attached to the C-donor ligands [2.584(4) Å] is 0.04-0.06 Å shorter than the remaining two. There appears to be less steric congestion in (3) than in (2): the conformation of the $Pt_3(\mu\text{-dppm})_3$ is such that only two dppm methylene carbon atoms lie on the nitrile side of the Pt_3 plane.

A recent paper by Evans provides an elegant rationalisation of these results in terms of extended Huckel (EHMO) theory.[57] This predicts that the addition of a second terminal CO to a $Pt_3(\mu_3\text{-CO})(\mu\text{-dppm})_3^{2+}$ cluster will be stabilised by the π-acidic properties of the μ-CO ligand (Figure 5(c)). The Mulliken population analysis predicts little change in Pt-Pt bond lengths but a strengthening of the $(\mu_3\text{-CO})$-Pt bonding to the metal atom bearing the terminal carbonyl at the expense of the other $(\mu_3\text{-CO})$-Pt bonds. From Tables 4.1 and 5.1 it is apparent that the parent 42-electron cation and the adducts with L = I^-, $CF_3CO_2^-$, SCN^-, $P(OPh)_3$ and CNC_6H_{11} show a gradual transition from symmetrical μ_3-CO towards a terminal CO with little change in Pt-Pt bond lengths.

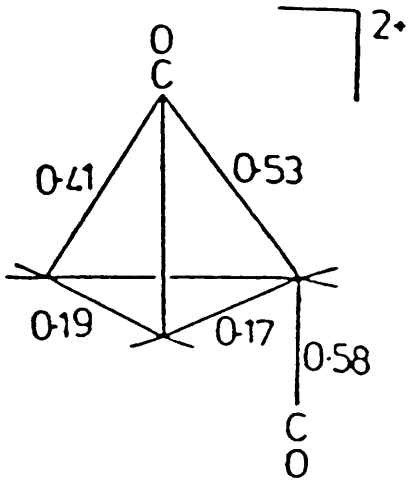


Figure 5(c). Mulliken population analysis of addition of terminal CO to the $Pt_3(\mu_3\text{-CO})(dppm)_3^{2+}$ cluster.[57]

Evans also compared the stability of the cluster with CO added terminally with that of a $Pt_3(\mu_3\text{-CO})_2(\mu\text{-dppm})_3^{2+}$ 44-electron cluster. The greater stability due to extra Pt-C bonding in the latter is more than offset by weaker metal-metal bonding but the difference in stability is not great. Infra-red and N.M.R. studies confirm that there is a rapid equilibrium between the two types of CO bonding in solution.[58] Although $Pt_3(\mu_3\text{-X})_2(\mu\text{-dppm})_3$ 44-electron clusters with μ_3-bridging ligands containing first or second row donor atoms have not been obtained so far the structure of $[Pt_3(\mu_3\text{-CO})(\mu_3\text{-SnF}_3)(\mu\text{-dppm})_3]^+$, for example, shows that such systems can be stabilised with bulkier bridging donor atoms (see Chapter 7).

Experimental

Broadly similar methods were used for all the analyses described in this Section. Full details of a typical

analysis are given below for complex (2) and details pertinent to each of the remaining analyses are given in their respective chapters. Table 5.6 summarises crystal data for complexes (2) and (3).

$[Pt_3(CO)(P(OPh)_3)(dppm)_3][PF_6]_2$ (2)

Data Collection. All measurements were made using Mo-Kα radiation on an Enraf Nonius CAD4F diffractometer equipped with a graphite monochromator. The crystal was a red plate, size 0.36x0.24x0.16 mm, mounted in a capillary. Cell dimensions were determined by a least-squares refinement of the setting angles of 23 automatically centred reflections with $8<\theta<12°$ (see Table 5.6). The intensities of 12262 reflections with $2\leq\theta\leq21°$ were measured by continuous $\omega/2\theta$ scans of 0.80° in ω, increased by 25% at each end to allow for background. The intensity standards, measured every two hours, showed no significant change. After correction for Lorentz, polarisation and absorption effects (empirical transmission factors on F 0.81-1.17),[59] and merging of eqivalent reflections, 9840 unique reflections were obtained; of these 3967 had $I\geq3\sigma(I)$ and were subsequently used.

Structure Analysis. The heavy atom positions were found from a Patterson synthesis and all other non-hydrogen atoms from subsequent difference syntheses. Two carbon atoms and one oxygen atom were introduced into the calculations to model two regions of diffuse electron density ascribed to disordered solvent. These atoms were included in the final refinement but are not allowed for in Table 5.6 because it

was not possible to establish the identity of the disordered solvent. Anisotropic displacement parameters were used for Pt and P atoms and isotropic displacement parameters were used for all the remaining atoms. A fixed contribution for the scattering of the hydrogen atoms was added to the structure factors assuming a C-H distance of 0.96 Å and a fixed isotropic U(H) = 0.05 $Å^2$. The phenyl rings were idealised, with C-C distances 1.380 Å and C-C-C angles 120°, and refined as groups. Similarly, P-F bond distances were fixed at 1.53 Å with F-P-F angles either 90 or 180° and each PF_6^- anion was refined as a group. Final parameters were obtained from full-matrix least-squares minimisation of $\Sigma w(|F_o|-|F_c|)^2$ with $w^{-1}=\sigma^2+0.00023F^2$ (where σ is derived from counting statistics), by adjustment of 351 parameters which convereged with R = 0.0475 and R_w = 0.0545.

All calculations were performed using the GX package,[60] on a GOULD-SEL 3227 computer. Neutral atom scattering factors and complex anomalous dispersion corrections were taken from ref. 61.

$[Pt_3(CO)(CNC_6H_{11})(dppm)_3][PF_6]_2$ (3).

Data Collection. Crystal mounted on a glass fibre.
Structure Analysis. The model used in the final refinement was $C_{82}F_6NP_8Pt_3$. Anisotropic displacement parameters were used for all Pt and P atoms with the exception of P(8). It and all other atoms used isotropic displacement parameters. Group refinement was used for all phenyl rings and for the $P(7)F_6^-$ anion with bond distances and angles idealised as

above.

Table 5.1. Comparison of geometries of $[M_3(X)(CO)(dppm)_3]^{n+}$ structures (distances in Å, angles in °) where X may be attached to one, two, or three M atoms.

M	Pt	Pt [a]	Pt [b]	Pt [c,3]	Pt	Pt	Pt
X	$P(OPh)_3$	CNC_6H_{11}	$CO/Cl/SnF_3^-$	dppa	S_2CNMe_2	$(SnF_3^-)_2$	$SnMe_3(PO_2F_2)^-$
n	2	2	1/0	2	1	0	1
	44	44	44	46	46	44	42
Pt(1)-Pt(2)	2.656(2)	2.584(4)	2.634(3)	2.628(1)	2.612(1)	2.639(1)	2.609(1)
Pt(1)-Pt(3)	2.626(2)	2.626(3)	-	2.648(1)	2.622(1)	2.609(2)	2.615(1)
Pt(2)-Pt(3)	2.636(2)	2.646(3)	-	2.620(1)	2.605(1)	2.622(1)	2.635(1)
Pt(1)-P(1)	2.341(8)	2.205(13)	2.268(15)	2.289(3)	2.298(3)	2.301(5)	2.272(4)
Pt(1)-P(6)	2.335(8)	2.251(15)	2.315(15)	2.342(3)	2.356(3)	2.303(5)	2.297(4)
Pt(2)-P(2)	2.323(8)	2.227(16)	-	2.246(3)	2.246(3)	2.304(6)	2.284(4)
Pt(2)-P(3)	2.290(8)	2.373(14)	-	2.256(3)	2.244(3)	2.313(5)	2.264(4)
Pt(3)-P(4)	2.288(8)	2.460(15)	-	2.291(3)	2.309(3)	2.278(5)	2.288(4)
Pt(3)-P(5)	2.300(8)	2.406(15)	-	2.319(3)	2.357(3)	2.308(5)	2.284(4)
mean Pt-Pt	2.639(15)	2.619(35)	2.634(3)	2.632(14)	2.613(9)	2.623(15)	2.620(14)
mean Pt-P	2.313(23)	2.32(14)	2.292(24)	2.291(31)	2.300(50)	2.301(12)	2.282(12)
Pt(1)-C	1.93(3)	-	2.142	2.049(8)	2.011(11)	-	-
Pt(2)-C	2.16(3)	-	-	-	2.671(11)	-	-
Pt(3)-C	2.27(3)	-	-	2.061(9)	2.023(11)	-	-
Pt(1)-C-O	154.6(21)	-	134.8	140.3(7)	137.1(8)	-	-
Pt(2)-C-O	121.1(19)	-	-	-	-	-	-
Pt(3)-C-O	119.9(20)	-	-	138.6(7)	140.9(8)	-	-
C-O	1.21(4)	-	1.129	1.194(10)	1.217(14)	-	-
Pt(1)-I	2.293(8)	1.88(5)	2.773(2)	2.355(3)	2.480(4)	2.746(2) 2.808(2)	2.766(2)
Pt(2)-I	-	-	-	-	3.58 3.54	2.801(2) 2.699(2)	2.739(2)
Pt(3)-I	-	-	-	2.372(3)	2.503(3)	2.783(2) 2.830(2)	2.702(2)
CH_2 to CO	ddd	ddu	ddd	ddd	udd	uud	uuu (to Sn)
mean P-CH_2	1.832(20)	1.84(16)	1.844(57)	1.830(4)	1.840(3)	1.836(30)	1.848(16)
mean P-C(Ph)	1.832(5)	1.82(6)	1.819(57)	1.805(5)	1.832(3)	1.832(24)	1.826(6)
MMP	93.2(2)- 98.2(2)	93.0(4)- 97.7(4)	95.8(4)	91.2(1)- 97.8(1)	89.3(1)- 98.0(1)	93.3(2)- 97.6(2)	89.5(1)- 97.6(1)
MPC	106.1(9)-112.2(9)	101.6(18)-110.8(16)	106.4(17)-106.5(15)	107.9(5)-111.7(3)	105.7(4)-110.5(4)	107.6(7)-110.9(6)	102.4(8)-112.7(5)
PCP	111.6(13)-121.5(14)	106.9(27)-124.8(34)	114.2(25)	97.4(10)-109.2(9)	109.1(6)-114.7(6)	112.9(10)-113.4(10)	107.5(8)-110.5(7)
MPCP	-34.7(11) 28.7(12)	51.9(19) -43.8(20)	49.5(22) -49.4(21)		34.4(5) -52.0(5)	39.6(8) -44.8(8)	-40.2(6) 48.1(6)
	-49.2(11) 50.6(11)	-38.0(30) 41.9(36)	- -		-37.6(4) 57.2(5)	46.6(8) -48.2(9)	-34.7(6) 52.3(7)
	-28.0(11) 46.2(12)	-51.1(24) 57.7(25)	- -		-47.1(5) 50.8(5)	-44.5(8) 46.0(8)	-39.1(6) 52.0(7)
mean Pt-C	2.12(17)	-	2.142	2.055(9)	2.017(11)	-	-

[a]Disordered - see page 25
[b]Disordered - see page 74

Table 5.2. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of compound (2).

	X/A	Y/B	Z/C	U[a]
PT(1)	-.24987(7)	.12158(6)	.28551(4)	.027
PT(2)	-.25422(7)	.13492(6)	.16332(4)	.029
PT(3)	-.16941(7)	.04082(6)	.24780(4)	.029
P(1)	-.3194(4)	.2190(4)	.2892(3)	.036
P(2)	-.3386(4)	.2251(4)	.1622(3)	.037
P(3)	-.2249(4)	.1021(4)	.1091(3)	.035
P(4)	-.1223(4)	-.0014(4)	.1848(3)	.037
P(5)	-.1260(4)	-.0255(4)	.3253(3)	.037
P(6)	-.1820(4)	.0953(4)	.3764(3)	.034
P(7)	-.3424(4)	.0409(4)	.2643(3)	.036
P(F1)	.2041(7)	.3890(7)	.5347(5)	.174
P(F2)	-.7078(7)	.1426(8)	.3778(8)	.324
O(1)	-.3440(10)	.0058(10)	.3175(7)	.046(6)
O(2)	-.4200(10)	.0755(9)	.2366(7)	.039(5)
O(3)	-.3423(10)	-.0278(9)	.2312(7)	.047(5)
O(4)	-.1176(11)	.1904(10)	.2663(7)	.049(6)
F(11)	.248(2)	.325(2)	.561(2)	.34(3)
F(12)	.161(2)	.453(2)	.508(2)	.31(2)
F(13)	.268(3)	.434(3)	.570(1)	.38(3)
F(14)	.140(3)	.344(3)	.500(1)	.44(4)
F(15)	.169(2)	.392(1)	.579(1)	.36(3)
F(16)	.239(2)	.386(1)	.490(1)	.26(2)
F(21)	-.689(3)	.103(1)	.334(2)	.54(6)
F(22)	-.727(3)	.182(1)	.422(2)	.79(9)
F(23)	-.694(2)	.211(1)	.354(2)	.43(3)
F(24)	-.721(2)	.075(1)	.402(2)	.27(2)
F(25)	-.626(2)	.140(4)	.415(2)	.36(3)
F(26)	-.789(2)	.145(4)	.341(2)	.39(3)
C(1)	-.3746(13)	.2393(12)	.2194(9)	.025(7)
C(2)	-.1950(14)	.0157(13)	.1159(10)	.031(7)
C(3)	-.1607(15)	.0038(14)	.3786(10)	.039(8)
C(4)	-.1715(16)	.1558(14)	.2621(10)	.038(8)
C(11)	-.3770(16)	-.0553(12)	.3255(8)	.039(8)
C(12)	-.3498(13)	-.1185(16)	.3177(12)	.061(10)
C(13)	-.3789(21)	-.1778(12)	.3311(15)	.076(11)
C(14)	-.4353(16)	-.1739(12)	.3523(8)	.113(15)
C(15)	-.4625(13)	-.1107(16)	.3601(12)	.152(19)
C(16)	-.4334(21)	-.0514(12)	.3467(15)	.093(13)
C(21)	-.4933(14)	.0486(22)	.2264(10)	.052(9)
C(22)	-.5404(24)	.0941(15)	.2384(10)	.107(14)
C(23)	-.6118(21)	.0743(16)	.2322(16)	.112(15)
C(24)	-.6360(14)	.0091(22)	.2138(10)	.131(17)
C(25)	-.5889(24)	-.0364(15)	.2018(10)	.104(14)
C(26)	-.5175(21)	-.0166(16)	.2080(16)	.060(10)
C(31)	-.3567(16)	-.0389(15)	.1769(7)	.030(7)
C(32)	-.3453(9)	-.1045(15)	.1613(11)	.053(9)
C(33)	-.3658(18)	-.1207(7)	.1067(13)	.076(11)
C(34)	-.3977(16)	-.0714(15)	.0677(7)	.074(11)
C(35)	-.4091(9)	-.0058(15)	.0833(11)	.061(10)
C(36)	-.3886(18)	.0104(7)	.1379(13)	.056(10)
C(A1)	-.3922(11)	.2186(11)	.3175(10)	.031(7)
C(A2)	-.3944(12)	.1659(13)	.3522(13)	.041(8)
C(A3)	-.4510(9)	.1631(9)	.3733(7)	.056(9)
C(A4)	-.5052(11)	.2131(11)	.3597(10)	.061(10)
C(A5)	-.5030(12)	.2658(13)	.3249(13)	.051(9)
C(A6)	-.4464(9)	.2685(9)	.3038(7)	.056(9)
C(B1)	-.2659(16)	.2955(13)	.3197(7)	.030(7)
C(B2)	-.2747(8)	.3256(10)	.3649(8)	.041(8)
C(B3)	-.2328(17)	.3822(9)	.3887(10)	.048(8)
C(B4)	-.1820(16)	.4067(13)	.3674(7)	.056(9)
C(B5)	-.1732(8)	.3786(10)	.3223(8)	.070(10)
C(B6)	-.2151(17)	.3219(9)	.2984(10)	.047(9)
C(C1)	-.4271(15)	.2249(20)	.1043(10)	.046(8)
C(C2)	-.4443(14)	.2740(14)	.0637(5)	.067(10)
C(C3)	-.5134(10)	.2743(13)	.0234(10)	.067(10)
C(C4)	-.5653(15)	.2255(20)	.0237(10)	.067(10)
C(C5)	-.5481(14)	.1764(14)	.0643(5)	.078(11)
C(C6)	-.4790(10)	.1761(13)	.1046(10)	.056(9)
C(D1)	-.2941(18)	.3070(14)	.1591(7)	.041(8)
C(D2)	-.2243(20)	.3066(12)	.1554(14)	.047(9)
C(D3)	-.1865(11)	.3675(18)	.1580(11)	.078(11)
C(D4)	-.2185(18)	.4289(14)	.1644(7)	.077(12)
C(D5)	-.2883(20)	.4293(12)	.1682(14)	.108(15)
C(D6)	-.3261(11)	.3683(18)	.1655(11)	.077(11)

Table 5.2(cont).

	X/A	Y/B	Z/C	U
C(E1)	-.2987(13)	.1017(17)	.0411(8)	.031(7)
C(E2)	-.3148(12)	.0454(12)	.0069(12)	.042(8)
C(E3)	-.3703(18)	.0492(11)	-.0435(10)	.063(10)
C(E4)	-.4097(13)	.1094(17)	-.0597(8)	.050(9)
C(E5)	-.3936(12)	.1657(12)	-.0255(12)	.058(10)
C(E6)	-.3381(18)	.1619(11)	.0249(10)	.050(9)
C(F1)	-.1509(11)	.1515(13)	.0957(8)	.041(8)
C(F2)	-.1438(20)	.1465(17)	.0451(6)	.065(10)
C(F3)	-.0873(17)	.1809(11)	.0348(9)	.068(10)
C(F4)	-.0379(11)	.2203(13)	.0751(8)	.081(12)
C(F5)	-.0451(20)	.2252(17)	.1257(6)	.075(11)
C(F6)	-.1016(17)	.1908(11)	.1360(9)	.065(10)
C(G1)	-.0384(11)	.0404(15)	.1821(10)	.038(7)
C(G2)	-.0169(20)	.0250(17)	.1382(6)	.050(9)
C(G3)	.0507(17)	.0474(8)	.1374(11)	.073(10)
C(G4)	.0969(11)	.0853(15)	.1805(10)	.087(12)
C(G5)	.0754(20)	.1007(17)	.2243(6)	.095(13)
C(G6)	.0077(17)	.0783(8)	.2251(11)	.069(10)
C(H1)	-.0981(16)	-.0912(10)	.1843(14)	.033(7)
C(H2)	-.1398(12)	-.1381(19)	.1465(11)	.060(9)
C(H3)	-.1177(19)	-.2059(16)	.1495(7)	.101(14)
C(H4)	-.0538(16)	-.2268(10)	.1903(14)	.055(9)
C(H5)	-.0121(12)	-.1798(19)	.2281(11)	.066(10)
C(H6)	-.0342(19)	-.1121(16)	.2251(7)	.056(9)
C(I1)	-.0251(14)	-.0209(20)	.3565(9)	.038(8)
C(I2)	.0154(15)	-.0722(11)	.3923(7)	.063(10)
C(I3)	.0895(11)	-.0621(16)	.4219(12)	.061(10)
C(I4)	.1231(14)	-.0008(20)	.4178(9)	.093(13)
C(I5)	.0827(15)	.0505(11)	.3840(7)	.073(11)
C(I6)	.0086(11)	.0404(16)	.3544(12)	.053(9)
C(J1)	-.1525(17)	-.1158(11)	.3209(11)	.028(7)
C(J2)	-.1478(20)	-.1526(16)	.3672(9)	.090(13)
C(J3)	-.1701(10)	-.2204(13)	.3628(8)	.093(13)
C(J4)	-.1971(17)	-.2514(11)	.3122(11)	.095(13)
C(J5)	-.2017(20)	-.2146(16)	.2660(9)	.084(12)
C(J6)	-.1794(10)	-.1468(13)	.2704(8)	.065(10)
C(K1)	-.0943(16)	.1410(18)	.4084(6)	.049(8)
C(K2)	-.0857(11)	.2064(19)	.3911(11)	.047(8)
C(K3)	-.0217(14)	.2428(8)	.4173(10)	.073(11)
C(K4)	.0337(16)	.2139(18)	.4607(6)	.084(12)
C(K5)	.0251(11)	.1484(19)	.4780(11)	.066(10)
C(K6)	-.0389(14)	.1120(8)	.4518(10)	.074(11)
C(L1)	-.2229(14)	.1061(7)	.4304(10)	.037(8)
C(L2)	-.2603(18)	.0533(10)	.4447(11)	.045(8)
C(L3)	-.2926(11)	.0638(10)	.4837(6)	.055(9)
C(L4)	-.2874(14)	.1272(7)	.5084(10)	.072(10)
C(L5)	-.2499(18)	.1801(10)	.4941(11)	.087(12)
C(L6)	-.2177(11)	.1696(10)	.4551(6)	.063(10)
O(S)	.2324(20)	.1313(20)	.5260(14)	.203(16)
C(S1)	-.518(4)	-.037(4)	-.493(4)	.24(4)
C(S2)	-.477(4)	.001(5)	-.458(3)	.23(3)

Table 5.2(cont).

	X/A	Y/B	Z/C	U
H(1A)	-.39163	.28714	.21768	.050
H(1B)	-.42214	.21197	.21015	.050
H(2A)	-.17596	.00452	.08481	.050
H(2B)	-.23844	-.01572	.10745	.050
H(3A)	-.12431	-.00686	.41443	.050
H(3B)	-.20540	-.02223	.37611	.050
H(12)	-.31054	-.12076	.30308	.050
H(13)	-.36059	-.22193	.32423	.050
H(14)	-.45720	-.21629	.35915	.050
H(15)	-.50371	-.10951	.37298	.050
H(16)	-.45371	-.00834	.35184	.050
H(22)	-.52265	.13708	.25447	.050
H(23)	-.64294	.10174	.24441	.050
H(24)	-.68383	-.00789	.21044	.050
H(25)	-.60446	-.08215	.18647	.050
H(26)	-.48419	-.04681	.19651	.050
H(32)	-.32173	-.13943	.18800	.050
H(33)	-.35903	-.16766	.09536	.050
H(34)	-.41363	-.08418	.02919	.050
H(35)	-.43085	.02755	.05563	.050
H(36)	-.39360	.05578	.14830	.050
H(A2)	-.35708	.13215	.36190	.050
H(A3)	-.45366	.12797	.39695	.050
H(A4)	-.54562	.21274	.37295	.050
H(A5)	-.54100	.30166	.31398	.050
H(A6)	-.44442	.30587	.27896	.050
H(B2)	-.30930	.30610	.38061	.050
H(B3)	-.23854	.40221	.42122	.050
H(B4)	-.15325	.44804	.38483	.050
H(B5)	-.13871	.39782	.30781	.050
H(B6)	-.20946	.30169	.26720	.050
H(C2)	-.40906	.30620	.06247	.050
H(C3)	-.52633	.30769	-.00565	.050
H(C4)	-.61512	.22585	-.00500	.050
H(C5)	-.58666	.14249	.06370	.050
H(C6)	-.46939	.14100	.13182	.050
H(D2)	-.20113	.26379	.15207	.050
H(D3)	-.13776	.36744	.15615	.050
H(D4)	-.19286	.47129	.16638	.050
H(D5)	-.31136	.47147	.17250	.050
H(D6)	-.37472	.36783	.16842	.050
H(E2)	-.28575	.00384	.01845	.050
H(E3)	-.37913	.00994	-.06734	.050
H(E4)	-.44654	.11167	-.09522	.050
H(E5)	-.42054	.20725	-.03732	.050
H(E6)	-.32720	.20112	.04846	.050
H(F2)	-.17641	.11860	.01802	.050
H(F3)	-.08141	.17769	.00010	.050
H(F4)	.00220	.24470	.06824	.050
H(F5)	-.00919	.25261	.15436	.050
H(F6)	-.10420	.19354	.17225	.050
H(G2)	-.04746	.00045	.10852	.050
H(G3)	.06865	.03692	.10897	.050
H(G4)	.14701	.09899	.18331	.050
H(G5)	.10927	.12458	.25717	.050
H(G6)	-.00685	.08811	.25671	.050
H(H2)	-.18317	-.12444	.11784	.050
H(H3)	-.14612	-.23958	.12365	.050
H(H4)	-.03850	-.27502	.19347	.050
H(H5)	.03209	-.19533	.25753	.050
H(H6)	-.00496	-.08023	.25176	.050
H(I2)	-.00919	-.11421	.39535	.050
H(I3)	.11630	-.09735	.44607	.050
H(I4)	.17408	.00606	.43858	.050
H(I5)	.10639	.09258	.38035	.050
H(I6)	-.01907	.07575	.32959	.050
H(J2)	-.12949	-.13342	.40162	.050
H(J3)	-.16665	-.24860	.39356	.050
H(J4)	-.21293	-.30016	.30744	.050
H(J5)	-.22209	-.23652	.22939	.050
H(J6)	-.18501	-.12133	.23746	.050
H(K2)	-.12425	.22705	.36187	.050
H(K3)	-.01667	.28989	.40688	.050

Table 5.2(cont).

	X/A	Y/B	Z/C	U
H(K4)	.07772	.24105	.48040	.050
H(K5)	.06448	.12938	.50898	.050
H(K6)	-.04310	.06654	.46396	.050
H(L2)	-.26179	.00897	.42882	.050
H(L3)	-.31409	.02617	.49640	.050
H(L4)	-.30578	.13388	.53794	.050
H(L5)	-.24510	.22436	.51190	.050
H(L6)	-.19279	.20715	.44433	.050

[a]Throughout this thesis U values quoted with standard deviations are refined isotropic displacement parameters and define an isotropic temperature factor of the form $\exp(-8\pi^2 U \sin^2\theta/\lambda^2)$. U valued without e.s.d.s are equivalent isotropic displacement parameters defined as:-

$$U = 1/3 \sum_{i=1}^{3} \sum_{j=1}^{3} U_{ij} a_i^* a_j^* (\underline{a}_i . \underline{a}_j).$$

For H-atoms only isotropic U were employed.

Anisotropic displacement parameters ($\AA^2$)

	U11	U22	U33	U12	U13	U23
PT(1)	.0260(6)	.0272(7)	.0238(7)	.0009(7)	.0077(6)	.0002(6)
PT(2)	.0282(8)	.0262(7)	.0278(7)	.0050(7)	.0102(6)	.0045(6)
PT(3)	.0268(7)	.0274(7)	.0294(7)	.0056(7)	.0102(6)	.0048(6)
P(1)	.021(5)	.039(5)	.042(5)	.002(4)	.010(4)	-.009(4)
P(2)	.034(5)	.035(5)	.038(5)	.018(5)	.010(4)	.008(4)
P(3)	.035(5)	.032(5)	.032(4)	.010(4)	.012(4)	.005(4)
P(4)	.028(5)	.033(5)	.046(5)	.008(4)	.012(4)	.004(4)
P(5)	.036(5)	.041(5)	.032(4)	.008(5)	.018(4)	.000(4)
P(6)	.032(5)	.036(5)	.031(4)	-.005(4)	.015(4)	-.003(4)
P(7)	.037(5)	.030(5)	.036(5)	-.001(5)	.014(4)	.004(4)
P(F1)	.251(21)	.122(13)	.133(12)	-.018(16)	.091(14)	.005(11)
P(F2)	.100(14)	.164(20)	.587(45)	-.032(15)	-.072(21)	.151(28)

Throughout this thesis the form of the anisotropic displacement factor was:-

$$\exp[-2\pi^2 \sum_{i=1}^{3} \sum_{j=1}^{3} U_{ij} h_i h_j a_i^* a_j^*].$$

Table 5.3. Selected bond distances (Å) and angles (°) of complex (2).

PT(1) - PT(2)	2.656(2)	PT(1) - PT(3)	2.626(2)
PT(1) - P(1)	2.341(8)	PT(1) - P(6)	2.335(8)
PT(1) - P(7)	2.293(8)	PT(1) - C(4)	1.93(3)
PT(2) - PT(3)	2.636(2)	PT(2) - P(2)	2.323(8)
PT(2) - P(3)	2.290(8)	PT(2) - C(4)	2.16(3)
PT(3) - P(4)	2.288(8)	PT(3) - P(5)	2.300(8)
PT(3) - C(4)	2.27(3)	P(1) - C(1)	1.81(3)
P(1) - C(A1)	1.80(3)	P(1) - C(B1)	1.83(3)
P(2) - C(1)	1.88(3)	P(2) - C(C1)	1.84(3)
P(2) - C(D1)	1.83(3)	P(3) - C(2)	1.76(3)
P(3) - C(E1)	1.85(3)	P(3) - C(F1)	1.85(3)
P(4) - C(2)	1.89(3)	P(4) - C(G1)	1.83(3)
P(4) - C(H1)	1.81(3)	P(5) - C(3)	1.83(3)
P(5) - C(I1)	1.84(3)	P(5) - C(J1)	1.82(3)
P(6) - C(3)	1.82(3)	P(6) - C(K1)	1.83(4)
P(6) - C(L1)	1.85(3)	P(7) - O(1)	1.56(2)
P(7) - O(2)	1.57(2)	P(7) - O(3)	1.59(2)
O(1) - C(11)	1.40(4)	O(2) - C(21)	1.44(4)
O(3) - C(31)	1.37(3)	O(4) - C(4)	1.21(4)

PT(2) - PT(1) - PT(3)	59.9(1)	PT(2) - PT(1) - P(1)	98.2(2)
PT(2) - PT(1) - P(6)	148.8(2)	PT(2) - PT(1) - P(7)	94.2(2)
PT(2) - PT(1) - C(4)	53.4(8)	PT(3) - PT(1) - P(1)	156.9(2)
PT(3) - PT(1) - P(6)	93.2(2)	PT(3) - PT(1) - P(7)	90.5(2)
PT(3) - PT(1) - C(4)	57.4(8)	P(1) - PT(1) - P(6)	105.1(3)
P(1) - PT(1) - P(7)	99.1(3)	P(1) - PT(1) - C(4)	104.7(9)
P(6) - PT(1) - P(7)	102.1(3)	P(6) - PT(1) - C(4)	100.1(8)
P(7) - PT(1) - C(4)	141.8(8)	PT(1) - PT(2) - PT(3)	59.5(1)
PT(1) - PT(2) - P(2)	95.1(2)	PT(1) - PT(2) - P(3)	153.3(2)
PT(1) - PT(2) - C(4)	45.9(8)	PT(3) - PT(2) - P(2)	154.6(2)
PT(3) - PT(2) - P(3)	93.9(2)	PT(3) - PT(2) - C(4)	55.5(8)
P(2) - PT(2) - P(3)	111.5(3)	P(2) - PT(2) - C(4)	107.9(8)
P(3) - PT(2) - C(4)	122.9(8)	PT(1) - PT(3) - PT(2)	60.6(1)
PT(1) - PT(3) - P(4)	156.3(2)	PT(1) - PT(3) - P(5)	95.0(2)
PT(1) - PT(3) - C(4)	45.7(8)	PT(2) - PT(3) - P(4)	95.7(2)
PT(2) - PT(3) - P(5)	155.2(2)	PT(2) - PT(3) - C(4)	51.6(7)
P(4) - PT(3) - P(5)	108.7(3)	P(4) - PT(3) - C(4)	120.3(7)
P(5) - PT(3) - C(4)	115.5(7)	PT(1) - P(1) - C(1)	106.2(9)
PT(1) - P(1) - C(A1)	123.5(8)	PT(1) - P(1) - C(B1)	115.7(10)
C(1) - P(1) - C(A1)	98.4(12)	C(1) - P(1) - C(B1)	107.9(11)
C(A1) - P(1) - C(B1)	103.1(12)	PT(2) - P(2) - C(1)	110.0(8)
PT(2) - P(2) - C(C1)	124.3(12)	PT(2) - P(2) - C(D1)	111.7(11)
C(1) - P(2) - C(C1)	99.5(12)	C(1) - P(2) - C(D1)	102.4(12)
C(C1) - P(2) - C(D1)	106.2(14)	PT(2) - P(3) - C(2)	110.4(9)
PT(2) - P(3) - C(E1)	118.8(9)	PT(2) - P(3) - C(F1)	116.6(8)
C(2) - P(3) - C(E1)	101.9(14)	C(2) - P(3) - C(F1)	105.6(12)
C(E1) - P(3) - C(F1)	101.8(11)	PT(3) - P(4) - C(2)	106.1(9)
PT(3) - P(4) - C(G1)	116.4(10)	PT(3) - P(4) - C(H1)	121.1(11)
C(2) - P(4) - C(G1)	105.0(12)	C(2) - P(4) - C(H1)	105.6(14)
C(G1) - P(4) - C(H1)	101.2(14)	PT(3) - P(5) - C(3)	112.2(9)
PT(3) - P(5) - C(I1)	113.0(10)	PT(3) - P(5) - C(J1)	118.6(10)
C(3) - P(5) - C(I1)	103.2(12)	C(3) - P(5) - C(J1)	100.4(13)
C(I1) - P(5) - C(J1)	107.7(16)	PT(1) - P(6) - C(3)	106.6(9)
PT(1) - P(6) - C(K1)	117.4(8)	PT(1) - P(6) - C(L1)	121.0(9)
C(3) - P(6) - C(K1)	107.3(15)	C(3) - P(6) - C(L1)	103.7(11)
C(K1) - P(6) - C(L1)	99.4(11)	PT(1) - P(7) - O(1)	109.8(8)
PT(1) - P(7) - O(2)	110.7(8)	PT(1) - P(7) - O(3)	124.0(8)
O(1) - P(7) - O(2)	106.9(11)	O(1) - P(7) - O(3)	96.9(11)
O(2) - P(7) - O(3)	106.8(10)	P(7) - O(1) - C(11)	131.1(15)
P(7) - O(2) - C(21)	130.1(20)	P(7) - O(3) - C(31)	131.3(18)
P(1) - C(1) - P(2)	121.5(14)	P(3) - C(2) - P(4)	111.6(13)
P(5) - C(3) - P(6)	114.6(15)	PT(1) - C(4) - PT(2)	80.7(11)
PT(1) - C(4) - PT(3)	76.8(10)	PT(1) - C(4) - O(4)	154.6(21)
PT(2) - C(4) - PT(3)	72.9(8)	PT(2) - C(4) - O(4)	121.1(19)
PT(3) - C(4) - O(4)	119.9(20)		

Table 5.4. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (3).

	X/A	Y/B	Z/C	U
PT(1)	0.37496(16)	0.22406(14)	0.29094(9)	0.036
PT(2)	0.23808(17)	0.30919(15)	0.22589(10)	0.038
PT(3)	0.26417(17)	0.12768(14)	0.27562(10)	0.038
P(1)	0.4150(12)	0.3554(10)	0.2888(6)	0.050
P(2)	0.3758(12)	0.4455(11)	0.2027(7)	0.064
P(3)	0.0950(10)	0.3341(10)	0.1628(7)	0.052
P(4)	0.1340(11)	0.1057(11)	0.2322(7)	0.059
P(5)	0.0379(11)	-0.0098(9)	0.3417(6)	0.046
P(6)	0.4739(11)	0.1013(10)	0.3468(6)	0.049
P(7)	0.1620(12)	0.2204(10)	0.5349(6)	0.091
P(8)	0.781(3)	0.200(3)	0.102(2)	0.25(2)
F(1)	0.094(2)	0.330(2)	0.517(2)	0.14(2)
F(2)	0.243(3)	0.255(3)	0.547(1)	0.14(2)
F(3)	0.215(4)	0.209(3)	0.479(1)	0.21(2)
F(4)	0.109(4)	0.233(3)	0.591(1)	0.18(2)
F(5)	0.230(2)	0.111(2)	0.553(2)	0.17(2)
F(6)	0.081(3)	0.186(3)	0.523(1)	0.22(3)
N(1)	0.105(3)	0.255(3)	0.355(2)	0.06(1)
C(1)	0.410(4)	0.421(3)	0.223(2)	0.05(2)
C(2)	0.050(4)	0.253(4)	0.208(2)	0.07(2)
C(3)	0.389(5)	0.038(4)	0.386(3)	0.08(2)
C(5)	0.170(3)	0.213(3)	0.324(2)	0.02(1)
C(A1)	0.545(3)	0.336(4)	0.294(3)	0.03(1)
C(A2)	0.623(5)	0.281(5)	0.259(1)	0.05(1)
C(A3)	0.724(5)	0.263(2)	0.262(2)	0.10(2)
C(A4)	0.748(3)	0.300(4)	0.301(3)	0.13(3)
C(A5)	0.671(5)	0.354(5)	0.337(1)	0.14(3)
C(A6)	0.569(5)	0.372(2)	0.333(2)	0.06(2)
C(B1)	0.341(6)	0.440(3)	0.336(3)	0.04(1)
C(B2)	0.286(4)	0.404(2)	0.378(2)	0.05(2)
C(B3)	0.220(3)	0.468(2)	0.413(2)	0.07(2)
C(B4)	0.209(6)	0.567(3)	0.408(3)	0.15(3)
C(B5)	0.264(4)	0.603(2)	0.366(2)	0.14(3)
C(B6)	0.330(3)	0.540(2)	0.330(2)	0.10(2)
C(C1)	0.179(5)	0.562(3)	0.231(3)	0.04(1)
C(C2)	0.186(4)	0.654(2)	0.221(2)	0.07(2)
C(C3)	0.120(4)	0.733(2)	0.248(2)	0.10(2)
C(C4)	0.045(5)	0.719(3)	0.286(3)	0.12(3)
C(C5)	0.037(4)	0.627(2)	0.297(2)	0.09(2)
C(C6)	0.104(4)	0.548(2)	0.269(2)	0.06(2)
C(D1)	0.290(6)	0.478(6)	0.131(2)	0.07(2)
C(D2)	0.217(6)	0.562(3)	0.108(4)	0.15(3)
C(D3)	0.232(4)	0.593(5)	0.055(4)	0.13(3)
C(D4)	0.322(6)	0.539(6)	0.026(2)	0.22(5)
C(D5)	0.396(6)	0.454(3)	0.049(4)	0.14(3)
C(D6)	0.380(4)	0.424(5)	0.102(4)	0.10(2)
C(E1)	0.113(8)	0.331(4)	0.113(2)	0.07(2)
C(E2)	0.212(6)	0.314(6)	0.089(4)	0.08(2)
C(E3)	0.234(5)	0.311(3)	0.036(4)	0.20(5)
C(E4)	0.158(3)	0.324(4)	0.006(2)	0.19(4)
C(E5)	0.059(6)	0.341(6)	0.030(4)	0.16(4)
C(E6)	0.037(5)	0.344(3)	0.083(4)	0.12(3)
C(F1)	-0.016(4)	0.454(2)	0.191(3)	0.04(1)
C(F2)	-0.035(5)	0.535(3)	0.152(2)	0.06(2)
C(F3)	-0.117(3)	0.625(4)	0.161(2)	0.09(2)
C(F4)	-0.179(4)	0.635(2)	0.208(3)	0.05(2)
C(F5)	-0.160(5)	0.554(3)	0.247(2)	0.12(3)
C(F6)	-0.078(3)	0.464(4)	0.238(2)	0.11(3)
C(G1)	0.046(3)	0.060(2)	0.270(2)	0.05(1)
C(G2)	0.000(4)	0.056(4)	0.324(2)	0.08(2)
C(G3)	-0.048(5)	0.022(4)	0.352(1)	0.09(2)
C(G4)	-0.101(3)	-0.007(2)	0.325(2)	0.07(2)
C(G5)	-0.084(4)	-0.003(4)	0.272(2)	0.07(2)
C(G6)	-0.011(5)	0.021(4)	0.244(1)	0.12(3)
C(H1)	0.193(6)	0.033(4)	0.178(3)	0.07(2)
C(H2)	0.242(5)	-0.067(5)	0.193(2)	0.11(2)
C(H3)	0.287(3)	-0.135(3)	0.156(3)	0.06(2)
C(H4)	0.283(6)	-0.099(4)	0.103(3)	0.10(2)

Table 5.4(cont).

	X/A	Y/B	Z/C	U
C(H5)	0.233(5)	0.003(5)	0.088(2)	0.14(3)
C(H6)	0.188(3)	0.069(3)	0.126(3)	0.11(3)
C(I1)	0.425(4)	-0.133(2)	0.325(3)	0.03(1)
C(I2)	0.438(3)	-0.157(5)	0.274(3)	0.08(2)
C(I3)	0.504(5)	-0.252(5)	0.262(1)	0.10(2)
C(I4)	0.556(4)	-0.324(2)	0.300(3)	0.09(2)
C(I5)	0.543(3)	-0.301(5)	0.351(3)	0.10(2)
C(I6)	0.478(5)	-0.205(5)	0.363(1)	0.09(2)
C(J1)	0.249(3)	-0.046(2)	0.387(2)	0.06(2)
C(J2)	0.207(5)	-0.007(4)	0.435(1)	0.08(2)
C(J3)	0.137(5)	-0.041(4)	0.467(2)	0.06(2)
C(J4)	0.110(3)	-0.112(2)	0.453(2)	0.12(3)
C(J5)	0.152(5)	-0.150(4)	0.406(1)	0.10(2)
C(J6)	0.222(5)	-0.117(4)	0.373(2)	0.10(2)
C(K1)	0.590(4)	0.003(2)	0.313(2)	0.04(1)
C(K2)	0.645(4)	-0.088(3)	0.340(1)	0.05(1)
C(K3)	0.729(3)	-0.159(3)	0.315(2)	0.06(2)
C(K4)	0.759(4)	-0.137(2)	0.262(2)	0.04(1)
C(K5)	0.704(4)	-0.046(3)	0.235(1)	0.10(2)
C(K6)	0.620(3)	0.025(3)	0.261(2)	0.07(2)
C(L1)	0.527(5)	0.129(4)	0.399(2)	0.06(2)
C(L2)	0.629(5)	0.115(2)	0.394(2)	0.04(1)
C(L3)	0.667(3)	0.138(4)	0.433(3)	0.09(2)
C(L4)	0.602(5)	0.175(4)	0.477(2)	0.09(2)
C(L5)	0.500(5)	0.189(2)	0.482(2)	0.10(2)
C(L6)	0.462(3)	0.166(4)	0.443(3)	0.06(2)
C(N1)	0.031(5)	0.321(4)	0.397(3)	0.07(2)
C(N2)	-0.060(5)	0.283(5)	0.402(3)	0.13(3)
C(N3)	-0.140(5)	0.357(5)	0.444(3)	0.09(2)
C(N4)	-0.135(4)	0.457(4)	0.428(2)	0.06(2)
C(N5)	-0.092(7)	0.480(6)	0.424(4)	0.14(3)
C(N6)	0.006(5)	0.422(4)	0.377(3)	0.08(2)

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
PT(1)	0.036(2)	0.034(1)	0.032(2)	-0.016(1)	-0.005(1)	-0.002(1)
PT(2)	0.035(1)	0.035(1)	0.035(2)	-0.011(1)	-0.006(1)	-0.002(1)
PT(3)	0.033(1)	0.033(1)	0.040(2)	-0.013(1)	-0.001(1)	-0.006(1)
P(1)	0.06(1)	0.04(1)	0.05(1)	-0.03(1)	0.00(1)	-0.01(1)
P(2)	0.06(1)	0.07(1)	0.05(1)	-0.04(1)	0.02(1)	-0.02(1)
P(3)	0.02(1)	0.06(1)	0.08(1)	-0.03(1)	-0.03(1)	0.00(1)
P(4)	0.04(1)	0.06(1)	0.07(1)	-0.01(1)	0.00(1)	-0.02(1)
P(5)	0.05(1)	0.04(1)	0.04(1)	-0.02(1)	0.00(1)	-0.02(1)
P(6)	0.04(1)	0.05(1)	0.05(1)	-0.02(1)	0.00(1)	-0.02(1)
P(7)	0.08(1)	0.11(1)	0.06(1)	-0.02(1)	0.00(1)	-0.02(1)

Table 5.5. Selected bond distances (Å) and angles (°) of complex (3).

PT(1) - PT(2)	2.584(4)	PT(1) - PT(3)	2.626(3)
PT(1) - P(1)	2.205(13)	PT(1) - P(6)	2.251(15)
PT(2) - PT(3)	2.646(3)	PT(2) - P(2)	2.227(16)
PT(2) - P(3)	2.373(14)	PT(3) - P(4)	2.460(15)
PT(3) - P(5)	2.406(15)	PT(3) - C(5)	1.88(5)
P(1) - C(1)	1.80(6)	P(1) - C(A1)	1.79(5)
P(1) - C(B1)	1.79(6)	P(2) - C(1)	1.95(6)
P(2) - C(C1)	1.88(6)	P(2) - C(D1)	1.83(5)
P(3) - C(2)	1.56(6)	P(3) - C(E1)	1.80(5)
P(3) - C(F1)	1.84(5)	P(4) - C(2)	2.00(6)
P(4) - C(G1)	1.77(5)	P(4) - C(H1)	1.82(7)
P(5) - C(3)	1.84(6)	P(5) - C(I1)	1.81(5)
P(5) - C(J1)	1.76(5)	P(6) - C(3)	1.88(7)
P(6) - C(K1)	1.89(5)	P(6) - C(L1)	1.84(5)
N(1) - C(5)	1.18(7)	N(1) - C(N1)	1.53(8)
C(N1) - C(N2)	1.59(10)	C(N1) - C(N6)	1.38(9)
C(N2) - C(N3)	1.63(11)	C(N3) - C(N4)	1.35(9)
C(N4) - C(N5)	1.47(11)		

PT(2) - PT(1) - PT(3)	61.0(1)	PT(2) - PT(1) - P(1)	96.2(4)
PT(2) - PT(1) - P(6)	157.5(4)	PT(3) - PT(1) - P(1)	156.4(4)
PT(3) - PT(1) - P(6)	96.7(4)	P(1) - PT(1) - P(6)	106.2(6)
PT(1) - PT(2) - PT(3)	60.3(1)	PT(1) - PT(2) - P(2)	94.4(5)
PT(1) - PT(2) - P(3)	157.5(4)	PT(3) - PT(2) - P(2)	154.6(5)
PT(3) - PT(2) - P(3)	97.7(4)	P(2) - PT(2) - P(3)	107.7(6)
PT(1) - PT(3) - PT(2)	58.7(1)	PT(1) - PT(3) - P(4)	153.0(4)
PT(1) - PT(3) - P(5)	93.0(4)	PT(1) - PT(3) - C(5)	80.5(13)
PT(2) - PT(3) - P(4)	94.3(4)	PT(2) - PT(3) - P(5)	151.4(4)
PT(2) - PT(3) - C(5)	77.8(13)	P(4) - PT(3) - P(5)	114.0(5)
P(4) - PT(3) - C(5)	96.3(13)	P(5) - PT(3) - C(5)	94.4(14)
PT(1) - P(1) - C(1)	108.8(17)	PT(1) - P(1) - C(A1)	119.5(20)
PT(1) - P(1) - C(B1)	115.6(22)	C(1) - P(1) - C(A1)	96.6(28)
C(1) - P(1) - C(B1)	111.4(25)	C(A1) - P(1) - C(B1)	103.4(32)
PT(2) - P(2) - C(1)	110.8(16)	PT(2) - P(2) - C(C1)	114.2(21)
PT(2) - P(2) - C(D1)	112.2(25)	C(1) - P(2) - C(C1)	107.8(27)
C(1) - P(2) - C(D1)	103.9(30)	C(C1) - P(2) - C(D1)	107.3(32)
PT(2) - P(3) - C(2)	109.2(23)	PT(2) - P(3) - C(E1)	119.1(33)
PT(2) - P(3) - C(F1)	114.9(20)	C(2) - P(3) - C(E1)	106.4(36)
C(2) - P(3) - C(F1)	103.1(28)	C(E1) - P(3) - C(F1)	102.8(33)
PT(3) - P(4) - C(2)	101.6(18)	PT(3) - P(4) - C(G1)	119.3(18)
PT(3) - P(4) - C(H1)	111.9(24)	C(2) - P(4) - C(G1)	106.1(21)
C(2) - P(4) - C(H1)	112.7(28)	C(G1) - P(4) - C(H1)	105.3(26)
PT(3) - P(5) - C(3)	107.2(19)	PT(3) - P(5) - C(I1)	121.7(24)
PT(3) - P(5) - C(J1)	115.7(14)	C(3) - P(5) - C(I1)	112.5(28)
C(3) - P(5) - C(J1)	98.6(26)	C(I1) - P(5) - C(J1)	98.8(23)
PT(1) - P(6) - C(3)	106.2(20)	PT(1) - P(6) - C(K1)	113.8(19)
PT(1) - P(6) - C(L1)	122.1(19)	C(3) - P(6) - C(K1)	109.1(23)
C(3) - P(6) - C(L1)	101.3(27)	C(K1) - P(6) - C(L1)	103.3(26)
C(5) - N(1) - C(N1)	170.1(47)	P(1) - C(1) - P(2)	106.9(27)
P(3) - C(2) - P(4)	124.8(34)	P(5) - C(3) - P(6)	109.1(34)
PT(3) - C(5) - N(1)	169.9(37)	P(1) - C(A1) - C(A2)	118.4(46)
P(1) - C(A1) - C(A6)	121.5(47)	P(1) - C(B1) - C(B2)	116.9(32)
P(1) - C(B1) - C(B6)	123.2(47)	P(2) - C(C1) - C(C2)	123.3(47)
P(2) - C(C1) - C(C6)	116.4(29)	P(2) - C(D1) - C(D2)	119.8(57)
P(2) - C(D1) - C(D6)	119.8(59)	P(3) - C(E1) - C(E2)	114.8(65)
P(3) - C(E1) - C(E6)	125.1(68)	P(3) - C(F1) - C(F2)	121.6(48)
P(3) - C(F1) - C(F6)	118.4(41)	P(4) - C(G1) - C(G2)	121.7(33)
P(4) - C(G1) - C(G6)	118.2(39)	P(4) - C(H1) - C(H2)	115.2(47)
P(4) - C(H1) - C(H6)	124.8(42)	P(5) - C(I1) - C(I2)	120.4(44)
P(5) - C(I1) - C(I6)	119.6(49)	P(5) - C(J1) - C(J2)	124.9(33)
P(5) - C(J1) - C(J6)	115.0(37)	P(6) - C(K1) - C(K2)	121.2(42)
P(6) - C(K1) - C(K6)	118.8(29)	P(6) - C(L1) - C(L2)	121.0(36)
P(6) - C(L1) - C(L6)	119.0(44)	N(1) - C(N1) - C(N2)	98.3(47)
N(1) - C(N1) - C(N6)	108.6(52)	C(N2) - C(N1) - C(N6)	114.9(54)
C(N1) - C(N2) - C(N3)	97.5(52)	C(N2) - C(N3) - C(N4)	119.7(61)
C(N3) - C(N4) - C(N5)	97.2(54)		

Table 5.6. Crystallographic details of the structure analyses of compounds (2) and (3).

Compound	$[Pt_3(CO)(P(OPh)_3)(dppm)_3][PF_6]$	$[Pt_3(CO)(CNC_6H_{11})(dppm)_3][PF_6]_2$
Formula	$C_{94}H_{81}F_{12}O_4P_9Pt_3$	$C_{83}H_{77}F_{12}NOP_8Pt_3$*
Formula Wt.	2366.7	2165.6
Crystal habit	red plate	red plate
Crystal size, mm	0.36x0.24x0.16	0.64x0.52x0.44
Crystal system	monoclinic	triclinic
Space group	$P\ 2_1/c$	$P\ \bar{1}$
a, Å	19.239(6)	14.300(11)
b, Å	19.461(10)	14.614(7)
c, Å	26.137(10)	26.088(7)
α, °	—	79.79(4)
β, °	110.28(3)	79.99(5)
γ, °	—	65.91(5)
Obtained from	23 refln, $8<\theta<12°$	25 refln, $10<\theta<15°$
V, $Å^3$	9179(7)	4867(5)
Z	4	2
F(000)	4616	2104
d calc, gcm^{-3}	1.713	1.478
T, K	293	297
μ(Mo-Kα), cm^{-1}	48.4	45.4
Absorption factors on F^2	0.81-1.17	0.73-1.45
Scan width, °	0.80	0.80
Max count time, s	120	95
Total refln measured	12262	12472
Unique refln	9840	11885
R_{INT}	0.050	0.030
Miller indicies h	0→19	0→15
measured, k	-19→ 7	-15→15
l	-26→26	-27→27
2θ range, °	4-42	4-44
Unique refln ≥ 3σ(I)	3967	5803
No. of parameters	351	292
R	0.0475	0.1017
R_w	0.0545	0.1530
$\|\Delta\rho\|_{max}$, $eÅ^{-3}$	1.31	3.54
Δ/σ_{max}	0.099	0.058

* Actual model used in final refinement was $C_{82}F_6NP_8Pt_3$

CHAPTER 6: 46-ELECTRON DERIVATIVES OF $[Pt_3(CO)(DPPM)_3]^{2+}$

The addition reactions of small organosulphur molecules and of alkynes to $[Pt_3(CO)(dppm)_3]^{2+}$ (1),[50] are particularly important as models for reactions on Pt(111) surfaces because of the participation of these small molecules in catalytic processes. The strong affinity of sulphur for some transition metals can be responsible for the poisoning of heterogeneous catalysts, while alkynes participate in many catalytic reactions. Professor Puddephatt's group has synthesised a number of 46-electron cluster products involving addition of sulphur or an alkyne to the parent 42-electron cluster. Their characterisation by X-ray analysis described below and elsewhere,[51,62] has established that there are two structurally distinct types of 46-electron cluster, dependant upon the nature of the incoming ligand L.

When L is a bidentate, 4-electron donor ligand, such as $Me_2NCS_2^-$ (Tables 6.1-6.3) or a diphosphine,[63] it bridges one of the Pt-Pt bonds longitudinally. The same bond is also bridged by a doubly, rather than triply, bridging carbonyl. Apart from rupture of one Pt-CO bond the $Pt_3(CO)P_6$ cluster unit remains intact.

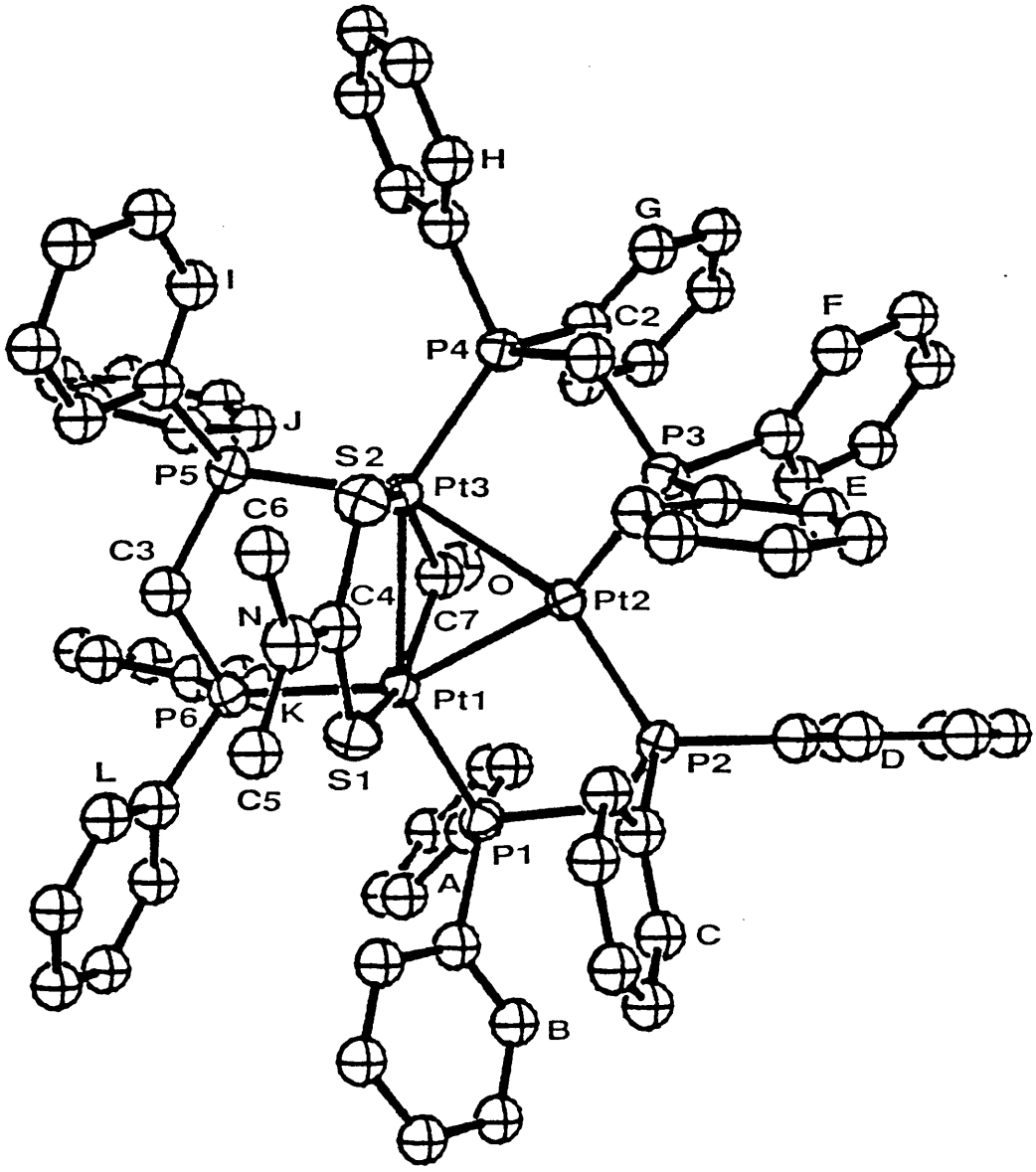
When L = HCCH (Tables 6.1, 6.4 and 6.5) or an organosulphur ligand,[51,62] the capping CO ligand is displaced by L which triply bridges the M_3 triangle. In this case the cluster geometry is more severely disrupted: two M-M bonds are ruptured and only the presence of the bridging dppm ligands stops disintegration of the cluster into mononuclear fragments.

Attachment of the dithiocarbamate ligand to the parent cluster (1) [50] produced the 46-electron species $[Pt_3(CO)(dppm)_3(S_2CNMe_2)]^+$ (2), (see Figure 6(a)). X-ray analysis of a crystal of the PF_6^- salt establishes that the unit cell contains equal numbers of the cation (2) and the anion $[PF_6]^-$ (see Experimental). Interionic distances are consistent with normal van der Waals radii.[52]

The incoming dithiocarbamate ligand is attached through Pt(1)-S(1) and Pt(3)-S(2) bonds of length 2.480(4) and 2.503(3) Å respectively, markedly shorter than the Pt-SCN ionic contact in Chapter 4 but still long for a Pt-S covalent bond. The lengths of such bonds are generally in the range 2.31-2.41 Å.[51] The C_2NCS_2 skeleton is approximately planar [C(5)NC(4)S(2) and C(6)NC(4)S(1) torsion angles are 176.3(15) and -176.1(14)° respectively], and the angle between the C(5)C(6)NC(4)S(1)S(2)Pt(1)Pt(3) and Pt(1)Pt(2)Pt(3) planes is 93.2°.

The average Pt-Pt bond length in (2), of 2.613(9) Å is comparable with those in (1) and in the 44-electron species discussed in previous chapters (see Tables 4.1 and 5.1), despite the presence of four more electrons than in the parent cation (1). The major effect of the extra electrons donated by the bidentate $S_2CNMe_2^-$ ligand is on the Pt-CO bonding. The bonds from carbonyl to Pt(1) and Pt(3), which are attached to the dithiocarbamate, have shortened significantly to 2.011(11) and 2.023(11) Å, compared with the corresponding mean Pt-C distance of 2.088(9) Å in (1), while the CO ligand is no longer attached to Pt(2). The carbonyl is now directly above the Pt(1)-Pt(3) edge and normal to the Pt_3 face (the angle between the Pt_3 and

Figure 6(a). The structure of cation (2). Hydrogen atoms are omitted and carbon atoms are presented as spheres of arbitrary size. 50% probability ellipsoids are used for all other atoms.



Pt(1)Pt(3)C(7)O planes being 90.1°).

The conformation of the $Pt_3(dppm)_3$ nucleus does not appear to be sterically constrained by the incoming ligand L = $S_2CNMe_2^-$ as it is by L = $P(OPh)_3$ (see Chapter 5): the Pt_3 face to which the dithiocarbamate is attached has four equatorial and two axial phenyl rings whereas there are six equatorial phenyl groups on the Pt_3 face carrying the phosphite (see Chapter 8). There appear to be three types of Pt-P bonds. The mean Pt(2)-P bond length is 2.245(3) Å, that for the Pt(1)-P and Pt(3)-P bonds *cis* to Pt(2) is longer at 2.304(3) Å, and the mean length of the Pt(1)-P and Pt(3)-P bonds which are *trans* to Pt(2) is longer still at 2.356(3) Å.

A structure similar to (2) is $[Pt_3(CO)(dmpm)_4]^{2+}$ (3) (dmpm = bis(dimethylphosphino)methane or $Me_2PCH_2PMe_2$),[63] also a 46-electron cluster. In this case the Pt_3 face with the extra dmpm ligand attached has six equatorial methyl groups (see Chapter 8). In (3) the CO ligand is μ_2-bonded, as in (2), and the Pt(1)Pt(3)C(5)O and Pt(1)Pt(3)P(7)P(8) planes are approximately normal to the Pt_3 plane (102 and 91° respectively). The average Pt-Pt bond length of 2.632(14) Å is comparable with the values for (1) and (2), and the latitudinal Pt-P bonds fall into the same three categories described for (2), average distances being 2.25, 2.29 and 2.33 Å respectively. The longest Pt-P bonds in (3) involve the longitudinal dmpm ligand, mean length 2.36 Å, which is consistent with the long Pt-S bonds found in (2).

These differences in the latitudinal Pt-P bonds are probably due to steric factors. The four-coordinate platinum atoms give the shortest bonds, as expected;

however, the reason for the difference in length of the two sets of Pt-P bonds involving the more highly substituted metal atoms is not so obvious. It is possible that the pseudo-axial Me/Ph substituents on P(5) and P(6) are subject to steric repulsion by the CO ligand. This would also explain why the effect is greater in (2) than (3). However, the different *trans*-influence experienced by the two sets of Pt-P bonds may also be significant.

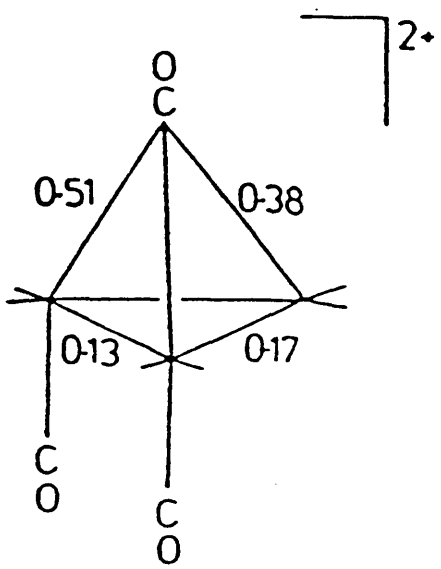


Figure 6(b). Mulliken population analysis of addition of two terminal CO ligands to the $Pt_3(\mu_3\text{-}CO)(dppm)_3^{2+}$ cation.

Structures (2) and (3) can be regarded as the products of the addition of two terminal 2-electron donor ligands to (1). Evans has performed EHMO calculations on such a 46-electron species formed by adding two terminal CO ligands to the parent cluster.[57] He predicts that population of the μ_3-CO π^* orbitals stabilises the attachment of incoming ligands to the M_3 triangle, resulting in the slipping of the μ_3-CO towards the pair of more highly substituted

platinum atoms (see Figure 6(b)). He also predicts only slight weakening of Pt-Pt bonds. A further calculation on $[Pt_3(dppm)_3(\mu_2\text{-}CO)(CO)_2]^{2+}$, where μ_2-CO is directly above the Pt-Pt edge, suggests that this model is Ø.2 eV more stable than the μ_3-CO isomer. This accords with the structures of (2) and (3).

Reaction of the monosulphur species H_2S and NCS^- with (1) gives products which are structurally different from (2) and (3). Thiocyanate reacts with $[Pd_3(\mu_3\text{-}CO)(dppm)_3]^{2+}$, (4)[1] first by attachment of the sulphur to the vacant face of the Pd_3 triangle, followed by cleavage of the S-C bond with transfer of CN to a Pd atom, loss of the CO and rupture of two Pd-Pd bonds.[51] When M = Pt, the second step is very slow and the intermediate SCN^- complex can be isolated (see Chapter 4). For M = Pd however, the second step is immediate and only $[Pd_3(S)(CN)(dppm)_3]^+$, (5) can be isolated.[51]

Reaction of H_2S with (1) gives a similar reaction,[62] the displacement of CO by sulphur, the rupture of two Pt-Pt bonds and attachment of hydrogen to the isolated platinum atom to give $[Pt_3(S)(H)(dppm)_3]^+$, (6). Similar reactions with molecules of type H_2E, E = Se, S, with (1) and (4), and HSR with (1), have also been observed using N.M.R.[62]

All the above structures are of the form $[M_3(\mu_3\text{-}S)(X)(dppm)_3]^+$ (see Figure 6(c)). The crystal structures of (5) and (6) show clearly there is only one M-M bond [length 2.579(1) and 2.597(4) Å respectively]. The other M-M distances [3.508(1) and 3.508(1) Å, and 3.574(2) and 3.678(7) Å respectively] are clearly non-bonding (Table 6.1). The side of the Pt_3 triangle with sulphur attached

has six equatorial dppm phenyl rings (see Chapter 8) in both (5) and (6) and ligand X is almost trans to the sulphur atom: 176.0(4)° for S-Pd-CN in (5) and 179(2)° for S-Pt-H in (6). The metal-sulphur bonds in (5) are equal at 2.297(3) Å whereas in (6) the Pt-S(trans to H) bond length of 2.375(6) Å is markedly longer than the others [2.294(5) and 2.311(3) Å] due to the high *trans* influence of hydrides.[51,62]

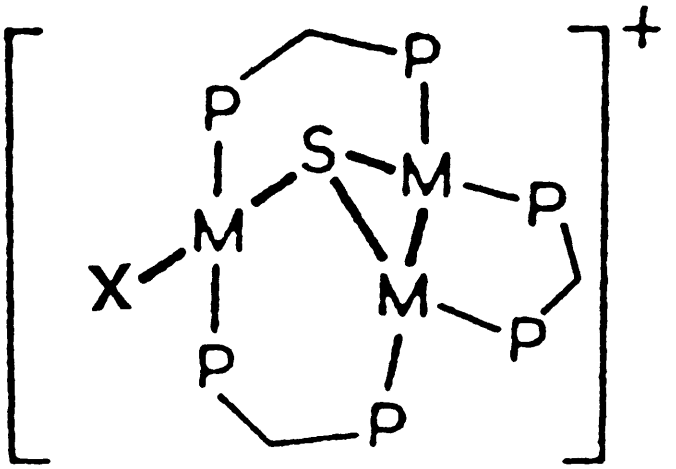


Figure 6(c). The structure of $[M_3(\mu_3\text{-}S)(X)(dppm)_3]^+$ cations.

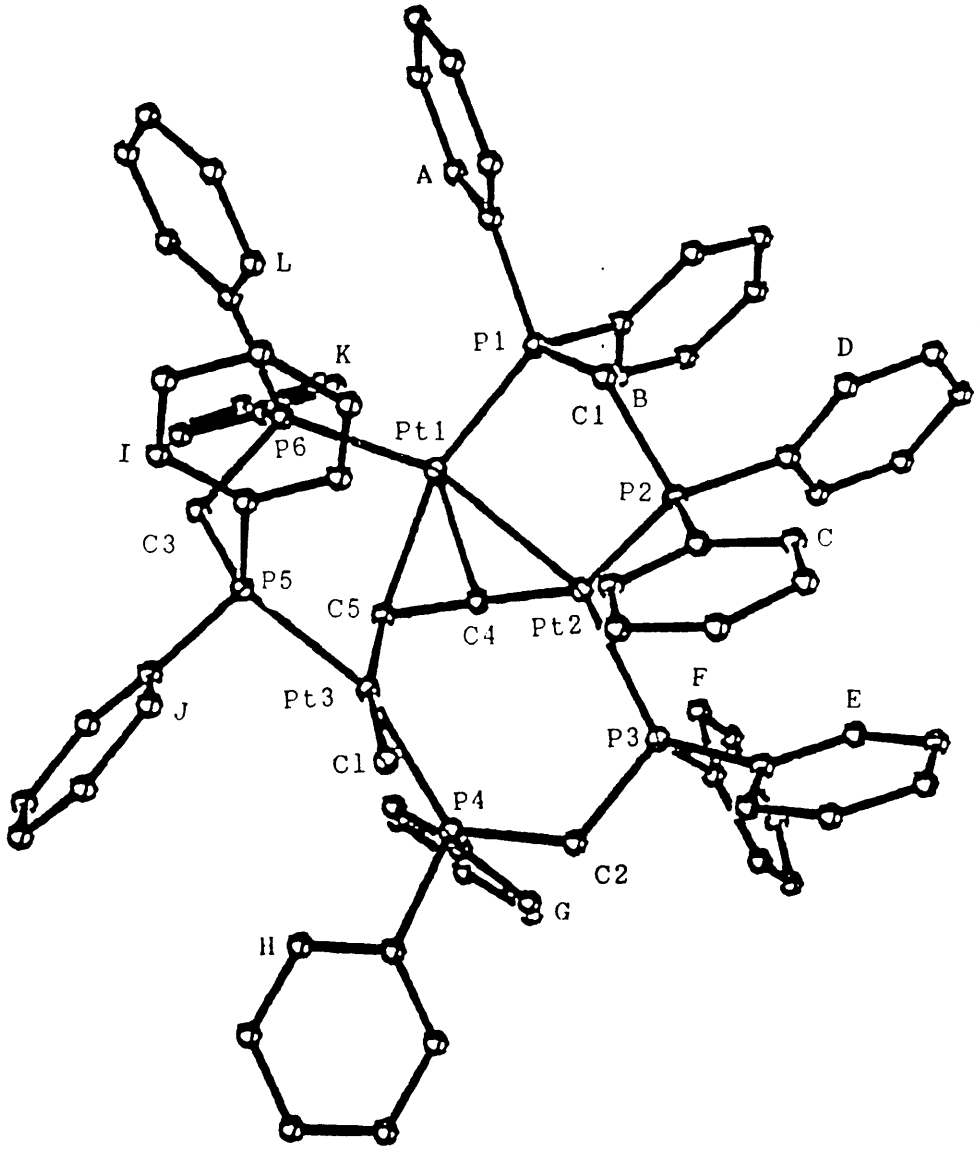
There are interesting similarities between the reaction of (1) with organosulphur compounds and the chemisorption of such compounds on Pt(111) surfaces. H_2S also displaces CO at Pt(111) surfaces with loss of hydrogen to give $Pt_3(\mu_3\text{-}S)$ units in which the Pt-S bond length of 2.28(3) Å found by LEED is comparable to the corresponding distances in μ_3-metal clusters.[28] However, addition of H_2S to (1) involves rupture of M-M bonds whereas there is no evidence that formation of $Pt_3(\mu_3\text{-}S)$ units on Pt(111) surfaces leads to weakening of the surface Pt-Pt bonds.[27,28]

The structures discussed here also provide confirmation of the important role of the capping CO ligand in stabilising these clusters. In 46-electron species which retain the CO ligand the M-M bonds retain their integrity whereas loss of the CO ligand and its empty π^* orbitals in the μ_3-S complexes involves rupture of two M-M bonds since anti-bonding cluster orbitals are now populated.

Addition of acetylene to (1) gives ultimately the cationic cluster $[Pt_3Cl(HC{\equiv}CH)(dppm)_3]^+$, (7) whose structure is shown in Figure 6(d). X-ray analysis of a crystal of the PF_6^- salt of (8) reveals that there are two distinct PF_6^- sites to one cation in each asymmetric unit. Both anion sites straddle crystallographic diad axes and one is disordered (see Experimental), giving overall a 1:1 ratio of cations to anions. Interionic contact distances are not significantly shorter than the sum of the appropriate van der Waals radii (Tables 6.1, 6.4 and 6.5).

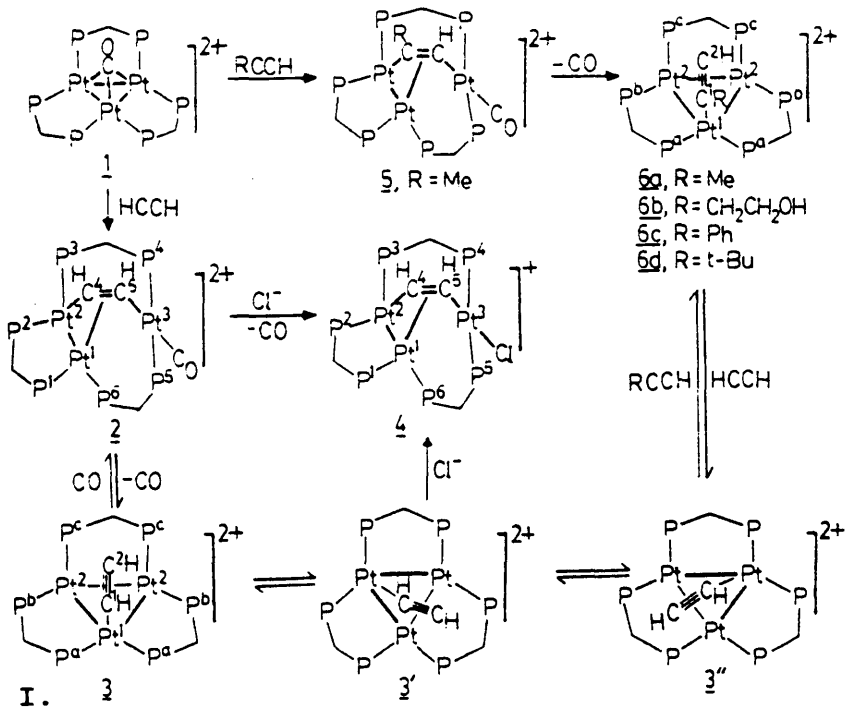
The Pt_3 triangle contains only one metal-metal bond, between Pt(1) and Pt(2) of length 2.631(2) Å. The other Pt...Pt distances [3.232(2) and 3.277(2) Å] are clearly non-bonding. The HC≡CH ligand lies over one face of the Pt_3 triangle. Each acetylenic carbon atom is σ-bonded to a platinum atom [Pt(2)-C(4) 2.05(3) Å and Pt(3)-C(5) 1.99(3)Å] and there is π-bonding between the acetylene and Pt(1) [Pt-C(4) 2.17(3) Å and Pt-C(5) 2.21(3) Å]. The chloro ligand is attached to the isolated Pt(3) atom and is *trans* to the acetylene [Pt(3)-Cl 2.408(9) Å]. The conformation of dppm ligands suggests there is little steric congestion within the cluster, the acetylene side of the Pt_3 triangle having two equatorial and four axial dppm

Figure 6(d). A view of the cation $[Pt_3Cl(HC{=}CH)(dppm)_3]^+$, (7). Hydrogen atoms are omitted for clarity and all other atoms are displayed as spheres of arbitrary size.



phenyl rings (see Chapter 8). Ring J is disordered (see Experimental), adopting two orientations [torsion angles Pt(3)-P(5)-C(J1)-C(J2) and Pt(3)-P(5)-C(SJ1)-C(SJ2) are 86(4) and 54(4)° respectively]. The Pt-P distances in (7) vary significantly from 2.241(9) to 2.333(8) Å but reasons for this are not obvious.

Scheme I shows the process by which acetylene dislodges the CO ligand in (1) to a terminal position. Subsequent replacement by chloride gives (7).[3] Reaction of acetylene with (1) and also with $[Pt_3(dppm)_3H]^+$, (8),[64] again suggests analogies with surface chemistry. The $Pt_3(HC{\equiv}CH)$ unit in (7) is an example of a μ_3-η^2-$\parallel$ bonding arrangement which is also favoured on Pt(111) surfaces. The alternative μ_3-η^2-$\perp$ arrangement is also found in clusters but not on surfaces.[3,26] N.M.R. studies of (8) have shown formation of the μ_3-η^2-$C{=}CH_2$ complex,[64] also found on Pt(111) surfaces after addition of acetylene.[26]



Scheme I.

The order of affinity of these small molecules for Pt_3 triangular units in clusters is the same as for Pt(111) surfaces: i.e. H_2S>HC≡CH>CO. Acetylene can displace CO, and H_2S can displace both CO and HC≡CH, while the reverse reactions do not occur.[3,64] It is possible, however, for one alkyne to replace another, as shown by the displacement of acetylene by propyne.

The breaking of Pt-Pt bonds in (7) can be ascribed to the population of antibonding orbitals, as with (5) and (6). In contrast, with $Pt_3(\mu_3\text{-}S)$ units, however, it has been suggested that when acetylene binds to a Pt(111) surface there is weakening of the Pt-Pt bonds,[65] but because metal atoms on a surface are held much tighter by lower layers and because they have a greater degree of coordinative unsaturation the effect is less marked.

Experimental

Because broadly similar methods were used for all analyses, full details are only given for the one analysis (see Experimental in Chapter 5). Any differences in procedure from that analysis are given below. Table 6.6 is a summary of the crystal data for the newly determined structures in this chapter.

$[Pt_3(CO)(S_2CNMe_2)(dppm)_3][PF_6]$ (2)

Data Collection. The crystal was mounted on a glass fibre and coated in araldite.

Structure Analysis. The phenyl hydrogen atoms contributed

to the group refinement of the C_6H_5 rings. The methyl and methylenic hydrogen atoms were constrained to ride on the parent carbon atoms with C-H = 0.96 Å. Hydrogen atom displacement parameters, U(H), were set at 1.2 times those of their parent carbon atoms and were not refined. Anisotropic displacement parameters were used for Pt, S, P and F atoms and isotropic parameters for all other atoms.

$[Pt_3Cl(HC{\equiv}CH)(dppm)_3][PF_6]$ (7)

Data Collection. The crystal was mounted on a glass fibre and coated in araldite.

Structure Analysis. Ring J (see Figure 6(d)) proved to be disordered and both orientations were refined as rigid groups (each with an occupancy of 0.5 and an isotropic group displacement parameter). All hydrogen atoms were placed in calculated positions, except those of the alkyne and of disordered ring J. Phenyl hydrogen atoms were included in group refinements of their respective rings, while the methylenic hydrogen atoms were constrained to ride on their parent carbon atoms. Pt, Cl and P atoms had anisotropic displacement parameters, with isotropic parameters for all others. U(H) values were set at and constrained to 1.2 times that of the parent carbon atoms. The two PF_6^- sites straddle two-fold axes but are crystallographically distinct. One phosphorus atom is on the axis (with occupancy 0.5) and as a consequence has only three independent fluorine atoms [F(71), F(72) and F(73)] associated with it. The other phosphorus site (occupancy 0.5) is disordered and is positioned just off the axis with

five associated fluorine sites: F(81), F(82), F(83), F(84), F(85), with occupancies of 1.0, 0.5, 0.5, 0.5 and 0.5 respectively.

Table 6.1. A comparison of selected bond distances (Å) of $[Pt_3(\mu_3\text{-}Y)(X)(dppm)_3]^{n+}$ structures.

M	Pt [62]	Pt	[a]Pd [51]
X	H	Cl	CN
Y	S	HCCH	S
Pt-Pt	2.597(4)	2.631(2)	2.579(1)
Pt...Pt	3.574(2)	3.232(2)	3.508(1)
Pt...Pt	3.678(7)	3.277(2)	-
Pt^{iso}-P	2.290(4)	2.33(1)	2.320(2)
	2.289(5)	2.25(1)	-
Pt-P(*trans* to Pt)	2.258(3)	2.24(1)	2.297(2)
	2.272(6)	2.28(1)	-
Pt-P(*cis* to Pt)	2.234(3)	2.25(1)	2.270(2)
	2.244(3)	2.28(1)	-
Pt^{iso}-X	2.15(8)	2.408(9)	2.059(12)
Pt^{iso}-S	2.375(6)		2.297(3)
Pt-S	2.294(5)		2.297(3)
	2.311(3)		-
Pt^{iso}-C_σ		1.99(3)	
Pt-C_σ		2.05(3)	
Pt-C_Π		2.17(3)	
Pt-C_Π		2.21(3)	

[a]Two Pt atoms are crystallographically eqivalent. Only one distance is listed for equivalent bonds.

Table 6.2. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of compound (2).

	X/A	Y/B	Z/C	U
PT(1)	.30328(2)	-.23601(3)	-.12626(1)	.028
PT(2)	.24238(2)	-.12841(3)	-.19044(1)	.029
PT(3)	.17035(2)	-.21360(3)	-.12533(1)	.027
S(1)	.32803(13)	-.08617(23)	-.07958(10)	.043
S(2)	.17351(13)	-.05513(22)	-.08085(10)	.040
P(1)	.39886(13)	-.26247(22)	-.17095(10)	.035
P(2)	.33917(13)	-.09260(22)	-.22866(9)	.032
P(3)	.15871(13)	-.03796(21)	-.22327(10)	.034
P(4)	.07265(12)	-.18084(21)	-.16901(9)	.031
P(5)	.15349(13)	-.28968(21)	-.05147(9)	.033
P(6)	.30893(13)	-.32700(22)	-.05547(9)	.033
P(7)	.72740(14)	.40578(27)	.36422(12)	.081
F(1)	.8054(2)	.4080(7)	.3614(3)	.131
F(2)	.6494(2)	.4036(7)	.3671(3)	.202
F(3)	.7307(6)	.4664(7)	.4097(2)	.166
F(4)	.7240(6)	.3452(7)	.3187(2)	.162
F(5)	.7314(2)	.3116(5)	.3935(3)	.117
F(6)	.7234(2)	.4999(5)	.3350(3)	.154
O	.2245(3)	-.3876(6)	-.1822(3)	.045(2)
N	.2627(4)	.0438(7)	-.0312(3)	.049(3)
C(1)	.3886(5)	-.2068(8)	-.2298(4)	.043(3)
C(2)	.0797(5)	-.0522(8)	-.1893(4)	.037(3)
C(3)	.2362(5)	-.2876(8)	-.0200(4)	.041(3)
C(4)	.2550(5)	-.0262(8)	-.0625(4)	.038(3)
C(5)	.3295(6)	.0714(10)	-.0106(4)	.065(4)
C(6)	.2043(6)	.0955(11)	-.0118(5)	.071(4)
C(7)	.2291(5)	-.3121(8)	-.1596(4)	.041(3)
C(A1)	.4145(6)	-.3908(4)	-.1856(4)	.040(3)
C(A2)	.4638(6)	-.4423(10)	-.1607(2)	.055(3)
C(A3)	.4699(3)	-.5421(10)	-.1669(4)	.068(4)
C(A4)	.4267(5)	-.5904(4)	-.1981(4)	.065(4)
C(A5)	.3775(5)	-.5388(10)	-.2230(2)	.072(4)
C(A6)	.3714(3)	-.4390(10)	-.2167(5)	.060(4)
C(B1)	.4821(5)	-.2182(11)	-.1496(3)	.046(3)
C(B2)	.5381(7)	-.2215(11)	-.1787(3)	.067(4)
C(B3)	.5998(5)	-.1839(4)	-.1634(4)	.078(4)
C(B4)	.6056(5)	-.1429(10)	-.1188(3)	.084(5)
C(B5)	.5496(7)	-.1396(8)	-.0897(3)	.095(5)
C(B6)	.4878(4)	-.1772(6)	-.1051(4)	.060(3)
C(C1)	.3930(6)	-.0004(8)	-.2014(2)	.036(3)
C(C2)	.4623(7)	.0054(5)	-.2095(4)	.051(3)
C(C3)	.5005(3)	.0790(7)	-.1888(4)	.059(3)
C(C4)	.4694(5)	.1470(7)	-.1600(2)	.055(3)
C(C5)	.4001(6)	.1413(4)	-.1519(4)	.068(4)
C(C6)	.3620(3)	.0676(8)	-.1726(3)	.049(3)
C(D1)	.3371(5)	-.0551(11)	-.2908(3)	.041(3)
C(D2)	.3321(7)	.0436(10)	-.3007(4)	.065(4)
C(D3)	.3310(5)	.0754(6)	-.3471(5)	.112(6)
C(D4)	.3348(4)	.0085(9)	-.3836(3)	.098(5)
C(D5)	.3398(7)	-.0902(8)	-.3737(4)	.087(5)
C(D6)	.3409(5)	-.1219(7)	-.3273(5)	.058(3)
C(E1)	.1743(6)	.0950(6)	-.2205(4)	.036(3)
C(E2)	.1822(7)	.1521(9)	-.2604(3)	.065(4)
C(E3)	.1969(4)	.2505(7)	-.2559(3)	.079(4)
C(E4)	.2035(5)	.2918(5)	-.2115(3)	.079(4)
C(E5)	.1956(6)	.2347(8)	-.1716(2)	.060(4)
C(E6)	.1809(3)	.1363(7)	-.1761(3)	.046(3)
C(F1)	.1303(6)	-.0600(10)	-.2843(2)	.038(3)
C(F2)	.0745(7)	-.0117(5)	-.3033(4)	.050(3)
C(F3)	.0505(3)	-.0363(8)	-.3479(4)	.062(4)
C(F4)	.0823(5)	-.1091(8)	-.3734(2)	.063(4)
C(F5)	.1381(5)	-.1574(4)	-.3543(4)	.062(4)
C(F6)	.1621(3)	-.1328(10)	-.3097(4)	.043(3)
C(G1)	.0540(7)	-.2467(9)	-.2238(2)	.035(3)
C(G2)	.0014(6)	-.2141(4)	-.2526(4)	.043(3)
C(G3)	-.0130(3)	-.2616(9)	-.2947(4)	.054(3)
C(G4)	.0252(6)	-.3417(8)	-.3080(2)	.060(3)
C(G5)	.0778(5)	-.3743(6)	-.2791(4)	.062(4)
C(G6)	.0922(4)	-.3268(10)	-.2371(4)	.052(3)
C(H1)	-.0129(4)	-.1871(7)	-.1424(4)	.040(3)
C(H2)	-.0511(5)	-.1057(6)	-.1310(2)	.056(3)
C(H3)	-.1163(5)	-.1168(5)	-.1137(4)	.077(4)

Table 6.2(cont).

	X/A	Y/B	Z/C	U
C(H4)	-.1432(3)	-.2092(6)	-.1078(3)	.069(4)
C(H5)	-.1051(5)	-.2906(5)	-.1191(3)	.059(4)
C(H6)	-.0399(6)	-.2796(6)	-.1364(5)	.049(3)
C(I1)	.0969(6)	-.2270(4)	-.0102(5)	.037(3)
C(I2)	.0301(7)	-.2146(9)	-.0251(3)	.054(3)
C(I3)	-.0145(4)	-.1606(10)	.0018(4)	.068(4)
C(I4)	.0076(5)	-.1189(4)	.0438(4)	.061(4)
C(I5)	.0744(6)	-.1313(9)	.0588(2)	.071(4)
C(I6)	.1190(3)	-.1854(10)	.0318(4)	.056(3)
C(J1)	.1258(6)	-.4172(6)	-.0493(4)	.043(3)
C(J2)	.1240(3)	-.4728(7)	-.0900(3)	.051(3)
C(J3)	.1045(6)	-.5698(9)	-.0881(3)	.071(4)
C(J4)	.0869(5)	-.6112(5)	-.0454(4)	.085(5)
C(J5)	.0887(4)	-.5556(8)	-.0046(2)	.102(5)
C(J6)	.1082(7)	-.4586(9)	-.0065(4)	.075(4)
C(K1)	.3024(6)	-.4614(5)	-.0569(4)	.040(3)
C(K2)	.3123(3)	-.5090(7)	-.0994(3)	.050(3)
C(K3)	.3091(6)	-.6098(7)	-.1014(3)	.058(3)
C(K4)	.2961(5)	-.6631(4)	-.0610(4)	.078(4)
C(K5)	.2862(4)	-.6155(7)	-.0186(2)	.081(4)
C(K6)	.2893(7)	-.5147(8)	-.0165(4)	.066(4)
C(L1)	.3833(5)	-.3097(12)	-.0159(4)	.039(3)
C(L2)	.3861(4)	-.2347(8)	.0167(5)	.050(3)
C(L3)	.4452(7)	-.2188(7)	.0427(4)	.070(4)
C(L4)	.5014(4)	-.2780(10)	.0360(3)	.076(4)
C(L5)	.4985(5)	-.3531(6)	.0034(5)	.075(4)
C(L6)	.4394(7)	-.3689(9)	-.0226(3)	.060(3)
H(11)	.36552	-.25264	-.25014	.051
H(12)	.43301	-.19341	-.24234	.051
H(21)	.04093	-.03583	-.20885	.045
H(22)	.08076	-.00931	-.16233	.045
H(31)	.23322	-.32991	.00699	.049
H(32)	.24472	-.22193	-.00940	.049
H(51)	.33508	.12282	.01227	.071
H(52)	.35700	.08909	-.03719	.071
H(53)	.34787	.01328	.00370	.071
H(61)	.20995	.14690	.01109	.079
H(62)	.17516	.04746	.00235	.079
H(63)	.18108	.12396	-.03856	.079
H(A2)	.49375	-.40876	-.13906	.071
H(A3)	.50409	-.57797	-.14962	.084
H(A4)	.43100	-.65981	-.20243	.077
H(A5)	.34750	-.57240	-.24462	.082
H(A6)	.33716	-.40318	-.23404	.068
H(B2)	.53406	-.24997	-.20974	.082
H(B3)	.63882	-.18624	-.18366	.096
H(B4)	.64860	-.11676	-.10818	.101
H(B5)	.55360	-.11112	-.05870	.104
H(B6)	.44885	-.17488	-.08477	.073
H(C2)	.48386	-.04191	-.22957	.059
H(C3)	.54862	.08301	-.19445	.070
H(C4)	.49594	.19825	-.14562	.064
H(C5)	.37853	.18852	-.13187	.077
H(C6)	.31378	.06357	-.16697	.056
H(D2)	.32942	.09016	-.27535	.077
H(D3)	.32748	.14405	-.35401	.122
H(D4)	.33401	.03062	-.41587	.121
H(D5)	.34246	-.13670	-.39908	.097
H(D6)	.34436	-.19061	-.32046	.071
H(E2)	.17752	.12338	-.29130	.077
H(E3)	.20240	.29019	-.28361	.093
H(E4)	.21371	.36027	-.20835	.089
H(E5)	.20021	.26350	-.14073	.072

Table 6.2(cont).

	X/A	Y/B	Z/C	U
H(E6)	.17533	.09666	-.14840	.053
H(F2)	.05245	.03892	-.28560	.057
H(F3)	.01174	-.00276	-.36115	.077
H(F4)	.06558	-.12626	-.40435	.072
H(F5)	.16016	-.20804	-.37200	.075
H(F6)	.20088	-.16634	-.29646	.054
H(G2)	-.02523	-.15835	-.24341	.050
H(G3)	-.04967	-.23885	-.31474	.067
H(G4)	.01514	-.37471	-.33722	.071
H(G5)	.10437	-.43003	-.28836	.072
H(G6)	.12885	-.34951	-.21706	.061
H(H2)	-.03234	-.04142	-.13519	.069
H(H3)	-.14285	-.06015	-.10584	.088
H(H4)	-.18857	-.21690	-.09575	.081
H(H5)	-.12383	-.35494	-.11498	.069
H(H6)	-.01332	-.33623	-.14435	.060
H(I2)	.01471	-.24355	-.05433	.063
H(I3)	-.06096	-.15194	-.00856	.077
H(I4)	-.02340	-.08131	.06256	.074
H(I5)	.08979	-.10235	.08796	.087
H(I6)	.16546	-.19398	.04219	.067
H(J2)	.13620	-.44397	-.11976	.061
H(J3)	.10322	-.60844	-.11652	.087
H(J4)	.07331	-.67868	-.04408	.100
H(J5)	.07644	-.58446	.02511	.119
H(J6)	.10945	-.41996	.02184	.089
H(K2)	.32134	-.47190	-.12748	.061
H(K3)	.31603	-.64287	-.13098	.070
H(K4)	.29392	-.73320	-.06245	.088
H(K5)	.27717	-.65258	.00956	.093
H(K6)	.28247	-.48161	.01308	.078
H(L2)	.34705	-.19348	.02137	.061
H(L3)	.44722	-.16660	.06544	.079
H(L4)	.54247	-.26698	.05413	.089
H(L5)	.53757	-.39424	-.00126	.096
H(L6)	.43742	-.42113	-.04533	.075

Anisotropic displacement parameters ($\mathring{A}^2$).

	U11	U22	U33	U12	U13	U23
PT(1)	.0270(2)	.0284(3)	.0274(2)	.0031(2)	.0000(2)	.0012(2)
PT(2)	.0281(2)	.0279(3)	.0295(2)	.0017(2)	0.0000(2)	.0037(2)
PT(3)	.0275(2)	.0274(3)	.0270(2)	.0016(2)	.0008(2)	-.0007(2)
S(1)	.040(2)	.040(2)	.048(2)	0.000(1)	-.004(1)	-.007(2)
S(2)	.043(2)	.036(2)	.043(2)	.004(1)	0.000(1)	-.009(1)
P(1)	.033(1)	.035(2)	.037(2)	.003(1)	.005(1)	.002(1)
P(2)	.033(1)	.033(2)	.029(2)	-.001(1)	.003(1)	.003(1)
P(3)	.036(1)	.026(2)	.039(2)	.001(1)	-.002(1)	.002(1)
P(4)	.030(1)	.028(2)	.037(2)	.002(1)	-.001(1)	-.002(1)
P(5)	.037(2)	.032(2)	.030(2)	-.002(1)	.003(1)	.000(1)
P(6)	.037(1)	.032(2)	.031(2)	.001(1)	-.003(1)	.004(1)
F(7)	.067(3)	.077(3)	.100(3)	.014(2)	-.017(2)	-.006(3)
F(1)	.070(6)	.165(11)	.158(9)	.011(7)	.009(6)	-.007(9)
F(2)	.052(5)	.227(16)	.326(17)	.008(8)	-.016(8)	.089(14)
F(3)	.166(10)	.201(14)	.133(9)	.050(10)	.002(8)	-.085(10)
F(4)	.271(15)	.122(10)	.093(7)	-.038(10)	-.045(9)	-.016(7)
F(5)	.125(8)	.094(8)	.131(8)	.003(7)	-.001(6)	.009(7)
F(6)	.208(12)	.100(9)	.154(10)	.042(9)	-.014(9)	.038(8)

Table 6.3. Selected bond distances (Å) and angles (°) of complex (2).

PT(1)	PT(2)	2.612(1)	PT(1)	PT(3)	2.622(1)
PT(1)	S(1)	2.480(4)	PT(1)	P(1)	2.298(3)
PT(1)	P(6)	2.356(3)	PT(1)	C(7)	2.011(11)
PT(2)	PT(3)	2.605(1)	PT(2)	P(2)	2.246(3)
PT(2)	P(3)	2.244(3)	PT(3)	S(2)	2.503(3)
PT(3)	P(4)	2.309(3)	PT(3)	P(5)	2.357(3)
PT(3)	C(7)	2.023(11)	S(1)	C(4)	1.722(11)
S(2)	C(4)	1.719(10)	P(1)	C(1)	1.836(12)
P(1)	C(A1)	1.828(8)	P(1)	C(B1)	1.834(12)
P(2)	C(1)	1.837(12)	P(2)	C(C1)	1.809(12)
P(2)	C(D1)	1.829(10)	P(3)	C(2)	1.841(10)
P(3)	C(E1)	1.844(9)	P(3)	C(F1)	1.829(7)
P(4)	C(2)	1.854(12)	P(4)	C(G1)	1.824(9)
P(4)	C(H1)	1.846(8)	P(5)	C(3)	1.838(11)
P(5)	C(I1)	1.831(13)	P(5)	C(J1)	1.826(9)
P(6)	C(3)	1.831(11)	P(6)	C(K1)	1.841(7)
P(6)	C(L1)	1.840(11)	O	C(7)	1.217(14)
N	C(4)	1.310(15)	N	C(5)	1.473(16)
N	C(6)	1.456(16)			

PT(2)	PT(1)	PT(3)	59.7(1)	PT(2)	PT(1)	S(1)	89.4(1)
PT(2)	PT(1)	P(1)	94.3(1)	PT(2)	PT(1)	P(6)	154.5(1)
PT(2)	PT(1)	C(7)	69.2(4)	PT(3)	PT(1)	S(1)	95.0(1)
PT(3)	PT(1)	P(1)	147.0(1)	PT(3)	PT(1)	P(6)	95.2(1)
PT(3)	PT(1)	C(7)	49.7(4)	S(1)	PT(1)	P(1)	105.4(1)
S(1)	PT(1)	P(6)	88.7(1)	S(1)	PT(1)	C(7)	144.2(4)
P(1)	PT(1)	P(6)	110.6(1)	P(1)	PT(1)	C(7)	104.5(4)
P(6)	PT(1)	C(7)	98.7(4)	PT(1)	PT(2)	PT(3)	60.3(1)
PT(1)	PT(2)	P(2)	94.3(1)	PT(1)	PT(2)	P(3)	157.3(1)
PT(3)	PT(2)	P(2)	154.6(1)	PT(3)	PT(2)	P(3)	98.0(1)
P(2)	PT(2)	P(3)	107.3(1)	PT(1)	PT(3)	PT(2)	60.0(1)
PT(1)	PT(3)	S(2)	95.0(1)	PT(1)	PT(3)	P(4)	146.5(1)
PT(1)	PT(3)	P(5)	96.1(1)	PT(1)	PT(3)	C(7)	49.3(3)
PT(2)	PT(3)	S(2)	87.6(1)	PT(2)	PT(3)	P(4)	89.3(1)
PT(2)	PT(3)	P(5)	154.7(1)	PT(2)	PT(3)	C(7)	69.2(4)
S(2)	PT(3)	P(4)	96.7(1)	S(2)	PT(3)	P(5)	86.6(1)
S(2)	PT(3)	C(7)	143.5(4)	P(4)	PT(3)	P(5)	115.8(1)
P(4)	PT(3)	C(7)	110.2(3)	P(5)	PT(3)	C(7)	102.4(4)
PT(1)	S(1)	C(4)	112.6(4)	PT(3)	S(2)	C(4)	111.6(4)
PT(1)	P(1)	C(1)	110.5(4)	PT(1)	P(1)	C(A1)	114.5(5)
PT(1)	P(1)	C(B1)	119.6(4)	C(1)	P(1)	C(A1)	102.1(6)
C(1)	P(1)	C(B1)	104.4(5)	C(A1)	P(1)	C(B1)	103.9(7)
PT(2)	P(2)	C(1)	105.7(4)	PT(2)	P(2)	C(C1)	116.0(4)
PT(2)	P(2)	C(D1)	120.8(4)	C(1)	P(2)	C(C1)	107.1(6)
C(1)	P(2)	C(D1)	103.2(6)	C(C1)	P(2)	C(D1)	102.7(5)
PT(2)	P(3)	C(2)	109.9(4)	PT(2)	P(3)	C(E1)	113.9(4)
PT(2)	P(3)	C(F1)	120.8(5)	C(2)	P(3)	C(E1)	102.8(6)
C(2)	P(3)	C(F1)	103.0(5)	C(E1)	P(3)	C(F1)	104.5(6)
PT(3)	P(4)	C(2)	106.6(4)	PT(3)	P(4)	C(G1)	121.0(5)
PT(3)	P(4)	C(H1)	121.6(4)	C(2)	P(4)	C(G1)	102.7(5)
C(2)	P(4)	C(H1)	103.9(5)	C(G1)	P(4)	C(H1)	98.6(6)
PT(3)	P(5)	C(3)	106.8(4)	PT(3)	P(5)	C(I1)	116.7(4)
PT(3)	P(5)	C(J1)	119.7(4)	C(3)	P(5)	C(I1)	102.8(6)
C(3)	P(5)	C(J1)	105.0(6)	C(I1)	P(5)	C(J1)	104.0(5)
PT(1)	P(6)	C(3)	106.2(4)	PT(1)	P(6)	C(K1)	120.3(5)
PT(1)	P(6)	C(L1)	118.5(5)	C(3)	P(6)	C(K1)	104.5(6)
C(3)	P(6)	C(L1)	104.2(5)	C(K1)	P(6)	C(L1)	101.3(7)
C(4)	N	C(5)	123.3(10)	C(4)	N	C(6)	121.5(10)
C(5)	N	C(6)	115.1(10)	P(1)	C(1)	P(2)	112.9(6)
P(3)	C(2)	P(4)	109.1(6)	P(5)	C(3)	P(6)	114.7(6)
S(1)	C(4)	S(2)	125.3(7)	S(1)	C(4)	N	116.5(8)
S(2)	C(4)	N	118.1(8)	PT(1)	C(7)	PT(3)	81.1(5)
PT(1)	C(7)	O	137.1(8)	PT(3)	C(7)	O	140.9(8)

Table 6.4. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of compound (7).

	X/A	Y/B	Z/C	U
PT(1)	.23817(6)	.34653(4)	-.19976(5)	.051
PT(2)	.30558(6)	.26932(5)	-.20803(4)	.050
PT(3)	.36899(6)	.36581(5)	-.15848(5)	.057
CL(1)	.4536(4)	.3741(3)	-.2129(4)	.092
P(1)	.1974(4)	.3204(3)	-.2741(3)	.069
P(2)	.2994(4)	.2552(4)	-.2949(3)	.077
P(3)	.3793(4)	.2199(3)	-.1864(3)	.050
P(4)	.4182(4)	.3045(3)	-.1134(3)	.048
P(5)	.3365(4)	.4406(4)	-.1792(4)	.092
P(6)	.2046(4)	.4215(3)	-.1753(3)	.061
P(7)	.7500	.0364(17)	.0000	.298
P(8)	.2754(11)	.0532(7)	-.4851(8)	.083
F(71)	.8135(24)	.0353(17)	.9790(18)	.32(3)
F(72)	.7604(24)	.0801(20)	1.0437(19)	.37(3)
F(73)	.7633(30)	-.0078(23)	1.0354(22)	.44(4)
F(81)	.2193(15)	.0524(11)	-.4609(13)	.201(13)
F(82)	.2718(16)	-.0036(13)	-.4840(12)	.089(12)
F(83)	.3343(24)	.0445(17)	-.4897(17)	.135(17)
F(84)	.2500	.1080(22)	-.5000	.274(24)
F(85)	.2774(21)	.0478(16)	-.4229(17)	.135(17)
C(1)	.2502(14)	.3024(10)	-.3219(10)	.062(9)
C(2)	.4399(11)	.2537(9)	-.1572(9)	.042(8)
C(3)	.2659(15)	.4574(12)	-.1498(12)	.086(11)
C(4)	.2760(12)	.3002(10)	-.1402(10)	.053(9)
C(5)	.2920(12)	.3483(11)	-.1286(10)	.056(9)
C(A1)	.1464(9)	.3582(15)	-.3099(18)	.100(13)
C(A2)	.0947(14)	.3679(12)	-.2846(9)	.075(10)
C(A3)	.0531(14)	.3966(7)	-.3082(14)	.105(13)
C(A4)	.0631(9)	.4156(12)	-.3571(15)	.144(17)
C(A5)	.1147(14)	.4059(9)	-.3824(7)	.134(16)
C(A6)	.1564(15)	.3772(10)	-.3588(17)	.136(16)
C(B1)	.1522(12)	.2679(8)	-.2616(8)	.059(9)
C(B2)	.1448(16)	.2488(13)	-.2124(7)	.076(10)
C(B3)	.1121(11)	.2071(11)	-.2054(8)	.084(11)
C(B4)	.0869(10)	.1844(7)	-.2478(8)	.091(11)
C(B5)	.0944(15)	.2035(12)	-.2970(6)	.099(12)
C(B6)	.1270(9)	.2452(10)	-.3039(8)	.086(11)
C(C1)	.3625(12)	.2618(10)	-.3356(13)	.099(12)
C(C2)	.3789(18)	.2300(14)	-.3746(8)	.144(16)
C(C3)	.4286(22)	.2390(11)	-.4032(14)	.170(20)
C(C4)	.4619(11)	.2797(10)	-.3928(11)	.150(17)
C(C5)	.4456(19)	.3115(13)	-.3538(10)	.157(18)
C(C6)	.3959(23)	.3026(10)	-.3252(15)	.092(12)
C(D1)	.2656(17)	.2008(12)	-.3115(11)	.093(12)
C(D2)	.2515(7)	.1916(10)	-.3628(11)	.126(15)
C(D3)	.2244(15)	.1484(15)	-.3761(8)	.148(17)
C(D4)	.2115(15)	.1144(11)	-.3382(10)	.105(13)
C(D5)	.2256(9)	.1237(11)	-.2869(10)	.128(15)
C(D6)	.2526(18)	.1669(16)	-.2736(7)	.102(13)
C(E1)	.4197(17)	.1863(8)	-.2362(12)	.055(9)
C(E2)	.3976(8)	.1423(7)	-.2533(9)	.103(12)
C(E3)	.4232(14)	.1185(9)	-.2947(8)	.136(15)
C(E4)	.4710(14)	.1387(7)	-.3191(10)	.095(12)
C(E5)	.4931(8)	.1827(8)	-.3020(7)	.069(10)
C(E6)	.4675(17)	.2064(10)	-.2606(10)	.069(10)
C(F1)	.3607(7)	.1706(7)	-.1423(7)	.046(8)
C(F2)	.3045(10)	.1690(11)	-.1235(14)	.085(11)
C(F3)	.2890(10)	.1342(10)	-.0872(11)	.108(13)
C(F4)	.3298(7)	.1011(7)	-.0696(7)	.085(11)
C(F5)	.3860(10)	.1028(11)	-.0884(13)	.102(13)
C(F6)	.4015(9)	.1375(9)	-.1248(11)	.079(10)
C(G1)	.3873(10)	.2775(8)	-.0547(5)	.047(8)
C(G2)	.4029(14)	.2317(6)	-.0372(12)	.070(10)
C(G3)	.3788(10)	.2134(8)	.0079(12)	.100(12)
C(G4)	.3393(9)	.2410(7)	.0357(5)	.093(12)
C(G5)	.3237(13)	.2868(6)	.0182(12)	.068(10)
C(G6)	.3478(9)	.3051(9)	-.0269(12)	.058(9)
C(H1)	.4877(13)	.3247(15)	-.0860(7)	.063(9)
C(H2)	.4971(9)	.3745(14)	-.0868(13)	.079(11)
C(H3)	.5481(14)	.3934(6)	-.0670(11)	.134(16)

Table 6.4(cont).

	X/A	Y/B	Z/C	U
C(H4)	.5897(11)	.3627(13)	-.0464(7)	.091(11)
C(H5)	.5803(11)	.3130(12)	-.0456(12)	.085(11)
C(H6)	.5292(16)	.2940(8)	-.0653(10)	.083(11)
C(I1)	.3305(12)	.4607(18)	-.2448(10)	.084(11)
C(I2)	.3232(19)	.5091(15)	-.2580(13)	.111(13)
C(I3)	.3169(14)	.5223(9)	-.3095(16)	.124(15)
C(I4)	.3179(11)	.4870(15)	-.3478(9)	.166(19)
C(I5)	.3252(18)	.4386(12)	-.3346(14)	.134(16)
C(I6)	.3315(12)	.4255(12)	-.2831(17)	.115(14)
C(J1)	.3920(24)	.4802(22)	-.1597(14)	.059(8)
C(J2)	.4373(30)	.4888(21)	-.1937(13)	.059
C(J3)	.4860(19)	.5137(10)	-.1770(17)	.059
C(J4)	.4895(24)	.5300(22)	-.1263(14)	.059
C(J5)	.4442(30)	.5213(21)	-.0923(13)	.059
C(J6)	.3955(19)	.4965(10)	-.1090(17)	.059
C(SJ1)	.3845(31)	.4922(23)	-.1307(10)	.068(8)
C(SJ2)	.4441(34)	.4872(10)	-.1344(23)	.068
C(SJ3)	.4802(16)	.5185(22)	-.1073(24)	.068
C(SJ4)	.4567(31)	.5547(23)	-.0766(10)	.068
C(SJ5)	.3971(34)	.5597(10)	-.0729(23)	.068
C(SJ6)	.3610(16)	.5285(22)	-.1000(24)	.068
C(K1)	.1562(11)	.4150(7)	-.1188(9)	.046(8)
C(K2)	.1212(17)	.3742(10)	-.1163(10)	.073(10)
C(K3)	.0843(12)	.3677(9)	-.0745(7)	.091(11)
C(K4)	.0824(10)	.4020(6)	-.0352(8)	.081(11)
C(K5)	.1174(15)	.4428(10)	-.0378(9)	.091(12)
C(K6)	.1543(11)	.4493(9)	-.0796(6)	.096(12)
C(L1)	.1669(8)	.4658(15)	-.2180(18)	.063(10)
C(L2)	.1857(16)	.4693(10)	-.2689(20)	.078(11)
C(L3)	.1599(16)	.5023(10)	-.3023(11)	.123(15)
C(L4)	.1153(8)	.5318(13)	-.2848(15)	.163(19)
C(L5)	.0965(16)	.5283(8)	-.2340(17)	.191(22)
C(L6)	.1223(16)	.4953(13)	-.2006(8)	.152(17)
H(11)	.27245	.33038	-.33244	.125
H(12)	.23031	.28940	-.35165	.125
H(21)	.46220	.26739	-.18519	.159
H(22)	.46385	.23129	-.13813	.159
H(31)	.25861	.49134	-.15630	.169
H(32)	.26819	.45218	-.11292	.169
H(A2)	.08776	.35470	-.25053	.090
H(A3)	.01712	.40336	-.29056	.126
H(A4)	.03407	.43554	-.37352	.173
H(A5)	.12169	.41909	-.41642	.160
H(A6)	.19234	.37041	-.37636	.163
H(B2)	.16235	.26457	-.18294	.091
H(B3)	.10690	.19379	-.17116	.101
H(B4)	.06421	.15536	-.24294	.110
H(B5)	.07686	.18768	-.32643	.119
H(B6)	.13225	.25847	-.33819	.103
H(C2)	.35570	.20171	-.38179	.173
H(C3)	.43994	.21682	-.43026	.204
H(C4)	.49650	.28585	-.41268	.179
H(C5)	.46878	.33983	-.34657	.188
H(C6)	.38449	.32469	-.29810	.110
H(D2)	.26045	.21518	-.38917	.152
H(D3)	.21462	.14194	-.41177	.178
H(D4)	.19268	.08438	-.34746	.126
H(D5)	.21654	.10006	-.26055	.153
H(D6)	.26239	.17330	-.23795	.122
H(E2)	.36434	.12822	-.23635	.124
H(E3)	.40780	.08789	-.30659	.164
H(E4)	.48880	.12219	-.34788	.114
H(E5)	.52636	.19670	-.31895	.083
H(E6)	.48295	.23703	-.24873	.082
H(F2)	.27610	.19197	-.13574	.102
H(F3)	.24992	.13310	-.07410	.129
H(F4)	.31908	.07701	-.04428	.102
H(F5)	.41436	.07978	-.07613	.123

Table 6.4(cont).

	X/A	Y/B	Z/C	U
H(F6)	.44055	.13860	-.13784	.095
H(G2)	.43039	.21259	-.05653	.084
H(G3)	.38957	.18156	.02003	.120
H(G4)	.32255	.22827	.06713	.112
H(G5)	.29621	.30594	.03754	.082
H(G6)	.33699	.33695	-.03905	.070
H(H2)	.46818	.39584	-.10115	.095
H(H3)	.55470	.42801	-.06758	.161
H(H4)	.62521	.37587	-.03263	.109
H(H5)	.60918	.29157	-.03122	.102
H(H6)	.52268	.25941	-.06478	.100
H(I2)	.32245	.53364	-.23133	.133
H(I3)	.31180	.55596	-.31872	.149
H(I4)	.31348	.49617	-.38368	.199
H(I5)	.32592	.41408	-.36130	.161
H(I6)	.33661	.39178	-.27393	.139
H(K2)	.12244	.35032	-.14362	.087
H(K3)	.05992	.33927	-.07278	.109
H(K4)	.05677	.39743	-.00614	.097
H(K5)	.11614	.46670	-.01050	.109
H(K6)	.17872	.47770	-.08136	.115
H(L2)	.21672	.44884	-.28102	.093
H(L3)	.17299	.50473	-.33766	.148
H(L4)	.09739	.55471	-.30805	.196
H(L5)	.06548	.54877	-.22183	.229
H(L6)	.10922	.49290	-.16517	.183

Anisotropic displacement parameters ($\AA^2$).

	U11	U22	U33	U12	U13	U23
PT(1)	.0520(9)	.0522(8)	.0502(7)	-.0061(8)	-.0117(7)	.0001(7)
PT(2)	.0585(9)	.0504(8)	.0403(7)	-.0043(8)	-.0081(7)	-.0083(7)
PT(3)	.0472(8)	.0499(8)	.0748(9)	.0000(9)	.0034(8)	.0077(8)
CL(1)	.060(6)	.094(7)	.123(8)	.017(6)	.030(6)	.040(6)
P(1)	.089(8)	.075(7)	.044(5)	.005(7)	-.025(5)	.002(5)
P(2)	.081(7)	.098(8)	.053(5)	.004(7)	-.007(6)	-.014(6)
P(3)	.056(6)	.042(5)	.052(5)	-.002(5)	.000(4)	-.010(4)
P(4)	.044(6)	.063(6)	.036(5)	-.003(5)	-.004(4)	-.014(4)
P(5)	.048(7)	.060(7)	.167(10)	-.012(6)	-.004(7)	.028(7)
P(6)	.035(6)	.057(6)	.091(6)	-.007(5)	-.010(5)	.006(5)
P(7)	.26(6)	.22(4)	.41(6)	.00	.06(5)	.00
P(8)	.10(2)	.07(1)	.07(2)	.04(1)	.01(1)	.02(1)

Table 6.5. Selected bond distances (Å) and angles (°) of complex (7).

PT(1) - PT(2)	2.631(2)	PT(1) - P(1)	2.245(9)
PT(1) - P(6)	2.283(9)	PT(1) - C(4)	2.17(3)
PT(1) - C(5)	2.21(3)	PT(2) - P(2)	2.271(9)
PT(2) - P(3)	2.241(9)	PT(2) - C(4)	2.05(3)
PT(3) - CL(1)	2.408(9)	PT(3) - P(4)	2.333(8)
PT(3) - P(5)	2.246(10)	PT(3) - C(5)	1.99(3)
P(1) - C(1)	1.80(4)	P(1) - C(A1)	1.81(4)
P(1) - C(B1)	1.80(3)	P(2) - C(1)	1.85(4)
P(2) - C(C1)	1.80(4)	P(2) - C(D1)	1.73(4)
P(3) - C(2)	1.83(3)	P(3) - C(E1)	1.83(4)
P(3) - C(F1)	1.81(3)	P(4) - C(2)	1.86(3)
P(4) - C(G1)	1.82(2)	P(4) - C(H1)	1.83(4)
P(5) - C(3)	1.85(4)	P(5) - C(I1)	1.78(4)
P(5) - C(J1)	1.75(6)	P(6) - C(3)	1.84(4)
P(6) - C(K1)	1.84(3)	P(6) - C(L1)	1.85(5)
P(7) - F(71)	1.56(15)	P(7) - F(72)	1.66(12)
P(7) - F(73)	1.55(12)	P(8) - F(81)	1.43(5)
P(8) - F(81')	1.39(4)	P(8) - F(82)	1.56(5)
P(8) - F(83)	1.38(7)	P(8) - F(84)	1.66(6)
P(8) - F(85)	1.60(5)	C(4) - C(5)	1.40(4)

PT(2) - PT(1) - P(1)	85.4(3)	PT(2) - PT(1) - P(6)	160.9(3)
PT(2) - PT(1) - C(4)	49.5(8)	PT(2) - PT(1) - C(5)	75.8(8)
P(1) - PT(1) - P(6)	112.3(4)	P(1) - PT(1) - C(4)	125.5(8)
P(1) - PT(1) - C(5)	161.0(8)	P(6) - PT(1) - C(4)	117.9(8)
P(6) - PT(1) - C(5)	86.7(8)	C(4) - PT(1) - C(5)	37.3(11)
PT(1) - PT(2) - P(2)	100.3(3)	PT(1) - PT(2) - P(3)	155.8(2)
PT(1) - PT(2) - C(4)	53.5(8)	P(2) - PT(2) - P(3)	100.9(4)
P(2) - PT(2) - C(4)	152.1(9)	P(3) - PT(2) - C(4)	106.8(8)
CL(1) - PT(3) - P(4)	88.0(3)	CL(1) - PT(3) - P(5)	92.5(4)
CL(1) - PT(3) - C(5)	165.2(9)	P(4) - PT(3) - P(5)	159.4(4)
P(4) - PT(3) - C(5)	93.8(9)	P(5) - PT(3) - C(5)	90.9(9)
PT(1) - P(1) - C(1)	112.8(11)	PT(1) - P(1) - C(A1)	121.2(15)
PT(1) - P(1) - C(B1)	110.0(8)	C(1) - P(1) - C(A1)	104.3(17)
C(1) - P(1) - C(B1)	107.0(13)	C(A1) - P(1) - C(B1)	100.0(14)
PT(2) - P(2) - C(1)	106.7(10)	PT(2) - P(2) - C(C1)	120.2(12)
PT(2) - P(2) - C(D1)	114.6(11)	C(1) - P(2) - C(C1)	101.8(14)
C(1) - P(2) - C(D1)	103.6(16)	C(C1) - P(2) - C(D1)	107.8(16)
PT(2) - P(3) - C(2)	111.7(9)	PT(2) - P(3) - C(E1)	120.9(11)
PT(2) - P(3) - C(F1)	115.3(7)	C(2) - P(3) - C(E1)	98.9(15)
C(2) - P(3) - C(F1)	107.5(11)	C(E1) - P(3) - C(F1)	100.5(11)
PT(3) - P(4) - C(2)	111.6(9)	PT(3) - P(4) - C(G1)	120.9(9)
PT(3) - P(4) - C(H1)	113.4(13)	C(2) - P(4) - C(G1)	107.5(11)
C(2) - P(4) - C(H1)	103.1(14)	C(G1) - P(4) - C(H1)	98.2(11)
PT(3) - P(5) - C(3)	115.0(11)	PT(3) - P(5) - C(I1)	122.2(16)
PT(3) - P(5) - C(J1)	104.8(20)	C(3) - P(5) - C(I1)	104.0(15)
C(3) - P(5) - C(J1)	111.7(21)	C(I1) - P(5) - C(J1)	97.8(19)
PT(1) - P(6) - C(3)	108.7(12)	PT(1) - P(6) - C(K1)	109.5(7)
PT(1) - P(6) - C(L1)	125.8(15)	C(3) - P(6) - C(K1)	103.6(13)
C(3) - P(6) - C(L1)	102.7(15)	C(K1) - P(6) - C(L1)	104.3(14)
P(1) - C(1) - P(2)	110.4(15)	P(3) - C(2) - P(4)	115.1(15)
P(5) - C(3) - P(6)	113.2(17)	PT(1) - C(4) - PT(2)	77.0(9)
PT(1) - C(4) - C(5)	72.8(16)	PT(2) - C(4) - C(5)	118.8(20)
PT(1) - C(5) - PT(3)	100.7(11)	PT(1) - C(5) - C(4)	69.9(16)
PT(3) - C(5) - C(4)	112.3(20)		

Table 6.6 Crystallographic and experimental details of the structure analyses of compounds (2) and (7).

Compound	$[Pt_3(CO)(S_2CN(CH_3)_2)(dppm)_3][PF_6]$	$[Pt_3(HC{\bullet}CH)(Cl)(dppm)_3][PF_6]$
Formula	$C_{79}H_{72}F_6NOP_7Pt_3S_2$	$C_{77}H_{68}ClF_6P_7Pt_3$
Formula Wt.	2031.7	1944.9
Crystal habit	purple plate	orange plate
Crystal size, mm	0.84x0.72x0.72	0.48x0.28x0.16
Crystal system	monoclinic	orthorhombic
Space group	$P\ 2_1/c$	Pnab (No. 60)
a, Å	19.583(3)	22.987(4)
b, Å	13.661(3)	27.408(9)
c, Å	28.245(5)	25.701(11)
β, °	90.63(2)	—
Obtained from	23 refln, 12<θ<14°	23 refln, 10<θ<14°
V, $Å^3$	7556(3)	16192(9)
Z	4	8
F(000)	3944	7520
d calc, gcm^{-3}	1.786	1.596
T, K	295	295
μ(Mo-Kα), cm^{-1}	58.6	54.5
Absorption factors on F^2	0.87-1.20	0.73-1.42
Scan width, °	0.80	(0.72+0.35tanθ)
Max count time, s	90	90
Total refln measured	12547	12136
Unique refln	9218	11189
R_{INT}	0.039	0.19
Miller indicies h	0→20	0→25
measured, k	-14→ 3	0→30
l	-29→29	0→28
2θ range, °	4-44	4-46
Unique refln ≥ 3σ(I)	6699	3925
No. of parameters	328	301
R	0.033	0.059
R_w	0.044	0.069
$\|\Delta\rho\|_{max}$, $eÅ^{-3}$	0.98	1.05
Δ/σ_{max}	0.023	0.203

CHAPTER 7: HETEROMETALLIC SPECIES OF HIGHER NUCLEARITY

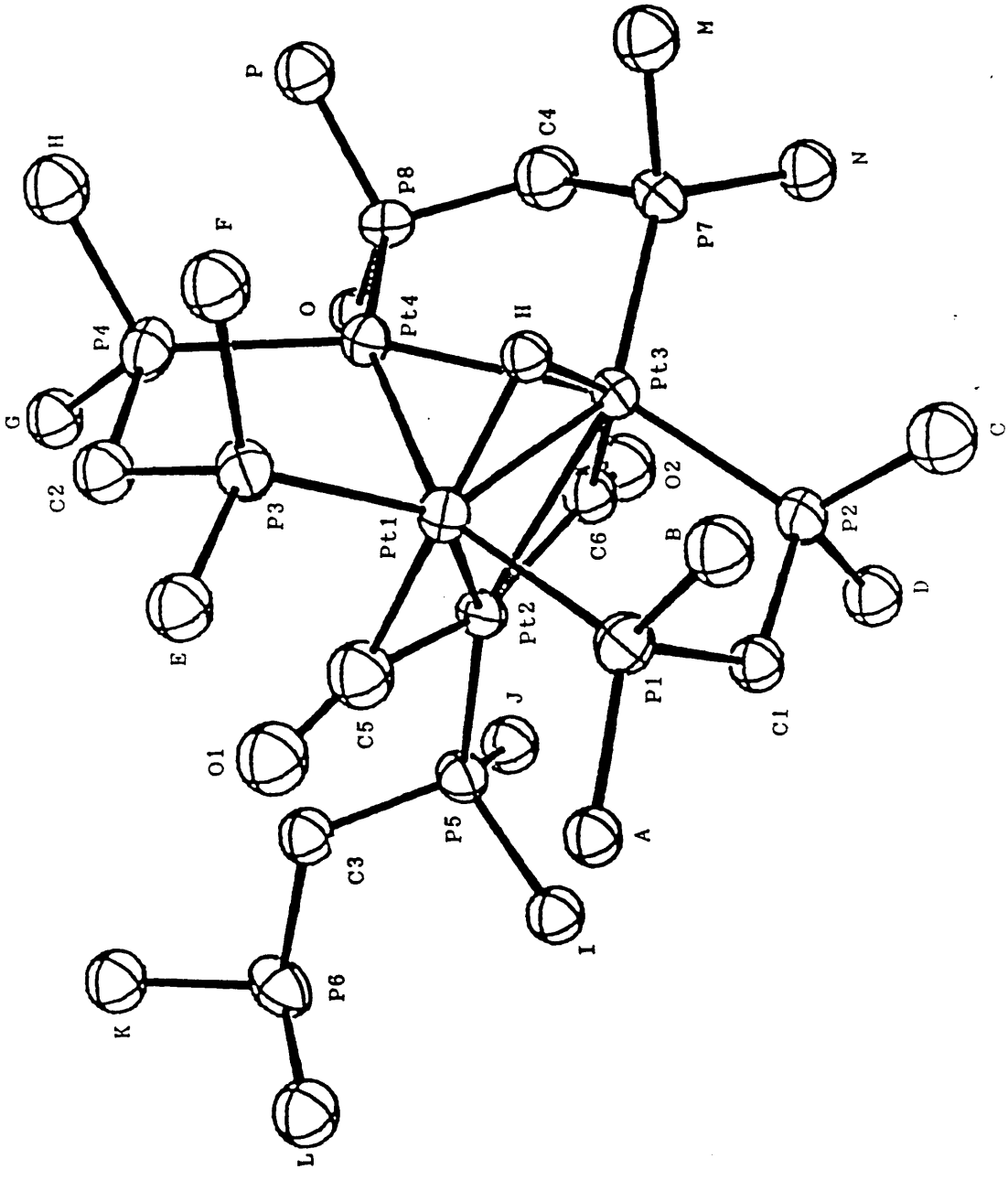
7.1 Introduction

The observation that the properties of both heterogeneous and homogeneous platinum catalysts can be usefully modified by the addition of other metals, notably gold and tin, underlies current interest in heterometallic platinum cluster chemistry.[29] In an attempt to develop this chemistry Professor Puddephatt has synthesised new types of clusters derived from the parent cation $[Pt_3(CO)(dppm)_3]^{2+}$, (1),[50] by addition of extra metal atoms. The characterisation of these new species by X-ray analysis is described here. The complexes fall into three categories: a) $[Pt_4H(CO)_2(\mu\text{-dppm})_3(dppm)]^+$, (2),[4] a 58-electron tetra-platinum cluster, b) $[Pt_3(\mu_3\text{-S})(AuPPh_3)(\mu_3\text{-AgCl})(\mu\text{-dppm})_3]^+$ a pentanuclear species with gold and silver heteroatoms,[5] and c) several compounds containing $\mu_3\text{-}SnX_3$ units attached to the basic Pt_3 triangle.[6] Apart from the strategic objective of establishing how additional metal atoms can be attached to the parent cation (1), the X-ray studies were necessary in order to understand the reactions involved in the formation of the new complexes. As will become apparent these reactions are often of a novel and unpredictable nature.

7.2 $[Pt_4(\mu\text{-H})(\mu\text{-CO})_2(\mu\text{-dppm})_3(dppm)][PF_6]$ (2)

Crystals of the PF_6^- salt of (2) were obtained by reaction of $[Pt(CF_3CO_2)_2(dppm)]$ with CO followed by anion

Figure 7(a). The structure of complex (2). For clarity only the ipso carbons of the phenyl rings are shown and all hydrogen atoms except the μ-H atom are omitted. Probability ellipsoids (50%) are displayed for all atoms shown.



exchange. X-ray analysis establishes that these crystals contain the monocationic tetranuclear cluster (2) (see Figure 7(a)) and the anion PF_6^-, in equal numbers. Interionic distances are consistent with normal van der Waals radii.[52] The structure of the cation (2) (see Tables 7.1 and 7.4) is based on the $Pt_3(\mu\text{-dppm})_3$ unit also found in (1) but with the μ_3-CO unit replaced by H^- and $Pt(CO)_2(dppm)$ units which lie above and below the Pt_3 face, doubly bridging the Pt(1)-Pt(3) bond.

The Pt_4 framework can be described as a distorted tetrahedron or "butterfly" structure, similar to other 58-electron Pt_4 clusters,[29,66-68] and is almost isomorphous with the neutral cluster $[Pt_4(CO)_2(Ph_2PCH_2P(O)Ph_2)(\mu\text{-dppm})_3]$. The hinge torsion angle Pt(2)-Pt(1)-Pt(3)-Pt(4) is 83.7(1)° which is larger than the 70.5° of a regular tetrahedron but less than the 89.4 and 98.6° found in the different crystalline forms of the butterfly cluster $[Pt_4(CO)_5(PMe_2Ph)_4]$.[66] The Pt(1)Pt(3)Pt(4) face is edge-bridged by three μ-dppm ligands with six equatorial phenyl rings on the $Pt(CO)_2(dppm)$ unit side of the Pt_3 triangle, thereby relieving steric congestion.

The Pt(2)-Pt(1) and Pt(2)-Pt(3) edges are bridged by μ-CO ligands displaced slightly [0.09(2) and 0.20(2) Å respectively], out of the Pt(1)Pt(2)Pt(3) plane towards Pt(4). The Pt(2)-CO bonds are significantly shorter [1.97(2) and 1.98(2) Å] than those from the carbonyl to Pt(1) and Pt(3) [2.09(2) and 2.15(2) Å]. This asymmetry could be of relevence in the fluxional behaviour of (2) in solution. The Pt-H distances of 1.69(12) and 2.02(13) Å, are based on a least-squares refinement of the hydrogen

atom position, initially obtained from a difference synthesis and are clearly of limited accuracy. The Pt-P distances lie in the range 2.250(5)-2.266(5) Å, except for those of Pt(1)-P(1) and Pt(3)-P(2) whose bond lengths are 2.360(4) and 2.329(5) Å respectively. The steric congestion brought about by the additional longitudinal bridging of the Pt(1)-Pt(3) bond may, at least partially, explain this.

Five of the six Pt-Pt vectors [2.613(1)-2.750(1) Å] are bonding, with the sixth Pt(2)...Pt(4) distance of 3.082(1) Å clearly non-bonding. The longest Pt-Pt bonds are those bridged by the carbonyls, followed by the hinge bond Pt(1)-Pt(3), while the shortest are those bonded to the Pt(4) atom, which has a lower coordination number than the other metal atoms (see Table 7.4). The differences in Pt-Pt bond lengths in (2) follow the trends discussed in Chapter 3: Pt-Pt bonds are lengthened by μ_2-bridging atoms, in this case carbon and hydrogen, and the bulkier the bridging atom the greater the lengthening.

Evans and Mingos [34] predicted that a stable Pt_4 tetrahedral cluster would have 56 bonding electrons with latitudinal ligands. On addition of further electrons, population of antibonding molecular orbitals would occur with a consequent disruption of the Pt_4 framework by lengthening or even breaking of a Pt-Pt bond. This clearly has occured, creating the "butterfly" structure seen in here in cluster (2) and in other 58-electron complexes.[29,66-68]

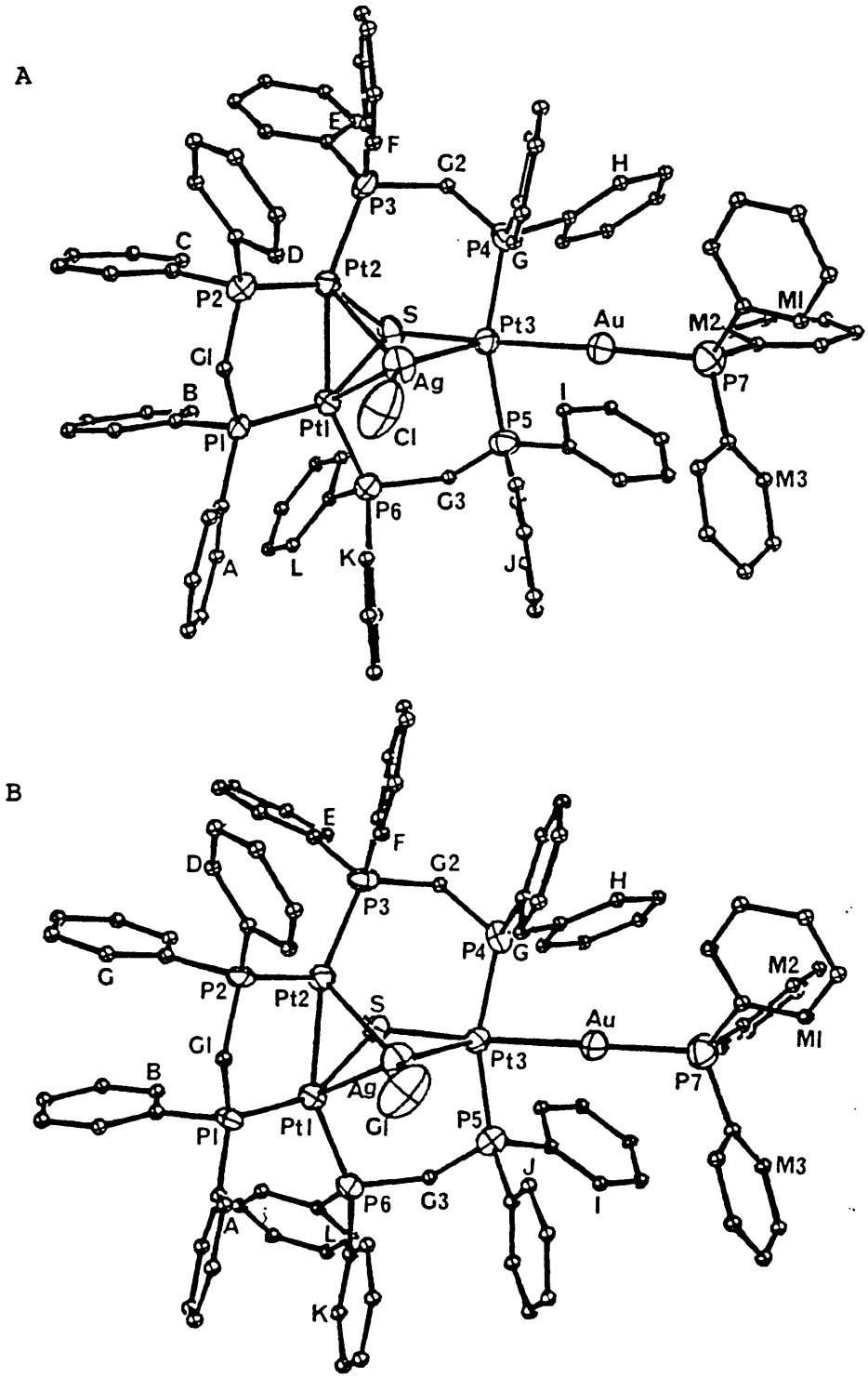
7.3 $[Pt_3(\mu_3\text{-}S)(AuPPh_3)(\mu_3\text{-}AgCl)(\mu\text{-}dppm)_3][PF_6]$ (3)

Cluster $[Pt_3(\mu_3\text{-}S)(AuPPh_3)(\mu_3\text{-}AgCl)(\mu\text{-}dppm)_3]^+$ (3), was formed when attempting to replace the hydride ligand in $[Pt_3H(\mu_3\text{-}S)(\mu\text{-}dppm)_3]^+$ (4),[62] by $AuPPh_3^+$, derived from $[AuCl(PPh_3)]$ and using $AgNO_3$ to remove the chloride. X-ray analysis of a crystal of the PF_6^- salt of (3) revealed the presence of four ion pairs in a centrosymmtric triclinic unit cell. There are therefore two crystallographically independant cations, A and B (see Figure 7(b)), as well as two independant anions. The analysis is based on the Type II reduced triclinic cell, and the Niggli matrix elements [A = 311.1, B = 347.9, C = 802.5, D = -44.5, E = -77.2 and F = -1.9 $Å^2$] indicate that no transformation to higher symmetry is possible (see Experimental).[69] Interionic distances are consistent with van der Waals radii.[52]

The cations A and B are chemically identical and their minor structural differences (see Tables 7.3 and 7.4) can be attributed to crystal packing. Each cation has a Pt_3 triangular face incorporating only one Pt-Pt bond. Each Pt-Pt edge is bridged latitudinally by a dppm ligand and opposite faces of the Pt_3 triangle are μ_3-bridged by AgCl and S groups. In addition, the isolated Pt(3) atom has attached a terminal $AuPPh_3$ ligand. The most obvious differences in the cations occur in the distances and angles involving the Ag and Cl atoms (see Table 7.4), the orientations of the PPh_3 phenyl rings and the orientations of the dppm phenyl rings, in particular ring L (see Figure 7(b)).

The $Pt_3(\mu_3\text{-}S)P_6$ skeleton in (3) shows only minor

Figure 7(b). Views of cations A and B of complex (3). Hydrogen atoms are omitted and the carbon atoms are represented by spheres of arbitrary size. Probability ellipsoids (50%) represent all other atoms shown.



changes from (4), with the average Pt(1)-Pt(2) bond length only slightly longer than the equivalent bond in (4) [2.617(2) Å compared to 2.597(4) Å], as are the non-bonded Pt(1)...Pt(3) and Pt(2)...Pt(3) distances of 3.631(2)-3.726(2) Å compared with 3.574(2) and 3.678(7) Å in (4). These increases are probably due to the extra steric demand of the added μ_3-AgCl ligand. Clusters $[Pd_3(\mu_3\text{-}S)(CN)(dppm)_3]^+$, (5),[51] and $[Pt_3Cl(HC{\equiv}CH)(dppm)_3]^+$, (6), which are structurally related to (4), also have shorter non-bonded M-M distances than in (3) (see Table 6.1), and seem to confirm this view.

The sulphur atom in (3) is 0.12 Å further from Pt(3) than it is from Pt(1) and Pt(2) [mean distances 2.389(6) and 2.272(5) Å respectively]. This may indicate a strong *trans*-influence exerted by the $AuPPh_3$ ligand on the Pt-S bond, similar to the effect of the hydride ligand in (4). In (5), however, the low *trans*-influence of CN^- leads to all Pd-S distances being equal.

Complex (3) affords the first example of an AgCl ligand triply bridging three metal atoms. The AgCl ligand is slightly closer to Pt(3) [Pt-Ag distances 2.780(4) and 2.768(4) Å for cations A and B respectively], than it is to Pt(1) and Pt(2) [Pt-Ag distances 2.808(4)-2.861(4) Å]. In B the silver atom is equidistant from Pt(1) and Pt(2) but in A the distances differ by 0.05 Å. These distances are similar to values found in complexes where a silver atom bridges two or more platinum atoms [2.74-3.06 Å].[70,71]

The Ag-Cl distances of 2.39(1) and 2.41(1) Å are comparable with the shortest Ag-Cl distances in $[Pt_2Ag_2Cl_4(C_6F_5)_4]^{2-}$, where the chlorine atom bridges the

Ag-Pt bonds.[71] The corresponding Pt-Ag-Cl angles in A and B with variations of up to 9° (see Table 7.4) suggest marked differences in the enviroments of the AgCl units in the different cations.

The conformations of the dppm ligands create a hydrophobic cavity in which the AgCl sits. In (4)[62] and (5)[51] the sulphur atom side of the Pt_3 triangle has six equatorial phenyl rings but in (3) it has only four equatorial and two axial rings (see Chapter 8), with the C(1) methylene being on the AgCl ligand side. The C(1) methylene group along with phenyl rings A, D, F, G, J, and K surround the AgCl unit, the shortest Ag...H and Cl...H distances being 2.79 and 2.77 Å respectively for cation A and 2.87 and 2.69 Å for cation B.

The bonding of $AuPPh_3$ to the cluster core is through a particularly short Pt-Au single bond [mean length 2.576(2) Å]. In general, gold tends to form Au-Au bonds or AuM_2 and AuM_3 clusters,[72,73] and any single bonds that are formed are usually ligand bridged.[74] This is clearly not the case in cluster (3), since the linearity of the Pt-Au-P unit [mean angle 174°] rules out any close contacts between the gold atom and surrounding phenyl rings [shortest Au-H(phenyl) distance 2.92 Å]. The Pt-Au bond distances in triangular[72,75] and linear[74] PtAu clusters range from 2.60-2.67 Å with 2.600(3) Å in $PtCl(AuPPh_3)_2(PEt_3)_2]^+$ [72] the shortest distance previously reported. While in butterfly[76] and tetrahedral[77] PtAu clusters the Pt-Au bonds are all longer than 2.71 Å.

The synthesis of complexes containing Pt-Au or Pt-Ag bonds has been growing rapidly in recent years.[72-78] This

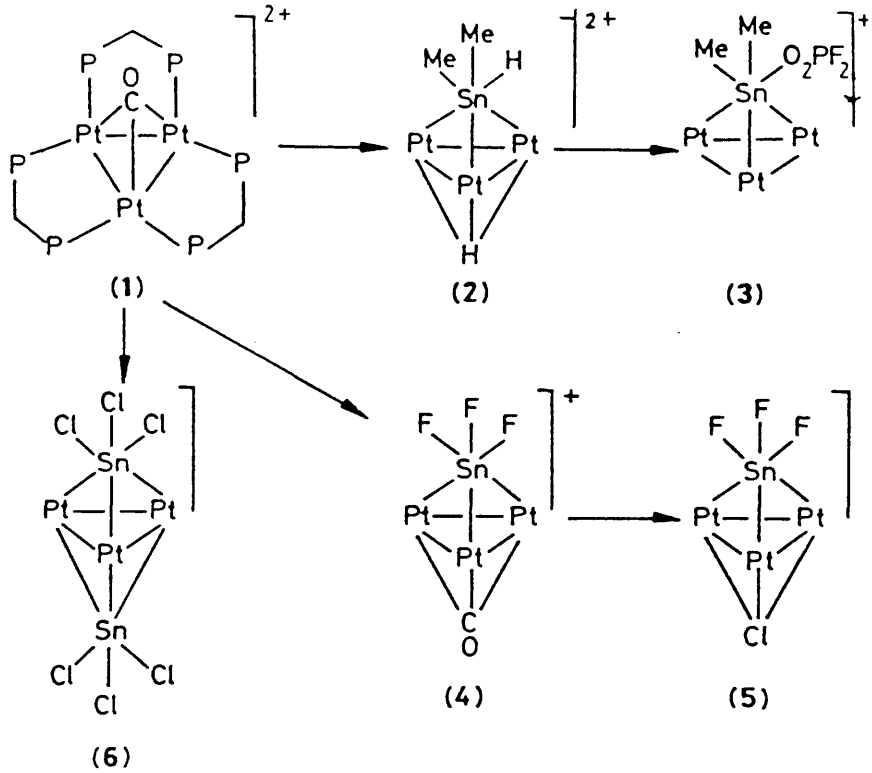
initial interest was because these complexes may serve as models for heterobimetallic catalysts where, in the case of gold added to platinum catalysts, changes in selectivity and catalytic activity were observed.[79] In addition to this primary aim, many interesting and often unexpected products have been formed in these reactions, e.g. complex (3) which displays some particularly interesting structural features.

Cluster (3) is the first PtAgAu cluster to be characterised, also the $Pt_3(\mu_3\text{-}AgCl)$ unit with only one Pt-Pt bond has not been observed before. The mode of attachment of the AgCl is also of chemical interest in building of higher nuclearity clusters. If (3) is formed from the addition of electron-poor AgCl to electron-rich $[Pt_3(\mu_3\text{-}S)(AuPPh_3)(dppm)_3]^+$ it is clear that the AgCl prefers to add via the electron rich platinum atoms rather than to the sulphur which has an exposed donor electron pair.[80]

7.4 Higher Nuclearity Clusters Containing Tin(II)

The use of Pt-Sn complexes and Pt-Sn/support combinations in homogeneous and heterogeneous catalysis respectively, has met with some success.[81,82] On platinum surface catalysts tin(II), as well as tin(Ø), species are known to exist.[83] Therefore, it was hoped to react tin(II) species with the cluster cation (1) in an attempt to model the coordination which occurs on such surfaces. Prior to this work the only Pt_3Sn complexes characterised by X-ray diffraction analysis were $[Pt_3(\mu_3\text{-}SnCl_3)_2(cod)_3]$ (cod =

cyclo-octa-1,5-diene)[47] and $[Pt_3(CO)_3(\mu_2\text{-}Sn(NR)_2)_3]$ (R = $SiMe_3$).[84] The first reactions carried out were between (1) and organotin compounds. Details are shown in Scheme II.[6]

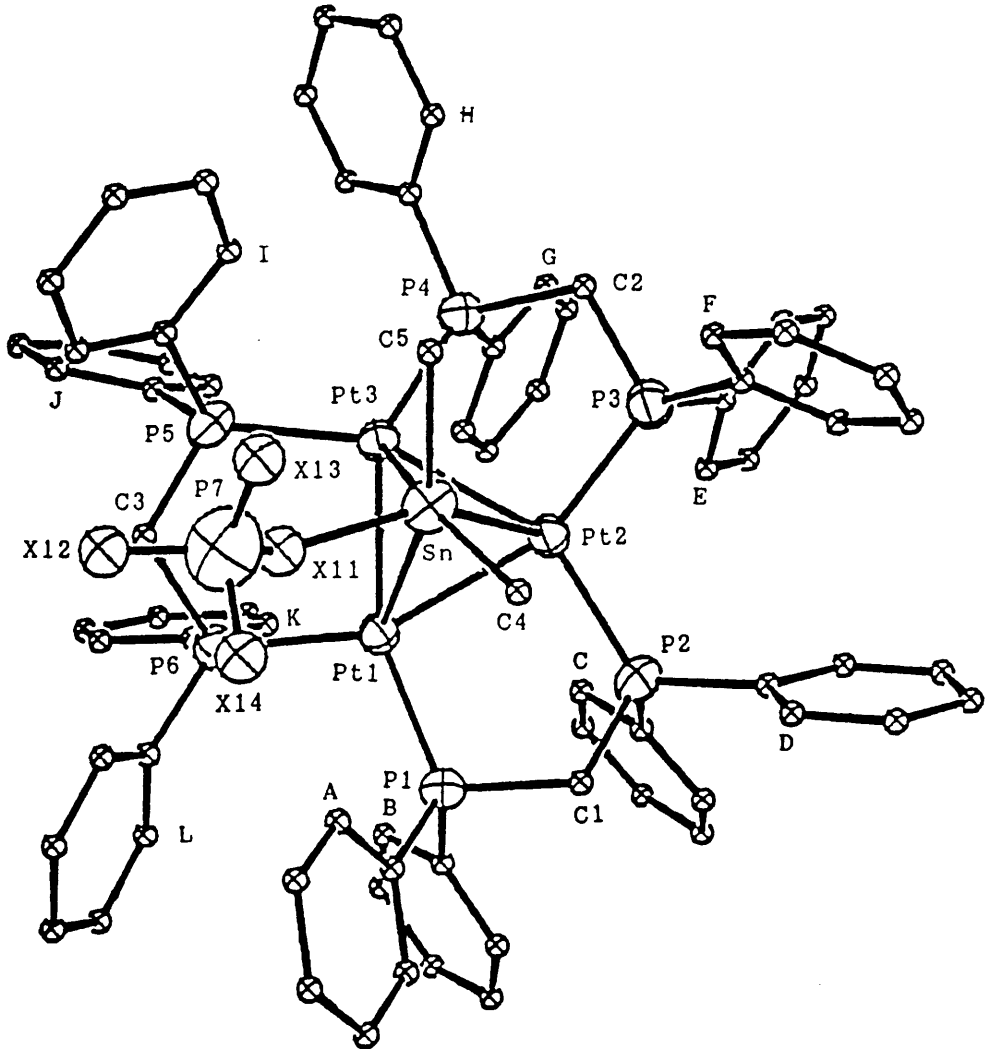


Scheme II.

Reaction of Me_2SnH_2 with the PF_6^- salt of the parent cation (1) initially formed $[Pt_3(\mu_3\text{-}SnMe_2H)(\mu_3\text{-}H)(dppm)_3]^{2+}$ which was characterised spectroscopically. X-ray analysis indicates that on slow crystallisation there was partial reaction with a PF_6^- group to give $PO_2F_2^-$ and that this attached itself to the tin atom, with rupture of the Sn-H and Pt-H bonds, to give crystals consisting of well separated cations $[Pt_3(\mu_3\text{-}SnMe_2(PO_2F_2))(\mu\text{-}dppm)_3]^+$, (7), (see Figure 7(c)) and PF_6^- anions in equal quantities (see Tables 7.5 and 7.6).

In the Pt_3 triangle of cation (7) all three Pt-Pt

Figure 7(c). Structure of cation (7). Hydrogen atoms are omitted and carbon atoms represented by spheres of arbitrary size. Otherwise 50% probability ellipsoids are displayed. The O and F atoms of the $PO_2F_2^-$ are represented by X(11)-X(14) as they could not be distinguished from one another in the structure analysis.



vectors are bonding and the mean Pt-Pt bond length of 2.620(14) Å is similar to that in the parent cation (see Table 4.1). The ability of μ_3-$SnMe_2(PO_2F_2)$ to replace CO in stabilising the 42-electron cluster (7) is particularly significant. The Sn-Pt bonds vary in length from 2.702(2) to 2.766(2) Å, slightly less than the 2.80(1) Å found in $[Pt_3(\mu_3\text{-}SnCl_3)_2(cod)_3]$.[47] The roughly octahedral coordination around the tin atom is completed by two methyl groups [Pt-C, 2.08(3) and 2.17(3) Å] and the $PO_2F_2^-$ unit [Sn-X(11), 2.12(2) Å, X = O or F]. The presence of the $PO_2F_2^-$ unit was finally confirmed by N.M.R. studies since X-ray analysis was unable to distinguish between the oxygen and the fluorine atoms attached to the phosphorus atom. P-X distances range from 1.48(3) to 1.53(2) Å, the longest being that involving the atom connecting the ligand to the tin atom.

Possibly because the μ_3-$SnMe_2(PO_2F_2)$ unit is much bulkier than the carbonyl, the dppm phenyl rings on its side of the Pt_3 triangle adopt a six equatorial mode in order to relieve steric congestion. In (1) there are four equatorial and two axial phenyl rings on the carbonyl side. However the Pt-P distances in (7) are very similar to those in (1) [mean distances 2.282(12) Å in (7) and 2.282(15) Å in (1)].

Reaction of (1) with Ph_3SnH also gave an unexpected product.[6] X-ray analysis carried out in this department by Dr.M.C. Jennings revealed a disordered structure of unusual type, in which cleavage of all three Sn-C(phenyl) bonds had occurred and were replaced by much more electronegative F^- ions. The cubic unit cell contains six cations $[Pt_3(\mu_3\text{-}$

$SnF_3)(\mu_3\text{-}CO)(\mu\text{-}dppm)_3]^+$, (8), six PF_6^- anions and two neutral clusters $[Pt_3(\mu_3\text{-}SnF_3)(\mu_3\text{-}Cl)(\mu\text{-}dppm)_3]$, (9). Clusters (8) and (9) occupy crystallographically eqivalent sites and differ only in the μ_3-capping ligand, CO or Cl^-. Cluster (8) is shown in Figure 7(d).

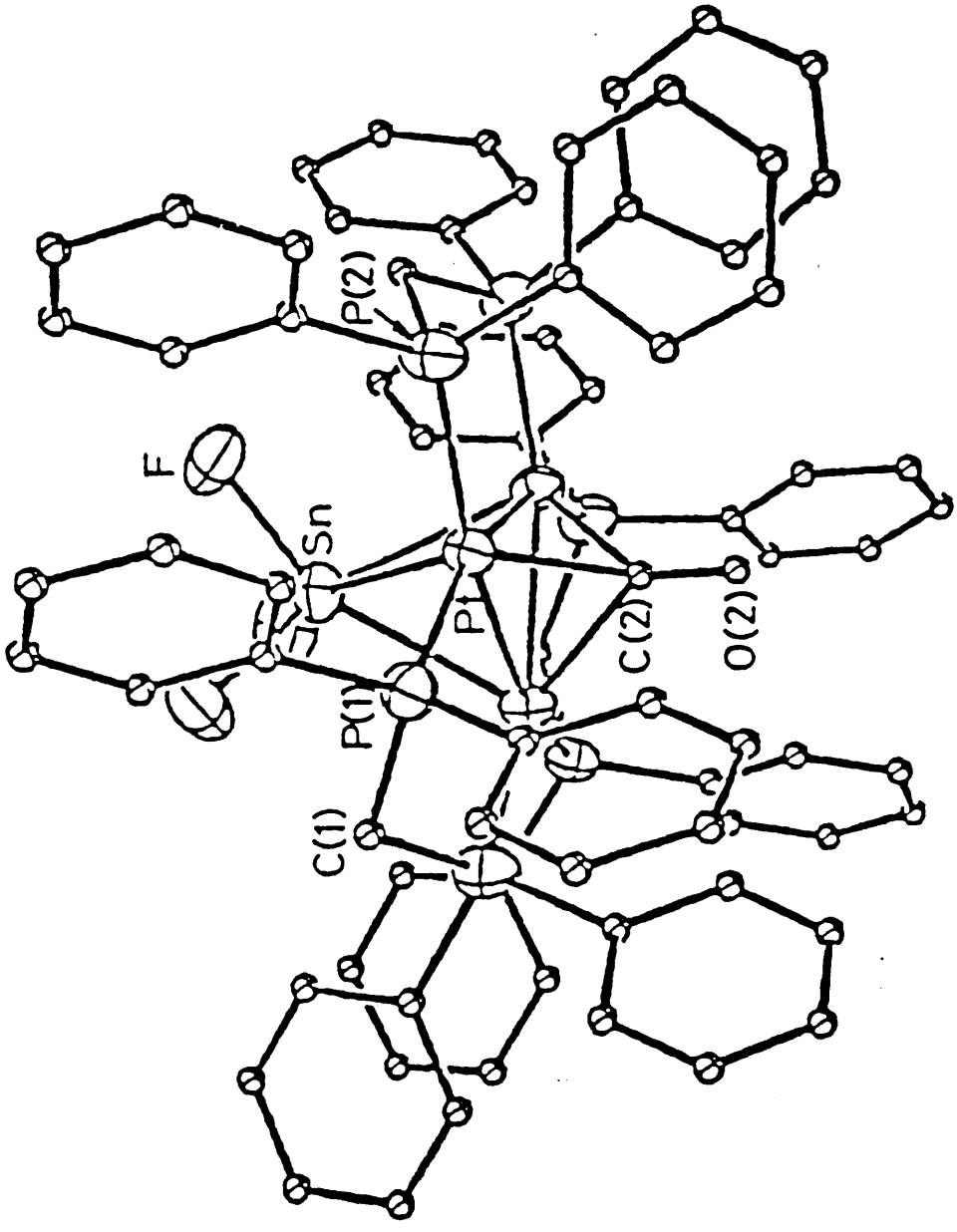
An attempt to synthesise cluster (8) by reaction of (1) with SnF_3^- provided crystals which on X-ray analysis gave almost identical unit cell dimensions to the previous crystal and a subsequent structural analysis showed them to be so (see Tables 7.7 and 7.8).

While the Pt-Pt bond distances in (8) and (9) are comparable with those in (7) [mean distance 2.634(4) and 2.620(14) Å respectively], the Pt-Sn distances do show a significant lengthening [distances 2.773(3) Å in (8) and (9) and 2.702(2)-2.766(2) Å in (7)], which may be ascribed to the increased number of bonding electrons in (8) and (9), i.e. 44 instead of 42.

The Pt-P bond distances in (8) and (9) also compare favourably with those of (7) [mean distances, 2.292(24) and 2.282(12) Å]. The much greater steric bulk of the $\mu_3\text{-}SnF_3^-$ ligand compared to the μ_3-CO and $\mu_3\text{-}Cl^-$ ligands is clearly indicated by the dppm ligands having six equatorial phenyl rings on its side of the Pt_3 triangle.

Reactions of (1) with excess $SnCl_3^-$ or SnF_3^- gave 44-electron clusters of the type $[Pt_3(\mu_3\text{-}SnX_3)_2(\mu\text{-}dppm)_3]$. In view of the disorder shown in the attempts to obtain crystals of (8), an X-ray analysis of $[Pt_3(\mu_3\text{-}SnF_3)_2(\mu\text{-}dppm)_3]$, (10), recrystallised from dichloromethane, was carried out in order to study, more clearly, the $\mu_3\text{-}SnF_3$ bonding to the Pt_3 triangle. The crystal structure

Figure 7(d). A view of cation (8). Hydrogen atoms are omitted and the carbon atoms and oxygen atom are presented as arbitrary spheres. All other atoms are represented by 50% probability ellipsoids.



contains three molecules of dichloromethane for every molecule of cluster (10). Two of these solvent molecules are heavily disordered (see Experimental). Intermolecular distances are consistent with van der Waals radii.[52] Cluster (10) is a neutral 44-electron cluster based on a Pt_3 triangle with SnF_3^- units μ_3-bonded to each face and dppm ligands latitudinally bridge each of the Pt-Pt edges (see Figure 7(e) and Tables 7.9 and 7.10).

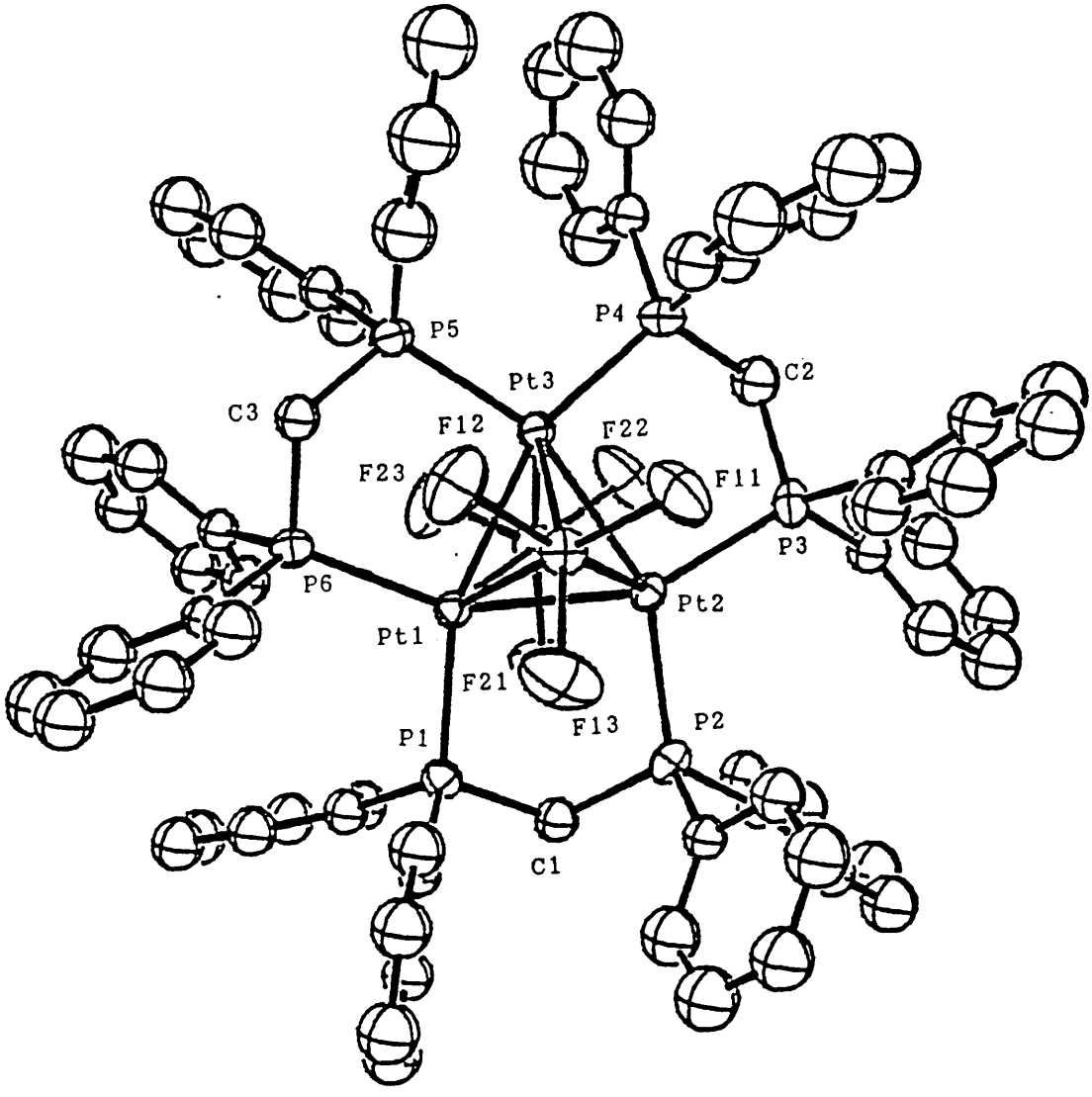
The Pt-Pt bond distances in (10) [2.609(2)-2.639(1) Å with mean distance 2.623(15) Å] are comparable to those found in (1) (see Table 4.1), despite the addition of an extra 2-electron donor ligand. However, comparison of Pt-Sn distances in (7), (8)/(9) and (10) shows that an additional two electrons in the cluster bonding does result in an increase in Pt-Sn bond lengths [mean distances 2.736(32), 2.773(3) and 2.778(65) Å respectively].

Three Sn-F bonds complete the roughly octahedral coordination around each tin atom. Distances range from 1.901(11) to 1.995(12) Å. When viewed along the normal to the Pt_3 plane, it is clear that the two sets of fluorine substituents virtually eclipse each other.

The dppm ligands have conformations such that one face has four equatorial and two axial phenyl rings surrounding it while the other has two equatorial and four axial rings, as is expected where two identical μ_3-units are bonded to the Pt_3 triangle. The Pt-P distances range from 2.278(5) to 2.313(5) Å and are therefore comparible with other similar compounds (see Table 5.1).

It appears that the $Pt_3(\mu_3\text{-}SnX_3)$ unit is the most favourable form of attachment for tin(II) complexes to Pt_3

Figure 7(e). The structure of cluster (10). Hydrogen atoms are omitted for clarity. 50% probability ellipsoids are displayed for all atoms shown.



triangles, particularly if X is an electronegative substituent such as F^-. As noted previously it appears that the SnX_3^- unit can stabilise the $Pt_3(dppm)_3^{2+}$ framework in a similar fashion to the carbonyl ligand in (1). On addition of a further ligand to the metal cluster, the SnX_3^- unit can accomodate additional electrons in empty π^* orbitals, hence the slight lengthening of the Pt-Sn bonds. The more electronegative X is, the less there is need to occupy antibonding orbitals, since X can pull electron density from the cluster bonding.

These model compounds suggest $Pt_3(\mu_3\text{-}SnX_3)$ units may occur on Pt-Sn/support catalyst surfaces where, for example, X could be the oxygen of the tin(II) aluminiate support.[83]

7.5 Experimental

Because fairly similar methods were used in all of the analyses in this section, full details of only one analysis has been given (see the Experimental in Chapter 5). Details of the analyses of structures in this chapter which differ from the model analysis are given below. Summaries of the crystal data of each is given in Table 7.11.

$[Pt_4(\mu\text{-}H)(\mu\text{-}CO)_2(\mu\text{-}dppm)_3(dppm)][PF_6]$ (2)

Data Collection. The crystal was mounted on a glass fibre. Structure analysis. The heavy atom positions were found using direct methods.[85] Anisotropic displacement parameters were used for Pt, P and F atoms and isotropic parameters

for all other atoms. The hydridic hydrogen atom was detected in a difference synthesis and its position and isotropic displacement parameters were refined. All the other hydrogen atoms were positioned geometrically (C-H = 0.96 Å).

$[Pt_3(\mu_3\text{-}S)(AuPPh_3)(\mu_3\text{-}AgCl)(\mu\text{-}dppm)_3][PF_6]$ (3)

Data Collection. The crystal was mounted on a glass fibre. In a Type II reduced triclinic cell there are two crystallographically independant ion pairs but the Niggli matrix elements [A = 311.1, B = 347.9, C = 802.5, D = -44.5, E = -77.2 and F = -1.9 $Å^2$] show that no transformation to higher symmetry is possible.[69] Collection of the 36-44° 2θ shell was discontinued because the reflections were too weak.

Structure Analysis. Heavy atom positions were determined using direct methods.[85] All the hydrogen atoms were positioned geometrically (C-H = 0.96 Å) and given a common isotropic displacement parameter U(H) = 0.10 $Å^2$. Anisotropic displacement parameters were used for Au, Ag, Pt, Cl, S and P atoms and isotropic parameters for the F and C atoms. The structure was refined using full-matrix least-squares, adjusting the parameters of cation A and the two PF_6^- anions and then those of cation B in alternate calculations (see 7.6 Program Modifications).

$[Pt(\mu_3\text{-}SnMe_2(PO_2F_2))(\mu\text{-}dppm)_3][PF_6]$ (7)

Data Collection. The crystal was mounted on a glass fibre.

A shell of 4-16° in 2θ with h+k = 2n+1 was collected to check that those reflections were systematically absent. Otherwise, measurements were made only for reflections with h+k = 2n.

Structure Analysis. All the hydrogen positions were calculated (C-H = 0.96 Å) and given U(H) = 1.2U(C_{iso}) Å. There were two distinct PF_6^- sites, each with the phosphorus atom on a two-fold axes and associated with only three independant fluorine atoms. The oxygen and fluorine atoms of the $PO_2F_2^-$ ligand could not be distinguished by X-ray analysis and each was assigned a fluorine scattering factor. The absolute structure was established by refining η, the coefficient of the imaginary component of the anomalous scattering factor.[86] For the coordinates in Table 7.5 the refined η value was 1.05(3). The platinum, tin and phosphorus atoms were given anisotropic displacement parameters, isotropic displacement parameters being used for the remaining atoms.

$[Pt_3(\mu_3\text{-}SnF_3)(\mu\text{-}dppm)_3(\mu_3\text{-}CO)]_{0.75}[Pt_3(\mu_3\text{-}SnF_3)(\mu\text{-}dppm)_3(\mu_3\text{-}Cl)]_{0.25}[PF_6]_{0.25}$ (8)/(9)

Data Collection. The crystal was mounted on a glass fibre. An initial shell of data, 2θ range 4-16°, was collected in order to determine the space group. At higher angle only unique reflections were collected. A Gaussian absorption correction was carried out.[87]

Structure Analysis. The heavy atom positions were found using direct methods.[85] Anisotropic thermal parameters were used for the Pt, Sn, P(1), P(2) and F(1) atoms, and

isotropic parameters were used for all other atoms.

The cation is positioned around a three fold axis with the tin atom and the carbonyl/Cl^- both on the axes. The positions of the carbonyl group and the chlorine atom were fixed with the chlorine and oxygen atoms sitting on the same position.

All hydrogen atoms were positioned geometrically, with the phenyl hydrogen positions refined as part of the rigid phenyl groups, while the methylene hydrogens were set to ride on their attached carbon atoms. All hydrogen atoms were given an isotropic displacement parameter U(H) = 0.10 $Å^2$ which was not refined. The PF_6^- phosphorus atom lay at the intersection of three two fold-axes and each of the three fluorine sites was on a two-fold axis.

For the coordinates given in Table 7.7 the refined η value was 1.09(6).

$[Pt_3(\mu_3\text{-}SnF_3)(\mu\text{-}dppm)_3].CH_2Cl_2$ (10)

Data Collection. The crystal was mounted on a glass fibre. Structure Analysis. A fixed contribution was used for the scattering of geometrically positioned hydrogen atoms, calculated using C-H = 0.96 Å and U(H) = 0.075 $Å^2$. Anisotropic displacement parameters were used for all non-hydrogen atoms except C atoms which were assigned isotropic parameters.

There were three molecules of solvent detected in difference syntheses. One molecule was clearly identified as CH_2Cl_2 and refined as such; it is included in Table 7.11. The other two molecules, however, were heavily

disordered. Distances and angles between electron density peaks suggested they were also CH_2Cl_2 molecules but the disorder could not be modelled satisfactorily. Five atomic sites for each molecule were used in the refinement. They were assigned chlorine scattering factors, and given a fixed isotropic displacement parameter of 0.16 $\AA^2$ and only their positions and occupancies refined [occupancies were 0.51(2), 0.54(2), 0.38(2), 0.36(2) and 0.28(2) for one molecule and 0.51(2), 0.49(2), 0.24(2), 0.33(2) and 0.29(2) for the other]. These molecules were not accounted for in Table 7.11.

7.6 Program Modifications

The size of the structures discussed above led to some problems with the GX program package. In particular $[Pt_3(AuPPh_3)(AgCl)(S)(dppm)_3][PF_6]$ with 390 atoms in the asymmetric unit caused difficulty since GX has a limit of 200 atoms per asymmetric unit. Accordingly the following new features were added to the RBLS refinement program.

(1) Provision for 400 rather than 350 refined parameters.

(2) Output of a file of fixed structure factor contributions.

(3) Addition of fixed contributions calculated in (2) to structure factors.

(4) Addition of fixed contributions and creation of an augmented set of fixed contributions.

Thus for the Pt_3AuAg structure hydrogen contributions were first calculated, then contributions for molecule A and the two PF_6^- anions were added using (4) and finally the

augmented contributions were used in the refinement of molecule B. Although this facility was added to overcome a specific difficulty the ability to use fixed contributions has proved generally useful, especially in dealing with disordered structures where trial full matrix calculations on disordered models can be quickly carried out with the ordered portion of the structure included as a fixed contribution.

Table 7.1. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (2).

	X/A	Y/B	Z/C	U
PT(1)	.30279(3)	.09876(2)	.33122(2)	.027
PT(2)	.24673(3)	.13707(2)	.40280(2)	.028
PT(3)	.17853(3)	.08408(2)	.34727(2)	.028
PT(4)	.21659(3)	.15875(2)	.30775(2)	.028
P(1)	.3342(2)	.0271(1)	.3605(1)	.035
P(2)	.1926(2)	.0172(1)	.3879(2)	.036
P(3)	.3692(2)	.1278(1)	.2807(1)	.031
P(4)	.2839(2)	.2106(1)	.2785(1)	.036
P(5)	.2608(2)	.1687(1)	.4683(1)	.033
P(6)	.3493(2)	.2396(2)	.5184(2)	.047
P(7)	.0831(2)	.0882(1)	.3150(1)	.035
P(8)	.1194(2)	.1910(1)	.3067(1)	.033
P(9)	.1916(3)	.4053(2)	.4777(3)	.112
F(1)	.1951(10)	.3530(3)	.4838(8)	.266
F(2)	.1457(10)	.3987(10)	.4401(5)	.275
F(3)	.2376(10)	.4119(10)	.5153(5)	.179
F(4)	.1882(10)	.4577(3)	.4716(8)	.252
F(5)	.1358(8)	.4075(3)	.5090(7)	.353
F(6)	.2475(8)	.4031(3)	.4464(7)	.300
O(1)	.3833(5)	.1625(4)	.3870(4)	.052(3)
O(2)	.1046(6)	.1354(4)	.4162(4)	.053(3)
C(1)	.2775(7)	.0105(4)	.3994(5)	.030(4)
C(2)	.3670(7)	.1908(5)	.2836(5)	.036(4)
C(3)	.3141(7)	.2182(5)	.4676(5)	.037(4)
C(4)	.0569(8)	.1486(5)	.3173(5)	.045(5)
C(5)	.3334(8)	.1432(5)	.3800(6)	.046(5)
C(6)	.1543(8)	.1258(5)	.4020(5)	.036(4)
C(A1)	.4080(5)	.0236(7)	.3912(5)	.030(4)
C(A2)	.4511(4)	.0590(5)	.3864(5)	.045(5)
C(A3)	.5070(6)	.0584(4)	.4093(3)	.054(5)
C(A4)	.5199(5)	.0224(7)	.4371(5)	.053(5)
C(A5)	.4768(4)	-.0130(5)	.4419(5)	.057(5)
C(A6)	.4209(6)	-.0124(4)	.4190(3)	.059(5)
C(B1)	.3352(10)	-.0225(5)	.3236(5)	.040(4)
C(B2)	.3413(6)	-.0141(4)	.2800(6)	.054(5)
C(B3)	.3453(7)	-.0506(6)	.2515(3)	.072(6)
C(B4)	.3431(10)	-.0954(5)	.2666(5)	.078(6)
C(B5)	.3370(6)	-.1037(4)	.3102(6)	.082(7)
C(B6)	.3330(7)	-.0673(6)	.3387(3)	.056(5)
C(C1)	.1745(11)	-.0394(5)	.3656(6)	.047(5)
C(C2)	.1702(10)	-.0771(7)	.3926(4)	.078(6)
C(C3)	.1647(4)	-.1209(5)	.3756(6)	.108(8)
C(C4)	.1635(11)	-.1271(5)	.3315(6)	.118(9)
C(C5)	.1678(10)	-.0894(7)	.3044(4)	.094(7)
C(C6)	.1733(4)	-.0456(5)	.3215(6)	.065(6)
C(D1)	.1548(9)	.0176(4)	.4407(5)	.038(4)
C(D2)	.1876(5)	.0109(5)	.4786(7)	.065(6)
C(D3)	.1568(8)	.0148(7)	.5177(5)	.078(6)
C(D4)	.0931(9)	.0254(4)	.5188(5)	.081(7)
C(D5)	.0602(5)	.0320(5)	.4808(7)	.076(6)
C(D6)	.0911(8)	.0282(7)	.4418(5)	.067(6)
C(E1)	.4550(4)	.1147(6)	.2843(6)	.036(4)
C(E2)	.4766(8)	.0738(6)	.2670(2)	.046(5)
C(E3)	.5378(9)	.0594(3)	.2749(6)	.066(6)
C(E4)	.5774(4)	.0859(6)	.3001(6)	.061(5)
C(E5)	.5558(8)	.1268(6)	.3175(2)	.053(5)
C(E6)	.4946(9)	.1413(3)	.3096(6)	.044(4)
C(F1)	.3544(8)	.1174(6)	.2228(3)	.040(4)
C(F2)	.3920(7)	.1400(5)	.1932(3)	.049(5)
C(F3)	.3811(4)	.1344(3)	.1496(3)	.066(6)
C(F4)	.3326(8)	.1062(6)	.1357(3)	.064(6)
C(F5)	.2950(7)	.0836(5)	.1654(3)	.061(5)
C(F6)	.3059(4)	.0892(3)	.2089(3)	.038(4)
C(G1)	.2870(10)	.2672(4)	.3047(6)	.037(4)
C(G2)	.3175(5)	.2729(6)	.3437(7)	.056(5)
C(G3)	.3116(8)	.3139(7)	.3660(4)	.065(6)
C(G4)	.2751(10)	.3492(4)	.3494(6)	.084(7)
C(G5)	.2445(5)	.3435(6)	.3104(7)	.064(5)
C(G6)	.2505(8)	.3025(7)	.2881(4)	.062(5)
C(H1)	.2767(8)	.2245(6)	.2214(4)	.045(4)
C(H2)	.3188(9)	.2541(7)	.2015(4)	.064(5)
C(H3)	.3130(5)	.2634(3)	.1581(3)	.081(7)
C(H4)	.2652(8)	.2431(6)	.1344(4)	.087(7)
C(H5)	.2232(9)	.2134(7)	.1543(4)	.090(7)

Table 7.1(cont).

	X/A	Y/B	Z/C	U
C(H6)	.2289(5)	.2042(3)	.1977(3)	.054(5)
C(I1)	.2971(3)	.1281(6)	.5052(6)	.036(4)
C(I2)	.2907(8)	.1330(3)	.5493(7)	.042(4)
C(I3)	.3198(8)	.1020(5)	.5767(3)	.071(6)
C(I4)	.3553(3)	.0662(6)	.5600(6)	.083(7)
C(I5)	.3617(8)	.0613(3)	.5160(7)	.067(6)
C(I6)	.3326(8)	.0923(5)	.4886(3)	.046(5)
C(J1)	.1902(7)	.1875(4)	.4971(6)	.042(4)
C(J2)	.1480(10)	.1535(3)	.5089(7)	.053(5)
C(J3)	.0933(6)	.1649(4)	.5308(3)	.077(6)
C(J4)	.0808(7)	.2105(4)	.5407(6)	.083(7)
C(J5)	.1231(10)	.2445(3)	.5289(7)	.071(6)
C(J6)	.1778(6)	.2330(4)	.5070(3)	.061(5)
C(K1)	.3888(6)	.2907(3)	.4964(4)	.048(5)
C(K2)	.4435(10)	.2882(4)	.4722(8)	.069(6)
C(K3)	.4698(7)	.3278(4)	.4553(6)	.088(7)
C(K4)	.4415(6)	.3700(3)	.4627(4)	.084(7)
C(K5)	.3868(10)	.3726(4)	.4870(8)	.091(7)
C(K6)	.3605(7)	.3329(4)	.5038(6)	.068(6)
C(L1)	.4166(5)	.2009(6)	.5282(8)	.051(5)
C(L2)	.4428(9)	.1722(7)	.4975(4)	.052(5)
C(L3)	.4947(11)	.1454(4)	.5077(7)	.064(6)
C(L4)	.5204(5)	.1473(6)	.5485(8)	.081(7)
C(L5)	.4942(9)	.1760(7)	.5792(4)	.103(8)
C(L6)	.4423(11)	.2028(4)	.5691(7)	.083(7)
C(M1)	.0764(11)	.0743(7)	.2585(4)	.043(4)
C(M2)	.0173(9)	.0750(4)	.2395(7)	.055(5)
C(M3)	.0111(7)	.0648(7)	.1962(7)	.079(7)
C(M4)	.0638(11)	.0540(7)	.1720(4)	.108(9)
C(M5)	.1229(9)	.0533(4)	.1911(7)	.14(1)
C(M6)	.1291(7)	.0634(7)	.2343(7)	.085(7)
C(N1)	.0139(4)	.0569(4)	.3366(4)	.041(4)
C(N2)	.0136(8)	.0096(4)	.3315(7)	.062(5)
C(N3)	-.0368(9)	-.0161(3)	.3466(6)	.075(6)
C(N4)	-.0869(4)	.0056(4)	.3668(4)	.072(6)
C(N5)	-.0865(8)	.0529(4)	.3719(7)	.069(6)
C(N6)	-.0361(9)	.0786(3)	.3568(6)	.055(5)
C(O1)	.1056(9)	.2323(4)	.3500(5)	.031(4)
C(O2)	.1555(6)	.2495(4)	.3738(6)	.048(5)
C(O3)	.1443(7)	.2809(6)	.4065(3)	.056(5)
C(O4)	.0833(9)	.2950(4)	.4153(5)	.058(5)
C(O5)	.0333(6)	.2777(4)	.3915(6)	.054(5)
C(O6)	.0445(7)	.2464(6)	.3589(3)	.047(5)
C(P1)	.0880(5)	.2209(7)	.2590(6)	.042(4)
C(P2)	.0853(10)	.2685(7)	.2579(4)	.056(5)
C(P3)	.0599(9)	.2906(3)	.2225(7)	.065(6)
C(P4)	.0370(5)	.2651(7)	.1883(6)	.099(8)
C(P5)	.0397(10)	.2175(7)	.1894(4)	.117(9)
C(P6)	.0652(9)	.1954(3)	.2248(7)	.079(7)
H(1)	.245(6)	.076(4)	.301(4)	.02(4)
H(11)	.28623	.02799	.42492	.050
H(12)	.28450	-.02168	.40524	.050
H(21)	.39208	.20367	.26071	.050
H(22)	.38420	.20084	.31074	.050
H(31)	.29111	.24354	.45516	.050
H(32)	.34875	.21036	.44886	.050
H(41)	.04000	.15434	.34558	.050
H(42)	.02383	.15281	.29644	.050
H(A2)	.44211	.08399	.36704	.050
H(A3)	.53698	.08306	.40596	.050
H(A4)	.55882	.02198	.45308	.050
H(A5)	.48571	-.03811	.46124	.050
H(A6)	.39085	-.03714	.42233	.050
H(B2)	.34268	.01700	.26947	.050
H(B3)	.34937	-.04485	.22116	.050
H(B4)	.34588	-.12077	.24679	.050
H(B5)	.33549	-.13489	.32071	.050
H(B6)	.32877	-.07305	.36903	.050
H(C2)	.17106	-.07278	.42333	.050
H(C3)	.16164	-.14712	.39448	.050
H(C4)	.15960	-.15757	.31970	.050
H(C5)	.16698	-.09371	.27378	.050

Table 7.1(cont).

	X/A	Y/B	Z/C	U
H(C6)	.17638	-.01939	.30265	.050
H(D2)	.23183	.00346	.47789	.050
H(D3)	.17948	.01004	.54410	.050
H(D4)	.07151	.02802	.54592	.050
H(D5)	.01588	.03950	.48155	.050
H(D6)	.06826	.03295	.41539	.050
H(E2)	.44899	.05534	.24942	.050
H(E3)	.55275	.03089	.26281	.050
H(E4)	.61990	.07589	.30565	.050
H(E5)	.58331	.14532	.33506	.050
H(E6)	.47961	.16981	.32162	.050
H(F2)	.42574	.15958	.20286	.050
H(F3)	.40722	.15005	.12901	.050
H(F4)	.32488	.10222	.10545	.050
H(F5)	.26111	.06393	.15571	.050
H(F6)	.27961	.07345	.22950	.050
H(G2)	.34279	.24841	.35525	.050
H(G3)	.33275	.31790	.39311	.050
H(G4)	.27093	.37776	.36484	.050
H(G5)	.21919	.36808	.29878	.050
H(G6)	.22926	.29859	.26095	.050
H(H2)	.35208	.26841	.21795	.050
H(H3)	.34235	.28412	.14429	.050
H(H4)	.26128	.24961	.10421	.050
H(H5)	.19004	.19928	.13784	.050
H(H6)	.19975	.18358	.21151	.050
H(I2)	.26595	.15764	.56082	.050
H(I3)	.31515	.10526	.60730	.050
H(I4)	.37532	.04453	.57911	.050
H(I5)	.38640	.03638	.50445	.050
H(I6)	.33714	.08890	.45798	.050
H(J2)	.15665	.12177	.50198	.050
H(J3)	.06391	.14125	.53903	.050
H(J4)	.04279	.21846	.55592	.050
H(J5)	.11444	.27620	.53583	.050
H(J6)	.20719	.25673	.49881	.050
H(K2)	.46327	.25882	.46716	.050
H(K3)	.50789	.32612	.43848	.050
H(K4)	.45986	.39767	.45100	.050
H(K5)	.36712	.40194	.49207	.050
H(K6)	.32247	.33467	.52072	.050
H(L2)	.42494	.17097	.46908	.050
H(L3)	.51303	.12559	.48624	.050
H(L4)	.55657	.12869	.55554	.050
H(L5)	.51208	.17728	.60763	.050
H(L6)	.42397	.22271	.59046	.050
H(M2)	-.01934	.08261	.25623	.050
H(M3)	-.02995	.06534	.18290	.050
H(M4)	.05950	.04686	.14191	.050
H(M5)	.15962	.04569	.17421	.050
H(M6)	.17022	.06288	.24754	.050
H(N2)	.04854	-.00550	.31749	.050
H(N3)	-.03690	-.04907	.34306	.050
H(N4)	-.12181	-.01234	.37731	.050
H(N5)	-.12130	.06795	.38596	.050
H(N6)	-.03585	.11147	.36035	.050
H(O2)	.19795	.23967	.36772	.050
H(O3)	.17909	.29287	.42300	.050
H(O4)	.07558	.31685	.43799	.050
H(O5)	-.00906	.28765	.39762	.050
H(O6)	.00984	.23445	.34233	.050
H(P2)	.10125	.28621	.28174	.050
H(P3)	.05810	.32378	.22176	.050
H(P4)	.01928	.28061	.16372	.050
H(P5)	.02364	.19991	.16566	.050
H(P6)	.06690	.16237	.22560	.050

Table 7.1(cont).

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
PT(1)	.0270(3)	.0260(3)	.0283(4)	-.0001(3)	.0010(3)	.0015(3)
PT(2)	.0258(4)	.0323(3)	.0248(4)	-.0021(3)	-.0013(3)	-.0012(3)
PT(3)	.0269(4)	.0274(3)	.0304(4)	-.0036(3)	-.0033(3)	.0015(3)
PT(4)	.0308(4)	.0247(3)	.0287(4)	-.0004(3)	-.0019(3)	.0017(3)
P(1)	.035(3)	.029(2)	.041(3)	.004(2)	-.005(2)	.002(2)
P(2)	.031(3)	.033(2)	.045(3)	-.004(2)	-.009(2)	.008(2)
P(3)	.033(3)	.032(2)	.029(3)	-.004(2)	.003(2)	-.003(2)
P(4)	.046(3)	.028(2)	.033(3)	-.002(2)	.003(2)	.002(2)
P(5)	.034(3)	.039(3)	.027(3)	-.007(2)	.001(2)	-.002(2)
P(6)	.043(3)	.058(3)	.040(3)	-.011(2)	.001(3)	-.013(2)
P(7)	.033(2)	.033(2)	.038(3)	-.007(2)	-.008(2)	-.002(2)
P(8)	.037(3)	.037(2)	.026(3)	-.002(2)	-.005(2)	.000(2)
P(9)	.065(4)	.077(5)	.194(9)	.000(4)	-.015(6)	-.059(5)
F(1)	.35(3)	.09(1)	.35(4)	-.02(2)	-.19(3)	-.06(2)
F(2)	.20(2)	.16(2)	.47(4)	.05(1)	-.22(3)	-.10(2)
F(3)	.21(2)	.13(1)	.20(2)	-.01(1)	-.12(2)	-.05(1)
F(4)	.21(2)	.10(1)	.44(4)	.01(1)	-.18(3)	-.05(2)
F(5)	.17(2)	.53(5)	.36(5)	-.02(3)	.16(3)	-.09(4)
F(6)	.16(2)	.56(5)	.18(3)	.10(3)	.03(2)	-.02(3)

Table 7.2. Selected bond distances ($Å$) and angles (°) of complex (2).

PT(1) - PT(2)	2.750(1)	PT(1) - PT(3)	2.705(1)
PT(1) - PT(4)	2.620(1)	PT(1) - P(1)	2.360(4)
PT(1) - P(3)	2.266(5)	PT(1) - C(5)	2.089(17)
PT(1) - H(1)	1.69(12)	PT(2) - PT(3)	2.720(1)
PT(2) - P(5)	2.250(5)	PT(2) - C(5)	1.971(18)
PT(2) - C(6)	1.980(17)	PT(3) - PT(4)	2.613(1)
PT(3) - P(2)	2.329(5)	PT(3) - P(7)	2.254(5)
PT(3) - C(6)	2.146(16)	PT(3) - H(1)	2.02(13)
PT(4) - P(4)	2.257(5)	PT(4) - P(8)	2.256(5)
P(1) - C(1)	1.766(16)	P(1) - C(A1)	1.830(14)
P(1) - C(B1)	1.836(16)	P(2) - C(1)	1.839(16)
P(2) - C(C1)	1.821(17)	P(2) - C(D1)	1.822(17)
P(3) - C(2)	1.826(15)	P(3) - C(E1)	1.855(10)
P(3) - C(F1)	1.847(11)	P(4) - C(2)	1.853(16)
P(4) - C(G1)	1.832(14)	P(4) - C(H1)	1.826(14)
P(5) - C(3)	1.825(15)	P(5) - C(I1)	1.811(17)
P(5) - C(J1)	1.819(18)	P(6) - C(3)	1.848(17)
P(6) - C(K1)	1.828(12)	P(6) - C(L1)	1.835(16)
P(7) - C(4)	1.837(16)	P(7) - C(M1)	1.803(13)
P(7) - C(N1)	1.845(11)	P(8) - C(4)	1.834(17)
P(8) - C(O1)	1.824(14)	P(8) - C(P1)	1.837(20)
O(1) - C(5)	1.212(21)	O(2) - C(6)	1.170(20)

Table 7.2(cont).

PT(2) - PT(1) - PT(3)	59.8(1)	PT(2) - PT(1) - PT(4)	70.0(1)
PT(2) - PT(1) - P(1)	99.5(2)	PT(2) - PT(1) - P(3)	132.5(2)
PT(2) - PT(1) - C(5)	45.6(5)	PT(2) - PT(1) - H(1)	107.3(41)
PT(3) - PT(1) - PT(4)	58.7(1)	PT(3) - PT(1) - P(1)	93.6(2)
PT(3) - PT(1) - P(3)	141.8(2)	PT(3) - PT(1) - C(5)	105.3(5)
PT(3) - PT(1) - H(1)	48.3(42)	PT(4) - PT(1) - P(1)	152.3(2)
PT(4) - PT(1) - P(3)	89.5(2)	PT(4) - PT(1) - C(5)	90.4(5)
PT(4) - PT(1) - H(1)	66.3(38)	P(1) - PT(1) - P(3)	114.8(2)
P(1) - PT(1) - C(5)	100.2(5)	P(1) - PT(1) - H(1)	94.3(38)
P(3) - PT(1) - C(5)	94.6(5)	P(3) - PT(1) - H(1)	102.0(42)
C(5) - PT(1) - H(1)	150.9(40)	PT(1) - PT(2) - PT(3)	59.3(1)
PT(1) - PT(2) - P(5)	146.9(2)	PT(1) - PT(2) - C(5)	49.2(5)
PT(1) - PT(2) - C(6)	110.3(5)	PT(3) - PT(2) - P(5)	150.7(2)
PT(3) - PT(2) - C(5)	108.4(5)	PT(3) - PT(2) - C(6)	51.4(5)
P(5) - PT(2) - C(5)	99.5(6)	P(5) - PT(2) - C(6)	102.0(5)
C(5) - PT(2) - C(6)	157.8(7)	PT(1) - PT(3) - PT(2)	60.9(1)
PT(1) - PT(3) - PT(4)	59.0(1)	PT(1) - PT(3) - P(2)	96.1(2)
PT(1) - PT(3) - P(7)	141.0(2)	PT(1) - PT(3) - C(6)	106.8(5)
PT(1) - PT(3) - H(1)	38.6(34)	PT(2) - PT(3) - PT(4)	70.6(1)
PT(2) - PT(3) - P(2)	93.4(2)	PT(2) - PT(3) - P(7)	136.5(2)
PT(2) - PT(3) - C(6)	46.2(5)	PT(2) - PT(3) - H(1)	98.9(34)
PT(4) - PT(3) - P(2)	154.5(2)	PT(4) - PT(3) - P(7)	91.3(2)
PT(4) - PT(3) - C(6)	88.8(4)	PT(4) - PT(3) - H(1)	63.2(31)
P(2) - PT(3) - P(7)	113.4(2)	P(2) - PT(3) - C(6)	94.1(5)
P(2) - PT(3) - H(1)	101.6(32)	P(7) - PT(3) - C(6)	96.2(5)
P(7) - PT(3) - H(1)	107.8(35)	C(6) - PT(3) - H(1)	142.8(33)
PT(1) - PT(4) - PT(3)	62.3(1)	PT(1) - PT(4) - P(4)	96.6(2)
PT(1) - PT(4) - P(8)	155.7(2)	PT(3) - PT(4) - P(4)	158.8(2)
PT(3) - PT(4) - P(8)	94.0(2)	P(4) - PT(4) - P(8)	107.0(2)
PT(1) - P(1) - C(1)	108.1(5)	PT(1) - P(1) - C(A1)	119.2(7)
PT(1) - P(1) - C(B1)	116.8(6)	C(1) - P(1) - C(A1)	101.9(7)
C(1) - P(1) - C(B1)	102.8(8)	C(A1) - P(1) - C(B1)	105.8(9)
PT(3) - P(2) - C(1)	108.5(5)	PT(3) - P(2) - C(C1)	121.1(7)
PT(3) - P(2) - C(D1)	115.2(5)	C(1) - P(2) - C(C1)	100.5(9)
C(1) - P(2) - C(D1)	104.7(8)	C(C1) - P(2) - C(D1)	104.8(8)

Table 7.3. Fractional atomic positions and displacement parameters ($Å^2$) of the crystal structure of compound (3).

Cation A

	X/A	Y/B	Z/C	U
AU	.61167(9)	.13628(8)	.27931(7)	.046
PT(1)	.94537(8)	.18177(7)	.26225(6)	.033
PT(2)	.87511(8)	.18892(7)	.17450(6)	.033
PT(3)	.73610(8)	.18777(7)	.25710(6)	.034
AG	.82940(16)	.07792(14)	.22862(13)	.051
CL	.8534(7)	-.0494(5)	.2267(5)	.100
S	.8438(5)	.2528(4)	.2398(4)	.041
P(1)	1.0445(5)	.1160(5)	.2433(4)	.036
P(2)	.9576(5)	.1166(5)	.1418(4)	.040
P(3)	.7799(5)	.2242(5)	.1175(4)	.039
P(4)	.6570(5)	.2013(5)	.1868(4)	.040
P(5)	.7757(5)	.1789(5)	.3374(4)	.039
P(6)	.9569(5)	.2004(5)	.3420(4)	.040
P(7)	.5019(6)	.0998(5)	.3048(4)	.051
C(1)	1.0134(19)	.0638(18)	.1859(15)	.051(11)
C(2)	.6947(18)	.2571(16)	.1447(14)	.040(10)
C(3)	.8651(18)	.2280(16)	.3626(14)	.039(10)
C(A1)	1.0965(12)	.0499(23)	.2822(17)	.055(12)
C(A2)	1.1391(25)	.0776(13)	.3249(16)	.061(12)
C(A3)	1.1818(25)	.0324(26)	.3543(8)	.082(15)
C(A4)	1.1818(12)	-.0405(23)	.3411(17)	.062(12)
C(A5)	1.1393(25)	-.0682(13)	.2984(16)	.082(14)
C(A6)	1.0966(25)	-.0230(26)	.2689(8)	.098(16)
C(B1)	1.1234(16)	.1773(17)	.2364(8)	.033(9)
C(B2)	1.1188(18)	.2499(15)	.2497(17)	.043(10)
C(B3)	1.1803(24)	.2953(11)	.2483(15)	.067(13)
C(B4)	1.2464(16)	.2682(17)	.2337(8)	.071(13)
C(B5)	1.2509(18)	.1956(15)	.2205(17)	.095(16)
C(B6)	1.1894(24)	.1502(11)	.2218(15)	.067(13)
C(C1)	1.0319(14)	.1663(16)	.1221(8)	.034(9)
C(C2)	1.0307(20)	.2402(14)	.1302(18)	.058(12)
C(C3)	1.0896(24)	.2818(11)	.1194(16)	.093(16)
C(C4)	1.1498(14)	.2495(16)	.1006(8)	.087(15)
C(C5)	1.1511(20)	.1755(14)	.0925(18)	.083(15)
C(C6)	1.0921(24)	.1339(11)	.1032(16)	.080(14)
C(D1)	.9220(24)	.0508(20)	.0934(10)	.039(10)
C(D2)	.8801(18)	-.0065(17)	.1044(8)	.050(11)
C(D3)	.8491(14)	-.0580(11)	.0687(9)	.077(14)
C(D4)	.8598(24)	-.0522(20)	.0220(10)	.078(14)
C(D5)	.9017(18)	.0052(17)	.0109(8)	.075(14)
C(D6)	.9327(14)	.0567(11)	.0466(9)	.046(11)
C(E1)	.8063(13)	.3034(10)	.0891(10)	.046(11)
C(E2)	.7693(17)	.3683(13)	.0912(15)	.054(11)
C(E3)	.7939(21)	.4251(14)	.0688(18)	.064(12)
C(E4)	.8555(13)	.4170(10)	.0443(10)	.082(15)
C(E5)	.8925(17)	.3521(13)	.0422(15)	.074(14)
C(E6)	.8680(21)	.2953(14)	.0646(18)	.066(13)
C(F1)	.7364(27)	.1662(27)	.0649(12)	.066(13)
C(F2)	.7318(15)	.0927(27)	.0672(15)	.065(13)
C(F3)	.7000(22)	.0488(12)	.0273(19)	.088(15)
C(F4)	.6729(27)	.0784(27)	-.0149(12)	.104(17)
C(F5)	.6775(15)	.1519(27)	-.0173(15)	.140(22)
C(F6)	.7092(22)	.1958(12)	.0226(19)	.090(15)
C(G1)	.6160(25)	.1206(18)	.1500(11)	.036(10)
C(G2)	.6376(17)	.0530(24)	.1628(12)	.033(9)
C(G3)	.6102(17)	-.0073(15)	.1334(16)	.058(12)
C(G4)	.5612(25)	-.0001(18)	.0912(11)	.078(14)
C(G5)	.5396(17)	.0675(24)	.0784(12)	.089(15)
C(G6)	.5670(17)	.1278(15)	.1078(16)	.069(13)
C(H1)	.5791(22)	.2606(14)	.2002(18)	.035(10)
C(H2)	.5020(27)	.2473(19)	.1843(11)	.070(13)
C(H3)	.4485(16)	.2956(24)	.1976(13)	.072(13)
C(H4)	.4722(22)	.3572(14)	.2267(18)	.093(16)
C(H5)	.5493(27)	.3705(19)	.2426(11)	.071(13)
C(H6)	.6028(16)	.3222(24)	.2293(13)	.059(12)
C(I1)	.7134(21)	.2343(12)	.3712(17)	.050(11)
C(I2)	.7027(12)	.3042(9)	.3594(8)	.046(11)
C(I3)	.6511(18)	.3471(13)	.3802(15)	.074(14)
C(I4)	.6103(21)	.3199(12)	.4127(17)	.074(14)
C(I5)	.6210(12)	.2500(9)	.4245(8)	.068(13)
C(I6)	.6725(18)	.2072(13)	.4037(15)	.060(12)
C(J1)	.7856(14)	.0951(14)	.3637(15)	.036(10)

Table 7.3(cont).

	X/A	Y/B	Z/C	U
C(J2)	.8115(23)	.0916(17)	.4120(13)	.047(11)
C(J3)	.8211(18)	.0256(22)	.4306(10)	.073(13)
C(J4)	.8048(14)	-.0369(14)	.4009(15)	.077(14)
C(J5)	.7789(23)	-.0333(17)	.3526(13)	.062(12)
C(J6)	.7693(18)	.0326(22)	.3341(10)	.059(12)
C(K1)	.9859(11)	.1254(16)	.3795(14)	.029(9)
C(K2)	.9745(19)	.0558(21)	.3588(8)	.036(10)
C(K3)	.9942(22)	-.0014(13)	.3858(13)	.056(12)
C(K4)	1.0254(11)	.0110(16)	.4335(14)	.051(11)
C(K5)	1.0368(19)	.0806(21)	.4543(8)	.083(15)
C(K6)	1.0171(22)	.1378(13)	.4273(13)	.052(11)
C(L1)	1.0227(24)	.2781(19)	.3610(9)	.040(10)
C(L2)	1.0948(18)	.2736(17)	.3874(17)	.058(12)
C(L3)	1.1399(17)	.3350(26)	.4005(15)	.082(14)
C(L4)	1.1128(24)	.4007(19)	.3872(9)	.079(14)
C(L5)	1.0407(18)	.4051(17)	.3607(17)	.092(16)
C(L6)	.9956(17)	.3438(26)	.3476(15)	.074(14)
C(M11)	.4376(25)	.0435(23)	.2605(9)	.046(11)
C(M12)	.3857(21)	-.0042(19)	.2732(8)	.070(13)
C(M13)	.3351(13)	-.0430(12)	.2381(8)	.074(14)
C(M14)	.3363(25)	-.0340(23)	.1904(9)	.086(15)
C(M15)	.3882(21)	.0137(19)	.1777(8)	.088(15)
C(M16)	.4388(13)	.0525(12)	.2128(8)	.077(14)
C(M21)	.4436(25)	.1746(14)	.3241(20)	.061(12)
C(M22)	.4673(12)	.2452(18)	.3241(14)	.066(13)
C(M23)	.4210(23)	.3004(14)	.3374(13)	.066(13)
C(M24)	.3511(25)	.2848(14)	.3507(20)	.077(14)
C(M25)	.3274(12)	.2142(18)	.3507(14)	.108(18)
C(M26)	.3737(23)	.1590(14)	.3374(13)	.093(16)
C(M31)	.5265(12)	.0510(21)	.3582(14)	.047(11)
C(M32)	.5098(19)	.0756(14)	.4027(19)	.063(12)
C(M33)	.5346(23)	.0383(16)	.4421(12)	.071(13)
C(M34)	.5761(12)	-.0236(21)	.4370(14)	.093(16)
C(M35)	.5929(19)	-.0481(14)	.3925(19)	.075(14)
C(M36)	.5680(23)	-.0109(16)	.3531(12)	.053(11)
H(11)	.98237	.02366	.19121	.100
H(12)	1.05781	.04617	.17328	.100
H(21)	.65380	.26269	.11876	.100
H(22)	.70855	.30325	.16143	.100
H(31)	.87215	.22493	.39665	.100
H(32)	.85752	.27737	.35610	.100
H(A2)	1.13911	.12830	.33420	.100
H(A3)	1.21135	.05159	.38409	.100
H(A4)	1.21143	-.07201	.36157	.100
H(A5)	1.13931	-.11890	.28911	.100
H(A6)	1.06707	-.04219	.23920	.100
H(B2)	1.07279	.26869	.25975	.100
H(B3)	1.17706	.34582	.25746	.100
H(B4)	1.28912	.29987	.23281	.100
H(B5)	1.29690	.17682	.21035	.100
H(B6)	1.19263	.09972	.21258	.100
H(C2)	.98886	.26269	.14336	.100
H(C3)	1.08875	.33327	.12509	.100
H(C4)	1.19079	.27842	.09309	.100
H(C5)	1.19286	.15304	.07928	.100
H(C6)	1.09299	.08246	.09762	.100
H(D2)	.87252	-.01052	.13695	.100
H(D3)	.81994	-.09785	.07642	.100
H(D4)	.83828	-.08799	-.00286	.100
H(D5)	.90929	.00919	-.02159	.100
H(D6)	.96186	.09654	.03895	.100
H(E2)	.72637	.37383	.10824	.100
H(E3)	.76797	.47016	.07030	.100
H(E4)	.87246	.45651	.02870	.100
H(E5)	.93541	.34655	.02511	.100
H(E6)	.89382	.25023	.06306	.100
H(F2)	.75058	.07211	.09660	.100
H(F3)	.69666	-.00226	.02896	.100
H(F4)	.65074	.04794	-.04272	.100
H(F5)	.65877	.17250	-.04674	.100
H(F6)	.71259	.24688	.02094	.100
H(G2)	.67156	.04797	.19224	.100
H(G3)	.62524	-.05429	.14233	.100
H(G4)	.54228	-.04202	.07072	.100
H(G5)	.50570	.07254	.04896	.100
H(G6)	.55205	.17482	.09887	.100

Table 7.3(cont).

	X/A	Y/B	Z/C	U
H(H2)	.48552	.20446	.16397	.100
H(H3)	.39483	.28630	.18652	.100
H(H4)	.43496	.39076	.23595	.100
H(H5)	.56577	.41332	.26290	.100
H(H6)	.65648	.33145	.24040	.100
H(I2)	.73096	.32310	.33665	.100
H(I3)	.64381	.39568	.37195	.100
H(I4)	.57450	.34969	.42718	.100
H(I5)	.59270	.23115	.44717	.100
H(I6)	.68005	.15857	.41189	.100
H(J2)	.82288	.13507	.43268	.100
H(J3)	.83909	.02317	.46418	.100
H(J4)	.81135	-.08279	.41384	.100
H(J5)	.76750	-.07683	.33201	.100
H(J6)	.75132	.03507	.30050	.100
H(K2)	.95282	.04724	.32554	.100
H(K3)	.98634	-.04977	.37132	.100
H(K4)	1.03924	-.02875	.45234	.100
H(K5)	1.05855	.08929	.48759	.100
H(K6)	1.02501	.18628	.44183	.100
H(L2)	1.11365	.22789	.39672	.100
H(L3)	1.19011	.33188	.41884	.100
H(L4)	1.14411	.44338	.39626	.100
H(L5)	1.02183	.45085	.35138	.100
H(L6)	.94540	.34688	.32923	.100
H(M12)	.38485	-.01052	.30639	.100
H(M13)	.29896	-.07617	.24695	.100
H(M14)	.30094	-.06089	.16599	.100
H(M15)	.38893	.02001	.14450	.100
H(M16)	.47489	.08564	.20393	.100
H(M22)	.51586	.25602	.31488	.100
H(M23)	.43743	.34950	.33747	.100
H(M24)	.31886	.32314	.36004	.100
H(M25)	.27874	.20333	.35998	.100
H(M26)	.35715	.10986	.33732	.100
H(M32)	.48097	.11866	.40624	.100
H(M33)	.52307	.05544	.47306	.100
H(M34)	.59340	-.04959	.46440	.100
H(M35)	.62172	-.09127	.38896	.100
H(M36)	.57965	-.02803	.32217	.100

Cation B

	X/A	Y/B	Z/C	U
AU	.47691(9)	.37094(8)	.78804(7)	.042
PT(1)	.80396(8)	.30868(7)	.75340(6)	.034
PT(2)	.71765(8)	.28921(7)	.66925(6)	.033
PT(3)	.59501(8)	.30886(7)	.76117(6)	.032
AG	.68732(16)	.41019(14)	.73040(13)	.050
CL	.6944(8)	.5373(5)	.7260(5)	.093
S	.6962(5)	.2375(4)	.7360(4)	.037
P(1)	.8971(5)	.3734(5)	.7298(4)	.037
P(2)	.7958(5)	.3542(5)	.6322(4)	.035
P(3)	.6131(5)	.2436(4)	.6164(4)	.034
P(4)	.5070(5)	.2763(4)	.6953(4)	.036
P(5)	.6446(5)	.3340(5)	.8391(4)	.038
P(6)	.8248(5)	.3085(5)	.8356(4)	.039
P(7)	.3707(6)	.4150(5)	.8152(4)	.051
C(1)	.8593(19)	.4129(17)	.6756(15)	.047(11)
C(2)	.5363(17)	.2155(15)	.6482(13)	.029(9)
C(3)	.7362(17)	.2898(15)	.8593(13)	.028(9)
C(A1)	.9487(24)	.4493(21)	.7671(8)	.045(11)
C(A2)	.9387(15)	.5206(24)	.7585(13)	.056(12)
C(A3)	.9825(18)	.5736(12)	.7875(15)	.067(13)
C(A4)	1.0362(24)	.5552(21)	.8251(8)	.068(13)
C(A5)	1.0463(15)	.4839(24)	.8337(13)	.065(13)
C(A6)	1.0025(18)	.4309(12)	.8047(15)	.051(11)
C(B1)	.9739(23)	.3207(18)	.7134(21)	.047(11)
C(B2)	.9707(13)	.2467(18)	.7131(11)	.064(13)
C(B3)	1.0300(25)	.2061(12)	.6993(17)	.092(16)
C(B4)	1.0925(23)	.2395(18)	.6860(21)	.105(17)
C(B5)	1.0956(13)	.3135(18)	.6863(11)	.117(19)
C(B6)	1.0363(25)	.3541(12)	.7001(17)	.097(16)
C(C1)	.8623(27)	.2996(14)	.6041(20)	.050(11)
C(C2)	.9169(26)	.3285(13)	.5808(17)	.087(15)

Table 7.3(cont).

	X/A	Y/B	Z/C	U
C(C3)	.9641(12)	.2837(15)	.5576(11)	.120(19)
C(C4)	.9568(27)	.2100(14)	.5579(20)	.138(22)
C(C5)	.9022(26)	.1811(13)	.5812(17)	.121(20)
C(C6)	.8550(12)	.2259(15)	.6043(11)	.065(13)
C(D1)	.7520(10)	.4148(20)	.5879(16)	.041(10)
C(D2)	.7524(22)	.3990(10)	.5395(18)	.059(12)
C(D3)	.7228(22)	.4471(19)	.5074(10)	.075(14)
C(D4)	.6927(10)	.5110(20)	.5236(16)	.080(14)
C(D5)	.6923(22)	.5268(10)	.5720(18)	.073(13)
C(D6)	.7219(22)	.4787(19)	.6042(10)	.073(14)
C(E1)	.6393(23)	.1617(10)	.5819(16)	.040(10)
C(E2)	.6263(15)	.0934(10)	.5946(10)	.057(12)
C(E3)	.6558(16)	.0346(10)	.5712(12)	.054(11)
C(E4)	.6982(23)	.0441(10)	.5351(16)	.055(12)
C(E5)	.7112(15)	.1124(10)	.5223(10)	.085(15)
C(E6)	.6817(16)	.1712(10)	.5456(12)	.065(13)
C(F1)	.5592(12)	.2894(23)	.5694(14)	.039(10)
C(F2)	.5665(24)	.3631(24)	.5694(7)	.038(10)
C(F3)	.5245(21)	.3983(10)	.5334(14)	.074(14)
C(F4)	.4753(12)	.3598(23)	.4974(14)	.101(17)
C(F5)	.4680(24)	.2861(24)	.4974(7)	.103(17)
C(F6)	.5099(21)	.2509(10)	.5334(14)	.046(11)
C(G1)	.4600(12)	.3444(19)	.6605(15)	.031(9)
C(G2)	.4859(20)	.4147(24)	.6713(10)	.070(13)
C(G3)	.4535(23)	.4681(14)	.6444(11)	.058(12)
C(G4)	.3950(12)	.4513(19)	.6066(15)	.085(15)
C(G5)	.3691(20)	.3809(24)	.5958(10)	.068(13)
C(G6)	.4016(23)	.3275(14)	.6227(11)	.053(11)
C(H1)	.4321(12)	.2210(11)	.7148(7)	.043(10)
C(H2)	.3551(14)	.2366(17)	.7111(15)	.064(13)
C(H3)	.3065(12)	.1938(20)	.7309(16)	.074(14)
C(H4)	.3348(12)	.1354(11)	.7544(7)	.066(13)
C(H5)	.4118(14)	.1198(17)	.7580(15)	.068(13)
C(H6)	.4604(12)	.1626(20)	.7382(16)	.056(12)
C(I1)	.5858(10)	.2843(11)	.8759(7)	.063(12)
C(I2)	.5555(24)	.3140(15)	.9151(13)	.060(12)
C(I3)	.5092(23)	.2726(13)	.9376(14)	.086(15)
C(I4)	.4933(10)	.2016(11)	.9210(7)	.064(12)
C(I5)	.5236(24)	.1719(15)	.8819(13)	.063(12)
C(I6)	.5698(23)	.2133(13)	.8594(14)	.062(12)
C(J1)	.6592(23)	.4229(14)	.8704(13)	.039(10)
C(J2)	.6306(20)	.4816(22)	.8474(9)	.056(12)
C(J3)	.6408(12)	.5498(17)	.8707(15)	.064(13)
C(J4)	.6795(23)	.5592(14)	.9171(13)	.068(13)
C(J5)	.7080(20)	.5005(22)	.9401(9)	.070(13)
C(J6)	.6978(12)	.4323(17)	.9168(15)	.033(9)
C(K1)	.8621(24)	.3945(15)	.8674(11)	.033(9)
C(K2)	.9135(14)	.3983(16)	.9095(15)	.045(11)
C(K3)	.9356(18)	.4644(23)	.9336(10)	.066(13)
C(K4)	.9062(24)	.5266(15)	.9154(11)	.062(12)
C(K5)	.8548(14)	.5228(16)	.8733(15)	.066(13)
C(K6)	.8327(18)	.4567(23)	.8492(10)	.043(10)
C(L1)	.8811(15)	.2349(20)	.8610(20)	.041(10)
C(L2)	.8698(23)	.2106(11)	.9041(19)	.086(15)
C(L3)	.9123(18)	.1543(18)	.9221(9)	.109(18)
C(L4)	.9661(15)	.1224(20)	.8970(20)	.082(15)
C(L5)	.9773(23)	.1467(11)	.8539(19)	.091(16)
C(L6)	.9348(18)	.2029(18)	.8359(9)	.084(15)
C(M11)	.3083(13)	.4699(22)	.7768(18)	.045(11)
C(M12)	.2562(24)	.5154(20)	.7948(10)	.070(13)
C(M13)	.2060(21)	.5530(11)	.7642(20)	.066(13)
C(M14)	.2078(13)	.5451(22)	.7154(18)	.081(14)
C(M15)	.2598(24)	.4996(20)	.6974(10)	.104(17)
C(M16)	.3101(21)	.4620(11)	.7281(20)	.070(13)
C(M21)	.3063(17)	.3412(14)	.8260(7)	.051(11)
C(M22)	.2283(14)	.3416(19)	.8102(16)	.061(12)
C(M23)	.1820(15)	.2860(24)	.8192(15)	.079(14)
C(M24)	.2138(17)	.2301(14)	.8439(7)	.073(13)
C(M25)	.2918(14)	.2297(19)	.8597(16)	.069(13)
C(M26)	.3380(15)	.2853(24)	.8507(15)	.078(14)
C(M31)	.3912(26)	.4717(23)	.8710(11)	.037(10)
C(M32)	.3781(18)	.4503(14)	.9145(12)	.062(12)
C(M33)	.4020(16)	.4938(18)	.9561(9)	.088(15)
C(M34)	.4389(26)	.5587(23)	.9541(11)	.094(16)
C(M35)	.4520(18)	.5800(14)	.9105(12)	.092(16)
C(M36)	.4281(16)	.5365(18)	.8690(9)	.080(14)

Table 7.3(cont).

	X/A	Y/B	Z/C	U
H(11)	.90170	.42723	.66080	.100
H(12)	.83139	.45483	.68414	.100
H(21)	.55268	.17215	.66242	.100
H(22)	.49174	.20502	.62458	.100
H(31)	.72640	.23903	.85300	.100
H(32)	.74756	.30138	.89345	.100
H(A2)	.90149	.53322	.73229	.100
H(A3)	.97550	.62313	.78146	.100
H(A4)	1.06656	.59211	.84531	.100
H(A5)	1.08369	.47119	.85994	.100
H(A6)	1.00960	.38131	.81082	.100
H(B2)	.92757	.22315	.72237	.100
H(B3)	1.02821	.15459	.69891	.100
H(B4)	1.13383	.21152	.67620	.100
H(B5)	1.13881	.33700	.67691	.100
H(B6)	1.03813	.40558	.70034	.100
H(C2)	.92217	.37962	.58065	.100
H(C3)	1.00210	.30356	.54141	.100
H(C4)	.98951	.17865	.54184	.100
H(C5)	.89695	.12982	.58148	.100
H(C6)	.81693	.20590	.62062	.100
H(D2)	.77322	.35446	.52832	.100
H(D3)	.72294	.43594	.47375	.100
H(D4)	.67196	.54432	.50126	.100
H(D5)	.67130	.57127	.58337	.100
H(D6)	.72159	.48980	.63798	.100
H(E2)	.59680	.08683	.61992	.100
H(E3)	.64673	-.01297	.58025	.100
H(E4)	.71865	.00302	.51897	.100
H(E5)	.74052	.11879	.49727	.100
H(E6)	.69052	.21858	.53693	.100
H(F2)	.60058	.38998	.59432	.100
H(F3)	.52947	.44951	.53319	.100
H(F4)	.44613	.38410	.47219	.100
H(F5)	.43384	.25913	.47237	.100
H(F6)	.50491	.19959	.53352	.100
H(G2)	.52668	.42623	.69756	.100
H(G3)	.47171	.51695	.65193	.100
H(G4)	.37262	.48853	.58786	.100
H(G5)	.32846	.36938	.56951	.100
H(G6)	.38347	.27865	.61514	.100
H(H2)	.33566	.27729	.69479	.100
H(H3)	.25296	.20479	.72828	.100
H(H4)	.30077	.10567	.76812	.100
H(H5)	.43124	.07905	.77442	.100
H(H6)	.51391	.15152	.74091	.100
H(I2)	.56673	.36317	.92662	.100
H(I3)	.48839	.29300	.96485	.100
H(I4)	.46131	.17261	.93666	.100
H(I5)	.51850	.12244	.87018	.100
H(I6)	.59083	.19260	.83194	.100
H(J2)	.60357	.47500	.81511	.100
H(J3)	.62066	.59060	.85462	.100
H(J4)	.68634	.60670	.93321	.100
H(J5)	.73489	.50717	.97230	.100
H(J6)	.71784	.39157	.93275	.100
H(K2)	.93403	.35512	.92236	.100
H(K3)	.97123	.46727	.96302	.100
H(K4)	.92132	.57265	.93214	.100
H(K5)	.83423	.56592	.86061	.100
H(K6)	.79707	.45381	.81994	.100
H(L2)	.83214	.23229	.92139	.100
H(L3)	.90440	.13700	.95193	.100
H(L4)	.99584	.08315	.90944	.100
H(L5)	1.01509	.12458	.83641	.100
H(L6)	.94284	.21988	.80587	.100
H(M12)	.25475	.52082	.82851	.100
H(M13)	.16968	.58461	.77644	.100
H(M14)	.17296	.57122	.69388	.100
H(M15)	.26129	.49403	.66344	.100
H(M16)	.34632	.43024	.71553	.100
H(M22)	.20613	.38048	.79279	.100
H(M23)	.12764	.28636	.80820	.100
H(M24)	.18147	.19156	.85031	.100

Table 7.3(cont).

	X/A	Y/B	Z/C	U
H(M25)	.31376	.19089	.87700	.100
H(M26)	.39222	.28504	.86165	.100
H(M32)	.35192	.40537	.91592	.100
H(M33)	.39265	.47921	.98633	.100
H(M34)	.45569	.58892	.98282	.100
H(M35)	.47803	.62478	.90889	.100
H(M36)	.43735	.55091	.83848	.100

$[PF_6]^-$ Anions

	X/A	Y/B	Z/C	U
P(F1)	.3570(6)	.2072(6)	.0294(5)	.109
F(11)	.4403(15)	.2276(24)	.0503(12)	.220(18)
F(12)	.2737(15)	.1866(24)	.0085(12)	.288(25)
F(13)	.3586(8)	.2607(15)	-.0085(11)	.198(17)
F(14)	.3555(8)	.1538(15)	.0674(11)	.243(21)
F(15)	.3293(26)	.2664(10)	.0631(16)	.199(16)
F(16)	.3848(26)	.1480(10)	-.0042(16)	.327(30)
P(F2)	.2530(8)	.1933(6)	.5031(6)	.161
F(21)	.2702(16)	.2703(8)	.4974(11)	.176(14)
F(22)	.2277(16)	.1163(8)	.5087(11)	.160(13)
F(23)	.1729(13)	.2198(14)	.5094(18)	.178(15)
F(24)	.3330(13)	.1668(14)	.4967(18)	.239(21)
F(25)	.2788(23)	.2055(20)	.5573(7)	.296(28)
F(26)	.2271(23)	.1811(20)	.4489(7)	.195(17)

Anisotropic displacement parameters ($Å^2$).

Cation A

	U11	U22	U33	U12	U13	U23
AU	.0392(10)	.0501(10)	.0468(14)	-.0053(8)	.0088(9)	.0103(9)
PT(1)	.0302(9)	.0355(9)	.0330(12)	.0014(7)	.0032(8)	.0048(8)
PT(2)	.0339(9)	.0341(9)	.0304(12)	.0048(7)	.0060(8)	.0042(8)
PT(3)	.0342(9)	.0350(9)	.0334(12)	.0036(7)	.0073(8)	.0042(8)
AG	.0474(20)	.0359(17)	.0683(29)	.0006(15)	.0134(19)	.0042(18)
CL	.136(11)	.050(7)	.118(14)	.002(7)	.075(10)	.014(7)
S	.032(6)	.031(5)	.059(9)	.007(5)	.011(6)	.008(5)
P(1)	.030(6)	.046(6)	.034(8)	.005(5)	.013(6)	.018(6)
P(2)	.047(7)	.041(6)	.032(8)	.001(5)	.010(6)	.002(6)
P(3)	.045(6)	.041(6)	.032(8)	.007(5)	.019(6)	.009(5)
P(4)	.025(6)	.048(6)	.045(9)	-.004(5)	-.002(6)	.006(6)
P(5)	.045(7)	.039(6)	.033(8)	.013(5)	.005(6)	.005(6)
P(6)	.035(6)	.049(6)	.035(8)	-.001(5)	.006(6)	.004(6)
P(7)	.047(7)	.038(6)	.067(10)	-.008(5)	.008(7)	.012(6)

Cation B

	U11	U22	U33	U12	U13	U23
AU	.0386(10)	.0457(10)	.0396(13)	.0075(8)	.0065(9)	-.0008(9)
PT(1)	.0322(9)	.0321(9)	.0365(13)	.0008(7)	.0019(9)	.0017(8)
PT(2)	.0352(9)	.0322(9)	.0308(12)	-.0013(7)	.0047(8)	.0008(8)
PT(3)	.0340(9)	.0324(9)	.0287(12)	.0014(7)	.0053(8)	.0033(8)
AG	.0518(20)	.0327(17)	.0632(28)	.0088(15)	.0096(19)	.0035(17)
CL	.150(12)	.042(7)	.089(12)	.013(7)	.049(10)	.004(7)
S	.038(6)	.043(6)	.030(7)	-.005(5)	.009(5)	.010(5)
P(1)	.024(6)	.048(6)	.034(8)	-.002(5)	-.006(6)	-.006(6)
P(2)	.033(6)	.042(6)	.027(8)	-.015(5)	-.001(6)	-.008(5)
P(3)	.037(6)	.031(6)	.030(8)	.006(5)	-.006(6)	.004(5)
P(4)	.030(6)	.032(6)	.046(8)	.002(5)	.009(6)	.018(6)
P(5)	.048(7)	.030(6)	.037(8)	.002(5)	.008(6)	.006(5)
P(6)	.028(6)	.055(7)	.032(8)	.008(5)	-.001(6)	.005(6)
P(7)	.049(7)	.053(7)	.051(9)	.013(6)	.011(7)	.008(6)

Table 7.3(cont). $[PF_6]^-$ Anions

	U11	U22	U33	U12	U13	U23
P(F1)	.069(10)	.108(11)	.154(18)	.028(8)	.054(11)	.018(11)
P(F2)	.201(21)	.086(11)	.181(26)	-.061(13)	-.054(17)	.052(13)

Table 7.4. Selected bond distances (Å) and angles (°) of cations A and B of complex (3).

	Cation A	Cation B		Cation A	Cation B
Au-Pt(3)	2.577(3)	2.575(3)	Au-P(7)	2.287(11)	2,265(11)
Pt(1)-Pt(2)	2.615(3)	2.619(3)	Pt(1)-P(1)	2.249(10)	2.249(10)
Pt(1)-Ag	2.808(4)	2.843(4)	Pt(2)-P(2)	2.241(10)	2.261(10)
Pt(2)-Ag	2.861(4)	2.832(4)	Pt(1)-P(6)	2.235(12)	2.301(12)
Pt(3)-Ag	2.780(4)	2.768(4)	Pt(2)-P(3)	2.284(10)	2.298(10)
Pt(1)-S	2.278(9)	2.278(9)	Pt(3)-P(4)	2.281(11)	2.272(11)
Pt(2)-S	2.257(11)	2.274(10)	Pt(3)-P(5)	2.294(11)	2.254(12)
Pt(3)-S	2.383(9)	2.394(9)	Ag-Cl	2.413(11)	2.388(10)
Pt(1)...Pt(3)	3.674(2)	3.726(2)	Au...Ag	4.414(3)	4.361(3)
Pt(2)...Pt(3)	3.642(2)	3.631(2)	P-C mean	1.828(4)	
Ag...S	3.255(8)	3.243(9)	P-C range	1.77(5) -	1.87(5)

	Cation A	Cation B		Cation A	Cation B
Pt(2)-Pt(1)-Ag	63.6(1)	62.3(1)	Pt(1)-Pt(2)-Ag	61.5(1)	62.7(1)
Pt(2)-Pt(1)-S	54.4(3)	54.8(3)	Pt(1)-Pt(2)-S	55.2(3)	55.0(3)
Pt(2)-Pt(1)-P(1)	96.7(3)	96.4(3)	Pt(1)-Pt(2)-P(2)	94.1(3)	94.4(3)
Pt(2)-Pt(1)-P(6)	154.2(3)	152.7(3)	Pt(1)-Pt(2)-P(3)	154.5(3)	154.4(3)
Ag-Pt(1)-S	78.8(3)	77.7(3)	Ag-Pt(2)-S	78.0(3)	78.0(3)
Ag-Pt(1)-P(1)	97.1(3)	94.8(3)	Ag-Pt(2)-P(2)	92.1(3)	92.4(3)
Ag-Pt(1)-P(6)	109.5(3)	106.7(3)	Ag-Pt(2)-P(3)	114.1(3)	114.8(3)
S-Pt(1)-P(1)	149.8(4)	150.6(4)	S-Pt(2)-P(2)	148.8(4)	149.0(4)
S-Pt(1)-P(6)	100.5(4)	99.6(4)	S-Pt(2)-P(3)	99.6(4)	99.5(4)
P(1)-Pt(1)-P(6)	109.0(4)	109.8(4)	P(2)-Pt(2)-P(3)	111.4(4)	111.3(4)
Au-Pt(3)-Ag	110.9(1)	109.4(1)	Ag-Pt(3)-P(4)	101.1(3)	103.9(3)
Au-Pt(3)-S	171.3(3)	172.9(3)	Ag-Pt(3)-P(5)	94.0(3)	93.5(3)
Au-Pt(3)-P(4)	81.7(3)	81.0(3)	S-Pt(3)-P(4)	97.0(4)	95.7(4)
Au-Pt(3)-P(5)	80.7(3)	82.4(3)	S-Pt(3)-P(5)	98.9(4)	99.3(4)
Ag-Pt(3)-S	77.7(3)	77.4(3)	P(4)-Pt(3)-P(5)	160.0(4)	159.1(4)
Pt(1)-Ag-Pt(2)	54.9(1)	55.0(1)	Cl-Ag-Pt(1)	122.2(4)	131.1(4)
Pt(1)-Ag-Pt(3)	82.2(1)	83.2(1)	Cl-Ag-Pt(2)	132.7(4)	134.1(4)
Pt(2)-Ag-Pt(3)	80.4(1)	80.8(1)	Cl-Ag-Pt(3)	145.5(4)	139.3(4)
Pt(3)-S-Pt(1)	104.0(4)	105.8(4)	Pt(3)-S-Pt(2)	103.4(4)	102.1(4)
Pt(1)-S-Pt(2)	70.4(3)	70.3(3)	Pt(3)-Au-P(7)	174.4(3)	174.1(3)
P(1)-C(1)-P(2)	113(2)	115(2)	P(5)-C(3)-P(6)	120(2)	122(2)
P(3)-C(2)-P(4)	118(2)	120(2)			

Table 7.5. Fractional atomic coordinates and displacement parameters ($Å^2$) for the crystal structure of complex (7).

	X/A	Y/B	Z/C	U
PT(1)	0.19860(2)	0.00000	0.29380(2)	0.033
PT(2)	0.19204(2)	-0.01483(7)	0.19556(2)	0.033
PT(3)	0.10112(2)	0.01972(6)	0.22621(2)	0.033
SN	0.17442(4)	0.18753(13)	0.23345(5)	0.046
P(1)	0.29188(13)	-0.03269(40)	0.32424(15)	0.041
P(2)	0.28273(15)	-0.07237(38)	0.21121(17)	0.042
P(3)	0.15027(14)	-0.02026(44)	0.10963(15)	0.045
P(4)	0.04779(14)	-0.03892(35)	0.14742(15)	0.037
P(5)	0.05208(14)	0.05657(38)	0.28500(17)	0.042
P(6)	0.15904(14)	-0.01354(40)	0.36159(14)	0.039
P(7)	0.17177(30)	0.38186(53)	0.32239(31)	0.088
P(8)	0.0000	-0.0044(12)	0.5000	0.109
P(9)	1.0000	0.3361(8)	1.0000	0.087
F(11)	0.1693(6)	0.2634(13)	0.3030(6)	0.096(4)
F(12)	0.1439(7)	0.3865(18)	0.3651(8)	0.139(6)
F(13)	0.1528(9)	0.4698(24)	0.2823(9)	0.189(9)
F(14)	0.2306(9)	0.4072(20)	0.3504(9)	0.163(8)
F(21)	0.0640(11)	-0.0021(31)	0.5126(10)	0.225(11)
F(22)	0.0063(12)	0.0679(35)	0.5467(12)	0.261(16)
F(23)	-0.0052(15)	-0.1281(34)	0.5286(13)	0.273(17)
F(31)	1.0182(12)	0.3336(31)	1.0604(12)	0.239(13)
F(32)	0.9623(13)	0.2332(40)	0.9915(16)	0.314(20)
F(33)	0.9618(13)	0.4436(37)	1.0026(14)	0.303(19)
C(1)	0.3262(5)	-0.0152(14)	0.2705(5)	0.036(3)
C(2)	0.0763(5)	0.0153(15)	0.0939(6)	0.045(3)
C(3)	0.0972(6)	0.0836(15)	0.3490(7)	0.046(4)
C(4)	0.2494(10)	0.2630(22)	0.2324(10)	0.082(7)
C(5)	0.1166(8)	0.3019(18)	0.1845(8)	0.064(5)
C(A1)	0.3298(14)	0.0680(23)	0.3699(7)	0.051(4)
C(A2)	0.3031(9)	0.1669(29)	0.3725(11)	0.108(9)
C(A3)	0.3303(11)	0.2487(17)	0.4056(13)	0.118(10)
C(A4)	0.3840(14)	0.2316(23)	0.4361(7)	0.102(8)
C(A5)	0.4107(9)	0.1328(29)	0.4335(11)	0.36(4)
C(A6)	0.3835(11)	0.0510(17)	0.4003(13)	0.123(11)
C(B1)	0.3157(7)	-0.1671(15)	0.3518(9)	0.044(4)
C(B2)	0.2773(6)	-0.2350(20)	0.3653(10)	0.083(7)
C(B3)	0.2938(6)	-0.3360(14)	0.3876(5)	0.108(9)
C(B4)	0.3488(7)	-0.3693(15)	0.3966(9)	0.089(7)
C(B5)	0.3872(6)	-0.3014(20)	0.3831(10)	0.119(10)
C(B6)	0.3707(6)	-0.2004(14)	0.3607(5)	0.072(6)
C(C1)	0.2925(7)	-0.2204(11)	0.2242(8)	0.046(4)
C(C2)	0.2491(6)	-0.2811(16)	0.2334(9)	0.056(5)
C(C3)	0.2561(5)	-0.3922(13)	0.2441(4)	0.091(7)
C(C4)	0.3064(7)	-0.4426(11)	0.2456(8)	0.097(8)
C(C5)	0.3497(6)	-0.3818(16)	0.2364(9)	0.073(6)
C(C6)	0.3428(5)	-0.2707(13)	0.2257(4)	0.065(5)
C(D1)	0.3230(5)	-0.0405(8)	0.1653(5)	0.042(3)
C(D2)	0.3530(8)	0.0564(11)	0.1699(7)	0.063(5)
C(D3)	0.3851(7)	0.0784(12)	0.1364(4)	0.065(5)
C(D4)	0.3871(5)	0.0034(8)	0.0983(5)	0.064(4)
C(D5)	0.3571(8)	-0.0936(11)	0.0937(7)	0.069(5)
C(D6)	0.3250(7)	-0.1155(12)	0.1273(4)	0.055(4)
C(E1)	0.1498(9)	-0.1501(12)	0.0733(7)	0.049(4)
C(E2)	0.1689(7)	-0.2448(19)	0.1007(4)	0.062(5)
C(E3)	0.1623(5)	-0.3456(15)	0.0760(8)	0.076(6)
C(E4)	0.1366(9)	-0.3516(12)	0.0237(7)	0.077(6)
C(E5)	0.1176(7)	-0.2569(19)	-0.0038(4)	0.074(6)
C(E6)	0.1242(5)	-0.1562(15)	0.0210(8)	0.074(6)
C(F1)	0.1782(6)	0.0831(12)	0.0729(4)	0.052(4)
C(F2)	0.1648(8)	0.1933(15)	0.0739(10)	0.086(7)
C(F3)	0.1930(10)	0.2707(13)	0.0530(10)	0.115(10)
C(F4)	0.2347(6)	0.2378(12)	0.0310(4)	0.107(9)
C(F5)	0.2480(8)	0.1276(15)	0.0299(10)	0.107(9)
C(F6)	0.2198(10)	0.0503(13)	0.0509(10)	0.077(6)
C(G1)	0.0495(7)	-0.1894(8)	0.1410(7)	0.038(3)
C(G2)	0.0223(4)	-0.2386(15)	0.0948(6)	0.052(4)
C(G3)	0.0228(8)	-0.3518(16)	0.0900(4)	0.078(6)
C(G4)	0.0505(7)	-0.4158(8)	0.1314(7)	0.070(6)
C(G5)	0.0778(4)	-0.3665(15)	0.1776(6)	0.061(5)
C(G6)	0.0773(8)	-0.2533(16)	0.1824(4)	0.053(4)

Table 7.5(cont).

	X/A	Y/B	Z/C	U
C(H1)	-0.0271(5)	-0.0104(19)	0.1235(8)	0.043(3)
C(H2)	-0.0463(4)	0.0761(11)	0.0902(4)	0.064(5)
C(H3)	-0.1029(4)	0.0989(16)	0.0742(8)	0.072(6)
C(H4)	-0.1402(5)	0.0352(19)	0.0914(8)	0.083(6)
C(H5)	-0.1210(4)	-0.0514(11)	0.1247(4)	0.073(6)
C(H6)	-0.0645(4)	-0.0742(16)	0.1408(8)	0.063(5)
C(I1)	0.0163(6)	0.1895(13)	0.2716(9)	0.043(4)
C(I2)	-0.0030(9)	0.2196(13)	0.2204(8)	0.060(5)
C(I3)	-0.0234(7)	0.3246(18)	0.2076(5)	0.079(6)
C(I4)	-0.0244(6)	0.3994(13)	0.2461(9)	0.072(6)
C(I5)	-0.0051(9)	0.3693(13)	0.2972(8)	0.095(8)
C(I6)	0.0153(7)	0.2643(18)	0.3100(5)	0.081(7)
C(J1)	-0.0002(5)	-0.0426(13)	0.2935(3)	0.044(4)
C(J2)	-0.0348(9)	-0.0175(12)	0.3245(8)	0.065(5)
C(J3)	-0.0733(7)	-0.0939(9)	0.3315(8)	0.078(6)
C(J4)	-0.0772(5)	-0.1954(13)	0.3075(3)	0.085(7)
C(J5)	-0.0427(9)	-0.2204(12)	0.2765(8)	0.080(6)
C(J6)	-0.0042(7)	-0.1440(9)	0.2696(8)	0.061(5)
C(K1)	0.1282(6)	-0.1475(11)	0.3686(5)	0.044(4)
C(K2)	0.1294(6)	-0.2327(9)	0.3349(6)	0.055(4)
C(K3)	0.1037(9)	-0.3316(12)	0.3395(7)	0.081(6)
C(K4)	0.0769(6)	-0.3454(11)	0.3779(5)	0.084(7)
C(K5)	0.0758(6)	-0.2602(9)	0.4116(6)	0.082(7)
C(K6)	0.1013(9)	-0.1612(12)	0.4070(7)	0.063(5)
C(L1)	0.2013(11)	0.0232(34)	0.4237(5)	0.054(4)
C(L2)	0.2327(14)	-0.0562(18)	0.4553(12)	0.128(11)
C(L3)	0.2691(8)	-0.0265(29)	0.5020(12)	0.189(17)
C(L4)	0.2739(11)	0.0826(34)	0.5171(5)	0.095(8)
C(L5)	0.2424(14)	0.1620(18)	0.4855(12)	0.178(17)
C(L6)	0.2061(8)	0.1323(29)	0.4388(12)	0.174(16)
H(11)	.36173	-.05222	.27939	.043
H(12)	.33210	.06174	.26563	.043
H(21)	.05679	-.01757	.06153	.054
H(22)	.07180	.09390	.09115	.054
H(31)	.07688	.07217	.37427	.055
H(32)	.11010	.15849	.35107	.055
H(41)	.26982	.28226	.26697	.098
H(42)	.27145	.21327	.21831	.098
H(43)	.24089	.32789	.21151	.098
H(51)	.09468	.31881	.20798	.077
H(52)	.10828	.36704	.16360	.077
H(53)	.09666	.24995	.15938	.077
H(A2)	.26576	.17684	.35108	.130
H(A3)	.31167	.31753	.40717	.140
H(A4)	.40276	.28855	.45905	.122
H(A5)	.44789	.12088	.45482	.400
H(A6)	.40199	-.01775	.39869	.148
H(B2)	.23901	-.21182	.35898	.099
H(B3)	.26703	-.38324	.39694	.130
H(B4)	.36026	-.43966	.41213	.107
H(B5)	.42546	-.32459	.38936	.143
H(B6)	.39738	-.15317	.35136	.086
H(C2)	.21417	-.24613	.23240	.067
H(C3)	.22595	-.43459	.25046	.109
H(C4)	.31121	-.51993	.25301	.117
H(C5)	.38470	-.41686	.23739	.087
H(C6)	.37293	-.22839	.21939	.078
H(D2)	.35150	.10851	.19635	.076
H(D3)	.40594	.14585	.13954	.078
H(D4)	.40947	.01882	.07498	.076
H(D5)	.35855	-.14561	.06725	.083
H(D6)	.30417	-.18297	.12412	.066
H(E2)	.18671	-.24081	.13718	.074
H(E3)	.17539	-.41150	.09515	.091
H(E4)	.13205	-.42160	.00647	.092
H(E5)	.09983	-.26091	-.04017	.089
H(E6)	.11100	-.09022	.00190	.089
H(F2)	.13585	.21618	.08927	.103
H(F3)	.18376	.34740	.05372	.139
H(F4)	.25435	.29176	.01640	.128
H(F5)	.27698	.10491	.01458	.128
H(F6)	.22907	-.02633	.05008	.092
H(G2)	.00292	-.19414	.06601	.063
H(G3)	.00385	-.38603	.05785	.093
H(G4)	.05089	-.49451	.12807	.084
H(G5)	.09708	-.41100	.20642	.074
H(G6)	.09618	-.21910	.21458	.063

Table 7.5(cont).

	X/A	Y/B	Z/C	U
H(H2)	-.02037	.12042	.07818	.077
H(H3)	-.11624	.15908	.05097	.087
H(H4)	-.17956	.05101	.08023	.099
H(H5)	-.14699	-.09577	.13673	.088
H(H6)	-.05113	-.13439	.16397	.075
H(I2)	-.00229	.16745	.19371	.072
H(I3)	-.03683	.34554	.17197	.095
H(I4)	-.03848	.47252	.23704	.086
H(I5)	-.00567	.42154	.32384	.114
H(I6)	.02877	.24344	.34562	.097
H(J2)	-.03206	.05304	.34112	.078
H(J3)	-.09731	-.07654	.35306	.093
H(J4)	-.10397	-.24857	.31247	.102
H(J5)	-.04541	-.29102	.25995	.096
H(J6)	.01988	-.16150	.24807	.073
H(K2)	.14802	-.22317	.30824	.066
H(K3)	.10454	-.39092	.31611	.097
H(K4)	.05909	-.41418	.38117	.100
H(K5)	.05709	-.26971	.43831	.098
H(K6)	.10050	-.10190	.43039	.076
H(L2)	.22881	-.13236	.44521	.154
H(L3)	.29032	-.08213	.52431	.228
H(L4)	.29919	.10304	.54952	.114
H(L5)	.24635	.23800	.49568	.212
H(L6)	.18485	.18776	.41651	.208

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
PT(1)	.0326(2)	.0323(3)	.0303(3)	.0007(2)	.0082(2)	-.0004(3)
PT(2)	.0328(2)	.0348(3)	.0302(3)	-.0020(2)	.0092(2)	-.0001(3)
PT(3)	.0311(2)	.0316(3)	.0327(3)	-.0004(2)	.0080(2)	0.0000(3)
SN	.0459(5)	.0303(6)	.0566(8)	-.0043(4)	.0147(5)	.0013(5)
P(1)	.0327(15)	.0506(26)	.0358(20)	-.0004(17)	.0056(14)	-.0023(20)
P(2)	.0321(16)	.0405(23)	.0505(26)	-.0011(16)	.0141(16)	.0016(19)
P(3)	.0409(17)	.0544(26)	.0377(20)	-.0051(20)	.0113(14)	-.0002(22)
P(4)	.0347(15)	.0358(22)	.0377(21)	-.0009(15)	.0075(14)	.0020(17)
P(5)	.0331(17)	.0386(22)	.0512(26)	.0047(16)	.0160(16)	.0033(19)
P(6)	.0422(16)	.0378(21)	.0354(18)	.0036(18)	.0111(14)	.0015(20)
P(7)	.103(5)	.046(3)	.109(6)	.000(3)	.033(4)	-.018(4)
P(8)	.081(5)	.091(8)	.135(9)	.000	-.017(5)	.000
P(9)	.133(8)	.048(5)	.072(6)	.000	.025(6)	.000

Table 7.6. Selected bond distances ($Å$) and angles (°) of complex (7).

PT(1)	PT(2)	2.609(1)	PT(1)	PT(3)	2.615(1)
PT(1)	SN	2.766(2)	PT(1)	P(1)	2.272(4)
PT(1)	P(6)	2.297(4)	PT(2)	PT(3)	2.635(1)
PT(2)	SN	2.739(2)	PT(2)	P(2)	2.284(4)
PT(2)	P(3)	2.264(4)	PT(3)	SN	2.702(2)
PT(3)	P(4)	2.288(4)	PT(3)	P(5)	2.284(5)
SN	F(11)	2.118(16)	SN	C(4)	2.08(3)
SN	C(5)	2.17(3)	P(1)	C(1)	1.877(13)
P(1)	C(A1)	1.81(3)	P(1)	C(B1)	1.82(2)
P(2)	C(1)	1.804(14)	P(2)	C(C1)	1.833(15)
P(2)	C(D1)	1.826(14)	P(3)	C(2)	1.820(14)
P(3)	C(E1)	1.853(17)	P(3)	C(F1)	1.844(15)
P(4)	C(2)	1.886(16)	P(4)	C(G1)	1.835(11)
P(4)	C(H1)	1.829(13)	P(5)	C(3)	1.812(17)
P(5)	C(I1)	1.829(17)	P(5)	C(J1)	1.829(15)
P(6)	C(3)	1.891(17)	P(6)	C(K1)	1.828(15)
P(6)	C(L1)	1.773(19)	P(7)	F(11)	1.526(17)
P(7)	F(12)	1.49(3)	P(7)	F(13)	1.50(3)
P(7)	F(14)	1.48(3)	P(8)	F(21)	1.53(3)
P(8)	F(22)	1.51(4)	P(8)	F(23)	1.71(5)
P(9)	F(31)	1.56(4)	P(9)	F(32)	1.54(5)
P(9)	F(33)	1.62(5)			

Table 7.6(cont).

PT(2) - PT(1) - PT(3)	60.6(1)	PT(2) - PT(1) - SN	61.2(1)
PT(2) - PT(1) - P(1)	97.6(1)	PT(2) - PT(1) - P(6)	151.1(1)
PT(3) - PT(1) - SN	60.2(1)	PT(3) - PT(1) - P(1)	158.1(2)
PT(3) - PT(1) - P(6)	92.6(1)	SN - PT(1) - P(1)	113.2(2)
SN - PT(1) - P(6)	116.9(2)	P(1) - PT(1) - P(6)	108.2(2)
PT(1) - PT(2) - PT(3)	59.8(1)	PT(1) - PT(2) - SN	62.2(1)
PT(1) - PT(2) - P(2)	92.6(2)	PT(1) - PT(2) - P(3)	157.2(1)
PT(3) - PT(2) - SN	60.3(1)	PT(3) - PT(2) - P(2)	151.0(2)
PT(3) - PT(2) - P(3)	97.4(1)	SN - PT(2) - P(2)	117.0(2)
SN - PT(2) - P(3)	109.3(2)	P(2) - PT(2) - P(3)	109.7(2)
PT(1) - PT(3) - PT(2)	59.6(1)	PT(1) - PT(3) - SN	62.7(1)
PT(1) - PT(3) - P(4)	144.2(1)	PT(1) - PT(3) - P(5)	95.9(2)
PT(2) - PT(3) - SN	61.7(1)	PT(2) - PT(3) - P(4)	89.5(1)
PT(2) - PT(3) - P(5)	155.3(2)	SN - PT(3) - P(4)	120.7(2)
SN - PT(3) - P(5)	106.0(2)	P(4) - PT(3) - P(5)	114.8(2)
PT(1) - SN - PT(2)	56.6(1)	PT(1) - SN - PT(3)	57.1(1)
PT(1) - SN - F(11)	83.9(5)	PT(1) - SN - C(4)	108.5(8)
PT(1) - SN - C(5)	152.5(6)	PT(2) - SN - PT(3)	57.9(1)
PT(2) - SN - F(11)	140.5(5)	PT(2) - SN - C(4)	99.0(8)
PT(2) - SN - C(5)	119.6(6)	PT(3) - SN - F(11)	101.1(4)
PT(3) - SN - C(4)	156.6(8)	PT(3) - SN - C(5)	96.7(6)
F(11) - SN - C(4)	95.0(9)	F(11) - SN - C(5)	94.0(7)
C(4) - SN - C(5)	99.1(9)	PT(1) - P(1) - C(1)	109.4(5)
PT(1) - P(1) - C(A1)	114.8(11)	PT(1) - P(1) - C(B1)	119.3(6)
C(1) - P(1) - C(A1)	100.8(11)	C(1) - P(1) - C(B1)	104.5(9)
C(A1) - P(1) - C(B1)	106.1(11)	PT(2) - P(2) - C(1)	111.7(5)
PT(2) - P(2) - C(C1)	114.1(6)	PT(2) - P(2) - C(D1)	120.1(5)
C(1) - P(2) - C(C1)	101.0(9)	C(1) - P(2) - C(D1)	102.2(6)
C(C1) - P(2) - C(D1)	105.6(7)	PT(2) - P(3) - C(2)	112.7(5)
PT(2) - P(3) - C(E1)	119.9(7)	PT(2) - P(3) - C(F1)	113.1(5)
C(2) - P(3) - C(E1)	102.5(9)	C(2) - P(3) - C(F1)	102.4(8)
C(E1) - P(3) - C(F1)	104.2(8)	PT(3) - P(4) - C(2)	110.9(5)
PT(3) - P(4) - C(G1)	112.0(6)	PT(3) - P(4) - C(H1)	123.1(7)
C(2) - P(4) - C(G1)	104.6(8)	C(2) - P(4) - C(H1)	102.8(8)
C(G1) - P(4) - C(H1)	101.7(10)	PT(3) - P(5) - C(3)	112.6(5)
PT(3) - P(5) - C(I1)	110.9(7)	PT(3) - P(5) - C(J1)	119.1(5)
C(3) - P(5) - C(I1)	99.8(10)	C(3) - P(5) - C(J1)	106.2(7)
C(I1) - P(5) - C(J1)	106.4(7)	PT(1) - P(6) - C(3)	108.2(6)
PT(1) - P(6) - C(K1)	115.2(5)	PT(1) - P(6) - C(L1)	117.4(9)
C(3) - P(6) - C(K1)	103.3(8)	C(3) - P(6) - C(L1)	104.9(13)
C(K1) - P(6) - C(L1)	106.5(13)	F(11) - P(7) - F(12)	108.4(11)
F(11) - P(7) - F(13)	116.7(13)	F(11) - P(7) - F(14)	108.2(12)
F(12) - P(7) - F(13)	113.9(13)	F(12) - P(7) - F(14)	101.3(12)
F(13) - P(7) - F(14)	107.1(14)	F(21) - P(8) - F(21')	177.9(23)
F(21) - P(8) - F(22)	86.4(17)	F(21) - P(8) - F(22')	92.4(17)
F(21) - P(8) - F(23)	96.7(19)	F(21) - P(8) - F(23')	85.2(19)
F(22) - P(8) - F(22')	108.7(23)	F(22) - P(8) - F(23)	98.0(20)
F(22) - P(8) - F(23')	152.3(20)	F(23) - P(8) - F(23')	57.0(18)
F(31) - P(9) - F(31')	177.8(21)	F(31) - P(9) - F(32)	97.7(21)
F(31) - P(9) - F(32')	80.6(21)	F(31) - P(9) - F(33)	88.8(19)
F(31) - P(9) - F(33')	92.9(19)	F(32) - P(9) - F(32')	71.6(21)
F(32) - P(9) - F(33)	108.7(19)	F(32) - P(9) - F(33')	169.3(21)
F(33) - P(9) - F(33')	73.2(19)	SN - F(11) - P(7)	134.8(10)
P(1) - C(1) - P(2)	110.5(7)	P(3) - C(2) - P(4)	107.5(8)
P(5) - C(3) - P(6)	108.7(9)	P(1) - C(A1) - C(A2)	117.0(22)
P(1) - C(A1) - C(A6)	123.0(22)	P(1) - C(B1) - C(B2)	118.0(14)
P(1) - C(B1) - C(B6)	121.9(14)	P(2) - C(C1) - C(C2)	119.2(13)
P(2) - C(C1) - C(C6)	120.7(12)	P(2) - C(D1) - C(D2)	120.0(11)
P(2) - C(D1) - C(D6)	119.8(9)	P(3) - C(E1) - C(E2)	118.3(14)
P(3) - C(E1) - C(E6)	121.2(13)	P(3) - C(F1) - C(F2)	121.4(13)
P(3) - C(F1) - C(F6)	117.8(12)	P(4) - C(G1) - C(G2)	119.8(13)
P(4) - C(G1) - C(G6)	120.2(13)	P(4) - C(H1) - C(H2)	120.8(12)
P(4) - C(H1) - C(H6)	119.2(16)	P(5) - C(I1) - C(I2)	116.7(15)
P(5) - C(I1) - C(I6)	122.6(17)	P(5) - C(J1) - C(J2)	120.5(12)
P(5) - C(J1) - C(J6)	119.5(11)	P(6) - C(K1) - C(K2)	120.9(11)
P(6) - C(K1) - C(K6)	119.0(11)	P(6) - C(L1) - C(L2)	119.8(27)
P(6) - C(L1) - C(L6)	120.0(23)		

Symmetry code:-

' -x y -z

Table 7.7. Fractional atomic positions and displacement parameters ($Å^2$) of the crystal structure of complexes (8)/(9).

	X/A	Y/B	Z/C	U
PT	-0.2763(1)	-0.1957(1)	-0.2513(1)	0.031
SN	-0.2925(2)	-0.2925	-0.2925	0.040
CL	-0.18270	-0.18270	-0.18270	0.03(1)
P(1)	-0.3479(6)	-0.1759(5)	-0.2061(5)	0.034
P(2)	-0.2701(6)	-0.1397(6)	-0.3198(6)	0.048
P(3)	-0.50000	0.00000	-0.50000	0.044(9)
F(1)	-0.370(1)	-0.299(1)	-0.282(1)	0.082
F(31)	-0.564(1)	0.000	-0.500	0.06(1)
F(32)	-0.500	0.000	-0.563(1)	0.05(1)
F(33)	-0.500	-0.057(2)	-0.500	0.08(2)
O(2)	-0.18270	-0.18270	-0.18270	0.030
C(1)	-0.370(2)	-0.237(2)	-0.173(2)	0.04(2)
C(2)	-0.20770	-0.20770	-0.20770	0.02(3)
C(A1)	-0.343(4)	-0.132(2)	-0.155(1)	0.10(3)
C(A2)	-0.295(3)	-0.117(1)	-0.138(3)	0.12(3)
C(A3)	-0.291(2)	-0.084(2)	-0.097(2)	0.08(2)
C(A4)	-0.334(3)	-0.065(1)	-0.074(1)	0.09(2)
C(A5)	-0.382(2)	-0.079(2)	-0.092(3)	0.07(2)
C(A6)	-0.386(3)	-0.113(2)	-0.132(2)	0.16(3)
C(B1)	-0.403(1)	-0.150(3)	-0.245(2)	0.07(2)
C(B2)	-0.405(2)	-0.100(3)	-0.259(1)	0.08(2)
C(B3)	-0.446(2)	-0.082(1)	-0.287(2)	0.09(2)
C(B4)	-0.484(1)	-0.115(2)	-0.302(2)	0.06(2)
C(B5)	-0.482(2)	-0.166(2)	-0.288(1)	0.08(2)
C(B6)	-0.442(2)	-0.183(2)	-0.259(2)	0.10(2)
C(C1)	-0.233(2)	-0.083(2)	-0.305(2)	0.06(2)
C(C2)	-0.226(1)	-0.069(1)	-0.255(1)	0.08(2)
C(C3)	-0.200(2)	-0.025(2)	-0.243(1)	0.07(2)
C(C4)	-0.181(1)	0.006(1)	-0.281(1)	0.08(2)
C(C5)	-0.188(1)	-0.008(2)	-0.332(1)	0.04(2)
C(C6)	-0.214(2)	-0.052(2)	-0.343(1)	0.03(2)
C(D1)	-0.329(1)	-0.121(3)	-0.353(2)	0.03(2)
C(D2)	-0.363(2)	-0.157(2)	-0.371(2)	0.12(3)
C(D3)	-0.405(2)	-0.142(2)	-0.399(1)	0.08(2)
C(D4)	-0.412(1)	-0.091(2)	-0.409(1)	0.07(2)
C(D5)	-0.378(2)	-0.055(1)	-0.391(2)	0.11(3)
C(D6)	-0.336(2)	-0.070(3)	-0.363(1)	0.11(3)
H(11)	-0.37339	-0.25893	-0.20299	0.100
H(12)	-0.40193	-0.23475	-0.15616	0.100
H(A2)	-0.265(4)	-0.131(2)	-0.154(4)	0.100
H(A3)	-0.258(3)	-0.075(3)	-0.085(3)	0.100
H(A4)	-0.331(5)	-0.042(2)	-0.046(1)	0.100
H(A5)	-0.412(3)	-0.066(2)	-0.076(4)	0.100
H(A6)	-0.419(3)	-0.122(4)	-0.145(3)	0.100
H(B2)	-0.378(3)	-0.077(4)	-0.249(1)	0.100
H(B3)	-0.447(3)	-0.047(1)	-0.297(2)	0.100
H(B4)	-0.512(1)	-0.103(4)	-0.322(2)	0.100
H(B5)	-0.509(3)	-0.189(3)	-0.298(1)	0.100
H(B6)	-0.440(3)	-0.219(2)	-0.249(3)	0.100
H(C2)	-0.239(1)	-0.090(2)	-0.228(2)	0.100
H(C3)	-0.195(2)	-0.016(3)	-0.208(1)	0.100
H(C4)	-0.163(2)	0.036(2)	-0.273(2)	0.100
H(C5)	-0.175(1)	0.013(2)	-0.358(2)	0.100
H(C6)	-0.219(3)	-0.062(3)	-0.379(1)	0.100
H(D2)	-0.358(3)	-0.193(2)	-0.364(3)	0.100
H(D3)	-0.428(3)	-0.167(3)	-0.412(1)	0.100
H(D4)	-0.441(1)	-0.080(4)	-0.429(2)	0.100
H(D5)	-0.383(3)	-0.019(1)	-0.398(3)	0.100
H(D6)	-0.313(3)	-0.045(3)	-0.350(1)	0.100

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
PT	0.030(1)	0.027(1)	0.036(1)	0.004(1)	0.004(1)	0.005(2)
SN	0.040(2)	0.040	0.040	-0.002	-0.002	-0.002(2)
P(1)	0.05(1)	0.03(1)	0.02(1)	0.02(1)	0.00(1)	0.01(1)
P(2)	0.06(2)	0.05(1)	0.04(1)	-0.01(1)	0.00(1)	0.01(1)
F(1)	0.12(3)	0.02(2)	0.11(3)	-0.02(2)	0.03(2)	-0.02(2)

Table 7.8. Selected bond distances (Å) and angles (°) of complexes (8)/(9).

Pt	- Pt'	2.634(4)	Pt	- Sn	2.773(3)
Pt	- Cl	3.045(1)	Pt	- P(1)	2.268(15)
Pt	- P(2)	2.315(16)	Pt	- C(2)	2.142(3)
Sn	- F(1)	2.06(3)	P(1)	- C(1)	1.90(5)
P(1)	- C(A1)	1.76(4)	P(1)	- C(B1)	1.88(5)
P(2)	- C(1)	1.79(5)	P(2)	- C(C1)	1.81(5)
P(2)	- C(D1)	1.82(4)	P(3)	- F(31)	1.66(4)
P(3)	- F(32)	1.65(4)	P(3)	- F(33)	1.50(5)
O(2)	- C(2)	1.129			

Pt'	- Pt	- Pt"	60.0	Pt'	- Pt	- Sn	61.7(1)
Pt'	- Pt	- P(1)	95.8(4)	Pt'	- Pt	- P(2)	155.7(5)
Pt'	- Pt	- C(2)	52.1(1)	Pt"	- Pt	- P(1)	155.7(4)
Pt"	- Pt	- P(2)	95.8(5)	Sn	- Pt	- P(1)	106.5(4)
Sn	- Pt	- P(2)	106.6(4)	Sn	- Pt	- C(2)	101.5(2)
P(1)	- Pt	- P(2)	108.3(6)	P(1)	- Pt	- C(2)	116.5(4)
P(2)	- Pt	- C(2)	116.3(5)	Pt	- Sn	- Pt'	56.7(1)
Pt	- Sn	- F(1)	100.0(8)	Pt	- Sn	- F(1')	155.4(8)
Pt	- Sn	- F(1")	105.6(8)	F(1)	- Sn	- F(1')	93.7(12)
Pt	- P(1)	- C(1)	106.5(8)	Pt	- P(1)	- C(A1)	118.6(34)
Pt	- P(1)	- C(B1)	115.8(15)	C(1)	- P(1)	- C(A1)	103.7(22)
C(1)	- P(1)	- C(B1)	108.1(25)	C(A1)	- P(1)	- C(B1)	103.1(35)
Pt	- P(2)	- C(1)	106.4(17)	Pt	- P(2)	- C(C1)	112.9(16)
Pt	- P(2)	- C(D1)	118.0(19)	C(1)	- P(2)	- C(C1)	107.8(22)
C(1)	- P(2)	- C(D1)	101.0(24)	C(C1)	- P(2)	- C(D1)	109.6(28)
P(1)	- C(1)	- P(2)	114.2(26)	Pt	- C(2)	- Pt'	75.9(1)
Pt	- C(2)	- O(2)	134.8(1)				

Symmetry code:-

'	z	x	y
"	y	z	x

Table 7.9. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (10).

	X/A	Y/B	Z/C	U
PT(1)	.19606(5)	.11103(5)	.20386(3)	.024
PT(2)	.29846(5)	.13848(5)	.29008(3)	.025
PT(3)	.22125(5)	.27533(5)	.21642(3)	.026
SN(1)	.07564(9)	.19459(9)	.30860(6)	.033
SN(2)	.40535(9)	.14772(9)	.16875(6)	.032
CL(1)	-.2837(7)	.3617(7)	.1717(4)	.124
CL(2)	-.2123(9)	.3359(7)	.0404(5)	.152
P(1)	.2272(3)	-.0458(3)	.2164(2)	.030
P(2)	.3344(3)	-.0142(4)	.3230(2)	.032
P(3)	.3838(4)	.2250(4)	.3367(2)	.034
P(4)	.2865(4)	.3841(3)	.2529(2)	.034
P(5)	.1227(4)	.3491(3)	.1429(2)	.034
P(6)	.0962(4)	.1568(3)	.1266(2)	.031
F(11)	.0280(9)	.2649(8)	.3852(6)	.070
F(12)	-.0556(8)	.2535(9)	.2793(6)	.069
F(13)	.0043(10)	.1009(9)	.3543(6)	.079
F(21)	.4995(8)	.0274(7)	.1625(6)	.058
F(22)	.5247(10)	.2068(9)	.1736(6)	.083
F(23)	.4354(9)	.1720(10)	.0794(5)	.079
C(1)	.3384(13)	-.0853(12)	.2588(8)	.035(4)
C(2)	.4059(14)	.3272(14)	.2837(9)	.044(5)
C(3)	.0319(13)	.2780(12)	.1331(8)	.033(4)
C(4)	-.2762(27)	.3005(25)	.1087(18)	.129(12)
C(A1)	.2722(16)	-.1001(12)	.1421(6)	.038(5)
C(A2)	.3782(12)	-.1149(15)	.1113(7)	.047(5)
C(A3)	.4062(12)	-.1462(8)	.0517(9)	.051(5)
C(A4)	.3281(16)	-.1627(12)	.0229(6)	.061(6)
C(A5)	.2220(12)	-.1479(15)	.0537(7)	.052(6)
C(A6)	.1941(12)	-.1166(8)	.1133(9)	.044(5)
C(B1)	.1262(7)	-.1115(7)	.2578(5)	.029(4)
C(B2)	.0275(14)	-.0677(7)	.2881(9)	.049(5)
C(B3)	-.0484(14)	-.1178(8)	.3205(10)	.056(6)
C(B4)	-.0256(7)	-.2117(7)	.3226(5)	.060(6)
C(B5)	.0731(14)	-.2556(7)	.2923(9)	.058(6)
C(B6)	.1489(14)	-.2055(8)	.2599(10)	.043(5)
C(C1)	.2388(11)	-.0550(9)	.3899(5)	.033(4)
C(C2)	.1988(14)	-.0002(9)	.4394(7)	.050(5)
C(C3)	.1338(19)	-.0312(12)	.4935(8)	.068(7)
C(C4)	.1088(11)	-.1170(9)	.4981(5)	.064(6)
C(C5)	.1488(14)	-.1719(9)	.4485(7)	.068(7)
C(C6)	.2138(19)	-.1409(12)	.3944(8)	.060(6)
C(D1)	.4653(10)	-.0648(15)	.3449(11)	.034(4)
C(D2)	.5572(10)	-.0559(14)	.3005(7)	.046(5)
C(D3)	.6563(11)	-.0957(6)	.3136(7)	.055(6)
C(D4)	.6634(10)	-.1443(15)	.3710(11)	.068(7)
C(D5)	.5714(10)	-.1532(14)	.4154(7)	.062(6)
C(D6)	.4723(11)	-.1134(6)	.4023(7)	.044(5)
C(E1)	.5193(10)	.1755(16)	.3521(11)	.035(4)
C(E2)	.5265(9)	.1133(8)	.4038(7)	.053(6)
C(E3)	.6249(9)	.0786(14)	.4195(9)	.068(7)
C(E4)	.7161(10)	.1061(16)	.3834(11)	.064(6)
C(E5)	.7089(9)	.1683(8)	.3317(7)	.062(6)
C(E6)	.6105(9)	.2031(14)	.3161(9)	.059(6)
C(F1)	.3216(19)	.2709(12)	.4132(8)	.039(5)
C(F2)	.2218(16)	.2547(15)	.4443(5)	.054(6)
C(F3)	.1748(10)	.2905(10)	.5015(8)	.074(7)
C(F4)	.2278(19)	.3425(12)	.5276(8)	.071(7)
C(F5)	.3276(16)	.3587(15)	.4965(5)	.070(7)
C(F6)	.3745(10)	.3229(10)	.4393(8)	.049(5)
C(G1)	.2046(20)	.4523(10)	.3164(10)	.047(5)
C(G2)	.0960(18)	.4514(17)	.3307(5)	.056(6)
C(G3)	.0311(11)	.4978(13)	.3803(10)	.081(8)
C(G4)	.0748(20)	.5450(10)	.4157(10)	.082(8)
C(G5)	.1834(18)	.5459(17)	.4014(5)	.076(7)
C(G6)	.2483(11)	.4995(13)	.3518(10)	.059(6)
C(H1)	.3375(9)	.4682(11)	.1926(6)	.036(4)
C(H2)	.4175(17)	.4391(10)	.1422(11)	.067(7)
C(H3)	.4477(18)	.5003(9)	.0921(10)	.090(8)
C(H4)	.3978(9)	.5906(11)	.0923(6)	.063(6)
C(H5)	.3178(17)	.6197(10)	.1427(11)	.083(8)
C(H6)	.2876(18)	.5585(9)	.1929(10)	.060(6)
C(I1)	.0375(19)	.4566(8)	.1641(11)	.036(5)
C(I2)	-.0595(12)	.4582(8)	.2058(7)	.064(6)
C(I3)	-.1195(14)	.5401(8)	.2260(9)	.077(7)
C(I4)	-.0824(19)	.6203(8)	.2045(11)	.085(8)

Table 7.9(cont).

	X/A	Y/B	Z/C	U
C(I5)	.0146(12)	.6187(8)	.1628(7)	.075(7)
C(I6)	.0746(14)	.5369(8)	.1426(9)	.063(6)
C(J1)	.1858(14)	.3771(12)	.0606(5)	.035(4)
C(J2)	.1228(14)	.4236(11)	.0193(11)	.054(6)
C(J3)	.1670(10)	.4365(16)	-.0442(10)	.063(6)
C(J4)	.2741(14)	.4030(12)	-.0664(5)	.070(7)
C(J5)	.3370(14)	.3565(11)	-.0251(11)	.068(7)
C(J6)	.2929(10)	.3436(16)	.0384(10)	.058(6)
C(K1)	.1686(14)	.1504(10)	.0439(6)	.031(4)
C(K2)	.1273(13)	.2027(10)	-.0048(10)	.048(5)
C(K3)	.1841(9)	.1974(14)	-.0663(8)	.063(6)
C(K4)	.2820(14)	.1398(10)	-.0790(6)	.050(5)
C(K5)	.3232(13)	.0875(10)	-.0303(10)	.048(5)
C(K6)	.2665(9)	.0928(14)	.0311(8)	.047(5)
C(L1)	-.0218(9)	.1047(12)	.1298(6)	.027(4)
C(L2)	-.1003(17)	.1123(15)	.1841(5)	.053(6)
C(L3)	-.1918(14)	.0766(9)	.1889(7)	.056(6)
C(L4)	-.2049(9)	.0334(12)	.1394(6)	.056(6)
C(L5)	-.1264(17)	.0258(15)	.0851(5)	.068(7)
C(L6)	-.0349(14)	.0615(9)	.0803(7)	.053(6)
H(11)	.40676	-.08626	.22940	.075
H(12)	.33699	-.14776	.27699	.075
H(21)	.46573	.31178	.24878	.075
H(22)	.42765	.37090	.30679	.075
H(31)	.00299	.30061	.09530	.075
H(32)	-.02860	.28226	.16870	.075
H(41)	-.35471	.29886	.10438	.075
H(42)	-.25046	.23467	.11852	.075
H(A2)	.43239	-.10291	.13072	.075
H(A3)	.47948	-.15513	.02939	.075
H(A4)	.34707	-.18392	-.01911	.075
H(A5)	.16756	-.16050	.03371	.075
H(A6)	.12046	-.10829	.13507	.075
H(B2)	.01137	-.00240	.28651	.075
H(B3)	-.11749	-.06737	.34113	.075
H(B4)	-.07880	-.24671	.34475	.075
H(B5)	.08876	-.32105	.29368	.075
H(B6)	.21766	-.23607	.23911	.075
H(C2)	.21566	.05965	.43598	.075
H(C3)	.10552	.00720	.52778	.075
H(C4)	.06379	-.13865	.53587	.075
H(C5)	.13216	-.23203	.45212	.075
H(C6)	.24230	-.17961	.36032	.075
H(D2)	.55248	-.02238	.26064	.075
H(D3)	.72050	-.08931	.28288	.075
H(D4)	.73264	-.17198	.38017	.075
H(D5)	.57668	-.18785	.45520	.075
H(D6)	.40863	-.12088	.43296	.075
H(E2)	.46362	.09392	.42880	.075
H(E3)	.63050	.03560	.45559	.075
H(E4)	.78510	.08265	.39450	.075
H(E5)	.77275	.18796	.30674	.075
H(E6)	.60586	.24629	.28001	.075
H(F2)	.18491	.21860	.42670	.075
H(F3)	.10556	.27927	.52377	.075
H(F4)	.19538	.36760	.56787	.075
H(F5)	.36458	.39520	.51497	.075
H(F6)	.44391	.33452	.41791	.075
H(G2)	.06534	.41932	.30596	.075
H(G3)	-.04476	.49770	.39022	.075
H(G4)	.02937	.57737	.45039	.075
H(G5)	.21357	.57866	.42632	.075
H(G6)	.32365	.50033	.34208	.075
H(H2)	.45256	.37696	.14210	.075
H(H3)	.50434	.48106	.05740	.075
H(H4)	.41950	.63407	.05786	.075
H(H5)	.28305	.68303	.14308	.075
H(H6)	.23123	.57892	.22776	.075
H(I2)	-.08623	.40306	.22006	.075
H(I3)	-.18806	.54184	.25424	.075
H(I4)	-.12471	.67778	.21830	.075
H(I5)	.04051	.67496	.14825	.075
H(I6)	.14239	.53618	.11415	.075
H(J2)	.04859	.44686	.03466	.075

Table 7.9(cont).

	X/A	Y/B	Z/C	U
H(J3)	.12328	.46937	-.07295	.075
H(J4)	.30501	.41308	-.11069	.075
H(J5)	.41204	.33431	-.04078	.075
H(J6)	.33732	.31178	.06682	.075
H(K2)	.05922	.24274	.00362	.075
H(K3)	.15577	.23370	-.10050	.075
H(K4)	.32190	.13593	-.12191	.075
H(K5)	.39148	.04732	-.03918	.075
H(K6)	.29492	.05636	.06492	.075
H(L2)	-.09190	.14214	.21874	.075
H(L3)	-.24742	.08235	.22647	.075
H(L4)	-.26947	.00938	.14234	.075
H(L5)	-.13596	-.00380	.05044	.075
H(L6)	.01958	.05599	.04268	.075

	X/A	Y/B	Z/C	U
CLS(11)	.678(2)	.413(2)	.348(1)	.51(2)
CLS(12)	.659(2)	.343(1)	.480(1)	.54(2)
CLS(13)	.760(2)	.409(2)	.447(2)	.38(2)
CLS(14)	.755(3)	.442(2)	.376(2)	.36(2)
CLS(15)	.763(3)	.333(3)	.407(2)	.28(2)
CLS(21)	.547(2)	.351(2)	.660(1)	.51(2)
CLS(22)	.419(2)	.292(2)	.778(1)	.49(2)
CLS(23)	.445(4)	.445(4)	.737(2)	.24(2)
CLS(24)	.512(3)	.350(3)	.745(2)	.33(2)
CLS(25)	.426(3)	.325(3)	.696(2)	.29(2)

Anisotropic displacement parameters ($\AA^2$).

	U11	U22	U33	U12	U13	U23
PT(1)	.0240(4)	.0233(4)	.0236(4)	-.0049(3)	-.0043(3)	-.0015(3)
PT(2)	.0251(4)	.0264(4)	.0220(4)	-.0029(3)	-.0044(3)	-.0013(3)
PT(3)	.0252(4)	.0231(4)	.0273(4)	-.0053(3)	-.0076(3)	.0002(3)
SN(1)	.0269(6)	.0375(8)	.0313(7)	-.0048(6)	.0001(6)	-.0047(7)
SN(2)	.0277(6)	.0370(8)	.0275(7)	-.0067(6)	.0014(5)	-.0036(6)
CL(1)	.129(7)	.129(8)	.108(7)	-.046(6)	-.035(5)	-.003(6)
CL(2)	.209(10)	.124(8)	.121(8)	-.072(8)	-.054(7)	-.006(6)
P(1)	.028(2)	.029(3)	.029(3)	-.009(2)	-.003(2)	-.003(2)
P(2)	.028(2)	.036(3)	.029(3)	-.001(2)	-.007(2)	.002(2)
P(3)	.032(3)	.040(3)	.028(3)	-.003(2)	-.009(2)	-.009(2)
P(4)	.033(3)	.025(3)	.039(3)	-.005(2)	-.005(2)	0.000(2)
P(5)	.035(3)	.027(3)	.037(3)	-.006(2)	-.011(2)	.003(2)
P(6)	.030(2)	.028(3)	.030(3)	-.006(2)	-.004(2)	.000(2)
F(11)	.059(7)	.059(9)	.090(10)	-.021(7)	-.019(7)	-.024(8)
F(12)	.040(6)	.095(11)	.064(8)	.005(7)	-.014(6)	.004(8)
F(13)	.094(9)	.064(9)	.068(9)	-.040(8)	.028(8)	-.013(7)
F(21)	.049(6)	.034(7)	.077(9)	.007(6)	.011(6)	-.012(6)
F(22)	.075(8)	.083(10)	.091(10)	-.047(8)	.002(8)	-.037(8)
F(23)	.052(7)	.126(13)	.043(7)	.014(8)	-.002(6)	.004(8)

Table 7.10. Selected bond distances (Å) and angles (°) of complex (10).

PT(1) - PT(2)	2.639(1)	PT(1) - PT(3)	2.609(2)
PT(1) - SN(1)	2.746(2)	PT(1) - SN(2)	2.808(2)
PT(1) - P(1)	2.301(5)	PT(1) - P(6)	2.303(5)
PT(2) - PT(3)	2.622(1)	PT(2) - SN(1)	2.801(2)
PT(2) - SN(2)	2.699(2)	PT(2) - P(2)	2.304(6)
PT(2) - P(3)	2.313(5)	PT(3) - SN(1)	2.783(2)
PT(3) - SN(2)	2.830(2)	PT(3) - P(4)	2.278(5)
PT(3) - P(5)	2.308(5)	SN(1) - F(11)	1.995(13)
SN(1) - F(12)	1.957(11)	SN(1) - F(13)	1.901(13)
SN(2) - F(21)	1.969(11)	SN(2) - F(22)	1.965(13)
SN(2) - F(23)	1.901(12)	CL(1) - C(4)	1.72(4)
CL(2) - C(4)	1.63(4)	P(1) - C(1)	1.844(18)
P(1) - C(A1)	1.824(15)	P(1) - C(B1)	1.817(11)
P(2) - C(1)	1.844(18)	P(2) - C(C1)	1.826(14)
P(2) - C(D1)	1.856(16)	P(3) - C(2)	1.836(21)
P(3) - C(E1)	1.854(16)	P(3) - C(F1)	1.831(18)
P(4) - C(2)	1.837(19)	P(4) - C(G1)	1.829(21)
P(4) - C(H1)	1.818(16)	P(5) - C(3)	1.806(18)
P(5) - C(I1)	1.811(17)	P(5) - C(J1)	1.834(14)
P(6) - C(3)	1.852(19)	P(6) - C(K1)	1.840(15)
P(6) - C(L1)	1.844(15)		

PT(2) - PT(1) - PT(3)	59.9(1)	PT(2) - PT(1) - SN(1)	62.6(1)
PT(2) - PT(1) - SN(2)	59.3(1)	PT(2) - PT(1) - P(1)	97.6(2)
PT(2) - PT(1) - P(6)	154.3(2)	PT(3) - PT(1) - SN(1)	62.6(1)
PT(3) - PT(1) - SN(2)	62.9(1)	PT(3) - PT(1) - P(1)	156.8(2)
PT(3) - PT(1) - P(6)	94.5(2)	SN(1) - PT(1) - SN(2)	113.9(1)
SN(1) - PT(1) - P(1)	114.5(2)	SN(1) - PT(1) - P(6)	104.8(2)
SN(2) - PT(1) - P(1)	101.9(2)	SN(2) - PT(1) - P(6)	113.7(2)
P(1) - PT(1) - P(6)	108.2(2)	PT(1) - PT(2) - PT(3)	59.5(1)
PT(1) - PT(2) - SN(1)	60.5(1)	PT(1) - PT(2) - SN(2)	63.5(1)
PT(1) - PT(2) - P(2)	93.3(2)	PT(1) - PT(2) - P(3)	153.4(2)
PT(3) - PT(2) - SN(1)	61.7(1)	PT(3) - PT(2) - SN(2)	64.2(1)
PT(3) - PT(2) - P(2)	152.8(2)	PT(3) - PT(2) - P(3)	94.5(2)
SN(1) - PT(2) - SN(2)	115.7(1)	SN(1) - PT(2) - P(2)	108.3(2)
SN(1) - PT(2) - P(3)	114.3(2)	SN(2) - PT(2) - P(2)	103.9(2)
SN(2) - PT(2) - P(3)	101.9(2)	P(2) - PT(2) - P(3)	112.3(2)
PT(1) - PT(3) - PT(2)	60.6(1)	PT(1) - PT(3) - SN(1)	61.1(1)
PT(1) - PT(3) - SN(2)	62.0(1)	PT(1) - PT(3) - P(4)	156.8(2)
PT(1) - PT(3) - P(5)	96.5(2)	PT(2) - PT(3) - SN(1)	62.3(1)
PT(2) - PT(3) - SN(2)	59.2(1)	PT(2) - PT(3) - P(4)	96.4(2)
PT(2) - PT(3) - P(5)	156.8(2)	SN(1) - PT(3) - SN(2)	112.1(1)
SN(1) - PT(3) - P(4)	113.3(2)	SN(1) - PT(3) - P(5)	104.7(2)
SN(2) - PT(3) - P(4)	104.6(2)	SN(2) - PT(3) - P(5)	115.6(2)
P(4) - PT(3) - P(5)	106.7(2)	PT(1) - SN(1) - PT(2)	56.8(1)
PT(1) - SN(1) - PT(3)	56.3(1)	PT(1) - SN(1) - F(11)	163.6(4)
PT(1) - SN(1) - F(12)	102.1(4)	PT(1) - SN(1) - F(13)	102.3(4)
PT(2) - SN(1) - PT(3)	56.0(1)	PT(2) - SN(1) - F(11)	108.1(4)
PT(2) - SN(1) - F(12)	152.3(4)	PT(2) - SN(1) - F(13)	110.7(4)
PT(3) - SN(1) - F(11)	111.3(4)	PT(3) - SN(1) - F(12)	98.2(4)
PT(3) - SN(1) - F(13)	158.2(4)	F(11) - SN(1) - F(12)	89.8(5)
F(11) - SN(1) - F(13)	88.7(6)	F(12) - SN(1) - F(13)	90.1(6)
PT(1) - SN(2) - PT(2)	57.2(1)	PT(1) - SN(2) - PT(3)	55.1(1)
PT(1) - SN(2) - F(21)	105.2(4)	PT(1) - SN(2) - F(22)	155.6(4)
PT(1) - SN(2) - F(23)	107.4(4)	PT(2) - SN(2) - PT(3)	56.6(1)
PT(2) - SN(2) - F(21)	102.6(4)	PT(2) - SN(2) - F(22)	102.5(4)
PT(2) - SN(2) - F(23)	161.4(4)	PT(3) - SN(2) - F(21)	156.1(4)

Table 7.10(cont).

PT(3)	SN(2)	F(22)	103.5(4)
F(21)	SN(2)	F(22)	91.9(5)
F(22)	SN(2)	F(23)	89.2(6)
PT(1)	P(1)	C(A1)	113.9(6)
C(1)	P(1)	C(A1)	104.4(9)
C(A1)	P(1)	C(B1)	101.0(8)
PT(2)	P(2)	C(C1)	116.6(5)
C(1)	P(2)	C(C1)	104.8(7)
C(C1)	P(2)	C(D1)	102.4(9)
PT(2)	P(3)	C(E1)	118.7(8)
C(2)	P(3)	C(E1)	103.2(9)
C(E1)	P(3)	C(F1)	99.3(11)
PT(3)	P(4)	C(G1)	120.8(8)
C(2)	P(4)	C(G1)	104.5(10)
C(G1)	P(4)	C(H1)	103.9(8)
PT(3)	P(5)	C(I1)	115.7(8)
C(3)	P(5)	C(I1)	104.8(10)
C(11)	P(5)	C(J1)	101.9(10)
PT(1)	P(6)	C(K1)	117.0(6)
C(3)	P(6)	C(K1)	105.2(8)
C(K1)	P(6)	C(L1)	104.0(8)
P(3)	C(2)	P(4)	112.9(10)
CL(1)	C(4)	CL(2)	116.4(21)

PT(3)	SN(2)	F(23)	106.9(5)
F(21)	SN(2)	F(23)	91.3(6)
PT(1)	P(1)	C(1)	109.0(6)
PT(1)	P(1)	C(B1)	123.4(4)
C(1)	P(1)	C(B1)	103.2(7)
PT(2)	P(2)	C(1)	110.9(6)
PT(2)	P(2)	C(D1)	120.0(7)
C(1)	P(2)	C(D1)	100.0(9)
PT(2)	P(3)	C(2)	108.7(7)
PT(2)	P(3)	C(F1)	121.3(8)
C(2)	P(3)	C(F1)	103.4(9)
PT(3)	P(4)	C(2)	107.6(7)
PT(3)	P(4)	C(H1)	115.1(5)
C(2)	P(4)	C(H1)	103.2(8)
PT(3)	P(5)	C(3)	108.7(6)
PT(3)	P(5)	C(J1)	122.1(6)
C(3)	P(5)	C(J1)	101.6(8)
PT(1)	P(6)	C(3)	109.4(6)
PT(1)	P(6)	C(L1)	118.7(6)
C(3)	P(6)	C(L1)	100.5(8)
P(1)	C(1)	P(2)	113.4(10)
P(5)	C(3)	P(6)	113.0(9)

Table 7.11. Crystallographic and experimental details of the structure analyses of complexes (2), (3), (7), (10) and (8)/(9).

Compound	$[Pt_4(H)(CO)_2(dppm)_4][PF_6]$	$[Pt_3(AgCl)(S)(dppm)_3(AuPPh_3)][PF_6]$
Formula	$C_{102}H_{89}F_6O_2P_9Pt_4$	$C_{93}H_{81}AgAuClF_6P_8Pt_3S$
Formula Wt.	2519.9	2518.1
Crystal habit	red plate	red plate
Crystal size, mm	0.48x0.48x0.08	0.32x0.36x0.40
Crystal system	orthorhombic	triclinic
Space group	Pcab (No. 61)	P $\bar{1}$
a, Å	21.120(6)	17.639(5)
b, Å	28.962(4)	18.651(5)
c, Å	31.026(4)	28.328(6)
α, °	—	94.83(2)
β, °	—	98.88(2)
γ, °	—	90.33(3)
Obtained from	25 refln, 12<θ<15°	22 refln, 11<θ<14°
V, $Å^3$	18978(6)	9173(4)
Z	8	4
F(000)	9744	4824
d calc, gcm^{-3}	1.764	1.823
T, K	295	295
μ(Mo-Kα), cm^{-1}	61.5	66.5
Absorption factors on F^2	0.81-1.43	0.76-1.57
Scan width, °	0.70	0.80
Max count time, s	100	100
Total refln measured	14235	15618
Unique refln	13174	15020
R_{INT}	0.050	0.036
Miller indicies h	0→23	-15→15
measured, k	0→31	-16→ 9
l	0→34	-24→24
2θ range, °	4-46	4-36
Unique refln ≥ 3σ(I)	6261	8006
No. of parameters	385	673
R	0.038	0.061
R_w	0.045	0.079
$\|\Delta\rho\|_{max}$, $eÅ^{-3}$	0.97	2.03
Δ/σ_{max}	0.30	0.157

Table 7.11(cont).

Compound	$[Pt_3(SnMe_2[PO_2F_2])(dppm)_3][PF_6]$	$[Pt_3(SnF_3)_2(dppm)_3].CH_2Cl_2$
Formula	$C_{77}H_{72}F_8O_2P_8Pt_3Sn$	$C_{76}H_{68}Cl_2F_6P_6Pt_3Sn_2$
Formula Wt.	2133.2	2174.8
Crystal habit	purple plate	orange plate
Crystal size, mm	0.76x0.20x0.48	0.56x0.40x0.40
Crystal system	monoclinic	triclinic
Space group	C2	P $\bar{1}$
a, Å	24.808(5)	13.002(3)
b, Å	12.136(3)	15.027(3)
c, Å	26.890(6)	21.744(5)
α, °	——	83.05(2)
β, °	105.64(2)	77.29(2)
γ, °	——	78.30(2)
Obtained from	23 refln, $12<\theta<14°$	22 refln, $11<\theta<16°$
V, $Å^3$	7796(3)	4045(2)
Z	4	2
F(000)	4104	2072
d calc, gcm^{-3}	1.817	1.786
T, K	295	292
μ(Mo-Kα), cm^{-1}	59.7	60.7
Absorption factors on F^2	0.80-1.43	0.69-1.39
Scan width, °	0.90	0.90
Max count time, s	90	60
Total refln measured	11055	12311
Unique refln	10528	11215
R_{INT}	0.051	0.044
Miller indicies h	0→31	-14→14
measured, k	-15→ 1	-16→16
l	-34→34	-23→ 3
2θ range, °	4-54	4-46
Unique refln ≥ 3σ(I)	7579	6860
No. of parameters	314	372
R	0.043	0.051
R_w	0.057	0.059
$\|\Delta\rho\|_{max}$, $eÅ^{-3}$	1.35	3.25
Δ/σ_{max}	0.12	0.195

Table 7.11(cont).

Compound	$[Pt_3(dppm)_3(SnF_3)(CO)]_{0.75}[Pt_3Cl(SnF_3)(dppm)_3]_{0.25}[PF_6]_{0.75}$
Formula	$C_{75.75}H_{66}Cl_{0.25}F_{7.5}O_{0.75}P_{6.75}Pt_3Sn$
Formula Wt.	2052.7
Crystal habit	orange plate
Crystal size, mm	0.18x0.32x0.36
Crystal system	cubic
Space group	P43n (No. 218)
a, Å	26.081(5)
b, Å	——
c, Å	——
α, °	——
β, °	——
γ, °	——
Obtained from	22 refln, 10<θ<14°
V, $Å^3$	17740(6)
Z	8
F(000)	7868
d calc, gcm^{-3}	1.537
T, K	295
μ(Mo-Kα), cm^{-1}	52.24
Absorption factors on F^2	0.153-0.395
Scan width, °	0.90
Max count time, s	90
Total refln measured	7772
Unique refln	4644
R_{INT}	0.055
Miller indicies h	0→36
measured, k	0→36
l	0→36
2θ range, °	4-60
Unique refln ≥ 3σ(I)	944
No. of parameters	102
R	0.058
R_w	0.065
$\|\Delta\rho\|_{max}$, $eÅ^{-3}$	1.95
Δ/σ_{max}	0.043

CHAPTER 8: SOME COMMENTS ON DPPM CONFORMATIONS IN $M_3(\mu\text{-DPPM})_3$ COMPLEXES

8.1 M_2P_2C Ring Conformations

In previous chapters it has been repeatedly observed that in $M_3(\mu\text{-dppm})_3$ complexes the M_2P_2C rings formed by a bridging dppm ligand attached to a pair of metal atoms show a preference for envelope conformations. The dppm methylene carbon atom defines the flap of the envelope and the M_2P_2 unit is roughly planar. We argue here that this conformation is the lowest in energy compatible with acceptable M-M bonding distances.

A survey of the structures reveals the following means and ranges for the M_2P_2C ring bond lengths and angles.

Table 8.1

		Mean	Range
M-P	Å	2.30	2.24-2.36
$P-CH_2$	Å	1.84	1.83-1.85*
$M-P-CH_2$	°	109	102-113
$P-CH_2-P$	°	111	108-122

* For the mean $P-CH_2$ in a given structure.

Although there are some outliers most of the ring angles at the phosphorus and carbon atoms are within 3° of the tetrahedral angle and we conclude that the formation of a M_2P_2C ring in $M_3(dppm)_3$ species does not usually involve significant deformation of bond lengths or angles. If we take the mean distances and angles in the above table as

typical of M_2P_2C rings we can calculate the values of the two M-P-C-P torsion angles, ω_1 and ω_2, which yield a given M-M distance. The curves in Figure 8(a) give the values of ω_1 and ω_2 which yield M-M = 2.6 Å (inner curve) and 3.0 Å (outer curve). For M-M = 2.6 Å a slightly flattened envelope conformation with $\omega_1 = 47°$, $\omega_2 = -47°$ (or vice versa) gives the smallest deformations from ideal staggering across P-C bonds [$|\omega| = 60°$]. For rings with M-M bonds (i.e. M-M ca. 2.60 Å) the experimental points (marked as crosses) cluster around these values of ω_1 and ω_2. The lack of any points representing a C_2 conformation with $\omega_1 = \omega_2 = \pm 23°$ on the M-M = 2.6 Å line is striking. Though such a conformation is geometrically possible the deviations from staggering across P-C bonds evidently impose too great a price in conformational energy.

Figure 8(a) also gives some insight into the ability of the $M_3(\mu\text{-dppm})_3$ unit to retain its identity after rupture of two of the M-M bonds. When M-M = 3.0 Å an envelope conformation with $\omega_1 = 60°$, $\omega_2 = -60°$, i.e. with no P-C-P-H torsional strain, is possible. Interestingly, the points corresponding to M_2P_2C rings without M-M bonding (circles in Figure 8(a)) lie close to the M-M = 3.0 Å line although the observed M-M distances are in the range 3.0-3.5 Å. These points typically have $\omega_1 \approx -65°$ and ω_2 in the range 30-50° suggesting that rupture of an M-M bond and consequent increase in the M-M separation does not require substantial costs in M-P-C-P torsional strain.

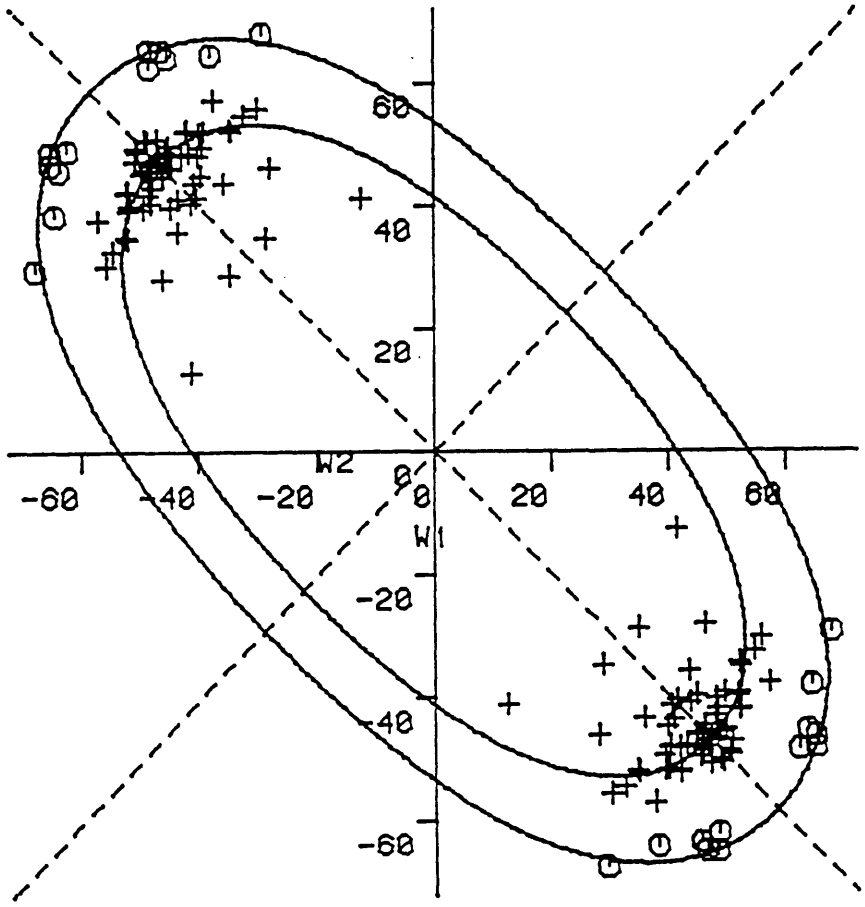


Figure 8(a). Values of P-C-P-M torsion angles(°), ω_1 and ω_2, in M_2P_2C rings with M-M = 2.6 Å (inner curve) and 3.0 Å (outer curve). Mean distances in Table 8.1 were used to generate the curves. Crosses represent experimental torsion angles in M_2P_2C rings with M-M bonds and circles values for rings without M-M bonds. Mirror operations across the broken diagonal lines connect energetically equivalent conformations.[88]

8.2 Latitudinal $M_3(\mu\text{-dppm})_3$ Conformations

In the $M_3(\mu\text{-dppm})_3$ complexes described in previous chapters electronic factors require a latitudinal and thus

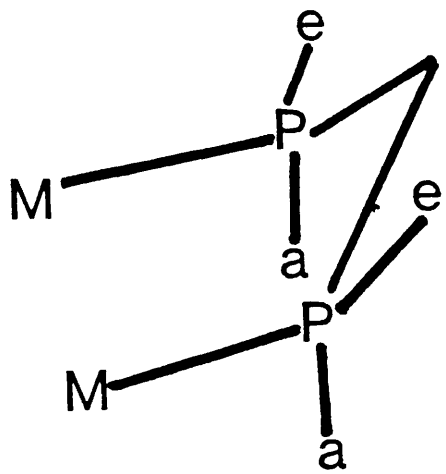


Figure 8(b). The equatorial (e) and axial (a) positions at the phosphorus atoms of the M_2P_2C ring.

roughly planar M_3P_6 core. This, together with the envelope conformation of the M_2P_2C rings, allows the dppm phenyl rings to be classed as axial (P-C bond roughly parallel with the triad axis of the M_3 triangle) or equatorial (P-C bond roughly normal to the triad axis) as shown in Figure 8(b).

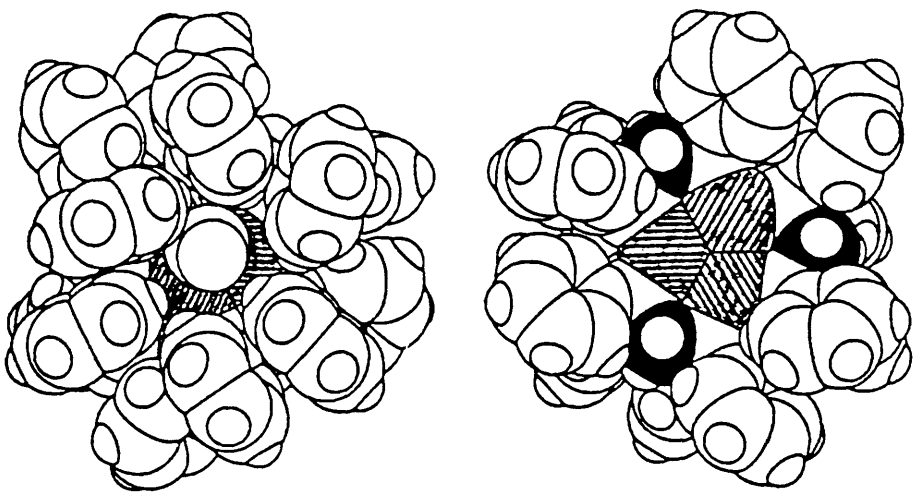


Figure 8(c). Space filled views of the cation $[Pt_3(CO)(P(OPh)_3)(dppm)_3]^{2+}$ (Chapter 5) from either side of the M_3 plane, using van der Waals radii[52] to calculate the shells. The $P(OPh)_3$ ligand has been removed for clarity.

For the complex as a whole two arrangements are possible. All three methylene carbon atoms can lie on one side of the M_3 plane (Figure 8(c)) as do the six equatorial phenyl rings. The six axial phenyl groups point out from the other side of the plane. Alternatively, two methylene carbon atoms lie on one side of the M_3 plane and one on the other side (Figure 8(d)). In this case four equatorial and two axial phenyl groups lie on one side, with two equatorial and four axial phenyl groups on the other side.

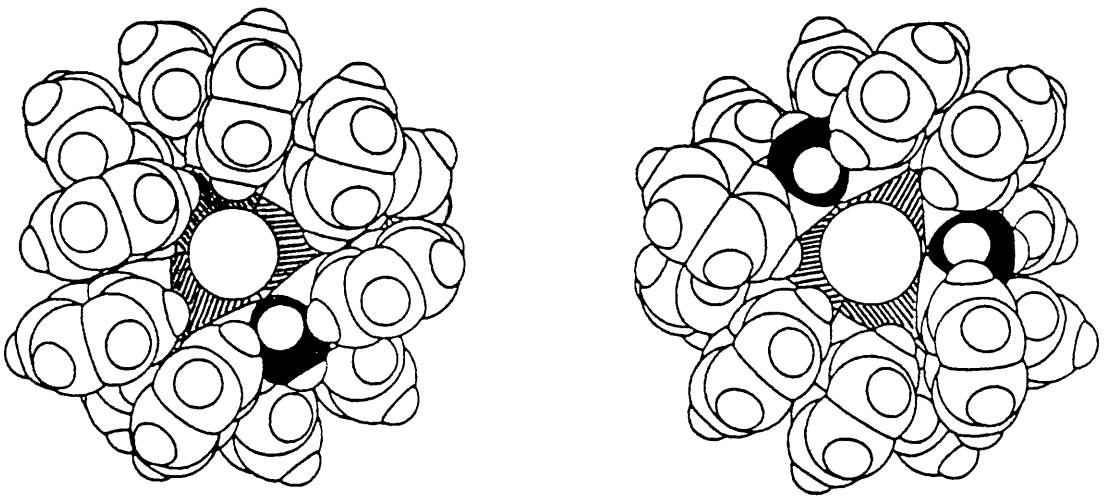


Figure 8(d). Space filled views of $[PdI(CO)(dppm)_3]^+$ [49] from either side of the M_3 plane, using van der Waals radii to calculate the shells.[52]

In neither case is the same steric enviroment found above and below the M_3 triangle. Axial phenyl groups tend to shield the M_3 triangle and there is therefore a tendency for faces carrying bulky longitudinal ligands to have mainly or exclusively equatorial phenyl groups projecting towards the ligand.

SECTION II: DERIVATIVES OF $[(C_5H_5)MX(F_3CC_2CF_3)_2]$, M= Mo, W, AND RELATED COMPOUNDS

CHAPTER 1: INTRODUCTORY COMMENTS ON TRANSITION METAL CATALYSIS

The bulk of the structural work presented in Section II relates to the characterisation of the products of the apparently simple addition reaction:

$$[CpM(SR)(hfb)_2] + R'C{\equiv}CR'' \longrightarrow [CpM(SR)(hfb)_2(R'C{\equiv}CR'')]$$

where M = Mo or W, Cp = η^5-C_5H_5, R = alkyl or aryl and hfb = $F_3CC{\equiv}CCF_3$, hexafluorobut-2-yne. As we shall see, the tris(alkyne) adduct formed by this reaction can adopt many different structural forms. The structural characterisation of these different species is clearly of interest in understanding transition metal mediated oligomerisation and polymerisation of alkynes. Before considering what was known of the above reaction at the inception of this work some general comments on transition metal catalysis are appropriate.

1.1 Catalysis by Transition Metals

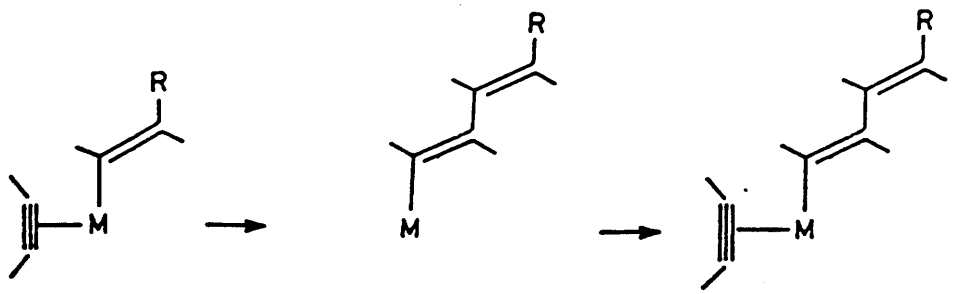
For many years transition metal complexes have been used to catalyse the conversion of unsaturated hydrocarbons obtained from natural gas or petroleum into commercially useful chemicals. Two of the major early discoveries which emphasised the commercial significance of transition metal catalysis were that of low pressure polymerisation of ethylene and propylene, giving polyalkenes and rubbers, by Zeigler and Natta and that of palladium-catalysed oxidation

of alkenes by Smidt.[89]

It is now recognised that complexes which are effective in homogeneous catalysis are usually coordinatively unsaturated, so that one or more vacant sites are available to incoming ligand substrates. Catalysis often involves such processes as oxidative addition (and the reverse process, reductive elimination), insertion into the metal-ligand bonds and attacks on coordinated ligands.[89,90]

Reactions for which transition metal complexes are effective catalysts include hydrogenation, hydroformylation, alkene isomerisation and metathesis and polymerisation/oligomerisation of alkenes and alkynes. The last of these is particularly relevant to the structural work described in later chapters.

The mechanism of alkene and alkyne polymerisation has been much discussed. For alkynes the Cossee and Arlman mechanism of polymerisation (see Scheme I)[91] has been widely accepted. It involves insertion of the incoming alkyne into a σ-alkenyl-metal bond, thereby lengthening the polyene chain by two carbon atoms.



Scheme I.

Alternative mechanisms, some involving cooperative effects between two metal centres, have also been proposed.[92]

1.2 Earlier Work on Alkyne Complexes of Molybdenum and Tungsten

Collaboration between the Crystallography Laboratory in Glasgow and Dr.J.L. Davidson of Heriot-Watt University on molybdenum and tungsten organometallics has been of long standing. The starting point of the work described below was the study, in 1979, of the addition of hfb to [CpW(SMe)$(CO)_3$].[93] X-ray analysis showed that that the adduct contained a $C(CF_3)C(CF_3)C(O)SMe$ ligand attached to the metal through the central carbon atoms of the incoming hfb ligand. One W-C bond, of length 2.193(7) Å, appeared to be a typical σ-W-C bond but the other, of 1.962(8) Å, was much shorter, being comparable in length to W-C(CO) bonds. The resulting cyclopropene-like W=C-C metallacycle was the first example of an η^2-vinyl ligand in organometallic chemistry.

Subsequent work [94-96] was directed towards understanding the addition of nucleophiles to $[CpM(hfb)_2X]$. Formally, this is a coordinatively unsaturated 16-electron species if the alkynes are viewed as two-electron donors. However, it is now well established [97] that alkynes may use between two and four π-electrons in bonding to metals so that the stability of species like $[CpM(hfb)_2X]$ is less surprising. In general it was found that two-electron donors, e.g. PR_3, added not to the metal but to coordinated

hfb to give η^2-vinyl $C(CF_3)C(CF_3)L$ ligands. In some cases, e.g. the addition of CO to $[CpMo(hfb)_2X]$, (see also Chapter 5),[98] a metal-promoted cyclisation was triggered by the incoming ligand. In others, e.g. addition of $CNBu^t$ to $[CpM(hfb)_2X]$,[96] initial formation of an η^2-vinyl was followed by cyclisation on addition of a second $CNBu^t$. More unusually the addition gave an η^1-vinyl, e.g. on addition of $P(OMe)_3$ to $[WBr_2(CO)(hfb)_2]$.[95] This work established that η^2-vinyls are often the product of reactions of molybdenum- or tungsten-alkyne complexes.

A particularly significant observation [99] was that the bis-alkyne thiolato species $[CpM(SR)(hfb)_2]$ could exist either as a bis-alkyne species (2) or as the isomeric η^2-vinyl (1) in which an hfb has undergone internal nucleophilic attack. In general structure (2) is shown when R is aryl and (1) when R is the more electron releasing alkyl (see Figure 1(a)).

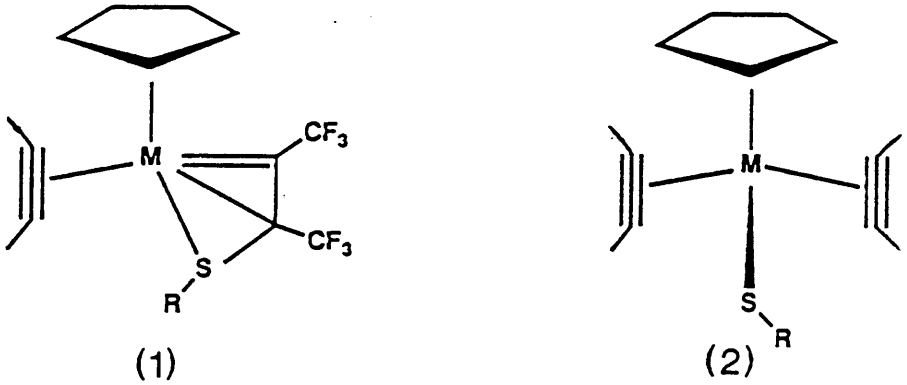


Figure 1(a). The two isomers of the bis-alkyne species $[CpM(SR)(hfb)_2]$

The addition of a third alkyne to species such as (1) or (2) is of obvious relevance to the question of alkyne oligomerisation mechanisms. Preliminary work [100] on the

addition of $MeC{\equiv}CMe$ and $MeO_2CC{\equiv}CCO_2Me$ (dmad) to the η^2-vinyl species $[CpW(SPr^i)(hfb)_2]$ established that these reactions are of some complexity. Addition of $MeC{\equiv}CMe$ gave complex (6) whereas dmad gave products (8a), (8b) and (9) [100] (the numbering scheme is that of Scheme III, in Chapter 3).

Complex $[CpW(SPr^i)(hfb)_2(MeC{\equiv}CMe)]$, (6), differs from the starting complex (1) in that the incoming ligand has inserted into the $Pr^iS-C(CF_3)$ bond, and the W-S bond has subsequently ruptured, forming an η^4-butadienyl ligand. Bond lengths and the planarity of this ligand suggest that it is attached to the tungsten atom through a W=C(carbene) bond, an η^2-alkene-W interaction and a σ-W-C bond.[100] The η^2-alkyne and the cyclopentadienyl ring complete the 18-electron configuration about the metal atom.

In $[CpW(SPr^i)(hfb)_2(dmad)]$, (8), the incoming dmad ligand has linked between the η^2-alkyne and η^2-vinyl units to form the chain $Pr^iSC(CF_3)C(CF_3)C(CO_2Me)C(CO_2Me)C(CF_3)=C-CF_3^-$. This chain is bonded to the central tungsten atom through the sulphur atom, the next four carbon atoms and also the final carbon atom of the C_6 part of the chain. Isomers (8a) and (8b) differ only by the orientation of the alkyl group on the sulphur atom. Relative to the cyclopentadienyl ring they are syn and anti respectively.

The structure of $[CpW(SPr^i)(hfb)_2(dmad)]$, (9), contains a chain similar to that in (8) except there has been a novel transfer of a fluorine atom (from the $-CF_3$ group attached to the final carbon of the chain) to the tungsten atom. The oligomer is bonded to the tungsten atom through the sulphur atom, a π-allylic interaction with the first

three carbon atoms and a σ-W-C(alkenyl) bond to the final carbon atom.

These structures are all consistent with the reaction of the incoming alkyne with the η^2-vinyl unit by insertion into the W=C bond followed, in the case of (6), by migration of the thiolate group, and in (8) and (9), by insertion of the η^2-alkyne initially present.[100]

1.3 Strategy of Structural and Chemical Work

The preliminary results discussed above led to a more systematic study of the addition reaction:

$$[CpM(SR)(hfb)_2] + R'C{\equiv}CR'' \longrightarrow [CpM(SR)(hfb)_2(R'C{\equiv}CR'')]$$

In general three factors appear to be of importance in determining the course of this reaction.

(i) The thiolato substituent R: as previously noted, when R = Me, Et, Pr^i and Bu^t the starting complex is an η^2-vinyl species, (1), whereas when R = MeC_6H_4 or C_6F_5 it is a bis(alkyne) species, (2).

(ii) The nature of the metal, M = Mo or W.

(iii) The nature of the incoming alkyne: in particular RC≡CMe, R = Me, Ph, gives different products from dimethyl-acetylenedicarboxylate (dmad).

Dr. Davidson has now completed chemical and spectroscopic studies on the products of the addition reaction and the crystal structures of several of these products are described below. The X-ray results have been of critical importance to establishing a sound structural

basis for the interpretation of the chemistry since at least twelve distinct product types can be distinguished. These often differ from each other in rather subtle ways which are difficult to establish from I.R. and N.M.R. spectra. Some of the structural results have already been published.[101-103]

In the following chapters the structures of tris(alkyne) adducts are first described. The chemical significance of the structural results is then considered. In addition, results on the structures of other molybdenum and tungsten organometallics related to the tris(alkyne) adducts are also presented.

CHAPTER 2: THERMOLYSIS OF η^2-VINYLS

2.1 Introduction

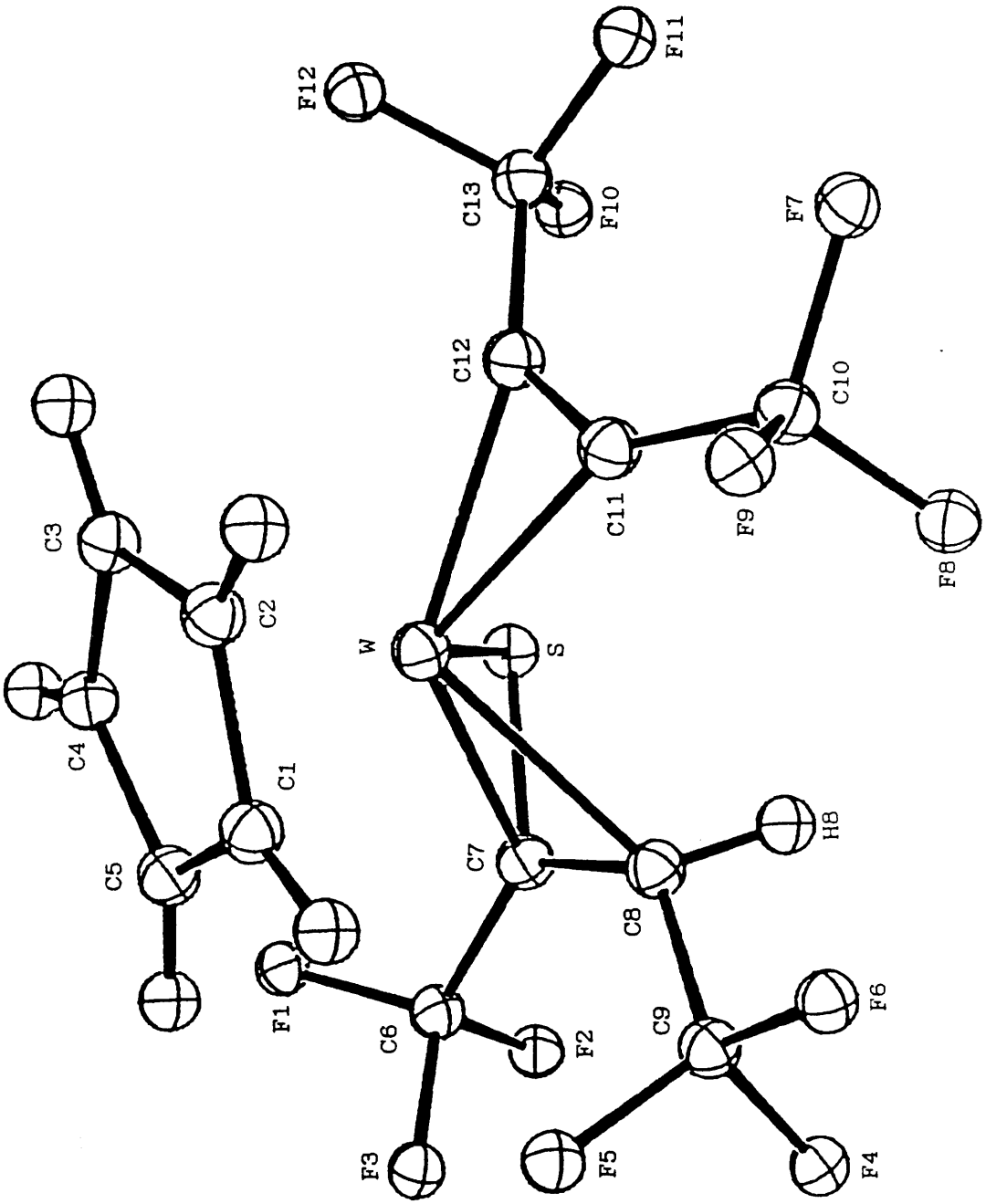
Transition metal complexes are well known for their ability to alter the stereochemistry of alkenes. A number of mechanisms have been proposed for these transformations. For isomerisation of vinyl ligands η^1-ionic and η^2-bonded intermediates have been suggested [104] and in isomerisation of butadienyl attached to palladium and rhodium a ring flip process has been proposed.[105,106] Thermolysis of the η^2-vinyl complex $[CpM(SR)(hfb)_2]$, (1),[99] M = W and R = Bu^t has now provided evidence of a ring flip mechanism which alters from *cis* to *trans* the arrangement of the trifluoromethyl substituents relative to the C=C double bond.

2.2 Results and Discussion

Thermolysis of (1), M = W, R = Bu^t, at 60 °C results in the formation of the complex $[CpW(hfb)(SC(CF_3)=C(H)CF_3)]$, (3), and the loss of butane gas. Complex (3) then isomerises to give the thermodynamically more stable complex (4). X-ray diffraction analysis was used to discover the structure of crystals of both (3) and (4). These crystals were found to contain discreet molecules of their respective isomer with contact distances comparable with van der Waal radii.[52] Structural information for the two isomers is given in Tables 2.1 - 2.5.

The structure of complex (3) (see Figure 2(a)) confirms the rupture of the S-Bu^t connection with transfer of a

Figure 2(a). A view of complex (3). All atoms are presented as spheres of arbitrary size.

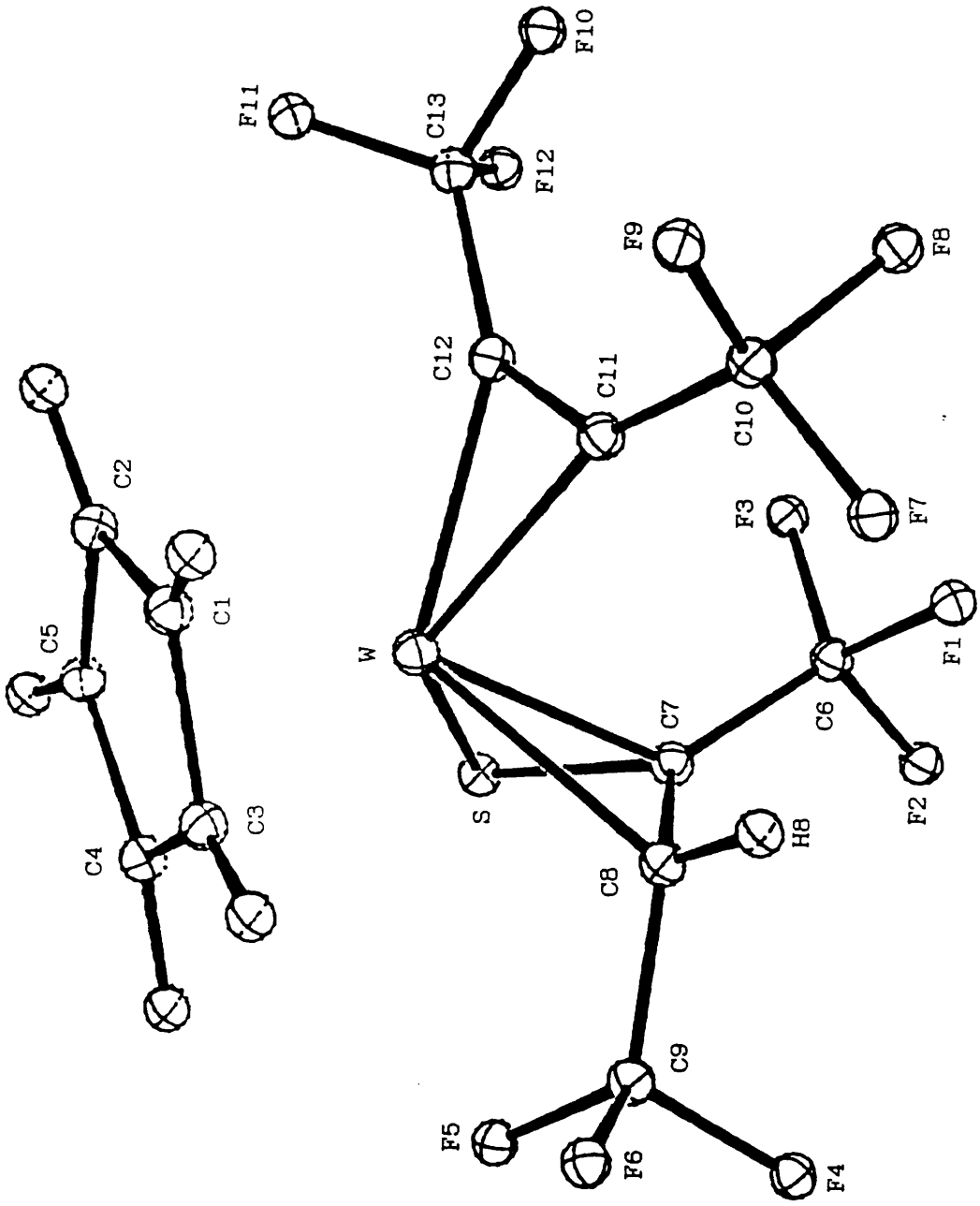


hydrogen atom to the carbon atom β to the sulphur atom of the η^2-vinyl ligand of (1). The $F_3CC(H)=C(CF_3)S^-$ ligand formed has the trifluoromethyl substituents mutually *cis*. The isomerisation to complex (4) (see Figure 2(b)) results in these substituents becoming *trans* [torsion angles C(6)-C(7)-C(8)-C(9) are -8(1) and -119(1)° respectively]. In each complex the bonding around the tungsten atom is completed by a cyclopentadienyl ring and a hexafluorobut-2-yne ligand. The CpW(η^2-hfb) geometries are almost identical in (3) and (4) (see Table 2.1).

In both isomers WSC(7)C(8) forms a butterfly skeleton. However, their orientations relative to the other ligands are distinctly different: e.g. the torsion angles Cp-W-C(7)-C(6) are 22 and 180 ° respectively for (3) and (4) (Cp is the centroid of the cyclopentadienyl ring). These different orientations can be described as the exo rotamer for the *cis* isomer and endo rotamer for the *trans*, as defined for related CpM(allyl) complexes.[107] The W-S distances in both (3) and (4) are much shorter than in (1) (see Table 2.1) while C(7) and C(8) are now nearly equidistant from the metal atom, C(8) no longer participating in a W-C multiple bond as it does in (1).

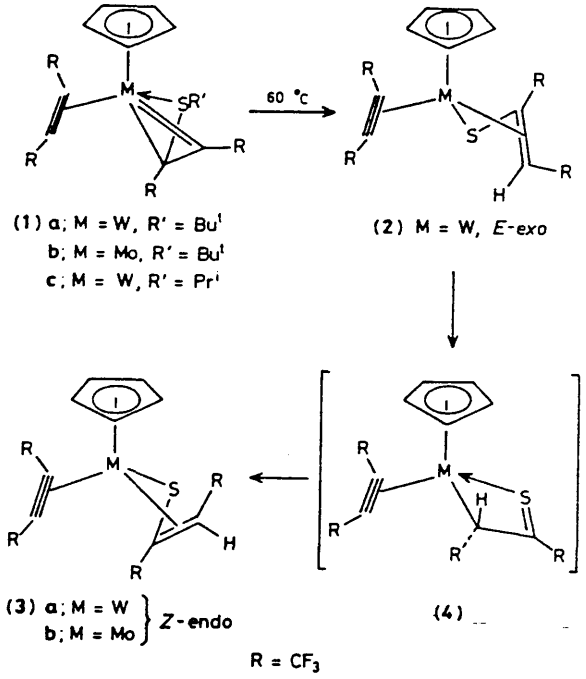
The formal electron count around the tungsten atom in (3) and (4) is 16 if the hfb ligand is considered a two electron donor. It would appear, from the shortness of the W-S distances, that these complexes are stabilised by considerable S→W π-electron donation rather than by donation from both sets of π-orbitals of the hfb ligand. There is little change in the W-C(alkyne) distances in (1), (3) and (4) [mean distances 2.08, 2.08 and 2.07 Å

Figure 2(b). The structure of complex (4) with all atoms presented as spheres of arbitrary size.



respectively] and this is consistent with the above observation.

Further reactions carried out on (3) and (4) with PPh_3 and with dioxygen have given products which ^{19}F N.M.R. suggested contain an η^1-$SC(CF_3)=C(H)CF_3$ ligand, always with retention of stereochemistry about the double bond.[101] These results together with the fact the exo/endo and *cis/trans* isomerisations occur simultaneously suggests the ring flip mechanism shown in Scheme II.



Scheme II.

2.3 Experimental

cis-[CpW(η^3-$SC(CF_3)=C(H)CF_3$)(hfb)] (3)

Data Collection:- A red needle of dimensions 0.52x0.16x0.16 mm was mounted on an Enraf-Nonius CAD4F diffractometer equipped with a graphite monochromator. All measurements

were made using Mo-Kα X-ray radiation. The cell dimensions were obtained by a least-squares refinement of the setting angles of 23 automatically centred reflections with $13<\theta<18°$ (see Table 2.6 for details). The intensities of 6322 reflections with $2\leq\theta\leq30°$ were determined by continuous $\omega/2\theta$ scans of 0.80° in ω, increased by 25% at each end to allow for background. After correction for crystal decomposition (about 40% linear reduction of intensity standards), Lp and absorption effects (empirical transmission factors on F 0.87 - 1.09),[59] symmetrically equivalent reflections were merged to give 3807 unique reflections. Of these 2610 with $I\geq3\sigma(I)$ were used subsequently.

Structure Analysis:- The structure was solved by Patterson and Fourier methods. Anisotropic displacement parameters were used for all non-hydrogen atoms. All hydrogen atom positions were determined from difference syntheses but they did not refine satisfactorily. Accordingly, the hydrogen positions were idealised with C-H distances 0.96 Å and the hydrogen atoms were set to ride on their parent carbon atoms. Hydrogen displacement parameters were set to 1.2 times the final isotropic displacement parameters of the parent carbon atom and not refined. Final atomic parameters (see Table 2.2) were obtained from full-matrix least-squares minimisation of $\Sigma w(|F_o|-|F_c|)^2$ with $w^{-1} = \sigma^2+ 0.0023F^2$ (where σ is derived from counting statistics). Adjustment of 244 parameters converged with R = 0.025 and R_w = 0.044.

Neutral atom scattering factors and complex anomalous dispersion corrections were taken from ref. 61. All

calculations were performed on a GOULD-3227 computer using the GX program package.[60]

trans-[CpW(η^3-SC(CF_3)=C(H)CF_3)(hfb)] (4)

For (4) and later structures in this part of the thesis data collection and structure analysis procedures closely follow those for (3) given above. Accordingly, here and in later experimental sections only variations from procedures used for (3) are explicitly mentioned.

Data Collection :- Cell dimensions and experimental parameters are given in Table 2.6. A decomposition correction was carried out: there was no decomposition in intensity standards forthe first 1400 reflection but a 9% linear decrease occured from that point to the end of data collection.

Structure Analysis:- All hydrogen atom positions were found from difference syntheses andsubsequently refined with their isotropic displacement parameters. Final atomic parameters are given in Table 2.4.

Table 2.1 Comparison of bond distances in complexes (1), (3) and (4) in (Å)

Bond		(1)	(3)	(4)
W - S		2.457(2)	2.303(2)	2.275(3)
W - C(Cp)	min	2.329(5)	2.302(7)	2.308(10)
	max	2.338(5)	2.378(7)	2.368(9)
W - C(7)		2.178(8)	2.166(6)	2.174(8)
W - C(8)		1.905(7)	2.211(6)	2.210(8)
W - C(11)		2.062(9)	2.074(6)	2.082(8)
W - C(12)		2.103(8)	2.079(7)	2.058(8)
S - C(7)		1.764(8)	1.757(7)	1.744(9)
C(7) - C(8)		1.417(10)	1.448(8)	1.440(12)
C(11)- C(12)		1.300(13)	1.266(9)	1.292(11)

Table 2.2. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (3).

	X/A	Y/B	Z/C	U
H(1)	.11995(1)	-.09841(3)	.12249(2)	.037
S(1)	.12900(5)	-.30423(24)	.25871(12)	.054
F(1)	.2035(1)	-.0991(7)	.3530(4)	.102
F(2)	.2217(2)	-.3811(7)	.3380(4)	.105
F(3)	.2342(1)	-.1664(8)	.2457(4)	.094
F(4)	.2152(2)	-.4497(7)	.0657(4)	.103
F(5)	.2089(1)	-.1514(7)	.0457(4)	.086
F(6)	.1700(1)	-.3373(7)	-.0604(3)	.096
F(7)	.0239(2)	-.3155(9)	-.1386(4)	.116
F(8)	.0804(2)	-.4359(7)	-.1091(4)	.141
F(9)	.0683(2)	-.1649(8)	-.1718(4)	.124
F(10)	.0323(2)	-.3232(14)	.1854(6)	.210
F(11)	-.0041(2)	-.2706(13)	.0424(5)	.155
F(12)	.0111(2)	-.0612(10)	.1378(7)	.177
C(1)	.1471(3)	.1358(8)	.0412(6)	.072
C(2)	.1071(2)	.1793(8)	.0199(5)	.064
C(3)	.0999(2)	.2178(9)	.1142(5)	.061
C(4)	.1349(2)	.1968(9)	.1938(5)	.065
C(5)	.1644(2)	.1495(9)	.1475(7)	.069
C(6)	.2068(2)	-.2272(12)	.2858(5)	.064
C(7)	.1687(2)	-.2705(8)	.2089(4)	.050
C(8)	.1608(2)	-.3183(8)	.1010(4)	.045
C(9)	.1888(2)	-.3122(11)	.0412(5)	.062
C(10)	.0621(2)	-.2812(11)	-.1026(5)	.065
C(11)	.0741(2)	-.1991(8)	.0015(4)	.046
C(12)	.0608(2)	-.1700(8)	.0770(4)	.050
C(13)	.0259(2)	-.2153(13)	.1108(7)	.075
H(1)	.16025	.10202	-.00875	.113
H(2)	.08806	.18206	-.04703	.088
H(3)	.07510	.25282	.12308	.081
H(4)	.13827	.21243	.26611	.119
H(5)	.19160	.13031	.18415	.071
H(8)	.15057	-.44123	.07828	.057

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
H(1)	.0368(2)	.0348(1)	.0360(1)	-.0012(1)	.0111(1)	-.0001(1)
S(1)	.058(1)	.058(1)	.043(1)	.000(1)	.019(1)	.010(1)
F(1)	.068(3)	.160(5)	.066(3)	-.005(3)	.003(3)	-.049(3)
F(2)	.081(4)	.135(5)	.081(3)	.025(3)	-.010(3)	.036(3)
F(3)	.045(3)	.162(5)	.068(3)	-.016(3)	.008(2)	.000(3)
F(4)	.085(4)	.128(4)	.091(3)	.063(3)	.033(3)	.013(3)
F(5)	.067(3)	.108(4)	.082(3)	-.005(3)	.036(3)	.006(2)
F(6)	.090(3)	.148(4)	.045(2)	.019(3)	.019(2)	-.013(3)
F(7)	.075(4)	.178(5)	.076(3)	-.030(4)	-.012(3)	-.032(4)
F(8)	.188(7)	.104(4)	.097(4)	.065(4)	-.021(4)	-.054(3)
F(9)	.163(6)	.141(5)	.053(3)	-.040(4)	.024(3)	.008(3)
F(10)	.076(4)	.315(10)	.232(8)	.028(5)	.071(5)	.202(8)
F(11)	.060(3)	.265(8)	.130(5)	-.062(5)	.023(4)	-.013(6)
F(12)	.139(7)	.172(7)	.227(9)	-.003(5)	.133(7)	-.034(6)
C(1)	.092(6)	.044(4)	.078(5)	-.010(3)	.043(5)	.005(3)
C(2)	.075(5)	.040(3)	.066(5)	-.003(3)	.010(4)	.013(3)
C(3)	.072(5)	.043(3)	.064(4)	.004(3)	.023(4)	.001(3)
C(4)	.080(5)	.040(3)	.063(5)	-.004(3)	.010(4)	-.010(3)
C(5)	.058(5)	.045(4)	.090(6)	-.017(3)	-.003(4)	.003(3)
C(6)	.054(4)	.088(5)	.041(4)	.006(4)	.003(3)	.001(4)
C(7)	.047(4)	.048(3)	.049(4)	.006(3)	.014(3)	.004(3)
C(8)	.045(4)	.046(3)	.038(3)	.007(3)	.009(3)	-.003(3)
C(9)	.053(5)	.075(5)	.051(4)	.021(4)	.009(3)	.005(4)
C(10)	.059(5)	.071(4)	.055(4)	0.000(4)	.005(4)	-.002(4)
C(11)	.038(3)	.048(3)	.045(4)	-.001(3)	.005(3)	.001(3)
C(12)	.048(4)	.055(4)	.043(4)	.001(3)	.015(3)	-.002(3)
C(13)	.052(5)	.086(5)	.081(6)	-.004(4)	.026(4)	-.007(5)

Table 2.3. Selected bond distances (Å) and angles (°) of complex (3).

W(1)	S(1)	2.303(2)	W(1)	C(1)	2.356(8)
W(1)	C(2)	2.378(7)	W(1)	C(3)	2.347(7)
W(1)	C(4)	2.302(7)	W(1)	C(5)	2.325(8)
W(1)	C(7)	2.166(6)	W(1)	C(8)	2.211(6)
W(1)	C(11)	2.074(6)	W(1)	C(12)	2.079(7)
S(1)	C(7)	1.757(7)	F(1)	C(6)	1.317(9)
F(2)	C(6)	1.326(10)	F(3)	C(6)	1.325(9)
F(4)	C(9)	1.327(10)	F(5)	C(9)	1.339(10)
F(6)	C(9)	1.357(8)	F(7)	C(10)	1.329(9)
F(8)	C(10)	1.293(10)	F(9)	C(10)	1.316(10)
F(10)	C(13)	1.237(13)	F(11)	C(13)	1.255(11)
F(12)	C(13)	1.312(12)	C(1)	C(2)	1.407(12)
C(1)	C(5)	1.396(12)	C(2)	C(3)	1.405(10)
C(3)	C(4)	1.397(11)	C(4)	C(5)	1.417(11)
C(6)	C(7)	1.480(9)	C(7)	C(8)	1.448(8)
C(8)	C(9)	1.464(9)	C(10)	C(11)	1.471(10)
C(11)	C(12)	1.266(9)	C(12)	C(13)	1.483(10)

S(1)	W(1)	C(7)	46.2(2)	S(1)	W(1)	C(8)	73.5(2)
S(1)	W(1)	C(11)	108.0(2)	S(1)	W(1)	C(12)	88.5(2)
C(7)	W(1)	C(8)	38.6(3)	C(7)	W(1)	C(11)	123.7(3)
C(7)	W(1)	C(12)	127.3(3)	C(8)	W(1)	C(11)	92.8(3)
C(8)	W(1)	C(12)	116.0(3)	C(11)	W(1)	C(12)	35.5(3)
W(1)	S(1)	C(7)	62.8(2)	C(2)	C(1)	C(5)	108.0(8)
C(1)	C(2)	C(3)	107.6(7)	C(2)	C(3)	C(4)	108.9(7)
C(3)	C(4)	C(5)	107.1(7)	C(1)	C(5)	C(4)	108.4(8)
F(1)	C(6)	F(2)	107.5(6)	F(1)	C(6)	F(3)	106.7(7)
F(1)	C(6)	C(7)	112.5(6)	F(2)	C(6)	F(3)	105.0(6)
F(2)	C(6)	C(7)	110.3(7)	F(3)	C(6)	C(7)	114.4(6)
W(1)	C(7)	S(1)	71.0(3)	W(1)	C(7)	C(6)	133.5(5)
W(1)	C(7)	C(8)	72.4(4)	S(1)	C(7)	C(6)	115.7(5)
S(1)	C(7)	C(8)	114.7(5)	C(6)	C(7)	C(8)	128.8(6)
W(1)	C(8)	C(7)	69.0(4)	W(1)	C(8)	C(9)	129.6(5)
C(7)	C(8)	C(9)	126.3(6)	F(4)	C(9)	F(5)	106.6(6)
F(4)	C(9)	F(6)	105.1(6)	F(4)	C(9)	C(8)	112.9(6)
F(5)	C(9)	F(6)	104.8(6)	F(5)	C(9)	C(8)	116.4(7)
F(6)	C(9)	C(8)	110.2(6)	F(7)	C(10)	F(8)	107.7(7)
F(7)	C(10)	F(9)	102.9(7)	F(7)	C(10)	C(11)	113.7(6)
F(8)	C(10)	F(9)	106.8(7)	F(8)	C(10)	C(11)	113.1(7)
F(9)	C(10)	C(11)	112.0(7)	W(1)	C(11)	C(10)	146.6(5)
W(1)	C(11)	C(12)	72.5(4)	C(10)	C(11)	C(12)	140.4(7)
W(1)	C(12)	C(11)	72.0(4)	W(1)	C(12)	C(13)	146.3(5)
C(11)	C(12)	C(13)	139.8(7)	F(10)	C(13)	F(11)	108.9(9)
F(10)	C(13)	F(12)	106.2(9)	F(10)	C(13)	C(12)	114.7(7)
F(11)	C(13)	F(12)	98.2(8)	F(11)	C(13)	C(12)	116.7(7)
F(12)	C(13)	C(12)	110.4(8)				

Table 2.4. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (4).

	X/A	Y/B	Z/C	U
W(1)	.42999(4)	.33720(2)	.25893(2)	.030
S(1)	.1955(3)	.2745(1)	.1702(2)	.050
F(1)	.2790(9)	.5017(4)	.0746(4)	.094
F(2)	.1018(10)	.4157(4)	-.0010(4)	.096
F(3)	.0555(10)	.4512(5)	.1378(5)	.105
F(4)	.5429(8)	.3004(4)	-.0365(3)	.085
F(5)	.5093(9)	.2089(4)	.0698(4)	.087
F(6)	.7545(7)	.2824(5)	.0725(4)	.092
F(7)	.6491(11)	.5452(4)	.1783(6)	.128
F(8)	.4524(13)	.6106(4)	.2340(7)	.138
F(9)	.6693(16)	.5695(6)	.3222(6)	.194
F(10)	.2443(23)	.5526(6)	.4109(11)	.263
F(11)	.2370(26)	.4474(9)	.4701(7)	.276
F(12)	.0690(14)	.4765(14)	.3725(11)	.268
C(1)	.6792(17)	.3206(8)	.3722(9)	.074
C(2)	.5255(15)	.2953(7)	.4154(6)	.063
C(3)	.4575(15)	.2271(7)	.3676(7)	.064
C(4)	.5634(16)	.2072(7)	.2941(7)	.066
C(5)	.7034(14)	.2673(7)	.2959(7)	.065
C(6)	.1856(14)	.4326(6)	.0835(6)	.058
C(7)	.3006(10)	.3595(5)	.1178(5)	.040
C(8)	.4946(11)	.3545(5)	.1109(5)	.041
C(9)	.5728(12)	.2861(7)	.0564(6)	.057
C(10)	.5630(15)	.5457(7)	.2552(7)	.066
C(11)	.4645(10)	.4679(5)	.2719(5)	.040
C(12)	.3399(10)	.4436(5)	.3249(5)	.040
C(13)	.2294(16)	.4789(8)	.3950(8)	.077
H(1)	.732(10)	.354(4)	.384(5)	.01(2)
H(2)	.497(13)	.320(5)	.476(6)	.07(3)
H(3)	.366(17)	.184(8)	.378(9)	.12(5)
H(4)	.558(16)	.162(7)	.235(7)	.11(5)
H(5)	.803(11)	.274(5)	.261(5)	.04(2)
H(8)	.565(9)	.406(4)	.099(4)	.02(2)

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
W(1)	.0303(2)	.0300(2)	.0308(2)	.0035(1)	.0029(1)	.0049(1)
S(1)	.0391(10)	.0448(13)	.0641(13)	-.0073(9)	-.0017(10)	-.0026(10)
F(1)	.114(5)	.046(4)	.117(5)	.005(3)	-.040(4)	.029(3)
F(2)	.126(5)	.079(4)	.076(4)	.023(4)	-.062(4)	-.008(3)
F(3)	.096(5)	.115(6)	.103(5)	.068(4)	.004(4)	.018(4)
F(4)	.104(4)	.116(5)	.035(3)	.010(4)	.009(3)	-.011(3)
F(5)	.119(5)	.056(4)	.088(4)	-.002(4)	.042(4)	-.022(3)
F(6)	.061(3)	.145(6)	.072(4)	.022(4)	.013(3)	-.033(4)
F(7)	.171(8)	.080(5)	.138(6)	-.061(5)	.087(6)	-.018(4)
F(8)	.178(8)	.040(4)	.197(9)	.002(5)	.035(7)	.020(5)
F(9)	.271(12)	.193(9)	.109(6)	-.191(9)	-.074(7)	.046(6)
F(10)	.385(20)	.085(7)	.337(17)	-.034(9)	.279(17)	-.096(9)
F(11)	.447(24)	.265(15)	.128(8)	.225(15)	.188(13)	.072(9)
F(12)	.091(7)	.473(27)	.242(15)	.046(11)	.051(8)	-.187(17)
C(1)	.057(7)	.070(9)	.091(9)	.013(6)	-.035(7)	.019(7)
C(2)	.080(7)	.073(8)	.036(5)	.020(6)	.001(5)	.013(5)
C(3)	.076(7)	.055(7)	.059(6)	.015(6)	.008(5)	.025(5)
C(4)	.086(7)	.055(7)	.057(6)	.030(6)	-.003(5)	.007(5)
C(5)	.054(6)	.087(8)	.054(6)	.036(6)	.011(5)	.023(6)
C(6)	.071(6)	.053(6)	.048(5)	.011(5)	-.024(5)	.000(4)
C(7)	.043(4)	.042(5)	.037(4)	-.001(3)	.000(3)	.000(3)
C(8)	.045(4)	.048(5)	.029(4)	.000(4)	.006(3)	.002(3)
C(9)	.055(5)	.074(7)	.042(5)	.002(5)	.006(4)	-.004(5)
C(10)	.084(7)	.047(6)	.067(7)	-.014(5)	.012(6)	-.007(5)
C(11)	.047(4)	.028(4)	.045(4)	-.005(3)	-.003(4)	.002(3)
C(12)	.048(4)	.036(5)	.036(4)	.010(4)	-.001(4)	-.005(3)
C(13)	.071(7)	.082(9)	.077(7)	.017(6)	.024(6)	-.026(6)

Table 2.5. Selected bond distances (Å) and angles (°) of complex (4).

W(1)	S(1)	2.275(3)	W(1)	C(1)	2.349(10)
W(1)	C(2)	2.368(9)	W(1)	C(3)	2.320(10)
W(1)	C(4)	2.308(10)	W(1)	C(5)	2.314(9)
W(1)	C(7)	2.174(8)	W(1)	C(8)	2.210(8)
W(1)	C(11)	2.082(8)	W(1)	C(12)	2.058(8)
S(1)	C(7)	1.744(9)	F(1)	C(6)	1.299(11)
F(2)	C(6)	1.329(10)	F(3)	C(6)	1.311(12)
F(4)	C(9)	1.339(10)	F(5)	C(9)	1.321(11)
F(6)	C(9)	1.337(11)	F(7)	C(10)	1.308(11)
F(8)	C(10)	1.327(13)	F(9)	C(10)	1.238(11)
F(10)	C(13)	1.187(14)	F(11)	C(13)	1.173(14)
F(12)	C(13)	1.196(15)	C(1)	C(2)	1.389(16)
C(1)	C(5)	1.394(16)	C(1)	H(1)	0.67(7)
C(2)	C(3)	1.345(15)	C(2)	H(2)	0.98(9)
C(3)	C(4)	1.389(15)	C(3)	H(3)	0.97(13)
C(4)	C(5)	1.398(15)	C(4)	H(4)	1.10(11)
C(5)	H(5)	0.92(8)	C(6)	C(7)	1.487(12)
C(7)	C(8)	1.440(12)	C(8)	C(9)	1.472(13)
C(8)	H(8)	0.98(7)	C(10)	C(11)	1.454(12)
C(11)	C(12)	1.292(11)	C(12)	C(13)	1.448(12)

S(1)	W(1)	C(7)	46.1(3)	S(1)	W(1)	C(8)	74.9(3)
S(1)	W(1)	C(11)	124.1(2)	S(1)	W(1)	C(12)	110.4(3)
C(7)	W(1)	C(8)	38.3(3)	C(7)	W(1)	C(11)	87.8(3)
C(7)	W(1)	C(12)	99.0(3)	C(8)	W(1)	C(11)	85.9(4)
C(8)	W(1)	C(12)	115.9(4)	C(11)	W(1)	C(12)	36.4(3)
W(1)	S(1)	C(7)	63.9(3)	C(2)	C(1)	C(5)	109.4(12)
C(2)	C(1)	H(1)	126.3(71)	C(5)	C(1)	H(1)	124.3(70)
C(1)	C(2)	C(3)	106.8(11)	C(1)	C(2)	H(2)	121.1(57)
C(3)	C(2)	H(2)	131.2(57)	C(2)	C(3)	C(4)	110.6(11)
C(2)	C(3)	H(3)	135.5(79)	C(4)	C(3)	H(3)	113.1(79)
C(3)	C(4)	C(5)	107.0(10)	C(3)	C(4)	H(4)	137.2(63)
C(5)	C(4)	H(4)	115.5(63)	C(1)	C(5)	C(4)	106.3(11)
C(1)	C(5)	H(5)	120.1(50)	C(4)	C(5)	H(5)	133.4(50)
F(1)	C(6)	F(2)	106.8(8)	F(1)	C(6)	F(3)	106.7(9)
F(1)	C(6)	C(7)	113.0(8)	F(2)	C(6)	F(3)	105.7(8)
F(2)	C(6)	C(7)	110.4(8)	F(3)	C(6)	C(7)	113.7(8)
W(1)	C(7)	S(1)	70.0(3)	W(1)	C(7)	C(6)	128.4(6)
W(1)	C(7)	C(8)	72.2(5)	S(1)	C(7)	C(6)	118.4(7)
S(1)	C(7)	C(8)	117.6(7)	C(6)	C(7)	C(8)	124.0(8)
W(1)	C(8)	C(7)	69.5(5)	W(1)	C(8)	C(9)	122.3(6)
W(1)	C(8)	H(8)	114.9(38)	C(7)	C(8)	C(9)	120.6(8)
C(7)	C(8)	H(8)	120.4(38)	C(9)	C(8)	H(8)	106.2(39)
F(4)	C(9)	F(5)	105.4(8)	F(4)	C(9)	F(6)	104.7(8)
F(4)	C(9)	C(8)	110.9(8)	F(5)	C(9)	F(6)	107.2(9)
F(5)	C(9)	C(8)	116.1(8)	F(6)	C(9)	C(8)	111.8(8)
F(7)	C(10)	F(8)	98.3(9)	F(7)	C(10)	F(9)	109.0(10)
F(7)	C(10)	C(11)	114.5(9)	F(8)	C(10)	F(9)	106.0(10)
F(8)	C(10)	C(11)	112.6(9)	F(9)	C(10)	C(11)	114.9(9)
W(1)	C(11)	C(10)	151.5(7)	W(1)	C(11)	C(12)	70.8(5)
C(10)	C(11)	C(12)	137.1(8)	W(1)	C(12)	C(11)	72.8(5)
W(1)	C(12)	C(13)	147.9(8)	C(11)	C(12)	C(13)	138.9(9)
F(10)	C(13)	F(11)	104.2(14)	F(10)	C(13)	F(12)	98.9(14)
F(10)	C(13)	C(12)	117.3(12)	F(11)	C(13)	F(12)	101.5(16)
F(11)	C(13)	C(12)	118.4(12)	F(12)	C(13)	C(12)	113.6(11)

Table 2.6. Crystallographic and experimental details of the structure analyses of complexes (3) and (4).

Compound	*cis*-[CpW(SC(CF$_3$)CCF$_3$)(hfb)] (3)	*trans*-[CpW(SC(CF$_3$)CCF$_3$)(hfb)] (4)
Formula	$C_{13}H_6F_{12}SW$	$C_{13}H_6F_{12}SW$
Formula Wt.	606.1	606.1
Crystal habit	red needle	red plate
Crystal size, mm	0.52x0.16x0.16	0.20x0.15x0.35
Crystal system	monoclinic	monoclinic
Space group	C 2/c	P 2_1/n
a, Å	35.551(5)	7.353(3)
b, Å	7.072(1)	15.764(12)
c, Å	13.548(2)	14.205(5)
β, °	107.00(1)	94.81(3)
Obtained from	25 refln, 13<θ<18°	25 refln, 11<θ<14°
V, Å^3	3282(1)	1641(2)
Z	8	4
F(000)	2256	1128
d calc, gcm^{-3}	2.453	2.454
T, K	297	295
μ(Mo-Kα), cm^{-1}	74.3	74.3
Absorption factors on F^2	0.87-1.09	0.81-1.39
Scan width, °	0.95	0.96
Max count time, s	90	120
Total refln measured	6322	5203
Unique refln	3807	2886
R_{INT}	0.024	0.025
Miller indicies h	0→50	0→ 8
measured, k	-9→ 9	-18→18
l	-19→19	-16→16
2θ range, °	4-60	4-50
Unique refln ≥ 3σ(I)	2610	2167
No. of parameters	244	268
R	0.025	0.027
R_w	0.031	0.034
$\|\Delta\rho\|_{max}$, eÅ^{-3}	0.86	0.97
Δ/σ_{max}	0.024	0.030

CHAPTER 3: STRUCTURES OF [CpM(SR)(hfb)$_2$(L-L)] COMPLEXES

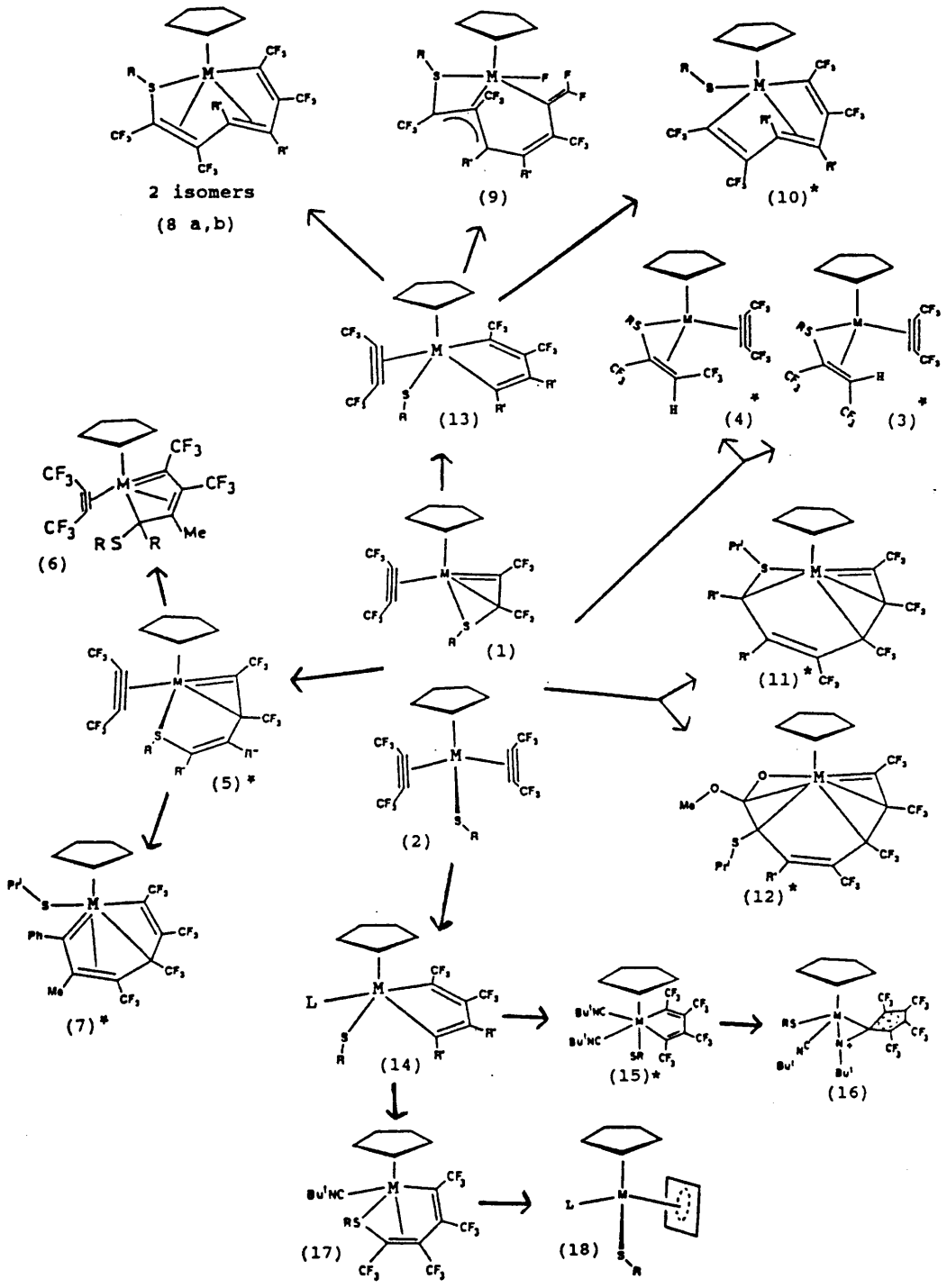
3.1 Introduction

In this chapter the structures are presented of six complexes of general formula [CpM(SR)(hfb)$_2$(L-L)], where L-L is either a third alkyne ligand or two isocyanide ligands. The molecules discussed are:

	M	R	L-L
(5)	Mo	Pr^i	PhC≡CMe
(7)	W	Pr^i	PhC≡CMe
(10)	W	4-MeC_6H_4	dmad
(11)	Mo	Pr^i	dmad
(12)	Mo	Pr^i	dmad
(15)	W	Pr^i	(4-MeC_6H_4NC)$_2$

The formulation of each compound, based on its X-ray analysis is shown in Scheme III and the molecular geometries are compared in Table 3.1. The structures are first considered individually (Section 3.2) and the chemical implications of the structural results are then presented (Sections 3.3 and 3.4).

Scheme III.



3.2 Description of Structures

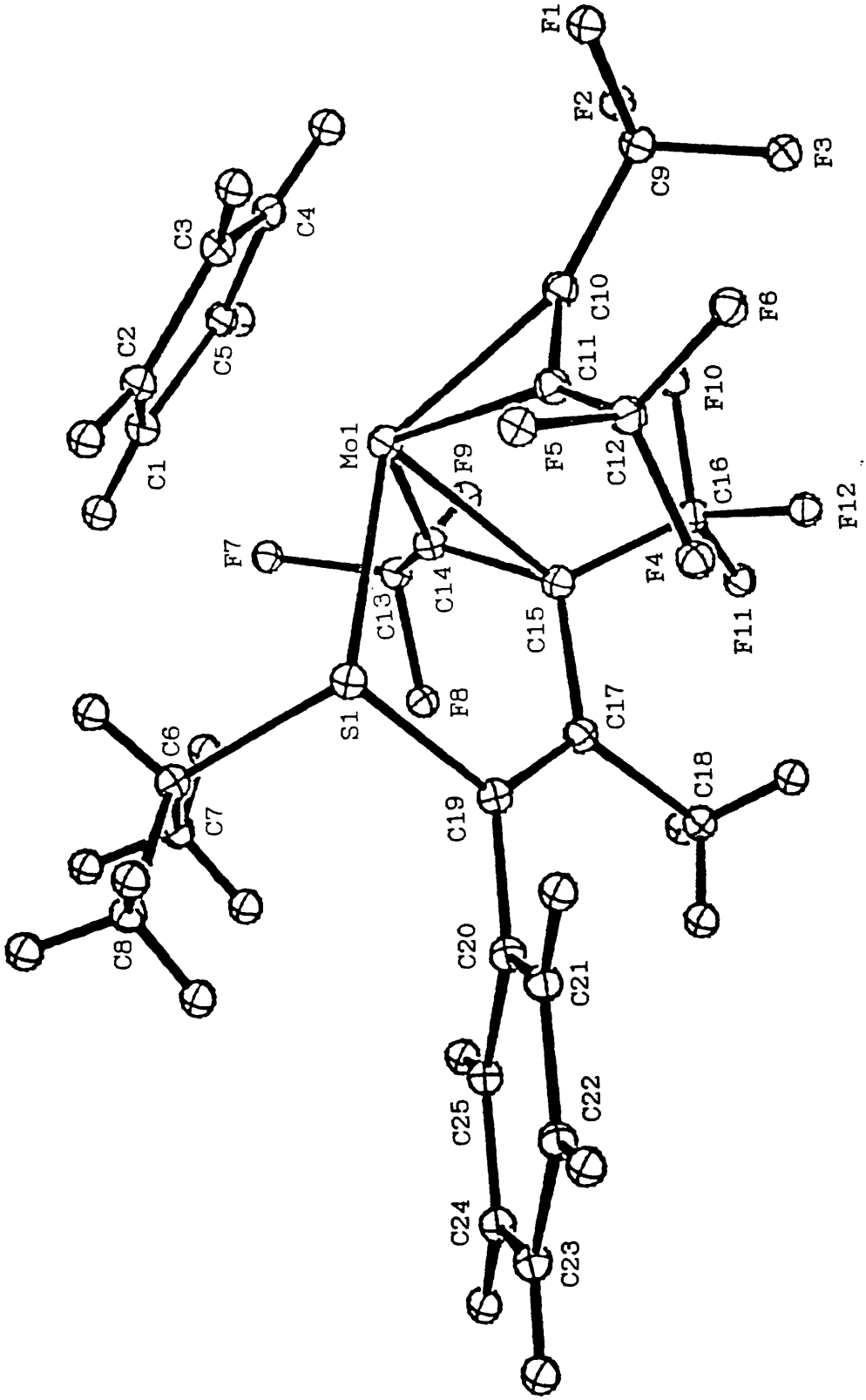
[CpMo(Pr^iSC(Ph)=C(Me)C(CF_3)CCF_3)(hfb)] (5)

The structure of (5) (see Figure 3(a)) was determined using X-ray diffraction analysis. The crystal used was shown to contain discreet molecules of complex (5) with intermolecular distances consistent with the appropriate sum of van der Waal radii.[52] Complex (5) differs formally from the starting complex (1) only by the insertion of PhC≡CMe into the S-C bond of the η^3-Pr^iSC(CF_3)CCF_3 ligand of (1).[99] A comparison of bonding distances between the two structures (see Tables 2.1 and 3.1) shows their remarkable similarity despite the different metal atom in each and the additional alkyne unit in complex (5).

In (5) the Mo-C(14) and Mo-C(15) distances [1.915(5) and 2.239(5) Å respectively] show only minor differences to the corresponding M-C bonds of the η^2-vinyl ligand in (1), the former clearly showing multiple bonding character and the latter obviously single in nature. The C(14)-C(15) bond length [1.426(7) Å] is short for a single C-C bond,[108] but is similar to that in (1) of 1.417(10) Å. This appears normal for η^2-vinylic bonding and is probably due to slight delocalisation of the Mo-C(14) π-bonding. The M-S distances are also closely comparable.

The C(15)-C(17), C(19)-C(17) and C(19)-S bond distances of 1.514(7), 1.338(7) and 1.798(6) Å and a S-C(19)-C(17)-C(15) torsion angle of -4.1(5)° suggest strongly that C(19)-C(17) is a localised double bond connected to atoms C(15) and S by single bonds. Atoms C(19) and C(17) are not

Figure 3(a). A view of complex (5) with all atoms presented as spheres of arbitrary size.



bonded to the molybdenum atom (see Table 3.1).

The Mo-C and C-C bond lengths in the cyclopentadienyl ring agree well with those in other structures in this series (see Table 3.1). The bonding of the η^2-hfb ligand to the Mo atom is similar to that of other such 2-electron donor ligands.[94,99] All other bonds and angles also appear unexceptional (see Tables 3.1 and 3.3), the main point of note being the wide range of C-F bond distances [1.25(1)-1.35(1) Å]. The fluorine atoms involved in the shortest of these bonds all have large thermal displacement parameters which could be caused by disorder of their atomic positions.

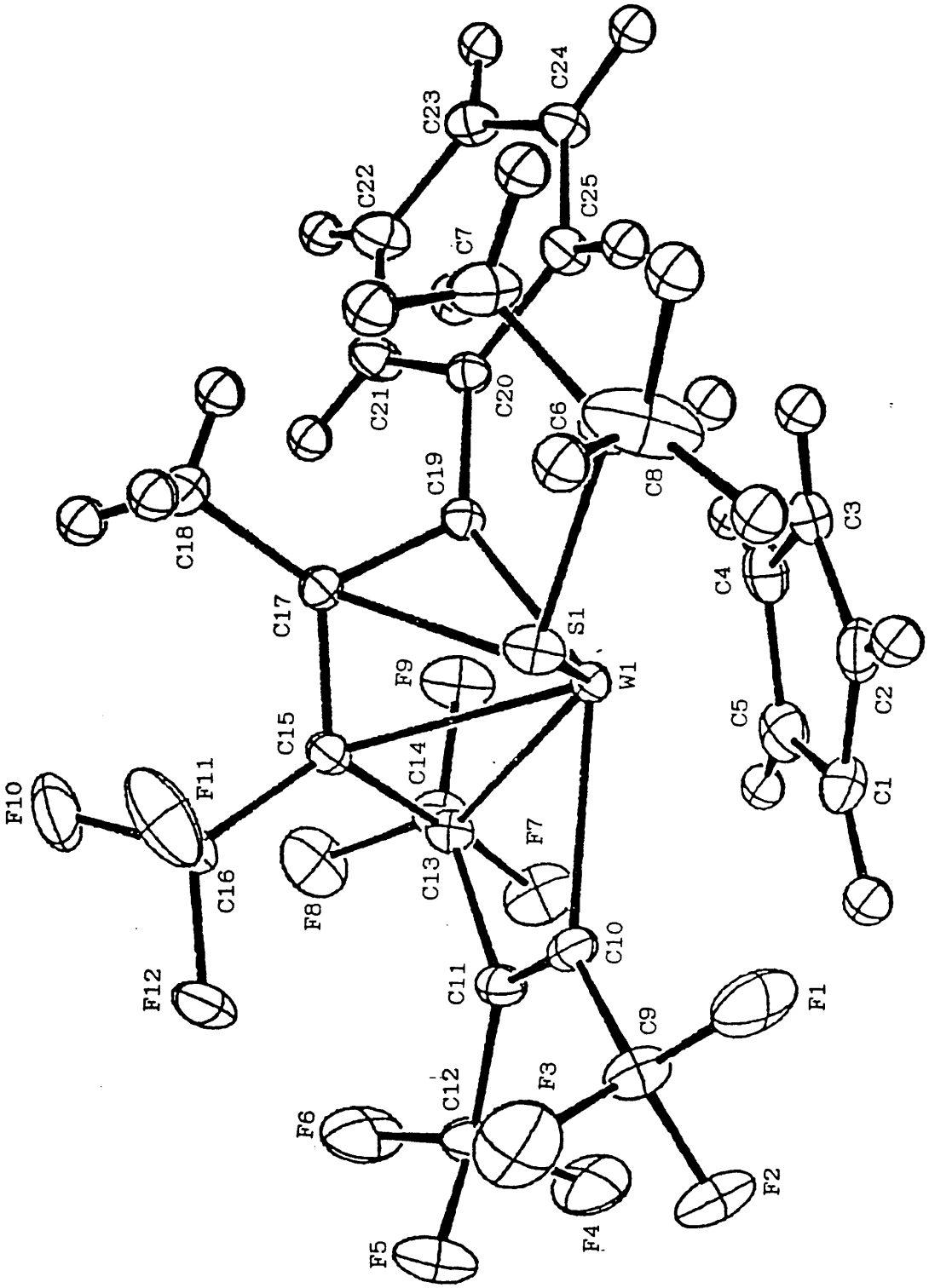
$[CpW(SPr^i)(PhCC(Me)C(CF_3)C(CF_3)C(CF_3)=CCF_3]$ (7)

X-ray analysis of a crystal of compound (7) showed it to contain well separated molecules. The tungsten atom in complex (7) has bonded to it a cyclopentadienyl ring, the thiolate group, SPr^i, and a carbon chain consisting of the three alkyne units. The thiolate group is not bonded to this oligomer (see Figure 3(b)).

In complex (7) the M-S distance is clearly shorter than in complex (5). This is probably due to the sulphur being only mono-substituted whereas in complex (5) it was attached to the carbon chain as well as to an alkyl group. There is a wide variation in C-H bond distances. However, this is not unusual when hydrogen atom positions are refined.

The carbon oligomer is bonded to the tungsten atom through five of the six carbon atoms in the chain (see Table 3.1). The C(13)-C(15)-C(17)-C(19) section is a

Figure 3(b). The structure of complex (7). 50% probability ellipsoids are displayed for all atoms.



roughly planar η^4-butadienyl unit [torsion angle -22.4(3)°]. W-C(19) is a multiple bond, length 2.Ø17(3) Å, which is longer than the similar bond in complex (5) but is clearly much shorter than a M-C single bond. The bonding from atoms C(17) and C(15) to the tungsten atom is similar to that of an η^2-alkene, as in complexes (3) and (4). However, the C(17)-C(19) and C(15)-C(17) bonds are both much shorter than C-C single bonds, suggesting some delocalisation of charge over atoms C(15), C(17) and C(19). The W-C(13) bond completes the bonding of the η^4-unit and appears single in nature, as does the C(13)-C(15) bond (see Tables 3.1 and 3.5).

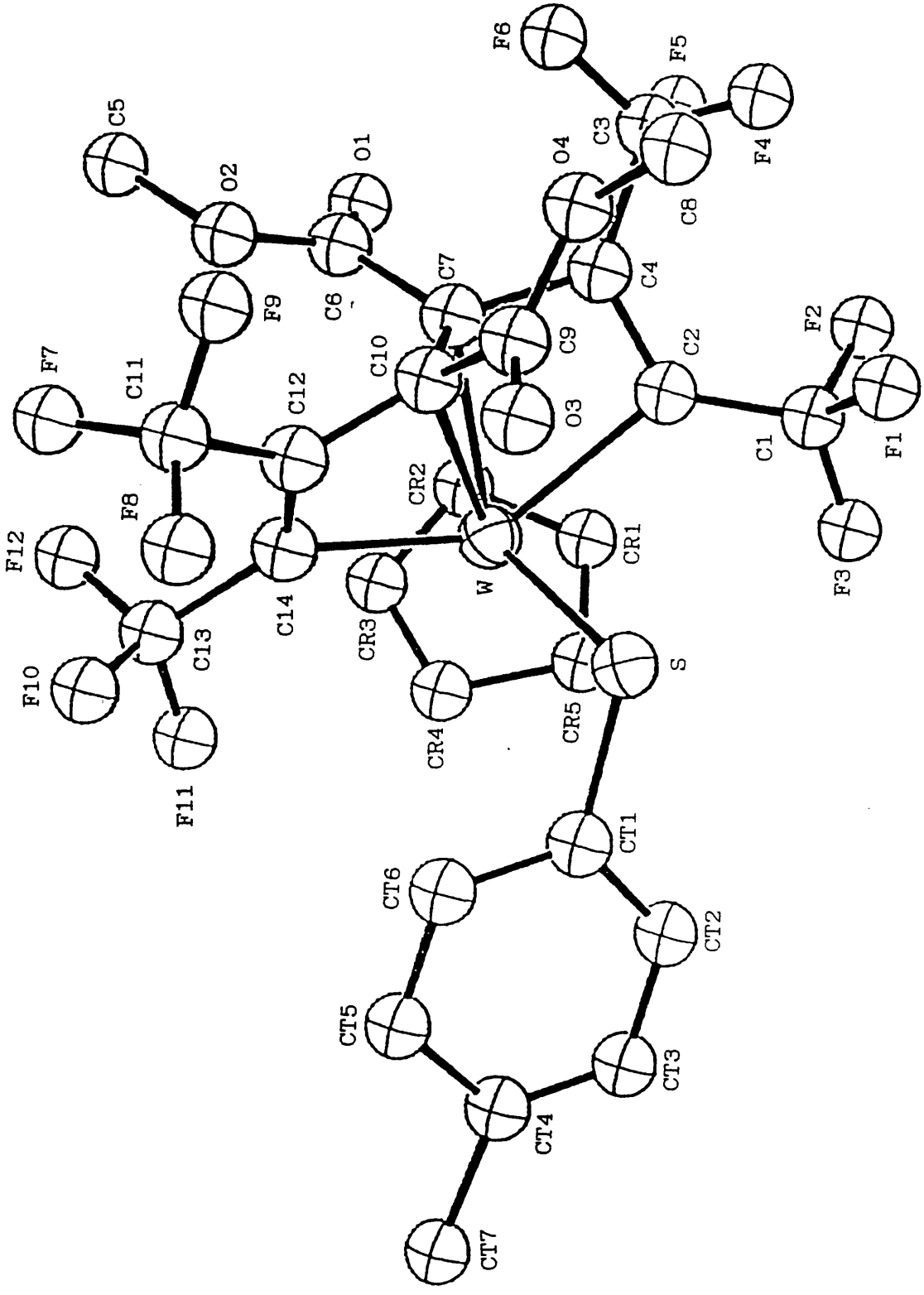
The final C_2 unit of the oligomer is bonded to the η^4-butadienyl with a C(11)-C(13) single bond and to the metal centre through a W-C(alkenyl) single bond. The torsion angle C(9)-C(1Ø)-C(11)-C(12) of -4.9(4)° and a bond length of 1.321(5) Å suggests that C(1Ø)-C(11) is a localised double bond.

[CpW(STol)(F_3CC=C(CF_3)C(CO_2Me)=C(CO_2Me)C(CF_3)=CCF_3)] (1Ø)

X-ray analysis of a crystal of complex (1Ø) showed it to be made up of discrete molecules of separated by distances consistent with those of the apprpriate van der Waals radii.[52]

Complex (1Ø) consists of a cyclopentadienyl ring, a 4-methylbenzenethiolate ligand and a carbon chain constructed from the three alkyne units, with the added dmad again separating the two hfb ligands. These ligands are all attached to the central tungsten atom (see Figure 3(c) and Tables 3.1 and 3.7).

Figure 3(c). The structure of complex (10). Hydrogen atoms are omitted. All atoms shown are displayed as spheres of arbitrary size.



The oligomer appears to be bonded to the tungsten atom through two M-C σ-bonds from the end carbons C(2) andC(14). The bond lengths [2.24(2) and 2.12(2) Å] are consistent with other such bonds (e.g. W-C(1Ø) 2.242(4) Å in complex (7)). The chain is also bonded through an η^2-alkenyl interaction from atoms C(7) and C(1Ø). The other carbon atoms C(4) and C(12) are clearly not bonded to the tungsten atom [distances are 2.79(2) and 2.67(2) Å respectively].

Bonds C(2)-C(4) and C(12)-C(14) with lengthsof 1.35(3) and 1.34(3) Å respectively, appear to be localised double bonds. Distances of 1.5Ø(3) Å for bond C(4)-C(7) and 1.47(2) Å for bond C(1Ø)-C(12) suggest that they are single in nature. The C(7)-C(1Ø) bond length is 1.44(3) Å and is consistent with other η^2-M-C(alkene) interactions e.g. in complexes (2) and (3) (see Table 2.1). The three C-C-C-C chain torsion angles [66(2), -166(2) and 51(2)°] seem to confirm this assesment and suggests that the C(7)-C(1Ø) double bond is *trans* in nature. This type of $M(CR)_6$ bonding has previously been observed for $Ni(CCF_3)_6$.[1Ø9] It is only the different nature of the chain bonding which distinguishes compound (1Ø) from the formally analogous complex (7).

The major point of note about the geometry of the other ligands is that the W-S distance [2.318(6) Å] is much shorter than the value for the monosubstituted thiolate group in complex (7). This could be due to the more electron withdrawing nature of the $4\text{-}MeC_6H_4$ substituent compared to isopropyl, but is more likely to be due to stabilisation of the 16-electron tungsten atom by π-electron donation from the sulphur atom. Of the compounds

discussed here (10) is the only one not to contain an 18-electron configuration.

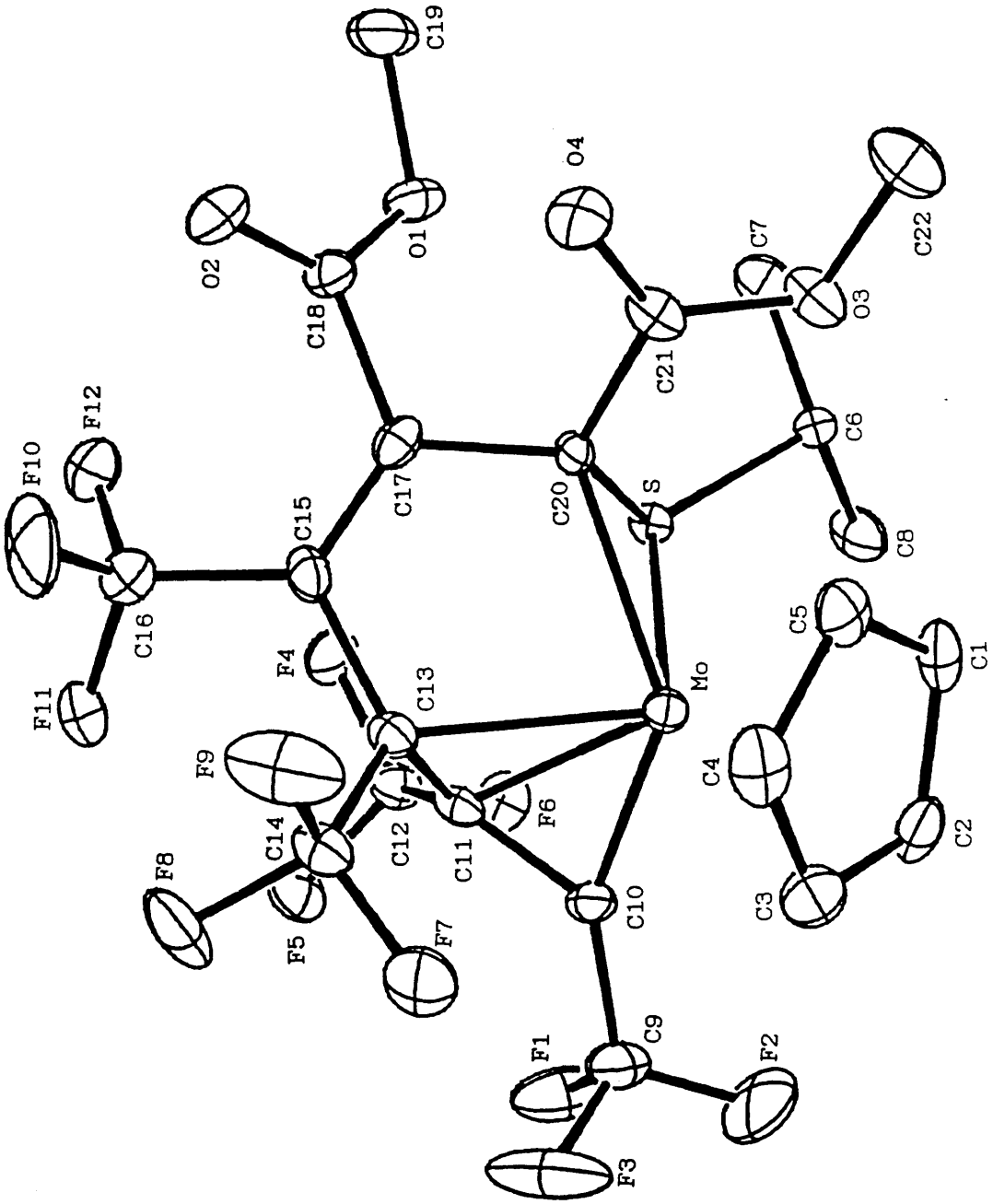
$[CpMo(Pr^{i}SC(CO_2Me)C(CO_2Me)=C(CF_3)C(CF_3)=C(CF_3)CCF_3)]$ (11)

Complex (11) was characterised using X-ray diffraction analysis. This showed the crystal to contain two crystallographically different molecules of (11) separated by distances consistent with van der Waals radii.[52] While the molecules are crystallographically different, chemically they are identical with only small differences in geometry which can be attributed to crystal packing (see Table 3.9).

In complex (11) there are only two discrete ligands attached to the molybdenum atom: the cyclopentadienyl ring which again has unexceptional geometry and an oligomer containing the three alkyne units and the thiolate group (see Figure 3(d)).

The oligomer is bonded to the molybdenum atom through the C(10), C(11), C(13), C(20) and S atoms. Atoms C(15) and C(17) are clearly non-bonding [Mo...C 3.192(8) and 3.169(8) Å respectively in molecule A and 3.177(8) and 3.162(8) Å in molecule B]. C(10), C(11) and C(13) are bonded in a similar fashion to the first three carbon atoms of the η^4-butadienyl unit in complex (7) (see C-C and M-C distances for C_a, C_b and C_c in Table 3.1), i.e. Mo-C(10) is a multiple bond and the Mo-C attachement of atoms C(11) and C(13) is a M-η^2-alkene interaction but with some delocalisation of π-bonding over all three carbon atoms. The attachment of the molybdenum atom to the oligomer is completed by σ-bond interactions with C(20) and S atoms.

Figure 3(d). A view of complex (11). Hydrogen atoms are omitted and 50% probability ellipsoids are shown for all other atoms.



Atom C(15) is connected to C(13) by a single bond as is C(17) to C(20) [mean bond distances 1.522(10) and 1.483(10) Å]. However, C(15)-C(17) is clearly a localised double bond [mean bond distance 1.318(10) Å and mean C(13)-C(15)-C(17)-C(20) torsion angle 1.9(6)°].

In complex (11) the methyl ester substituents are no longer on the central alkyne unit of the oligomer as in compound (10) but are now on the alkyne unit attached to the thiolate group.

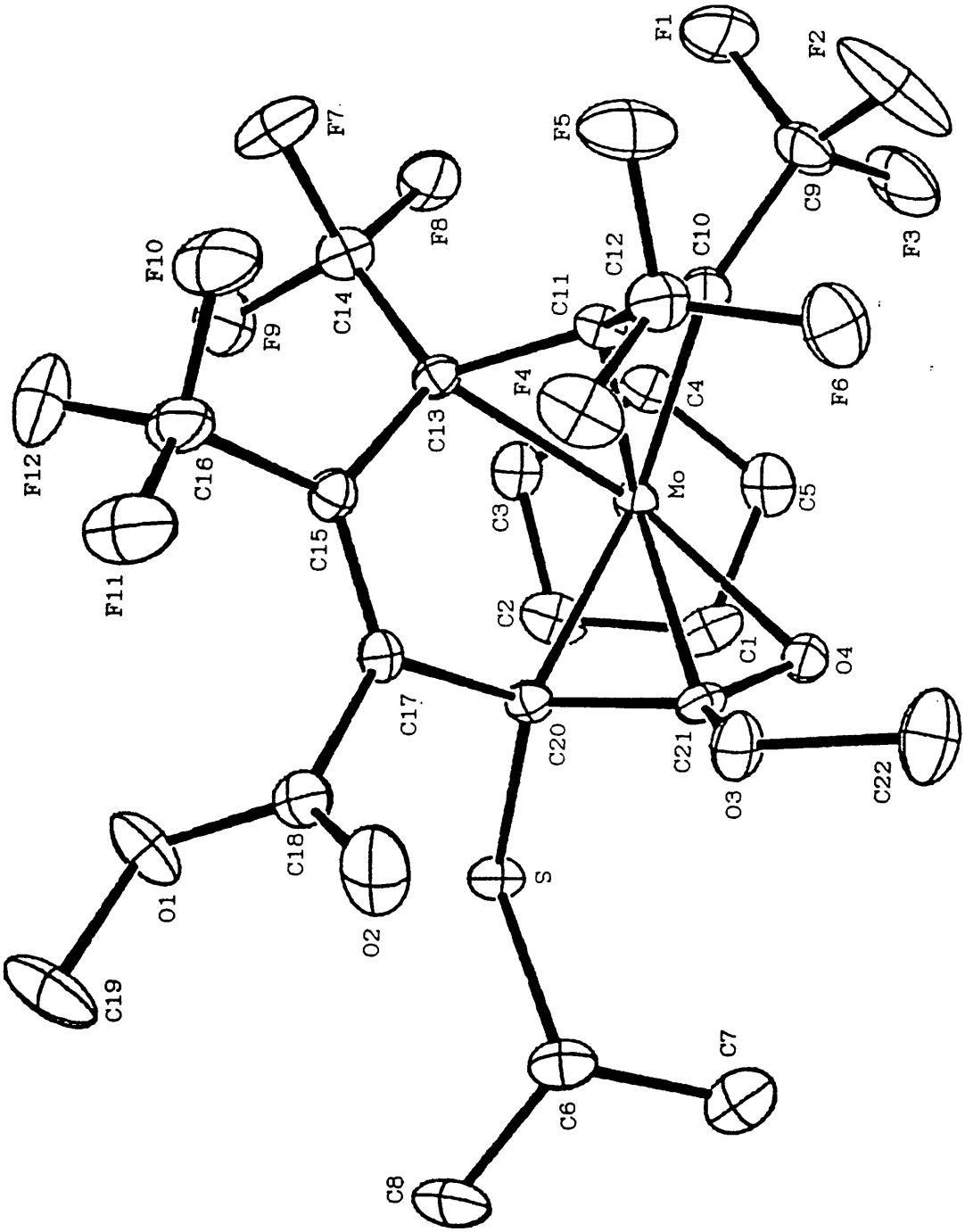
$[CpMo(F_3CCC(CF_3)C(CF_3)C(CF_3)=C(CO_2Me)C(SPr^i)C(OMe)=O)]$ (12)

X-ray diffraction analysis of a crystal of complex (12) shows it to be made up of discrete molecules separated by distances consistent with van der Waals radii.[52]

The structure of compound (12) shows it to be an isomer of complex (11), and like (11) it has a cyclopentadienyl ring and the same oligomer, consisting of the three alkyne units and the thiolate group, bonded to the molybdenum atom (see Figure 3(e)). The cyclopentadienyl rings geometry is again consistent with others in this series (see Tables 3.1 and 3.11).

The bonding within the carbon chain and to the molybdenum atom is remarkably similar to that in complex (11) (see Table 3.1 for comparison of M-C and C-C bond distances and C-C-C-C torsion angles), and can be regarded as identical. The structures differ in that there has been a rotation of the substituents attached to C(20) so that in complex (12) the sulphur atom is no longer bonded to the molybdenum atom and Mo-C(21) and Mo-O(4) distances [2.477(6) and 2.125(4) Å respectively] suggest the methyl

Figure 3(e). A view of complex (12). For clarity, hydrogen atoms have been omitted. 50% probability ellipsoids are displayed for all other atoms.



ester group is now attached to the molybdenum atom through the carbonyl group. Comparison of the two methyl ester geometries in complex (12) shows there has been a lengthening of the C=O bond [C(21)-O(4) 1.248(9) Å and C(16)-O(2) 1.178(10) Å] characteristic of η^2-C=O π-bonding to the metal centre. Evidence that the C(21)-O(4) interaction is no longer a localised double bond is seen in the Mo(1)-O(4)-C(21)-C(20) torsion angle being 32.2(5)°.

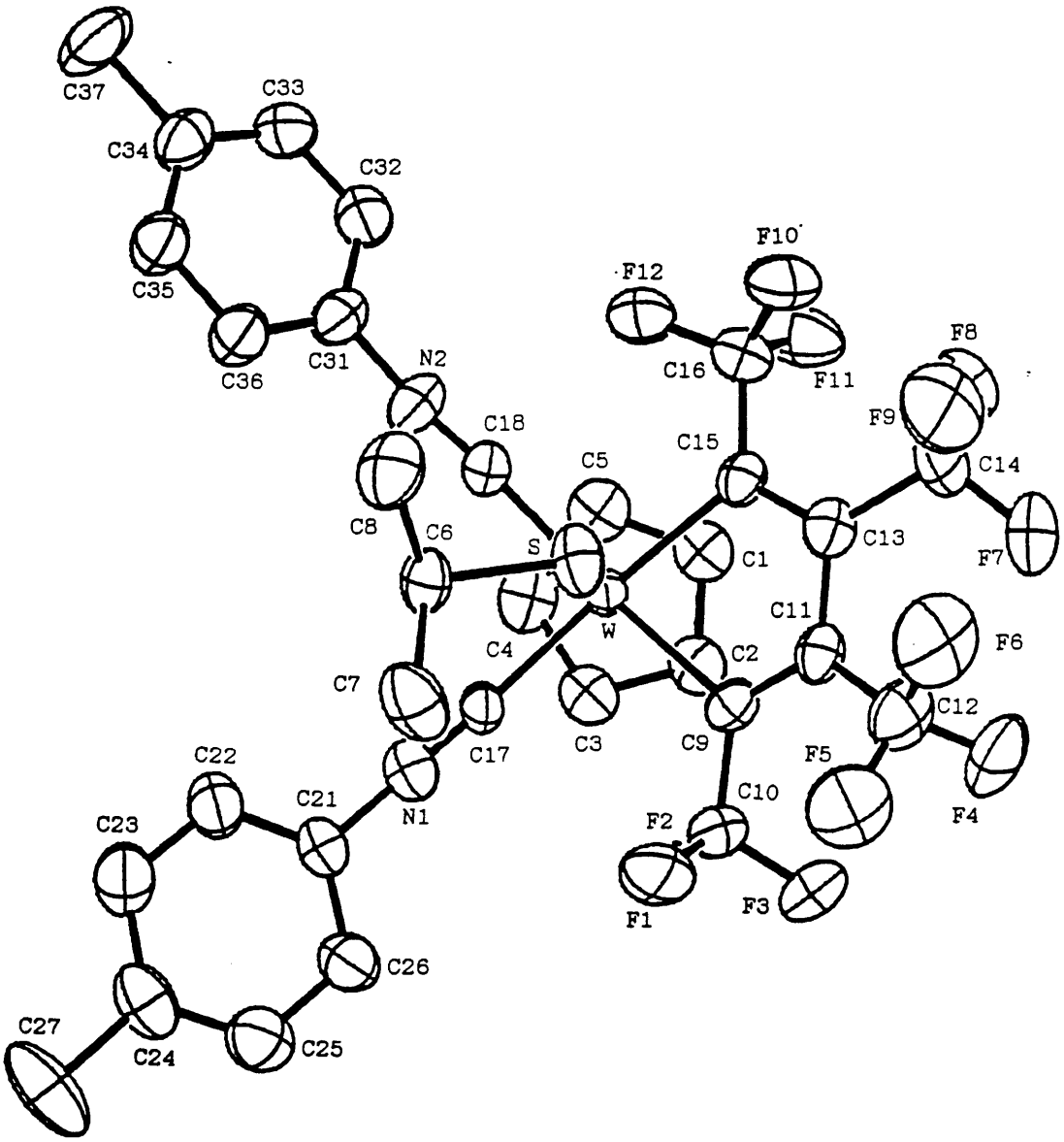
$[CpW(SPr^i)(F_3CC{=}C(CF_3)C(CF_3){=}CCF_3)(4\text{-}MeC_6H_4NC)_2]$ (15)

X-ray diffraction analysis was used to study the crystals of complex (15). They were found to contain well separated molecules of the compound with all intermolecular contacts consistent with van der waals radii.[52] Complex (15) contains a $W(CCF_3)_4$ metallacycle, with a cyclopentadienyl ring, an isopropylthiolate ligand and two 4-MeC_6H_4NC ligands also bonded to the tungsten atom (see Figure 3(f) and Tables 3.1 and 3.13).

The 18-electron bonding around the tungsten(IV) atom is roughly octahedral with the cyclopentadienyl ring occupying a single vertex *trans* to the thiolato-sulphur atom. The equatorial plane is made up of the two mutually *cis* 4-MeC_6H_4NC ligands and the $C_4(CF_3)_4^{2-}$ unit. This means the molecule has an approximate mirror plane which passes through the midpoints of C(1)-C(2) and C(11)-C(13) bonds and atoms W, S and C(4).

The W-C(cyclopentadienyl) bond lengths are comparable with those in the [CpM(SR)$(hfb)_2$(R'C≡CR")] complexes (see Table 3.1). However the W-S distance of 2.561(2) Å and the W-CNR distances of 2.081(6) and 2.090(6) Å are longer than

Figure 3(f). The structure of complex (15). Hydrogen atoms are omitted. Probability ellipsoids of 50% are displayed for all atoms shown.



for those in the comparable tungsten(II) structure $[CpW(SPr^i)(CNBu^t)(\eta^2\text{-}C_4(CF_3)_4CNBu^t)]$ [W-S 2.374(3) Å and W-CNR 2.Ø17(9) Å].[110] The bonding within these ligands in the two structures does not show any major differences.

The geometry of the metallacycle suggests that the W-C_α bonds are single in nature [mean distance 2.21Ø(4) Å] whereas the C_α-C_β bond lengths are clearly in the range of localised double bonds [1.354(8) and 1.359(8) Å] and the C_β-C_β bond appears to be single [1.472(8) Å]. The internal torsion angles are all 12° or less.

This is clearly different from the WC_4 metallacycle of $[CpW(C(CF_3)C(CF_3)C(CF_3)C(CF_3))(CO)_2Co(CO)_2]$,[111] in which the cobalt atom is bonded to the tungsten atom and is roughly equidistant from all four butadiene carbons. The C-C distances in this structure are all in the range 1.42(1)-1.44(1) Å i.e. all effectively the same length. There is one other type of bonding possible for the ring i.e. when the W-C_α and C_β-C_β bonds are localised double bonds and C_α-C_β bonds are single in nature.

Experimental

The same basic experimental procedure was carried out for the structures in this Chapter as for those in Chapter 2. Therefore only differences from the procedure given in Chapter 2 are mentioned below.

$[CpMo(SPr^i)(hfb)_2(PhCCMe)]$ (5)

Data Collection. Cell dimensions and experimental parameters are given in Table 3.14. Severe non-linear decomposition (intensity standards fell by 70%) meant even after correction, standards varied by ±10%. As a result a Gaussian rather than empirical absorption correction was carried out.[87]

Structure Analysis. All hydrogen atoms save one methyl hydrogen were found in the difference synthesis. Independent refinement of hydrogen parameters was not satisfactory. Accordingly, hydrogen positions were idealised (C-H = 0.96Å) and the hydrogen atoms were constrained to ride on their parent carbon atoms with U(H) = 1.2 U(C). Final atomic parameters were obtained (see Table 3.2) by refinement of blocks of the 351 parameters.

$[CpW(SPr^i)(hfb)_2(PhCCMe)]$ (7)

Data Collection. Cell dimensions and experimental parameters are given in Table 3.14. No decomposition correction was necessary.

Structure Analysis. All hydrogen atom positions were found and refined, as were their isotropic displacement parameters. Final atomic parameters for all atoms (Table 3.4) were obtained by refinement of blocks of the 432 parameters. All reflections were used in the final refinement because of a marked improvement in the e.s.d.s of the atomic parameters.

[CpW(STol)$(hfb)_2$(dmad)] (10)

Data Collection. Cell dimensions and experimental parameters are given in Table 3.14. No decomposition correction was necessary.

Structure Analysis. Anisotropic displacement parameters were used for the W and S atoms. All other non-hydrogen atoms used isotropic parameters. Although it proved impossible to locate hydrogen positions in the difference synthesis these were calculated geometrically. Refinement of the chirality factor η from both +1 and -1 gave a convergance to the physically meaningless value of η = -0.10(6). Final atomic positions and displacement parameters are given in Table 3.6.

[CpMo(SPr^i)$(hfb)_2$(dmad)] (11)

Data Collection. Cell dimensions and experimental parameters are given in Table 3.14. The Type I triclinic cell has two molecules per asymmetric unit. It does not transform to a higher symmetry cell [A = 118.8, B = 259.9, C = 305.6, D = 124.4, E = 55.3 and F = 55.9]. No decomposition correction was necessary.

Structure Analysis. No hydrogen atom positions were found and hence they were calculated geometrically. Final atomic positions and displacement parameters (Table 3.8) were obtained by refinement of blocks of the 721 parameters.

$[CpMo(SPr^i)(hfb)_2(dmad)]$ (12)

Data Collection. The cell dimensions and experimental parameters are given in Table 3.14. No decomposition correction was applied.

Structure Analysis. Final atomic positions and thermal displacement parameters are given in Table 3.1Ø.

$[CpW(SPr^i)(hfb)_2(CNTol)_2]$ (15)

Data Collection. The cell dimensions and experimental parameters are listed in Table 3.14. A decomposition correction was applied to correct a 1Ø% linear decay of the intensity standards.

Structure Analysis. Hydrogen thermal displacement parameters were set at U(H) = Ø.Ø5 $Å^2$ and were not refined. Final atomic positions and displacement parameters were obtained by refinement of blocks of the 433 parameters (see Table 3.12).

3.3 Reaction Scheme and Discussion

Scheme III shows the intermediates and products, in the reaction of alkynes with complexes (1) and (2), elucidated during and prior to this period of research. The * denotes structures which were characterised using X-ray diffraction analysis by the author. The thermolysis products (3) and (4) were referred to in Chapter 2, while all other compounds are discussed below and their geometries have been described more fully in 3.2.

Insertion of R'C≡CMe

The reactions of the bis(alkyne) species (2), M = W, R = 4-MeC_6H_4 and the η^2-vinyl complexes (1), M = Mo, W, R = Pr^i, with an incoming alkyne of the form R'C≡CMe, R' = Me, Ph at room temperature, lead initially to the same species (5) irrespective of the metal or incoming alkyne used.

The structure of the 18-electron complex (5), M = Mo, R = Pr^i, R' = Ph is formally derived from (1) by insertion of the incoming PhC≡CMe into the S-C bond of the η^3-$C(CF_3)C(CF_3)SPr^i$ ligand with the phenyl substituent on the carbon adjacent to sulphur and involves virtually no change in metal-ligand coordination. Indeed there are no major variations in the metal-ligand bonding between the two complexes (1) and (5) (cf Tables 2.1 and 3.1).

On heating complex (5) can isomerise to either compound (6) or (7), both 18-electron structures, depending on the nature of the metal atom, of the thiolate group or of the incoming alkyne.

Complex (6), M = W, R = Pr^i, R' = Me, was characterised

by X-ray diffraction analysis previously.[100] It differs from complex (5) only in the rearrangement of the SC_4 chain where cleavage of the metal-sulphur bond and attachment of the previously non-bonded chain carbons to form an η^4-butadienyl ligand has occurred. The η^2-alkyne and cyclopentadienyl ring remain essentially unaffected.

The structure of complex (7), M = W, R = Pr^i, R' = Ph, (see 3.2 for geometrical description) is derived from complex (5) by incorporation of the η^2-alkyne into the oligomer and by scission of the S-C(oligomer) bond to form a WC_6 metallacycle and so that the thiolate group remains bonded to the metal only. The oligomer is attached to the metal through a roughly planar η^4-butadienyl unit, similar to that found in complex (6), and a σ-M-C(alkenyl) bond.

Insertion of $MeO_2CC{\equiv}CCO_2Me$ (dmad)

The reaction of complex (1), M = W, R = Pr^i, with dmad produced the isomers (8a) and (8b), which differ only in the orientation of the isopropyl group on the sulphur atom relative to the cyclopentadienyl ring, and the novel complex (9), which has undergone transfer of a fluorine atom from a trimethylfluoro group to the metal atom. These structures were all characterised previously using X-ray diffraction analysis,[100] and their bonding is described in 1.2.

The main points of note are that, in both complex (8) and (9), all three alkynes are linked in a continuous chain, with the incoming dmad ligand in the middle position and with the thiolate attached at one end. The differences in structures occur in the mode of bonding of

this oligomer around the metal atom and in the transfer, in complex (9), of the fluorine atom to the tungsten atom.

Reaction of dmad with complex (2), M = W, R = 4-MeC_6H_4, results in a structurally different product (10). In complex (10) (see 3.2 for geometrical description), as in complexes (8) and (9) the three alkynes are connected in a continuous chain around the metal atom with dmad the central unit. However in complex (10) the CO_2Me substituents are clearly *trans* relative to each other whereas in complex (8) they are *cis*. Also in complex (10) there is no bonding between the carbon chain and the thiolate group. The chain is bonded to tungsten atom through the η^2-alkene type interaction from the central alkyne unit and two σ-M-C(alkenyl) bonds from the outer carbons of the end alkyne units of the C_6 chain. Complex (10) also differs from (8) and (9) in that it is a 16-electron structure rather than having 18-electrons around the tungsten atom.

The reaction of dmad with complex (1), M = Mo, R = Pr^i, produced structurally different complexes from those above. Complexes (11) and (12) are isomers (geometrical details in 3.2). In both complexes the three alkyne units are again connected in a continuous chain. In this case, however, the dmad unit is at one end of the chain and the thiolate group is attached to it.

In complex (11) the oligomer is attached to the molybdenum atom through bonding from the sulphur atom, the carbon atom adjacent to sulphur by a single σ-M-C(alkyl) interaction, and following two clearly non-bonding carbons of the chain through a η^2-alkene interaction from the next

two carbons and by a M-C(carbene) interaction from the final carbon.

The Mo-C bonding of the oligomer in complex (12) is very similar to that of structure (11). However (12) differs from (11) formally in that there has been a rotation of the groups attached to the first carbon as mentioned above. There has been scission of the Mo-S bond and the methyl-ester substituent is now attached to the molybdenum atom through a η^2-Mo-C=O interaction.

It has been established by Dr.J.L. Davidson using N.M.R. and I.R. spectroscopy that all the above reactions involving dmad proceed via an intermediate which is unstable above -30°C and it has been predicted that this intermediate has structure (13). Unfortunately this has not as yet been confirmed using X-ray diffraction analysis because suitable crystals have not yet been obtained.

It appears that the 16-electron complex (13) has a metallacyclic ring involving the incoming alkyne and one of the hexafluorobut-2-yne ligands already attached. The thiolate group and the other hfb ligand are attached only to the metal centre.

Addition of R'NC

Attachment of ligands other than alkynes to complexes (1) and (2) can also result in the formation of metallacycles. The reaction of (1) and (2) with R'NC when R' = Bu^t is one such example.[96,112]

Reaction of RNC with (1) led to the formation of complex (14) which is similar in structure to (13) but with the η^2-hfb ligand replaced by the iso-nitrile. Addition of

a further R'NC ligand produced complex (15). X-ray diffraction analysis of crystals of this compound, M = W, R = Pr^i, R' = 4-MeC_6H_4 has been carried out (see 3.2 for geometrical and experimental details).

Bonded to the tungsten atom are two molecules of 4-MeC_6H_4NC, a cyclopentadienyl ring, the thiolate group SPr^i and a carbon chain comprising of the two hfb ligands. The last of these ligands creates a metallacycle with the tungsten atom similar to that thought to be present in complexes (13) and (14). The bonding in the metallacycle comprises two W-C(alkenyl) single bonds to the end carbons of the C_4 chain, two localised C-C double bonds with a C-C single bond separating these.

Reaction of the R'NC ligand with complex (2) can also produce (15), however it is also possible, in this case, for the incoming ligand to attach itself to one of the η^2-alkynes to form an η^2-vinyl species which on reaction with a further R'NC unit forms complex (15) but not by way of complex (14) as above.[112]

On heating complex (15) rearranges to form the novel complex (16), in which a five membered carbon ring has been formed by cyclisation of the carbon chain with a nitrile carbon.[96]

3.4 Conclusions

It is clear from this study that reaction of different alkynes R'C≡CR" with the η^2vinyl structure (1) and its isomer (2) can create a large number of products, dependant on the nature of the metal atom, the alkylidene groups and

the thiolato substituent R.

Complexes containing η^2-vinyl species appear to play an important part in these processes and the thiolate group also appears crucial because of its ability not only to bond to the alkyne ligands but also to stabilise 16-electron structures, as in complex (10).

The reactions appear to proceed initially by metalla-cyclisation of one of the co-ordinated alkyne ligands and the incoming ligand. The incoming ligand seems always to be preferred to the other co-ordinated alkyne ligand. On addition of dmad this intermediate has been detected by N.M.R. and I.R. spectroscopy by Dr.J.L. Davidson, i.e. complex (13), but not as yet when using alkynes of the form R'C≡CMe for which complex (5) is the first intermediate detected. However it is likely that complex (5) is formed with attack by R'C≡CMe at the M=C bond in (1) with resultant cleavage of the S-C bond and formation of a metallacycle similar to (13). Then immediate attachment of the thiolate group to the new ligand side of the metallacycle forms complex (5).

The products obtained by heating intermediates (5) and (13) also depend on the factors mentioned above. In complex (5) the η^2-vinyl ligand can isomerise to give the η^4-butadienyl ligand of complex (6) and cleavage of the M-S bond. Alternatively the η^2-alkyne can insert into the M=C bond to produce an oligomer comprising three alkyne units, with cleavage of the S-C(oligomer) bond giving complex (7). X-ray diffraction analysis has shown that when M = W, R = Pr^i and R' = Me structure (6) is produced[100] and when M = W, R = Pr^i and R' = Ph it is structure (7) that is formed

suggesting that substituent R' has an effect on what products are formed. Similarly spectroscopic data [102] suggest molybdenum complexes are more likely to form complex (6) than (7) compared with tungsten complexes.

When dmad was the incoming ligand used it is clear that there is selective thiolate migration onto either the hfb or dmad metal coordinated carbon of the metallacycle of complex (13) depending on whether the metal centre was a tungsten or molybdenum atom. This means that the product of further insertion of an alkyne into the carbon chain is selective. When M = Mo the sequence of substituents on the carbon chain is $CF_3CF_3CF_3CF_3CO_2MeCO_2MeSR$ and when M = W the sequence is $CF_3CF_3CO_2MeCO_2MeCF_3CF_3SR$ as can be seen in structures (11) and (12), and (8), (9) and (10) respectively.

Altering the thiolato substituent, R, of the starting complex also appears to have an effect on the final product, e.g. with M = W and dmad the incoming ligand, when R is the aryl group, C_6H_5, complex (10) has been formed where the thiolate group is attached only to the metal centre, whereas when the thiolate substituent is the alkyl group, Pr^i, complexes (8) and (9) have been isolated where the sulphur atom is attached to the oligomer as well as the metal atom.

It can be seen that formation of both *cis* and *trans* oligomers is possible. While the first insertion always occurs with *cis* geometry, because of the metallacyclopentadiene intermediate, the final product can keep this *cis* orientation, as in complex (8),[100] or it can change to include a *trans* bond as in complexes (7), (10), (11) and

(12) (see Table 3.1). The ability to change orientation is probably due to the formation of η^4-butadiene or η^2-vinyl intermediates whereas an η^1-bonding mode would lead to an all *cis* structure.

It is also possible for cyclisation reactions to occur if ligands other than alkynes are added to complexes (1) and (2). An example of this is the reaction pathway (14)→(15)→(16) in Scheme III where on addition of two R'NC ligands a five membered ring was formed consisting of the two alkyne ligands and a carbon atom from one of the isonitriles.[112] A cyclobutadienyl ring can also be formed, as in complex (18), by cyclisation of the two alkyne ligands after addition of PR'_3 to complex (1). This reaction proceeds via intermediates (14) and (17). A similar cyclobutadienyl complex (19) is described in Chapter 4.

From this work there are at least two important generalisations which can be made. First, it is clear that polymerisation of alkynes by transition metals can involve many different intermediates. Secondly, although the initial step in the oligomerisation reactions discussed here is formation of a metallacyclopentadiene with mutually *cis* double bonds, the final polyene obtained may either retain this configuration if only M-C scission occurs, or it may have a *trans* arrangement of double bonds if further steps involve coordination of several chain atoms to the metal e.g. as η^2-vinyl or η^4-butadienyl units.

Table 3.1. A comparison of the geometries of the $[CpM(SR)(hfb)_2(L\text{-}L)]$ structures (distances in Å, angles in °).

Complex		(5)	(7)	(10)	(11)		(12)	(15)
M		Mo	W	W	Mo		Mo	W
R		Pr^i	Pr^i	MeC_6H_4	Pr^i		Pr^i	MeC_6H_4
L-L		PhC_2Me	PhC_2Me	dmad	dmad		dmad	$(TolNC)_2$
M-C(Cp)	min	2.342(6)	2.333(5)	2.32(2)	2.310(8)		2.314(8)	2.255(7)
	max	2.410(7)	2.356(5)	2.37(3)	2.378(7)		2.367(7)	2.360(6)
C-C(Cp)	min	1.381(10)	1.396(6)	1.34(3)	1.389(14)		1.383(11)	1.397(9)
	max	1.423(9)	1.419(6)	1.47(3)	1.434(12)		1.416(12)	1.417(9)
C-F	min	1.25(1)	1.294(5)	1.25(4)	1.269(14)		1.273(9)	1.322(9)
	max	1.35(1)	1.341(5)	1.38(4)	1.358(10)		1.345(9)	1.351(9)
M-S		2.468(2)	2.374(1)	2.318(6)	2.400(2)	2.405(2)	-	2.561(2)
S-R		1.866(6)	1.840(4)	1.78(2)	1.833(7)	1.846(7)	1.839(8)	1.839(6)
S-C(chain)		1.798(6)	-	-	1.784(7)	1.789(6)	1.819(7)	-
M-C_a		1.915(5)	2.017(3)	2.24(2)	1.915(8)	1.921(6)	1.918(7)	2.207(6)
M-C_b		2.239(5)	2.489(3)	[2.79(2)]	2.179(8)	2.176(7)	2.195(7)	-
M-C_c		[3.216(5)]	2.351(4)	2.21(2)	2.273(8)	2.273(8)	2.266(7)	-
M-C_d		[3.343(5)]	2.195(4)	2.29(2)	[3.192(8)	3.177(8)]	[3.187(7)]	2.213(6)
M-C_e		{2.133(6)}	[2.766(4)]	[2.67(2)]	[3.169(8)	3.162(8)]	[3.203(7)]	-
M-C_f		{2.156(6)}	2.242(4)	2.12(2)	2.267(6)	2.282(7)	2.249(7)	-
C_a-C_b		1.426(7)	1.400(5)	1.35(3)	1.411(11)	1.410(11)	1.410(10)	1.354(8)
C_b-C_c		1.514(7)	1.404(5)	1.50(3)	1.449(10)	1.434(9)	1.431(9)	1.472(8)
C_c-C_d		1.338(7)	1.475(5)	1.44(3)	1.533(10)	1.510(11)	1.517(10)	1.359(8)
C_d-C_e		-	1.509(5)	1.47(2)	1.316(10)	1.320(10)	1.316(9)	-
C_e-C_f		1.267(8)	1.321(5)	1.34(3)	1.489(11)	1.477(10)	1.503(10)	-
C_a-C_b-C_c-C_d		-62.5(6)	-22.4(3)	66(2)	152.0(9)	151.2(9)	152.9(8)	7.7(5)
C_b-C_c-C_d-C_e		-	149.0(5)	-166(2)	-78.9(8)	-79.0(8)	-70.7(7)	-
C_c-C_d-C_e-C_f		-	-64.3(4)	51(2)	1.4(6)	2.4(6)	-3.9(6)	-

C_a - C_f are the carbon atoms of the oligomer chain, and C_a is the end carbon atom of the chain not attached to the sulphur atom (when applicable).
[] signify the distance is non-bonding.
{} signify the carbon atoms are not part of the oligomer.

Table 3.2. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (5).

	X/A	Y/B	Z/C	U
MO(1)	.05682(5)	-.35608(2)	.30362(2)	.034
S(1)	.18982(15)	-.23586(7)	.37348(5)	.039
F(1)	.0548(9)	-.3790(3)	.1168(2)	.142
F(2)	.0571(7)	-.5099(3)	.1599(2)	.118
F(3)	.2711(7)	-.4511(5)	.1451(2)	.171
F(4)	.4581(5)	-.2291(4)	.2691(3)	.131
F(5)	.2760(7)	-.1484(3)	.2317(3)	.147
F(6)	.3720(10)	-.2404(5)	.1766(3)	.209
F(7)	-.1012(4)	-.5212(2)	.4120(2)	.082
F(8)	.1355(5)	-.5433(3)	.4513(2)	.086
F(9)	.0402(5)	-.6187(2)	.3709(2)	.089
F(10)	.2297(4)	-.5569(2)	.2701(2)	.065
F(11)	.3912(4)	-.5917(2)	.3491(2)	.071
F(12)	.4539(4)	-.4866(2)	.2861(2)	.068
C(1)	-.1927(7)	-.3321(4)	.3349(3)	.059
C(2)	-.1653(7)	-.2526(4)	.2996(3)	.059
C(3)	-.1579(7)	-.2797(4)	.2400(3)	.061
C(4)	-.1819(8)	-.3785(4)	.2369(3)	.062
C(5)	-.2049(7)	-.4110(4)	.2945(3)	.062
C(6)	.0744(7)	-.2064(3)	.4373(3)	.056
C(7)	.0586(9)	-.2870(4)	.4813(3)	.074
C(8)	.1366(9)	-.1165(4)	.4688(3)	.072
C(9)	.1346(10)	-.4285(5)	.1608(3)	.084
C(10)	.1497(7)	-.3781(3)	.2196(2)	.051
C(11)	.2193(6)	-.3055(3)	.2437(2)	.046
C(12)	.3320(8)	-.2348(4)	.2287(3)	.067
C(13)	.0426(6)	-.5350(3)	.3978(3)	.049
C(14)	.1011(6)	-.4585(3)	.3601(2)	.039
C(15)	.2602(6)	-.4418(3)	.3490(2)	.038
C(16)	.3340(7)	-.5180(3)	.3145(3)	.049
C(17)	.3784(6)	-.3905(3)	.3947(2)	.039
C(18)	.5227(7)	-.4424(4)	.4226(3)	.053
C(19)	.3570(6)	-.3005(3)	.4108(2)	.043
C(20)	.4658(7)	-.2428(3)	.4543(2)	.048
C(21)	.5375(8)	-.1628(4)	.4339(3)	.062
C(22)	.6388(9)	-.1081(4)	.4732(3)	.078
C(23)	.6672(10)	-.1331(5)	.5337(4)	.092
C(24)	.5967(10)	-.2116(5)	.5548(3)	.081
C(25)	.4955(8)	-.2664(4)	.5158(3)	.064
H(1)	-.20187	-.33293	.37780	.035
H(2)	-.15372	-.18878	.31454	.045
H(3)	-.13982	-.23823	.20718	.042
H(4)	-.18203	-.41675	.20099	.050
H(5)	-.22476	-.47538	.30521	.039
H(6)	-.03079	-.18930	.41955	.089
H(7A)	-.01315	-.26940	.50951	.120
H(7B)	.16128	-.29980	.50326	.120
H(7C)	.02002	-.34311	.45973	.120
H(8A)	.15001	-.06869	.43897	.118
H(8B)	.23697	-.12905	.49262	.118
H(8C)	.06479	-.09201	.49505	.118
H(18A)	.58488	-.45999	.39108	.046
H(18B)	.49242	-.49828	.44293	.046
H(18C)	.58537	-.40274	.45168	.046
H(21)	.51530	-.14530	.39166	.073
H(22)	.68870	-.05321	.45854	.094
H(23)	.73614	-.09459	.56143	.106
H(24)	.61887	-.22862	.59716	.104
H(25)	.44619	-.32145	.53054	.093

Table 3.2(cont).

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
MO(1)	.0305(2)	.0317(2)	.0407(2)	-.0036(2)	.0051(1)	.0028(2)
S(1)	.0443(7)	.0308(4)	.0413(7)	-.0031(4)	.0054(5)	.0019(4)
F(1)	.230(7)	.145(4)	.045(2)	-.001(4)	-.013(3)	.002(2)
F(2)	.169(5)	.098(3)	.081(3)	-.028(3)	-.009(3)	-.035(2)
F(3)	.138(5)	.262(7)	.115(4)	.002(5)	.052(4)	-.106(4)
F(4)	.062(3)	.171(4)	.155(5)	-.048(3)	-.012(3)	.050(4)
F(5)	.125(4)	.076(3)	.239(6)	-.024(3)	.036(4)	.068(3)
F(6)	.285(9)	.227(6)	.126(4)	-.172(6)	.134(5)	-.048(4)
F(7)	.064(2)	.079(2)	.107(3)	-.001(2)	.045(2)	.033(2)
F(8)	.081(3)	.099(2)	.074(2)	-.021(2)	.003(2)	.039(2)
F(9)	.112(3)	.039(1)	.119(3)	-.019(2)	.052(3)	-.002(2)
F(10)	.062(2)	.051(2)	.079(2)	.001(1)	.006(2)	-.025(1)
F(11)	.071(2)	.044(1)	.095(3)	.021(1)	.008(2)	.001(1)
F(12)	.049(2)	.079(2)	.077(2)	.002(2)	.030(2)	-.011(2)
C(1)	.034(3)	.061(3)	.082(4)	.008(2)	.019(3)	.007(3)
C(2)	.040(3)	.046(3)	.089(5)	.007(2)	.006(3)	.006(3)
C(3)	.039(3)	.065(3)	.075(4)	.001(3)	-.009(3)	.018(3)
C(4)	.046(4)	.068(4)	.067(4)	-.004(3)	-.014(3)	-.003(3)
C(5)	.037(3)	.048(3)	.099(5)	-.008(2)	.000(3)	.008(3)
C(6)	.066(4)	.044(2)	.057(4)	.001(2)	.023(3)	-.005(2)
C(7)	.099(6)	.060(3)	.066(4)	-.001(3)	.040(4)	.003(3)
C(8)	.105(6)	.045(3)	.066(4)	.005(3)	.016(4)	-.011(2)
C(9)	.095(6)	.102(5)	.053(4)	-.003(4)	.010(4)	-.008(3)
C(10)	.054(4)	.057(3)	.041(3)	-.004(2)	.008(3)	0.000(2)
C(11)	.042(3)	.051(3)	.046(3)	-.003(2)	.012(3)	.006(2)
C(12)	.064(4)	.078(4)	.059(4)	-.016(3)	.019(3)	.018(3)
C(13)	.041(3)	.043(2)	.064(3)	-.004(2)	.013(3)	.009(2)
C(14)	.040(3)	.034(2)	.044(3)	-.004(2)	.009(2)	0.000(2)
C(15)	.036(3)	.031(2)	.047(3)	.001(2)	.007(2)	.002(2)
C(16)	.043(3)	.045(2)	.060(3)	.002(2)	.012(3)	-.006(2)
C(17)	.036(3)	.041(2)	.040(3)	-.004(2)	.009(2)	.006(2)
C(18)	.041(3)	.055(3)	.060(4)	.005(2)	-.002(3)	.005(2)
C(19)	.046(3)	.040(2)	.042(3)	-.009(2)	-.001(2)	.007(2)
C(20)	.051(4)	.044(2)	.047(3)	-.008(2)	-.005(3)	.001(2)
C(21)	.066(4)	.060(3)	.057(4)	-.017(3)	-.002(3)	.004(2)
C(22)	.085(6)	.064(3)	.080(5)	-.034(4)	-.010(4)	.001(3)
C(23)	.098(6)	.081(4)	.090(5)	-.036(4)	-.032(5)	-.006(4)
C(24)	.094(6)	.088(4)	.054(4)	-.015(4)	-.027(4)	.005(3)
C(25)	.081(5)	.052(3)	.055(4)	-.013(3)	-.008(3)	.008(2)

Table 3.3. Selected bond distances (Å) and angles (°) of complex (5)

MO(1) - S(1)	2.468(2)	MO(1) - C(1)	2.342(6)
MO(1) - C(2)	2.382(6)	MO(1) - C(3)	2.410(7)
MO(1) - C(4)	2.370(7)	MO(1) - C(5)	2.342(6)
MO(1) - C(10)	2.133(6)	MO(1) - C(11)	2.156(6)
MO(1) - C(14)	1.915(5)	MO(1) - C(15)	2.239(5)
S(1) - C(6)	1.866(6)	S(1) - C(19)	1.798(6)
F(1) - C(9)	1.320(9)	F(2) - C(9)	1.324(9)
F(3) - C(9)	1.294(11)	F(4) - C(12)	1.305(9)
F(5) - C(12)	1.315(8)	F(6) - C(12)	1.246(9)
F(7) - C(13)	1.317(7)	F(8) - C(13)	1.339(7)
F(9) - C(13)	1.320(6)	F(10) - C(16)	1.350(7)
F(11) - C(16)	1.345(6)	F(12) - C(16)	1.341(7)
C(1) - C(2)	1.405(8)	C(1) - C(5)	1.423(9)
C(2) - C(3)	1.381(10)	C(3) - C(4)	1.410(8)
C(4) - C(5)	1.390(10)	C(6) - C(7)	1.515(8)
C(6) - C(8)	1.510(8)	C(9) - C(10)	1.472(9)
C(10) - C(11)	1.267(8)	C(11) - C(12)	1.451(9)
C(13) - C(14)	1.489(7)	C(14) - C(15)	1.426(7)
C(15) - C(16)	1.502(7)	C(15) - C(17)	1.514(7)
C(17) - C(18)	1.493(8)	C(17) - C(19)	1.338(7)
C(19) - C(20)	1.488(7)	C(20) - C(21)	1.388(8)
C(20) - C(25)	1.390(8)	C(21) - C(22)	1.378(10)
C(22) - C(23)	1.374(11)	C(23) - C(24)	1.371(11)
C(24) - C(25)	1.374(10)		

S(1) - MO(1) - C(10)	116.9(2)	S(1) - MO(1) - C(11)	82.9(2)
S(1) - MO(1) - C(14)	94.4(2)	S(1) - MO(1) - C(15)	80.0(2)
C(10) - MO(1) - C(11)	34.4(2)	C(10) - MO(1) - C(14)	113.1(2)
C(10) - MO(1) - C(15)	87.6(2)	C(11) - MO(1) - C(14)	124.2(3)
C(11) - MO(1) - C(15)	86.2(2)	C(14) - MO(1) - C(15)	39.2(2)
MO(1) - S(1) - C(6)	112.5(2)	MO(1) - S(1) - C(19)	102.0(2)
C(6) - S(1) - C(19)	103.3(3)	C(2) - C(1) - C(5)	106.3(6)
C(1) - C(2) - C(3)	109.8(5)	C(2) - C(3) - C(4)	107.2(6)
C(3) - C(4) - C(5)	108.6(6)	C(1) - C(5) - C(4)	108.0(5)
S(1) - C(6) - C(7)	114.6(4)	S(1) - C(6) - C(8)	110.4(5)
C(7) - C(6) - C(8)	113.0(5)	F(1) - C(9) - F(2)	104.4(7)
F(1) - C(9) - F(3)	109.2(7)	F(1) - C(9) - C(10)	111.5(6)
F(2) - C(9) - F(3)	104.1(7)	F(2) - C(9) - C(10)	114.9(6)
F(3) - C(9) - C(10)	112.2(7)	MO(1) - C(10) - C(9)	147.0(5)
MO(1) - C(10) - C(11)	73.8(4)	C(9) - C(10) - C(11)	138.2(6)
MO(1) - C(11) - C(10)	71.8(4)	MO(1) - C(11) - C(12)	149.7(4)
C(10) - C(11) - C(12)	138.3(6)	F(4) - C(12) - F(5)	100.4(6)
F(4) - C(12) - F(6)	109.6(7)	F(4) - C(12) - C(11)	113.3(6)
F(5) - C(12) - F(6)	104.4(6)	F(5) - C(12) - C(11)	111.8(6)
F(6) - C(12) - C(11)	115.9(6)	F(7) - C(13) - F(8)	105.2(5)
F(7) - C(13) - F(9)	106.2(5)	F(7) - C(13) - C(14)	114.5(5)
F(8) - C(13) - F(9)	107.0(4)	F(8) - C(13) - C(14)	110.8(5)
F(9) - C(13) - C(14)	112.6(5)	MO(1) - C(14) - C(13)	149.4(4)
MO(1) - C(14) - C(15)	82.8(3)	C(13) - C(14) - C(15)	127.6(5)
MO(1) - C(15) - C(14)	58.0(3)	MO(1) - C(15) - C(16)	120.6(4)
MO(1) - C(15) - C(17)	116.6(3)	C(14) - C(15) - C(16)	116.0(4)
C(14) - C(15) - C(17)	121.8(5)	C(16) - C(15) - C(17)	113.3(5)
F(10) - C(16) - F(11)	104.6(4)	F(10) - C(16) - F(12)	105.3(5)
F(10) - C(16) - C(15)	112.4(5)	F(11) - C(16) - F(12)	106.3(5)
F(11) - C(16) - C(15)	114.2(5)	F(12) - C(16) - C(15)	113.3(4)
C(15) - C(17) - C(18)	118.7(4)	C(15) - C(17) - C(19)	122.0(5)
C(18) - C(17) - C(19)	119.3(5)	S(1) - C(19) - C(17)	119.2(4)
S(1) - C(19) - C(20)	114.0(4)	C(17) - C(19) - C(20)	126.6(5)
C(19) - C(20) - C(21)	119.9(5)	C(19) - C(20) - C(25)	121.3(5)
C(21) - C(20) - C(25)	118.8(5)	C(20) - C(21) - C(22)	121.1(6)
C(21) - C(22) - C(23)	119.1(7)	C(22) - C(23) - C(24)	120.6(7)
C(23) - C(24) - C(25)	120.5(7)	C(20) - C(25) - C(24)	119.9(6)

Table 3.4. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (7).

	X/A	Y/B	Z/C	U
W(1)	.07416(1)	.14326(1)	.23673(1)	.028
S(1)	.32053(10)	.20816(4)	.23689(6)	.040
F(1)	.3315(4)	.1448(1)	.0481(2)	.090
F(2)	.2954(4)	.0436(1)	.0128(2)	.083
F(3)	.4922(3)	.0696(2)	.0984(2)	.105
F(4)	.0849(4)	-.0691(1)	.0898(2)	.099
F(5)	.3423(4)	-.0640(1)	.1196(2)	.087
F(6)	.1724(4)	-.1010(1)	.2114(2)	.095
F(7)	-.1464(3)	-.0328(1)	.2303(2)	.079
F(8)	-.0151(4)	-.0590(1)	.3449(2)	.084
F(9)	-.1760(3)	.0258(1)	.3434(2)	.072
F(10)	.3773(3)	.0081(2)	.4218(2)	.090
F(11)	.4824(3)	.0810(2)	.3433(2)	.101
F(12)	.4048(4)	-.0122(2)	.2923(2)	.120
C(1)	-.0417(6)	.1496(2)	.0982(3)	.059
C(2)	-.0103(6)	.2150(2)	.1268(3)	.055
C(3)	-.1107(5)	.2280(2)	.1973(2)	.049
C(4)	-.2058(4)	.1697(2)	.2144(3)	.055
C(5)	-.1603(5)	.1211(3)	.1529(3)	.060
C(6)	.2724(5)	.2960(2)	.2640(2)	.043
C(7)	.2483(7)	.3056(3)	.3586(3)	.064
C(8)	.4087(9)	.3390(3)	.2292(6)	.096
C(9)	.3361(5)	.0821(2)	.0795(2)	.057
C(10)	.2225(4)	.0735(2)	.1545(2)	.041
C(11)	.1675(4)	.0158(2)	.1852(2)	.040
C(12)	.1908(6)	-.0547(2)	.1520(3)	.061
C(13)	.0789(4)	.0354(2)	.2662(2)	.036
C(14)	-.0641(5)	-.0066(2)	.2970(3)	.052
C(15)	.1923(4)	.0642(2)	.3309(2)	.035
C(16)	.3662(5)	.0363(2)	.3446(2)	.050
C(17)	.1344(4)	.1130(2)	.3884(2)	.034
C(18)	.2268(6)	.1361(3)	.4659(3)	.056
C(19)	-.0065(4)	.1469(2)	.3586(2)	.033
C(20)	-.1320(4)	.1761(2)	.4171(2)	.035
C(21)	-.1906(5)	.1376(2)	.4842(3)	.048
C(22)	-.3077(5)	.1629(2)	.5394(3)	.054
C(23)	-.3676(4)	.2270(2)	.5293(2)	.047
C(24)	-.3092(4)	.2663(2)	.4649(2)	.047
C(25)	-.1927(5)	.2414(2)	.4089(2)	.045
H(1)	.011(6)	.125(2)	.049(3)	.08(2)
H(2)	.061(6)	.247(3)	.106(3)	.09(2)
H(3)	-.097(5)	.270(2)	.230(3)	.07(1)
H(4)	-.292(6)	.160(3)	.260(3)	.09(2)
H(5)	-.198(5)	.081(2)	.151(2)	.04(1)
H(6)	.175(5)	.308(2)	.239(2)	.05(1)
H(7A)	.222(6)	.351(2)	.373(3)	.08(2)
H(7B)	.359(6)	.296(3)	.385(3)	.08(2)
H(7C)	.157(6)	.272(2)	.388(3)	.08(1)
H(8A)	.498(5)	.328(2)	.241(3)	.04(1)
H(8B)	.428(7)	.399(4)	.247(3)	.14(2)
H(8C)	.422(8)	.342(3)	.158(4)	.11(2)
H(18A)	.319(7)	.152(3)	.459(3)	.08(2)
H(18B)	.268(6)	.103(3)	.504(3)	.08(2)
H(18C)	.158(7)	.167(3)	.486(4)	.11(2)
H(21)	-.151(5)	.091(2)	.492(2)	.06(1)
H(22)	-.354(5)	.133(2)	.586(3)	.05(1)
H(23)	-.443(5)	.246(2)	.562(3)	.06(1)
H(24)	-.352(4)	.316(2)	.461(2)	.04(1)
H(25)	-.140(5)	.273(2)	.370(2)	.06(1)

Table 3.4(cont).

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
W(1)	.0280(1)	.0277(1)	.0278(1)	-.0001(1)	-.0001(0)	.0003(1)
S(1)	.0354(4)	.0336(4)	.0509(4)	-.0040(3)	.0095(3)	-.0044(3)
F(1)	.139(3)	.075(2)	.055(1)	-.020(2)	.046(2)	-.001(1)
F(2)	.108(2)	.092(2)	.049(1)	-.009(2)	.023(1)	-.029(1)
F(3)	.046(1)	.178(3)	.091(2)	-.006(2)	.022(1)	-.003(2)
F(4)	.118(2)	.081(2)	.097(2)	-.010(2)	-.017(2)	-.055(2)
F(5)	.093(2)	.061(2)	.108(2)	.022(2)	.027(2)	-.029(2)
F(6)	.145(3)	.034(1)	.105(2)	.004(2)	.030(2)	-.006(1)
F(7)	.075(2)	.072(2)	.089(2)	-.039(1)	.001(1)	-.020(1)
F(8)	.092(2)	.053(1)	.108(2)	-.009(1)	.015(2)	.031(1)
F(9)	.058(1)	.058(1)	.098(2)	-.019(1)	.034(1)	-.010(1)
F(10)	.088(2)	.098(2)	.082(2)	.037(2)	-.017(2)	.031(2)
F(11)	.034(1)	.090(2)	.179(3)	.003(1)	-.010(2)	.036(2)
F(12)	.109(2)	.141(3)	.110(2)	.094(2)	-.049(2)	-.072(2)
C(1)	.064(2)	.075(3)	.040(2)	.012(2)	-.016(2)	-.003(2)
C(2)	.063(2)	.059(2)	.043(2)	.007(2)	-.008(2)	.016(2)
C(3)	.053(2)	.047(2)	.046(2)	.013(2)	-.011(2)	.005(2)
C(4)	.034(2)	.068(3)	.063(3)	.005(2)	-.011(2)	.010(2)
C(5)	.052(2)	.057(2)	.070(3)	-.003(2)	-.026(2)	-.003(2)
C(6)	.045(2)	.032(2)	.053(2)	-.006(1)	.006(2)	-.003(1)
C(7)	.079(3)	.050(2)	.064(3)	.000(2)	.007(2)	-.016(2)
C(8)	.088(4)	.044(3)	.156(6)	-.018(3)	.072(4)	-.011(3)
C(9)	.063(2)	.061(3)	.046(2)	-.006(2)	.014(2)	-.011(2)
C(10)	.042(2)	.049(2)	.032(1)	.001(2)	.004(1)	-.009(1)
C(11)	.040(2)	.036(2)	.045(2)	.002(1)	0.000(1)	-.011(1)
C(12)	.075(3)	.040(2)	.068(3)	.003(2)	.006(2)	-.018(2)
C(13)	.034(1)	.033(2)	.042(2)	-.004(1)	.004(1)	-.003(1)
C(14)	.054(2)	.036(2)	.066(2)	-.009(2)	.008(2)	-.001(2)
C(15)	.036(1)	.032(1)	.037(2)	.005(1)	.003(1)	.002(1)
C(16)	.048(2)	.046(2)	.055(2)	.017(2)	-.005(2)	-.002(2)
C(17)	.035(1)	.035(2)	.032(1)	.001(1)	.003(1)	.003(1)
C(18)	.053(2)	.067(3)	.048(2)	.014(2)	-.012(2)	-.017(2)
C(19)	.034(1)	.031(1)	.034(1)	0.000(1)	.003(1)	.000(1)
C(20)	.033(1)	.037(2)	.036(2)	.003(1)	.004(1)	-.002(1)
C(21)	.054(2)	.039(2)	.051(2)	.007(2)	.017(2)	.005(2)
C(22)	.060(2)	.051(2)	.053(2)	.001(2)	.025(2)	.003(2)
C(23)	.035(2)	.055(2)	.052(2)	.000(2)	.012(1)	-.010(2)
C(24)	.047(2)	.043(2)	.053(2)	.010(2)	.005(2)	-.006(2)
C(25)	.046(2)	.041(2)	.047(2)	.004(2)	.010(2)	.005(1)

Table 3.5. Selected bond distances (Å) and angles (°) of complex (7).

W(1)	S(1)	2.374(1)	W(1)	C(1)	2.356(5)
W(1)	C(2)	2.333(5)	W(1)	C(3)	2.335(4)
W(1)	C(4)	2.348(4)	W(1)	C(5)	2.339(5)
W(1)	C(10)	2.242(4)	W(1)	C(13)	2.195(4)
W(1)	C(15)	2.351(4)	W(1)	C(17)	2.489(3)
W(1)	C(19)	2.017(3)	S(1)	C(6)	1.840(4)
F(1)	C(9)	1.341(5)	F(2)	C(9)	1.335(5)
F(3)	C(9)	1.318(5)	F(4)	C(12)	1.322(6)
F(5)	C(12)	1.341(6)	F(6)	C(12)	1.316(5)
F(7)	C(14)	1.339(5)	F(8)	C(14)	1.340(5)
F(9)	C(14)	1.330(5)	F(10)	C(16)	1.332(5)
F(11)	C(16)	1.294(5)	F(12)	C(16)	1.303(6)
C(1)	C(2)	1.400(7)	C(1)	C(5)	1.408(7)
C(2)	C(3)	1.396(6)	C(3)	C(4)	1.419(6)
C(4)	C(5)	1.413(7)	C(6)	C(7)	1.503(7)
C(6)	C(8)	1.500(8)	C(9)	C(10)	1.503(6)
C(10)	C(11)	1.322(5)	C(11)	C(12)	1.509(6)
C(11)	C(13)	1.509(5)	C(13)	C(14)	1.508(5)
C(13)	C(15)	1.476(5)	C(15)	C(16)	1.526(5)
C(15)	C(17)	1.404(5)	C(17)	C(18)	1.491(6)
C(17)	C(19)	1.401(5)	C(19)	C(20)	1.488(5)
C(20)	C(21)	1.384(5)	C(20)	C(25)	1.394(5)
C(21)	C(22)	1.379(6)	C(22)	C(23)	1.372(6)
C(23)	C(24)	1.361(6)	C(24)	C(25)	1.381(6)

S(1)	W(1)	C(10)	83.4(1)	S(1)	W(1)	C(13)	121.2(1)
S(1)	W(1)	C(15)	91.4(1)	S(1)	W(1)	C(17)	88.3(1)
S(1)	W(1)	C(19)	104.8(1)	C(10)	W(1)	C(13)	60.4(2)
C(10)	W(1)	C(15)	74.2(2)	C(10)	W(1)	C(17)	107.0(2)
C(10)	W(1)	C(19)	137.7(2)	C(13)	W(1)	C(15)	37.7(2)
C(13)	W(1)	C(17)	63.9(2)	C(13)	W(1)	C(19)	80.9(2)
C(15)	W(1)	C(17)	33.6(2)	C(15)	W(1)	C(19)	64.3(2)
C(17)	W(1)	C(19)	34.2(2)	W(1)	S(1)	C(6)	109.8(2)
C(2)	C(1)	C(5)	107.7(4)	C(1)	C(2)	C(3)	108.6(4)
C(2)	C(3)	C(4)	108.4(4)	C(3)	C(4)	C(5)	106.8(4)
C(1)	C(5)	C(4)	108.5(5)	S(1)	C(6)	C(7)	112.0(3)
S(1)	C(6)	C(8)	107.6(4)	C(7)	C(6)	C(8)	112.6(5)
F(1)	C(9)	F(2)	104.0(4)	F(1)	C(9)	F(3)	106.5(4)
F(1)	C(9)	C(10)	112.1(4)	F(2)	C(9)	F(3)	107.3(4)
F(2)	C(9)	C(10)	113.2(4)	F(3)	C(9)	C(10)	113.2(4)
W(1)	C(10)	C(9)	135.0(3)	W(1)	C(10)	C(11)	98.5(3)
C(9)	C(10)	C(11)	126.1(4)	C(10)	C(11)	C(12)	129.9(4)
C(10)	C(11)	C(13)	104.0(3)	C(12)	C(11)	C(13)	126.1(4)
F(4)	C(12)	F(5)	106.4(4)	F(4)	C(12)	F(6)	107.0(4)
F(4)	C(12)	C(11)	111.8(4)	F(5)	C(12)	F(6)	106.1(4)
F(5)	C(12)	C(11)	111.9(4)	F(6)	C(12)	C(11)	113.2(4)
W(1)	C(13)	C(11)	94.8(3)	W(1)	C(13)	C(14)	126.6(3)
W(1)	C(13)	C(15)	76.9(2)	C(11)	C(13)	C(14)	119.6(3)
C(11)	C(13)	C(15)	112.2(3)	C(14)	C(13)	C(15)	118.1(3)
F(7)	C(14)	F(8)	106.0(4)	F(7)	C(14)	F(9)	106.0(4)
F(7)	C(14)	C(13)	110.2(4)	F(8)	C(14)	F(9)	105.9(4)
F(8)	C(14)	C(13)	112.6(4)	F(9)	C(14)	C(13)	115.5(4)
W(1)	C(15)	C(13)	65.4(2)	W(1)	C(15)	C(16)	134.6(3)
W(1)	C(15)	C(17)	78.6(2)	C(13)	C(15)	C(16)	121.5(3)
C(13)	C(15)	C(17)	119.9(3)	C(16)	C(15)	C(17)	118.1(3)
F(10)	C(16)	F(11)	105.0(4)	F(10)	C(16)	F(12)	103.9(4)
F(10)	C(16)	C(15)	109.7(3)	F(11)	C(16)	F(12)	108.8(4)
F(11)	C(16)	C(15)	114.6(4)	F(12)	C(16)	C(15)	113.9(4)
W(1)	C(17)	C(15)	67.8(2)	W(1)	C(17)	C(18)	142.3(3)
W(1)	C(17)	C(19)	54.1(2)	C(15)	C(17)	C(18)	124.4(4)
C(15)	C(17)	C(19)	113.2(3)	C(18)	C(17)	C(19)	121.6(4)
W(1)	C(19)	C(17)	91.7(2)	W(1)	C(19)	C(20)	144.9(3)
C(17)	C(19)	C(20)	122.8(3)	C(19)	C(20)	C(21)	119.0(3)
C(19)	C(20)	C(25)	123.3(3)	C(21)	C(20)	C(25)	117.6(4)
C(20)	C(21)	C(22)	120.6(4)	C(21)	C(22)	C(23)	120.7(4)
C(22)	C(23)	C(24)	119.7(4)	C(23)	C(24)	C(25)	120.1(4)
C(20)	C(25)	C(24)	121.1(4)				

Table 3.6. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (10).

	X/A	Y/B	Z/C	U
W	.34260(8)	.06154(5)	.14820(4)	.036
S	.2244(7)	.1168(4)	.0569(3)	.056
F(1)	.3010(20)	-.0945(12)	-.0200(9)	.119(6)
F(2)	.5028(21)	-.1388(12)	.0107(8)	.117(6)
F(3)	.4701(18)	-.0061(11)	-.0125(8)	.104(5)
F(4)	.2801(16)	-.2498(10)	.0714(8)	.090(5)
F(5)	.4718(17)	-.2492(10)	.1298(7)	.100(5)
F(6)	.2639(16)	-.2552(10)	.1742(7)	.086(4)
F(7)	-.0423(17)	.0629(13)	.3119(8)	.111(5)
F(8)	-.1308(19)	.1156(11)	.2226(8)	.102(5)
F(9)	-.1149(16)	-.0233(9)	.2395(7)	.093(5)
F(10)	.0889(17)	.2178(10)	.2829(7)	.094(5)
F(11)	.3036(16)	.2401(10)	.2616(7)	.088(5)
F(12)	.2503(18)	.1458(11)	.3359(8)	.115(5)
O(1)	.4312(17)	-.1321(10)	.2686(7)	.069(4)
O(2)	.2128(16)	-.0806(11)	.2981(7)	.072(5)
O(3)	-.0641(16)	-.0068(10)	.1048(7)	.065(4)
O(4)	.0424(17)	-.1391(10)	.1161(7)	.067(4)
C(1)	.4081(31)	-.0691(23)	.0155(14)	.091(8)
C(2)	.3634(19)	-.0589(15)	.0856(8)	.049(4)
C(3)	.3441(34)	-.2204(15)	.1261(11)	.075(7)
C(4)	.3287(22)	-.1204(11)	.1305(8)	.041(5)
C(5)	.2448(36)	-.1071(22)	.3668(17)	.123(11)
C(6)	.3241(25)	-.0966(13)	.2569(10)	.055(6)
C(7)	.2748(19)	-.0676(15)	.1874(9)	.046(4)
C(8)	-.0603(28)	-.1774(17)	.0703(13)	.082(7)
C(9)	.0301(20)	-.0541(15)	.1246(9)	.051(5)
C(10)	.1425(20)	-.0218(11)	.1726(8)	.037(4)
C(11)	-.0568(27)	.0549(22)	.2505(13)	.084(7)
C(12)	.1013(18)	.0476(12)	.2192(9)	.039(4)
C(13)	.2173(32)	.1774(21)	.2800(15)	.088(8)
C(14)	.2133(22)	.1020(14)	.2285(11)	.043(5)
C(R1)	.5884(22)	.0452(14)	.1269(10)	.056(6)
C(R2)	.5708(28)	.0322(17)	.1944(13)	.076(8)
C(R3)	.5262(29)	.1128(18)	.2198(12)	.075(7)
C(R4)	.5160(26)	.1725(16)	.1704(11)	.072(7)
C(R5)	.5546(25)	.1275(16)	.1090(11)	.064(6)
C(T1)	.2497(21)	.2327(13)	.0585(10)	.049(5)
C(T2)	.3310(29)	.2753(14)	.0120(11)	.065(6)
C(T3)	.3575(27)	.3651(14)	.0169(10)	.062(6)
C(T4)	.3099(29)	.4100(17)	.0665(14)	.089(9)
C(T5)	.2122(28)	.3713(19)	.1128(13)	.086(8)
C(T6)	.1880(24)	.2801(15)	.1067(11)	.065(7)
C(T7)	.3315(34)	.5116(18)	.0752(13)	.102(9)
H(51)	.16681	-.09511	.39663	.148
H(52)	.32941	-.07590	.38118	.148
H(53)	.26464	-.16915	.36729	.148
H(81)	-.05025	-.23955	.06303	.098
H(82)	-.04663	-.14775	.02924	.098
H(83)	-.15690	-.16631	.08565	.098
H(R1)	.61987	-.00019	.09746	.068
H(R2)	.58989	-.01986	.21961	.092
H(R3)	.50230	.12568	.26454	.090
H(R4)	.48930	.23323	.17526	.086
H(R5)	.55348	.15270	.06588	.077
H(T2)	.37423	.24225	-.02296	.078
H(T3)	.40986	.39477	-.01717	.074
H(T5)	.16341	.40538	.14568	.103
H(T6)	.12855	.24953	.13789	.078
H(T71)	.29552	.54529	.11144	.122
H(T72)	.29050	.53868	.03694	.122
H(T73)	.43431	.52110	.07514	.122

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
W	.0356(3)	.0366(3)	.0367(4)	-.0018(5)	-.0006(5)	-.0040(5)
S	.067(3)	.044(3)	.057(4)	.000(3)	-.005(3)	.009(3)

Table 3.7. Selected bond distances (Å) and angles (°) of complex (10).

W	-	S	2.318(7)	W	-	C(2)	2.240(22)
W	-	C(7)	2.209(23)	W	-	C(10)	2.294(18)
W	-	C(14)	2.119(22)	W	-	C(R1)	2.324(21)
W	-	C(R2)	2.351(26)	W	-	C(R3)	2.370(27)
W	-	C(R4)	2.368(24)	W	-	C(R5)	2.340(24)
S	-	C(T1)	1.775(21)	F(1)	-	C(1)	1.286(34)
F(2)	-	C(1)	1.377(38)	F(3)	-	C(1)	1.253(37)
F(4)	-	C(3)	1.340(30)	F(5)	-	C(3)	1.261(35)
F(6)	-	C(3)	1.339(30)	F(7)	-	C(11)	1.265(31)
F(8)	-	C(11)	1.282(34)	F(9)	-	C(11)	1.322(35)
F(10)	-	C(13)	1.337(34)	F(11)	-	C(13)	1.297(35)
F(12)	-	C(13)	1.275(36)	O(1)	-	C(6)	1.151(28)
O(2)	-	C(5)	1.490(38)	O(2)	-	C(6)	1.351(27)
O(3)	-	C(9)	1.198(25)	O(4)	-	C(8)	1.453(30)
O(4)	-	C(9)	1.307(28)	C(1)	-	C(2)	1.497(33)
C(2)	-	C(4)	1.347(27)	C(3)	-	C(4)	1.528(29)
C(4)	-	C(7)	1.497(26)	C(6)	-	C(7)	1.552(28)
C(7)	-	C(10)	1.438(26)	C(9)	-	C(10)	1.510(26)
C(10)	-	C(12)	1.479(25)	C(11)	-	C(12)	1.598(31)
C(12)	-	C(14)	1.337(28)	C(13)	-	C(14)	1.555(38)
C(R1)	-	C(R2)	1.401(33)	C(R1)	-	C(R5)	1.339(32)
C(R2)	-	C(R3)	1.390(38)	C(R3)	-	C(R4)	1.360(36)
C(R4)	-	C(R5)	1.471(33)	C(T1)	-	C(T2)	1.373(31)
C(T1)	-	C(T6)	1.346(31)	C(T2)	-	C(T3)	1.389(30)
C(T3)	-	C(T4)	1.298(36)	C(T4)	-	C(T5)	1.433(39)
C(T4)	-	C(T7)	1.565(38)	C(T5)	-	C(T6)	1.408(37)

S	-	W	-	C(2)	82.9(5)	S	-	W	-	C(7)	118.7(5)
S	-	W	-	C(10)	89.7(5)	S	-	W	-	C(14)	104.6(6)
C(2)	-	W	-	C(7)	60.4(7)	C(2)	-	W	-	C(10)	75.1(7)
C(2)	-	W	-	C(14)	136.6(8)	C(7)	-	W	-	C(10)	37.2(7)
C(7)	-	W	-	C(14)	79.5(8)	C(10)	-	W	-	C(14)	62.5(8)
W	-	S	-	C(T1)	106.4(8)	C(5)	-	O(2)	-	C(6)	112.8(19)
C(8)	-	O(4)	-	C(9)	115.1(17)	F(1)	-	C(1)	-	F(2)	102.6(25)
F(1)	-	C(1)	-	F(3)	108.8(25)	F(1)	-	C(1)	-	C(2)	111.0(23)
F(2)	-	C(1)	-	F(3)	105.3(23)	F(2)	-	C(1)	-	C(2)	108.8(23)
F(3)	-	C(1)	-	C(2)	118.9(27)	W	-	C(2)	-	C(1)	130.8(19)
W	-	C(2)	-	C(4)	99.0(12)	C(1)	-	C(2)	-	C(4)	130.1(23)
F(4)	-	C(3)	-	F(5)	110.2(21)	F(4)	-	C(3)	-	F(6)	103.6(22)
F(4)	-	C(3)	-	C(4)	109.9(19)	F(5)	-	C(3)	-	F(6)	109.7(20)
F(5)	-	C(3)	-	C(4)	115.4(23)	F(6)	-	C(3)	-	C(4)	107.4(20)
C(2)	-	C(4)	-	C(3)	128.8(18)	C(2)	-	C(4)	-	C(7)	103.7(17)
C(3)	-	C(4)	-	C(7)	127.5(17)	O(1)	-	C(6)	-	O(2)	127.4(20)
O(1)	-	C(6)	-	C(7)	125.1(20)	O(2)	-	C(6)	-	C(7)	107.2(17)
W	-	C(7)	-	C(4)	95.7(12)	W	-	C(7)	-	C(6)	120.0(14)
W	-	C(7)	-	C(10)	74.6(12)	C(4)	-	C(7)	-	C(6)	117.4(18)
C(4)	-	C(7)	-	C(10)	112.2(15)	C(6)	-	C(7)	-	C(10)	125.3(16)
O(3)	-	C(9)	-	O(4)	127.6(19)	O(3)	-	C(9)	-	C(10)	121.5(20)
O(4)	-	C(9)	-	C(10)	110.3(17)	W	-	C(10)	-	C(7)	68.2(11)
W	-	C(10)	-	C(9)	126.3(12)	W	-	C(10)	-	C(12)	87.4(11)
C(7)	-	C(10)	-	C(9)	124.3(17)	C(7)	-	C(10)	-	C(12)	115.5(16)
C(9)	-	C(10)	-	C(12)	118.4(16)	F(7)	-	C(11)	-	F(8)	115.3(26)
F(7)	-	C(11)	-	F(9)	107.3(24)	F(7)	-	C(11)	-	C(12)	107.8(20)
F(8)	-	C(11)	-	F(9)	110.8(22)	F(8)	-	C(11)	-	C(12)	111.0(22)
F(9)	-	C(11)	-	C(12)	104.0(21)	C(10)	-	C(12)	-	C(11)	123.1(18)
C(10)	-	C(12)	-	C(14)	109.5(17)	C(11)	-	C(12)	-	C(14)	127.4(20)
F(10)	-	C(13)	-	F(11)	102.9(24)	F(10)	-	C(13)	-	F(12)	110.1(24)
F(10)	-	C(13)	-	C(14)	110.3(22)	F(11)	-	C(13)	-	F(12)	112.9(25)
F(11)	-	C(13)	-	C(14)	111.0(23)	F(12)	-	C(13)	-	C(14)	109.5(24)
W	-	C(14)	-	C(12)	98.5(14)	W	-	C(14)	-	C(13)	136.3(17)
C(12)	-	C(14)	-	C(13)	124.7(20)	C(R2)	-	C(R1)	-	C(R5)	111.9(21)
C(R1)	-	C(R2)	-	C(R3)	106.1(22)	C(R2)	-	C(R3)	-	C(R4)	109.3(23)
C(R3)	-	C(R4)	-	C(R5)	107.8(22)	C(R1)	-	C(R5)	-	C(R4)	104.9(20)
S	-	C(T1)	-	C(T2)	121.8(17)	S	-	C(T1)	-	C(T6)	119.2(17)
C(T2)	-	C(T1)	-	C(T6)	119.0(20)	C(T1)	-	C(T2)	-	C(T3)	120.6(21)
C(T2)	-	C(T3)	-	C(T4)	120.9(23)	C(T3)	-	C(T4)	-	C(T5)	120.8(25)
C(T3)	-	C(T4)	-	C(T7)	124.2(25)	C(T5)	-	C(T4)	-	C(T7)	114.3(24)
C(T4)	-	C(T5)	-	C(T6)	116.5(24)	C(T1)	-	C(T6)	-	C(T5)	121.6(22)

Table 3.8. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (11).

	X/A	Y/B	Z/C	U
MO(A)	.13982(6)	.20293(4)	.49559(4)	.041
MO(B)	.32945(6)	.29559(4)	.00411(4)	.037
S(A)	.23296(17)	.27392(11)	.55408(12)	.040
S(B)	.54513(16)	.22779(11)	-.05649(11)	.037
F(A1)	-.2602(6)	.3203(5)	.5632(5)	.145
F(A2)	-.1849(6)	.3377(8)	.4359(5)	.199
F(A3)	-.2417(6)	.2152(5)	.5236(6)	.166
F(A4)	.0340(5)	.2037(3)	.7350(3)	.070
F(A5)	-.1628(5)	.2100(4)	.7312(3)	.088
F(A6)	-.0702(5)	.3248(3)	.6430(3)	.078
F(A7)	-.0442(6)	.0507(4)	.5592(4)	.103
F(A8)	-.0761(6)	-.0102(4)	.6921(4)	.109
F(A9)	.1054(5)	-.0565(4)	.6228(6)	.149
F(A10)	.1740(7)	-.1002(4)	.7964(4)	.116
F(A11)	.0043(5)	.0100(4)	.8057(4)	.095
F(A12)	.1815(6)	.0090(4)	.8345(3)	.101
F(B1)	.1106(6)	.1751(5)	-.0652(5)	.142
F(B2)	.0854(9)	.1548(7)	.0630(5)	.196
F(B3)	-.0110(5)	.2787(5)	-.0217(6)	.168
F(B4)	.4478(4)	.3014(3)	-.2374(3)	.065
F(B5)	.2550(5)	.2936(4)	-.2339(3)	.083
F(B6)	.3752(4)	.1774(3)	-.1474(3)	.065
F(B7)	.0566(4)	.4450(4)	-.0570(4)	.085
F(B8)	.0920(5)	.5116(4)	-.1917(4)	.102
F(B9)	.1613(5)	.5540(4)	-.1160(5)	.141
F(B10)	.3477(7)	.6040(4)	-.2922(4)	.131
F(B11)	.2984(5)	.4934(4)	-.3053(3)	.086
F(B12)	.4963(6)	.4999(4)	-.3321(3)	.099
O(A1)	.4538(5)	.1134(4)	.6929(4)	.061
O(A2)	.4316(6)	-.0369(4)	.7515(4)	.085
O(A3)	.4845(5)	.1978(3)	.4499(4)	.061
O(A4)	.5138(5)	.0509(4)	.5486(4)	.067
O(B1)	.7378(5)	.3931(4)	-.1932(4)	.063
O(B2)	.6250(6)	.5428(4)	-.2466(4)	.085
O(B3)	.6248(5)	.3017(4)	.0518(4)	.064
O(B4)	.6073(5)	.4498(4)	-.0475(4)	.065
C(A1)	.2518(8)	.2599(6)	.3519(5)	.062
C(A2)	.1158(10)	.2824(6)	.3509(5)	.078
C(A3)	.0720(10)	.1957(7)	.3856(5)	.076
C(A4)	.1825(10)	.1227(6)	.4046(6)	.075
C(A5)	.2938(8)	.1585(5)	.3859(5)	.060
C(A6)	.3297(7)	.3643(5)	.4870(5)	.048
C(A7)	.4296(9)	.3537(6)	.5364(6)	.080
C(A8)	.2261(9)	.4570(5)	.4698(6)	.072
C(A9)	-.1787(10)	.2785(7)	.5133(7)	.086
C(A10)	-.0461(7)	.2357(5)	.5332(5)	.050
C(A11)	-.0049(7)	.1864(5)	.6143(5)	.050
C(A12)	-.0471(8)	.2293(5)	.6809(5)	.055
C(A13)	.0751(7)	.0921(5)	.6261(5)	.045
C(A14)	.0180(8)	.0206(6)	.6253(6)	.061
C(A15)	.1739(7)	.0537(4)	.6873(5)	.045
C(A16)	.1363(9)	-.0075(6)	.7804(6)	.069
C(A17)	.2844(7)	.0834(5)	.6574(5)	.050
C(A18)	.3969(7)	.0451(6)	.7085(5)	.056
C(A19)	.5766(8)	.0860(7)	.7219(7)	.088
C(A20)	.3093(6)	.1539(4)	.5672(4)	.038
C(A21)	.4463(7)	.1286(5)	.5205(5)	.053
C(A22)	.6116(9)	.1743(7)	.3977(7)	.087
C(B1)	.3620(8)	.2375(6)	.1479(5)	.057
C(B2)	.2459(9)	.2143(6)	.1480(5)	.064
C(B3)	.1551(8)	.2992(7)	.1173(6)	.073
C(B4)	.2090(9)	.3757(6)	.0968(5)	.070
C(B5)	.3367(8)	.3383(6)	.1164(5)	.060
C(B6)	.6663(6)	.1370(4)	.0104(4)	.040
C(B7)	.8044(7)	.1476(6)	-.0415(6)	.072
C(B8)	.6378(8)	.0444(5)	.0237(6)	.075
C(B9)	.1016(9)	.2174(7)	-.0131(7)	.077
C(B10)	.2116(6)	.2616(5)	-.0346(5)	.045
C(B11)	.2790(6)	.3146(5)	-.1151(5)	.046
C(B12)	.3407(7)	.2725(5)	-.1841(5)	.055
C(B13)	.2801(7)	.4078(4)	-.1256(5)	.044
C(B14)	.1506(8)	.4776(6)	-.1217(6)	.060
C(B15)	.3964(7)	.4485(5)	-.1851(5)	.049

Table 3.8(cont).

	X/A	Y/B	Z/C	U
C(B16)	.3833(10)	.5134(7)	-.2790(6)	.077
C(B17)	.5076(7)	.4203(5)	-.1558(5)	.045
C(B18)	.6282(8)	.4614(6)	-.2055(5)	.055
C(B19)	.8601(9)	.4253(7)	-.2232(6)	.090
C(B20)	.5188(6)	.3477(4)	-.0678(4)	.035
C(B21)	.5869(7)	.3727(6)	-.0203(5)	.050
C(B22)	.6854(10)	.3248(7)	.1003(7)	.094
H(A1)	.30569	.30472	.33266	.064
H(A2)	.06163	.34496	.32971	.078
H(A3)	-.01615	.18963	.39377	.069
H(A4)	.18237	.05654	.42757	.080
H(A5)	.38074	.12217	.39548	.063
H(A6)	.37581	.35381	.43508	.048
H(A71)	.47228	.40612	.50713	.080
H(A72)	.49479	.29584	.54238	.080
H(A73)	.38359	.35279	.59259	.080
H(A81)	.16216	.46024	.44009	.069
H(A82)	.26467	.51127	.43722	.069
H(A83)	.18242	.46099	.52474	.069
H(A191)	.61843	.13543	.71054	.087
H(A192)	.63688	.04527	.69409	.087
H(A193)	.56327	.05093	.78345	.087
H(A221)	.60371	.13934	.36755	.081
H(A222)	.67694	.13635	.43379	.081
H(A223)	.63779	.23191	.35656	.081
H(B1)	.44170	.19410	.16595	.062
H(B2)	.23390	.15154	.16557	.071
H(B3)	.06778	.30453	.11137	.077
H(B4)	.16736	.44175	.07374	.084
H(B5)	.39727	.37430	.10945	.066
H(B6)	.65456	.14610	.06294	.046
H(B71)	.87097	.09839	-.01126	.072
H(B72)	.81729	.20801	-.05157	.072
H(B73)	.81158	.14446	-.09627	.072
H(B81)	.63591	.04860	-.03248	.068
H(B82)	.55227	.04036	.05888	.068
H(B83)	.70442	-.00916	.04935	.068
H(B191)	.86316	.46159	-.19288	.082
H(B192)	.87124	.46307	-.28421	.082
H(B193)	.93228	.37095	-.21388	.082
H(B221)	.71273	.27418	.15193	.080
H(B222)	.62356	.37446	.11649	.080
H(B223)	.76146	.34805	.06295	.080

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
MO(A)	.0430(4)	.0349(3)	.0344(4)	-.0132(3)	-.0085(3)	-.0123(3)
MO(B)	.0291(4)	.0344(3)	.0334(4)	-.0041(3)	-.0039(3)	-.0122(3)
S(A)	.037(1)	.031(1)	.039(1)	-.007(1)	-.008(1)	-.015(1)
S(B)	.031(1)	.032(1)	.036(1)	-.006(1)	-.006(1)	-.015(1)
F(A1)	.064(4)	.150(6)	.185(8)	.032(4)	-.060(4)	-.111(6)
F(A2)	.068(4)	.295(12)	.096(6)	-.004(6)	-.043(4)	.048(7)
F(A3)	.081(4)	.122(5)	.259(10)	-.014(4)	-.078(5)	-.090(6)
F(A4)	.069(3)	.069(3)	.052(3)	-.007(2)	-.016(3)	-.032(2)
F(A5)	.059(3)	.101(4)	.074(4)	-.021(3)	.014(3)	-.050(3)
F(A6)	.080(3)	.059(3)	.075(3)	-.005(2)	-.008(3)	-.044(3)
F(A7)	.118(5)	.088(4)	.085(4)	-.063(4)	-.022(4)	-.030(3)
F(A8)	.099(4)	.122(5)	.078(4)	-.082(4)	.017(3)	-.034(4)
F(A9)	.069(4)	.074(4)	.266(10)	-.004(3)	-.026(5)	-.103(5)
F(A10)	.154(6)	.053(3)	.082(4)	-.026(3)	-.004(4)	.017(3)
F(A11)	.067(4)	.106(4)	.068(4)	-.041(3)	.000(3)	-.004(3)
F(A12)	.087(4)	.126(5)	.046(3)	-.032(4)	-.026(3)	.001(3)

Table 3.8(cont).

	U11	U22	U33	U12	U13	U23
F(B1)	.083(4)	.152(6)	.165(7)	-.068(4)	.017(4)	-.102(6)
F(B2)	.197(8)	.228(9)	.106(6)	-.186(8)	-.029(6)	.020(6)
F(B3)	.038(3)	.133(5)	.286(11)	-.013(3)	-.013(5)	-.123(7)
F(B4)	.063(3)	.070(3)	.042(3)	-.022(2)	.004(2)	-.027(2)
F(B5)	.073(3)	.099(4)	.057(3)	-.015(3)	-.025(3)	-.039(3)
F(B6)	.072(3)	.044(3)	.058(3)	-.009(2)	-.003(2)	-.029(2)
F(B7)	.045(3)	.085(3)	.085(4)	.014(3)	-.005(3)	-.031(3)
F(B8)	.064(3)	.119(5)	.080(4)	.027(3)	-.045(3)	-.035(4)
F(B9)	.071(4)	.073(4)	.245(9)	.011(3)	-.046(5)	-.101(5)
F(B10)	.188(7)	.036(3)	.122(6)	-.015(3)	-.089(5)	.016(3)
F(B11)	.083(4)	.092(4)	.051(3)	-.029(3)	-.034(3)	.001(3)
F(B12)	.086(4)	.122(5)	.046(3)	-.055(4)	-.007(3)	.004(3)
O(A1)	.044(3)	.063(3)	.056(3)	-.001(3)	-.018(3)	-.028(3)
O(A2)	.069(4)	.056(4)	.084(5)	.003(3)	-.037(4)	.010(4)
O(A3)	.046(3)	.045(3)	.069(4)	-.014(2)	.015(3)	-.030(3)
O(A4)	.060(4)	.045(3)	.071(4)	.008(3)	-.011(3)	-.030(3)
O(B1)	.041(3)	.072(4)	.056(4)	-.028(3)	.008(3)	-.030(3)
O(B2)	.084(5)	.056(4)	.084(5)	-.043(3)	-.018(4)	.001(4)
O(B3)	.060(4)	.044(3)	.073(4)	.002(3)	-.034(3)	-.028(3)
O(B4)	.072(4)	.042(3)	.067(4)	-.017(3)	-.012(3)	-.028(3)
C(A1)	.065(6)	.060(5)	.044(5)	-.024(4)	-.007(4)	-.019(4)
C(A2)	.102(8)	.063(6)	.046(5)	-.023(5)	-.033(5)	-.009(5)
C(A3)	.083(7)	.083(6)	.046(5)	-.038(6)	-.021(5)	-.025(5)
C(A4)	.086(7)	.067(6)	.055(6)	-.038(6)	-.002(5)	-.030(5)
C(A5)	.072(6)	.057(5)	.036(4)	-.025(4)	.004(4)	-.025(4)
C(A6)	.040(4)	.041(4)	.048(5)	-.011(3)	-.002(4)	-.020(4)
C(A7)	.084(7)	.075(6)	.059(6)	-.044(5)	-.017(5)	-.014(5)
C(A8)	.072(6)	.033(4)	.077(6)	-.008(4)	-.004(5)	-.010(4)
C(A9)	.072(7)	.070(6)	.094(8)	-.015(5)	-.037(6)	-.029(6)
C(A10)	.042(5)	.046(4)	.044(5)	-.011(3)	-.016(4)	-.012(4)
C(A11)	.044(4)	.039(4)	.053(5)	-.019(3)	-.010(4)	-.014(4)
C(A12)	.051(5)	.048(5)	.046(5)	-.005(4)	-.001(4)	-.022(4)
C(A13)	.041(4)	.036(4)	.041(4)	-.018(3)	.004(4)	-.012(4)
C(A14)	.046(5)	.057(5)	.063(6)	-.025(4)	.006(5)	-.028(5)
C(A15)	.044(5)	.026(4)	.048(5)	-.005(3)	-.006(4)	-.008(3)
C(A16)	.066(7)	.058(6)	.047(6)	-.015(5)	-.004(5)	.004(5)
C(A17)	.049(5)	.028(4)	.054(5)	-.003(3)	-.011(4)	-.012(4)
C(A18)	.036(4)	.056(5)	.050(5)	-.002(4)	-.012(4)	-.011(5)
C(A19)	.038(5)	.113(8)	.084(7)	-.011(5)	-.022(5)	-.038(6)
C(A20)	.038(4)	.029(4)	.033(4)	-.005(3)	.001(3)	-.014(3)
C(A21)	.048(5)	.043(5)	.053(5)	-.014(4)	-.005(4)	-.026(4)
C(A22)	.059(6)	.083(6)	.086(7)	-.023(5)	.029(5)	-.049(6)
C(B1)	.062(6)	.054(5)	.029(4)	.009(4)	-.010(4)	-.013(4)
C(B2)	.068(6)	.061(5)	.034(5)	-.022(5)	.005(4)	-.006(4)
C(B3)	.050(5)	.084(7)	.057(6)	-.013(5)	.003(5)	-.029(5)
C(B4)	.066(6)	.066(6)	.049(5)	.016(5)	-.005(5)	-.032(5)
C(B5)	.058(5)	.066(5)	.038(5)	-.007(4)	-.003(4)	-.029(4)
C(B6)	.032(4)	.038(4)	.036(4)	-.011(3)	-.004(3)	-.013(3)
C(B7)	.036(5)	.069(5)	.078(7)	.004(4)	-.017(5)	-.022(5)
C(B8)	.069(6)	.042(4)	.091(7)	-.006(4)	-.041(5)	-.013(5)
C(B9)	.048(6)	.074(6)	.083(7)	-.027(5)	-.009(5)	-.020(6)
C(B10)	.028(4)	.034(4)	.056(5)	-.007(3)	-.009(4)	-.010(4)
C(B11)	.025(4)	.044(4)	.052(5)	.001(3)	-.014(4)	-.019(4)
C(B12)	.045(5)	.054(5)	.051(5)	-.014(4)	-.011(4)	-.024(4)
C(B13)	.038(4)	.032(4)	.049(5)	-.007(3)	-.015(4)	-.015(3)
C(B14)	.041(5)	.056(5)	.063(6)	-.003(4)	-.019(5)	-.023(4)
C(B15)	.055(5)	.032(4)	.044(5)	-.006(3)	-.022(4)	-.008(4)
C(B16)	.074(7)	.065(6)	.065(6)	-.035(5)	-.023(6)	-.001(5)
C(B17)	.053(5)	.032(4)	.038(4)	-.017(3)	.002(4)	-.015(3)
C(B18)	.056(5)	.048(5)	.045(5)	-.027(4)	-.009(4)	-.012(4)
C(B19)	.055(6)	.111(8)	.078(7)	-.041(5)	-.004(5)	-.039(6)
C(B20)	.037(4)	.023(3)	.034(4)	-.008(3)	-.013(3)	-.006(3)
C(B21)	.034(4)	.050(5)	.054(5)	.004(4)	-.011(4)	-.034(4)
C(B22)	.082(7)	.094(7)	.088(7)	-.012(6)	-.035(6)	-.054(6)

Table 3.9. Selected bond distances (Å) and angles (°) of complex (11).

Mo	- S	2.400(2)	2.405(2)	Mo	- C(1)	2.353(9)	2.355(7)
Mo	- C(2)	2.328(9)	2.322(9)	Mo	- C(3)	2.310(8)	2.319(10)
Mo	- C(4)	2.329(8)	2.356(9)	Mo	- C(5)	2.363(9)	2.378(7)
Mo	- C(10)	1.915(8)	1.921(6)	Mo	- C(11)	2.179(8)	2.176(7)
Mo	- C(13)	2.273(8)	2.273(8)	Mo	- C(20)	2.267(6)	2.282(7)
S	- C(6)	1.833(7)	1.846(7)	S	- C(20)	1.784(7)	1.789(6)
F(1)	- C(9)	1.300(14)	1.324(12)	F(2)	- C(9)	1.273(15)	1.269(14)
F(3)	- C(9)	1.326(11)	1.308(12)	F(4)	- C(12)	1.326(9)	1.334(9)
F(5)	- C(12)	1.350(10)	1.326(8)	F(6)	- C(12)	1.350(9)	1.345(9)
F(7)	- C(14)	1.334(10)	1.323(10)	F(8)	- C(14)	1.334(11)	1.358(10)
F(9)	- C(14)	1.313(11)	1.323(9)	F(10)	- C(16)	1.338(11)	1.316(11)
F(11)	- C(16)	1.352(11)	1.319(10)	F(12)	- C(16)	1.335(9)	1.330(12)
O(1)	- C(18)	1.320(9)	1.337(10)	O(1)	- C(19)	1.437(9)	1.454(10)
O(2)	- C(18)	1.194(11)	1.180(10)	O(3)	- C(21)	1.312(10)	1.340(10)
O(3)	- C(22)	1.461(12)	1.433(10)	O(4)	- C(21)	1.196(10)	1.189(9)
C(1)	- C(2)	1.413(13)	1.428(11)	C(1)	- C(5)	1.434(12)	1.426(12)
C(2)	- C(3)	1.433(13)	1.391(14)	C(3)	- C(4)	1.389(14)	1.394(12)
C(4)	- C(5)	1.400(12)	1.407(12)	C(6)	- C(7)	1.503(10)	1.533(11)
C(6)	- C(8)	1.525(11)	1.524(9)	C(9)	- C(10)	1.460(13)	1.460(10)
C(10)	- C(11)	1.411(11)	1.410(11)	C(11)	- C(12)	1.496(11)	1.526(11)
C(11)	- C(13)	1.449(10)	1.434(9)	C(13)	- C(14)	1.480(9)	1.504(11)
C(13)	- C(15)	1.533(10)	1.510(11)	C(15)	- C(16)	1.498(12)	1.527(13)
C(15)	- C(17)	1.316(10)	1.320(10)	C(17)	- C(18)	1.534(10)	1.517(11)
C(17)	- C(20)	1.489(11)	1.477(10)	C(20)	- C(21)	1.503(11)	1.498(8)

S	- Mo - C(10)	104.9(3)	104.4(2)	S	- Mo - C(11)	83.1(2)	83.3(2)
S	- Mo - C(13)	94.8(2)	94.5(2)	S	- Mo - C(20)	44.8(2)	44.8(2)
C(10)	- Mo - C(11)	39.7(3)	39.6(3)	C(10)	- Mo - C(13)	69.0(3)	69.2(3)
C(10)	- Mo - C(20)	130.8(3)	130.5(3)	C(11)	- Mo - C(13)	37.9(3)	37.5(3)
C(11)	- Mo - C(20)	92.3(3)	92.2(3)	C(13)	- Mo - C(20)	75.7(3)	75.5(3)
Mo	- S - C(6)	123.5(3)	123.1(3)	Mo	- S - C(20)	63.6(3)	64.0(2)
C(6)	- S - C(20)	118.1(3)	117.8(3)	C(18)	- O(1) - C(19)	117.3(7)	115.8(7)
C(21)	- O(3) - C(22)	117.0(6)	116.1(7)	C(2)	- C(1) - C(5)	107.4(7)	106.8(7)
C(1)	- C(2) - C(3)	108.5(8)	107.3(8)	C(2)	- C(3) - C(4)	106.4(8)	110.2(8)
C(3)	- C(4) - C(5)	111.0(8)	107.2(8)	C(1)	- C(5) - C(4)	106.7(7)	108.5(7)
S	- C(6) - C(7)	108.5(6)	108.2(5)	S	- C(6) - C(8)	103.3(5)	102.9(5)
C(7)	- C(6) - C(8)	114.5(7)	111.8(6)	F(1)	- C(9) - F(2)	106.2(9)	105.3(9)
F(1)	- C(9) - F(3)	101.4(8)	103.1(8)	F(1)	- C(9) - C(10)	115.8(9)	113.3(8)
F(2)	- C(9) - F(3)	104.0(9)	106.1(9)	F(2)	- C(9) - C(10)	115.1(9)	115.2(9)
F(3)	- C(9) - C(10)	112.8(8)	112.8(8)	Mo	- C(10) - C(9)	150.1(7)	148.6(7)
Mo	- C(10) - C(11)	80.3(5)	80.0(4)	C(9)	- C(10) - C(11)	129.6(8)	131.3(8)
Mo	- C(11) - C(10)	60.1(4)	60.4(4)	Mo	- C(11) - C(12)	135.8(5)	135.5(5)
Mo	- C(11) - C(13)	74.5(4)	74.9(4)	C(10)	- C(11) - C(12)	121.3(7)	119.8(6)
C(10)	- C(11) - C(13)	113.4(7)	115.1(7)	C(12)	- C(11) - C(13)	125.2(7)	125.1(7)
F(4)	- C(12) - F(5)	105.7(7)	106.2(7)	F(4)	- C(12) - F(6)	106.0(6)	106.5(6)
F(4)	- C(12) - C(11)	117.4(7)	115.7(6)	F(5)	- C(12) - F(6)	104.9(6)	106.9(6)
F(5)	- C(12) - C(11)	111.0(6)	110.4(6)	F(6)	- C(12) - C(11)	110.9(7)	110.8(7)
Mo	- C(13) - C(11)	67.5(4)	67.5(4)	Mo	- C(13) - C(14)	116.9(6)	115.7(6)
Mo	- C(13) - C(15)	112.6(5)	112.7(5)	C(11)	- C(13) - C(14)	119.4(6)	118.2(6)
C(11)	- C(13) - C(15)	115.8(6)	117.1(6)	C(14)	- C(13) - C(15)	115.7(6)	116.3(6)
F(7)	- C(14) - F(8)	100.6(6)	102.2(6)	F(7)	- C(14) - F(9)	105.6(8)	105.7(7)
F(7)	- C(14) - C(13)	114.8(7)	115.7(7)	F(8)	- C(14) - F(9)	104.8(8)	104.5(7)
F(8)	- C(14) - C(13)	116.2(7)	114.9(7)	F(9)	- C(14) - C(13)	113.4(6)	112.6(6)
C(13)	- C(15) - C(16)	119.3(7)	118.1(7)	C(13)	- C(15) - C(17)	118.1(7)	118.6(7)
C(16)	- C(15) - C(17)	122.3(7)	123.0(7)	F(10)	- C(16) - F(11)	105.6(7)	108.3(8)
F(10)	- C(16) - F(12)	108.6(8)	107.8(8)	F(10)	- C(16) - C(15)	113.3(7)	113.4(8)
F(11)	- C(16) - F(12)	104.6(7)	104.7(8)	F(11)	- C(16) - C(15)	111.0(7)	111.5(8)
F(12)	- C(16) - C(15)	113.1(7)	110.8(8)	C(15)	- C(17) - C(18)	123.8(7)	124.2(7)
C(15)	- C(17) - C(20)	120.1(7)	120.3(7)	C(18)	- C(17) - C(20)	116.0(6)	115.4(6)
O(1)	- C(18) - O(2)	126.0(7)	125.1(7)	O(1)	- C(18) - C(17)	110.7(7)	110.6(7)
O(2)	- C(18) - C(17)	123.1(7)	124.3(7)	Mo	- C(20) - S	71.5(3)	71.2(3)
Mo	- C(20) - C(17)	113.4(5)	112.8(5)	Mo	- C(20) - C(21)	118.1(5)	117.9(5)
S	- C(20) - C(17)	114.5(5)	115.6(5)	S	- C(20) - C(21)	120.8(5)	121.0(5)
C(17)	- C(20) - C(21)	112.6(6)	112.3(6)	O(3)	- C(21) - O(4)	124.1(7)	124.0(7)
O(3)	- C(21) - C(20)	115.1(6)	115.1(6)	O(4)	- C(21) - C(20)	120.7(7)	120.9(7)

Table 3.10. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (12).

	X/A	Y/B	Z/C	U
MO(1)	.21324(5)	.11628(4)	.21204(3)	.032
S(1)	-.06322(16)	.16672(13)	.06463(10)	.042
F(1)	.5628(5)	.1048(4)	.3809(4)	.115
F(2)	.4355(7)	.1035(4)	.4656(3)	.144
F(3)	.4416(5)	.0031(3)	.3814(3)	.100
F(4)	.1576(4)	.3116(3)	.3640(3)	.068
F(5)	.3533(4)	.2915(3)	.4389(3)	.083
F(6)	.2063(5)	.1978(3)	.4367(3)	.079
F(7)	.4986(4)	.3237(3)	.2533(3)	.085
F(8)	.5092(4)	.1952(3)	.2250(3)	.069
F(9)	.4181(4)	.2798(3)	.1242(3)	.083
F(10)	.3201(5)	.4225(3)	.2816(4)	.088
F(11)	.1368(5)	.4591(3)	.2062(4)	.100
F(12)	.2936(6)	.4350(4)	.1440(4)	.116
O(1)	-.0458(5)	.3940(3)	.0699(3)	.065
O(2)	-.1207(6)	.3634(4)	.1867(4)	.086
O(3)	-.0637(5)	.2053(3)	.2874(3)	.051
O(4)	.0409(4)	.0896(3)	.2566(3)	.039
C(1)	.1550(7)	-.0037(5)	.1261(5)	.061
C(2)	.1920(7)	.0566(5)	.0717(4)	.057
C(3)	.3221(7)	.0769(5)	.1040(4)	.050
C(4)	.3693(7)	.0262(5)	.1778(4)	.046
C(5)	.2660(8)	-.0229(5)	.1933(5)	.058
C(6)	-.2324(7)	.1789(5)	.0769(5)	.053
C(7)	-.2809(8)	.0988(7)	.1106(6)	.086
C(8)	-.3141(8)	.2011(7)	-.0125(7)	.107
C(9)	.4441(8)	.0862(6)	.3880(5)	.057
C(10)	.3415(6)	.1273(4)	.3198(4)	.042
C(11)	.2928(6)	.2104(4)	.3123(4)	.036
C(12)	.2508(7)	.2533(5)	.3862(4)	.052
C(13)	.2976(6)	.2482(4)	.2278(4)	.034
C(14)	.4284(7)	.2607(5)	.2085(5)	.053
C(15)	.1968(6)	.3162(4)	.1951(4)	.038
C(16)	.2350(8)	.4081(5)	.2054(6)	.064
C(17)	.0728(6)	.2952(4)	.1683(4)	.033
C(18)	-.0416(7)	.3543(4)	.1450(5)	.046
C(19)	-.1513(8)	.4546(6)	.0466(5)	.084
C(20)	.0416(6)	.2028(4)	.1666(4)	.032
C(21)	.0022(6)	.1635(4)	.2411(4)	.035
C(22)	-.0944(9)	.1629(6)	.3634(5)	.078
H(1)	.06969	-.02823	.11941	.064
H(2)	.13580	.07989	.02026	.066
H(3)	.37123	.11875	.08109	.060
H(4)	.45773	.02476	.21164	.049
H(5)	.26957	-.06214	.24018	.071
H(6)	-.23462	.22302	.11826	.064
H(7A)	-.22439	.08368	.16548	.098
H(7B)	-.27902	.05481	.06910	.098
H(7C)	-.36865	.10586	.11798	.098
H(8A)	-.29932	.15728	-.05120	.099
H(8B)	-.28406	.25360	-.03103	.099
H(8C)	-.40540	.20373	-.01229	.099
H(19A)	-.23263	.43040	.05243	.085
H(19B)	-.16043	.47415	-.01226	.085
H(19C)	-.13125	.50240	.08470	.085
H(22A)	-.14153	.19963	.39388	.078
H(22B)	-.01571	.14456	.40297	.078
H(22C)	-.14639	.11383	.34430	.078

Table 3.10(cont).

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
MO(1)	.0304(3)	.0302(3)	.0341(3)	.0037(4)	.0085(2)	.0001(3)
S(1)	.0309(9)	.0534(13)	.0379(8)	.0014(9)	.0045(7)	-.0066(9)
F(1)	.048(3)	.133(6)	.147(5)	.001(4)	-.027(3)	.052(5)
F(2)	.178(6)	.197(7)	.041(3)	.125(6)	-.012(3)	.007(4)
F(3)	.119(5)	.065(4)	.100(4)	.023(4)	-.024(3)	.032(3)
F(4)	.071(3)	.075(4)	.054(2)	.028(3)	.015(2)	-.019(2)
F(5)	.069(3)	.114(5)	.057(3)	-.005(3)	-.005(2)	-.039(3)
F(6)	.098(4)	.091(4)	.048(2)	.006(3)	.033(3)	.003(3)
F(7)	.049(3)	.076(4)	.124(4)	-.026(3)	.018(3)	-.027(3)
F(8)	.040(3)	.066(3)	.098(3)	.010(3)	.022(2)	.007(3)
F(9)	.067(3)	.117(5)	.065(3)	-.009(3)	.030(3)	.024(3)
F(10)	.077(4)	.045(3)	.129(4)	-.007(3)	-.015(3)	-.022(3)
F(11)	.069(4)	.032(3)	.180(6)	.007(3)	-.020(4)	-.018(3)
F(12)	.119(5)	.077(5)	.145(5)	-.035(4)	.035(4)	.038(4)
O(1)	.083(4)	.061(4)	.047(3)	.038(3)	.006(3)	.009(3)
O(2)	.079(4)	.066(5)	.117(5)	.038(4)	.058(4)	.029(4)
O(3)	.058(3)	.049(3)	.048(3)	.004(3)	.031(2)	.002(2)
O(4)	.037(3)	.038(3)	.041(2)	.000(2)	.011(2)	.005(2)
C(1)	.045(5)	.051(5)	.085(6)	-.009(4)	.022(4)	-.040(5)
C(2)	.057(5)	.068(6)	.042(4)	.021(5)	.012(3)	-.025(4)
C(3)	.057(5)	.048(5)	.046(4)	.008(4)	.031(4)	-.007(4)
C(4)	.042(4)	.049(5)	.046(4)	.012(4)	.010(3)	-.005(4)
C(5)	.072(6)	.031(4)	.068(5)	.016(4)	.027(4)	-.003(4)
C(6)	.039(4)	.058(6)	.059(4)	.004(4)	.007(3)	-.015(4)
C(7)	.063(6)	.096(8)	.095(7)	-.016(6)	.018(5)	.004(6)
C(8)	.038(5)	.155(11)	.119(8)	.017(6)	-.004(5)	.051(8)
C(9)	.052(5)	.058(6)	.055(4)	.016(5)	-.005(4)	.013(4)
C(10)	.036(4)	.043(5)	.045(3)	.004(4)	.011(3)	.003(3)
C(11)	.033(4)	.038(4)	.033(3)	.004(3)	.003(3)	-.002(3)
C(12)	.049(5)	.061(6)	.046(4)	-.001(4)	.013(4)	-.006(4)
C(13)	.027(4)	.036(4)	.039(3)	.000(3)	.010(3)	-.002(3)
C(14)	.046(5)	.055(5)	.056(4)	-.005(4)	.008(4)	.000(4)
C(15)	.039(4)	.032(4)	.042(4)	-.001(4)	.012(3)	0.000(3)
C(16)	.041(5)	.043(5)	.098(7)	.001(4)	-.002(5)	.003(5)
C(17)	.039(4)	.033(4)	.027(3)	.002(3)	.013(3)	-.001(3)
C(18)	.043(4)	.032(4)	.059(4)	.002(4)	.009(4)	-.005(4)
C(19)	.087(7)	.072(6)	.080(6)	.050(6)	-.020(5)	-.004(5)
C(20)	.026(3)	.031(4)	.037(3)	.005(3)	.008(3)	-.002(3)
C(21)	.022(3)	.042(4)	.039(3)	-.004(4)	.008(3)	-.002(3)
C(22)	.110(7)	.067(6)	.062(5)	-.005(6)	.060(5)	-.005(5)

Table 3.11. Selected bond distances (Å) and angles (°) of complex (12).

Mo(1) - O(4)	2.125(5)	Mo(1) - C(1)	2.336(9)
Mo(1) - C(2)	2.367(7)	Mo(1) - C(3)	2.339(7)
Mo(1) - C(4)	2.328(8)	Mo(1) - C(5)	2.314(8)
Mo(1) - C(10)	1.918(7)	Mo(1) - C(11)	2.195(7)
Mo(1) - C(13)	2.266(7)	Mo(1) - C(20)	2.249(7)
Mo(1) - C(21)	2.477(6)	S(1) - C(6)	1.839(8)
S(1) - C(20)	1.819(7)	F(1) - C(9)	1.310(10)
F(2) - C(9)	1.273(9)	F(3) - C(9)	1.324(11)
F(4) - C(12)	1.334(10)	F(5) - C(12)	1.345(9)
F(6) - C(12)	1.339(10)	F(7) - C(14)	1.342(10)
F(8) - C(14)	1.331(10)	F(9) - C(14)	1.341(9)
F(10) - C(16)	1.342(11)	F(11) - C(16)	1.313(10)
F(12) - C(16)	1.328(11)	O(1) - C(18)	1.332(9)
O(1) - C(19)	1.450(11)	O(2) - C(18)	1.178(10)
O(3) - C(21)	1.296(8)	O(3) - C(22)	1.470(10)
O(4) - C(21)	1.248(9)	C(1) - C(2)	1.398(12)
C(1) - C(5)	1.416(12)	C(2) - C(3)	1.383(11)
C(3) - C(4)	1.408(10)	C(4) - C(5)	1.401(11)
C(6) - C(7)	1.511(13)	C(6) - C(8)	1.513(13)
C(9) - C(10)	1.487(11)	C(10) - C(11)	1.410(10)
C(11) - C(12)	1.497(10)	C(11) - C(13)	1.471(9)
C(13) - C(14)	1.486(10)	C(13) - C(15)	1.517(10)
C(15) - C(16)	1.513(12)	C(15) - C(17)	1.316(9)
C(17) - C(18)	1.502(10)	C(17) - C(20)	1.503(10)
C(20) - C(21)	1.468(9)		

O(4) - Mo(1) - C(10)	101.8(3)	O(4) - Mo(1) - C(11)	96.4(2)
O(4) - Mo(1) - C(13)	119.3(2)	O(4) - Mo(1) - C(20)	63.0(2)
O(4) - Mo(1) - C(21)	30.2(2)	C(10) - Mo(1) - C(11)	39.4(3)
C(10) - Mo(1) - C(13)	69.0(3)	C(10) - Mo(1) - C(20)	125.2(3)
C(10) - Mo(1) - C(21)	106.7(3)	C(11) - Mo(1) - C(13)	38.5(3)
C(11) - Mo(1) - C(20)	87.7(3)	C(11) - Mo(1) - C(21)	82.6(3)
C(13) - Mo(1) - C(20)	74.6(3)	C(13) - Mo(1) - C(21)	92.5(3)
C(20) - Mo(1) - C(21)	35.8(3)	C(6) - S(1) - C(20)	106.2(4)
C(18) - O(1) - C(19)	114.1(6)	C(21) - O(3) - C(22)	117.9(6)
Mo(1) - O(4) - C(21)	90.7(4)	C(2) - C(1) - C(5)	108.0(7)
C(1) - C(2) - C(3)	108.8(7)	C(2) - C(3) - C(4)	107.6(7)
C(3) - C(4) - C(5)	108.7(7)	C(1) - C(5) - C(4)	106.8(7)
S(1) - C(6) - C(7)	111.0(6)	S(1) - C(6) - C(8)	106.5(6)
C(7) - C(6) - C(8)	110.9(7)	F(1) - C(9) - F(2)	108.0(7)
F(1) - C(9) - F(3)	102.7(7)	F(1) - C(9) - C(10)	112.7(7)
F(2) - C(9) - F(3)	106.6(7)	F(2) - C(9) - C(10)	113.6(8)
F(3) - C(9) - C(10)	112.5(7)	Mo(1) - C(10) - C(9)	147.7(6)
Mo(1) - C(10) - C(11)	81.0(4)	C(9) - C(10) - C(11)	131.3(7)
Mo(1) - C(11) - C(10)	59.7(4)	Mo(1) - C(11) - C(12)	137.5(5)
Mo(1) - C(11) - C(13)	73.4(4)	C(10) - C(11) - C(12)	121.8(6)
C(10) - C(11) - C(13)	111.8(6)	C(12) - C(11) - C(13)	126.3(7)
F(4) - C(12) - F(5)	106.5(7)	F(4) - C(12) - F(6)	106.1(6)
F(4) - C(12) - C(11)	116.2(6)	F(5) - C(12) - F(6)	105.6(6)
F(5) - C(12) - C(11)	110.4(6)	F(6) - C(12) - C(11)	111.4(7)
Mo(1) - C(13) - C(11)	68.2(4)	Mo(1) - C(13) - C(14)	117.3(5)
Mo(1) - C(13) - C(15)	113.3(5)	C(11) - C(13) - C(14)	117.5(6)
C(11) - C(13) - C(15)	115.6(6)	C(14) - C(13) - C(15)	116.2(6)
F(7) - C(14) - F(8)	103.4(6)	F(7) - C(14) - F(9)	105.2(7)
F(7) - C(14) - C(13)	114.6(7)	F(8) - C(14) - F(9)	105.9(7)
F(8) - C(14) - C(13)	115.7(7)	F(9) - C(14) - C(13)	111.2(6)
C(13) - C(15) - C(16)	120.2(6)	C(13) - C(15) - C(17)	119.4(7)
C(16) - C(15) - C(17)	119.8(7)	F(10) - C(16) - F(11)	104.5(8)
F(10) - C(16) - F(12)	105.7(7)	F(10) - C(16) - C(15)	111.5(7)
F(11) - C(16) - F(12)	107.7(8)	F(11) - C(16) - C(15)	114.0(7)
F(12) - C(16) - C(15)	112.8(8)	C(15) - C(17) - C(18)	126.7(7)
C(15) - C(17) - C(20)	116.6(6)	C(18) - C(17) - C(20)	116.5(6)
O(1) - C(18) - O(2)	123.4(7)	O(1) - C(18) - C(17)	112.0(6)
O(2) - C(18) - C(17)	124.5(7)	Mo(1) - C(20) - S(1)	111.6(3)
Mo(1) - C(20) - C(17)	115.8(4)	Mo(1) - C(20) - C(21)	80.6(4)
S(1) - C(20) - C(17)	114.1(5)	S(1) - C(20) - C(21)	110.3(5)
C(17) - C(20) - C(21)	120.1(6)	Mo(1) - C(21) - O(3)	150.8(5)
Mo(1) - C(21) - O(4)	59.1(4)	Mo(1) - C(21) - C(20)	63.6(4)
O(3) - C(21) - O(4)	124.3(6)	O(3) - C(21) - C(20)	121.0(6)
O(4) - C(21) - C(20)	114.7(6)		

Table 3.12. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (15).

	X/A	Y/B	Z/C	U
W	.13805(2)	.27768(1)	-.33947(1)	.031
S	.3e550(15)	.24149(8)	-.26773(9)	.049
F(1)	.1313(4)	.2727(2)	-.1329(2)	.076
F(2)	-.0419(4)	.3074(2)	-.203e(2)	.075
F(3)	-.0432(4)	.2005(2)	-.1504(2)	.078
F(4)	.0286(4)	.0425(2)	-.1711(2)	.086
F(5)	.1675(4)	.1235(2)	-.1186(2)	.086
F(6)	.2265(5)	.0338(2)	-.1795(2)	.089
F(7)	.0885(4)	-.0215(2)	-.2882(2)	.086
F(8)	.1215(5)	-.0038(2)	-.3964(2)	.094
F(9)	.2889(4)	-.0094(2)	-.3102(3)	.105
F(10)	.3027(4)	.0784(2)	-.4355(2)	.073
F(11)	.1055(4)	.1091(3)	-.4869(2)	.082
F(12)	.2624(5)	.1914(2)	-.4738(2)	.086
N(1)	.2115(5)	.4240(3)	-.2342(3)	.048
N(2)	.3629(5)	.3465(3)	-.4274(3)	.054
C(1)	-.0478(6)	.2404(3)	-.4241(3)	.051
C(2)	-.0965(5)	.2692(3)	-.3629(3)	.048
C(3)	-.0580(5)	.3464(3)	-.3547(3)	.047
C(4)	.0166(6)	.3651(3)	-.4106(3)	.054
C(5)	.0210(6)	.2993(4)	-.4533(3)	.052
C(6)	.4796(5)	.3224(3)	-.2427(3)	.044
C(7)	.4935(7)	.3382(4)	-.1613(3)	.066
C(8)	.6121(6)	.3028(4)	-.2648(4)	.066
C(9)	.0868(5)	.2094(3)	-.2476(3)	.039
C(10)	.0356(6)	.2460(4)	-.1841(3)	.053
C(11)	.1189(5)	.1340(3)	-.2473(3)	.040
C(12)	.1347(7)	.0837(4)	-.1799(4)	.062
C(13)	.1589(5)	.1038(3)	-.3147(3)	.042
C(14)	.1666(7)	.0174(3)	-.3283(4)	.066
C(15)	.1747(5)	.1566(3)	-.3665(3)	.039
C(16)	.2116(7)	.1332(3)	-.4387(3)	.056
C(17)	.1851(5)	.3712(3)	-.2705(3)	.040
C(18)	.2839(5)	.3193(3)	-.3972(3)	.042
C(21)	.2522(6)	.4853(3)	-.1868(3)	.043
C(22)	.3424(7)	.5370(4)	-.2041(3)	.057
C(23)	.3869(7)	.5964(4)	-.1574(4)	.062
C(24)	.3415(7)	.6023(3)	-.0918(4)	.057
C(25)	.2491(7)	.5498(4)	-.0744(3)	.063
C(26)	.2052(7)	.4906(3)	-.1215(4)	.058
C(27)	.3884(9)	.6648(5)	-.0385(4)	.098
C(31)	.4624(5)	.3695(3)	-.4667(3)	.045
C(32)	.4590(6)	.3443(4)	-.5372(3)	.055
C(33)	.5598(7)	.3677(4)	-.5751(3)	.061
C(34)	.6605(6)	.4152(3)	-.5444(3)	.052
C(35)	.6618(6)	.4400(4)	-.4728(3)	.054
C(36)	.5604(6)	.4173(4)	-.4349(3)	.055
C(37)	.7700(8)	.4408(4)	-.5831(4)	.082
H(1)	-.05998	.18918	-.44297	.050
H(2)	-.14629	.24105	-.33176	.050
H(3)	-.07940	.38099	-.31794	.050
H(4)	.05741	.41369	-.41773	.050
H(5)	.06388	.29536	-.49568	.050
H(6)	.44460	.36734	-.26889	.050
H(22)	.37610	.53110	-.24923	.050
H(23)	.44870	.63336	-.17097	.050
H(25)	.21625	.55379	-.02878	.050
H(26)	.14129	.45388	-.10981	.050
H(32)	.38857	.31163	-.55990	.050
H(33)	.55931	.35043	-.62425	.050
H(35)	.73317	.47212	-.45003	.050
H(36)	.55858	.43605	-.38648	.050
H(7A)	.55247	.38076	-.14868	.050
H(7B)	.52850	.29325	-.13512	.050
H(7C)	.40748	.34959	-.14876	.050
H(8A)	.67106	.34537	-.25212	.050
H(8B)	.60205	.29325	-.31624	.050
H(8C)	.64722	.25753	-.23917	.050
H(27A)	.35683	.66912	.00745	.050
H(27B)	.36746	.71252	-.06350	.050
H(27C)	.48348	.65957	-.02747	.050
H(37A)	.84054	.47414	-.56155	.050
H(37B)	.72827	.46605	-.62664	.050
H(37C)	.81218	.39467	-.59617	.050

Table 3.12(cont).

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
H	.0313(1)	.0297(1)	.0326(1)	-.0009(1)	.0050(1)	-.0002(1)
S	.0373(7)	.0383(7)	.0671(10)	-.0014(6)	-.0045(7)	.0022(7)
F(1)	.092(3)	.089(3)	.046(2)	-.016(2)	.010(2)	-.021(2)
F(2)	.091(3)	.066(2)	.070(2)	.025(2)	.037(2)	-.002(2)
F(3)	.087(3)	.079(3)	.071(2)	-.012(2)	.046(2)	.005(2)
F(4)	.101(3)	.070(3)	.088(3)	-.016(2)	.034(3)	.030(2)
F(5)	.107(3)	.095(3)	.051(2)	.005(3)	-.006(2)	.016(2)
F(6)	.094(3)	.083(3)	.087(3)	.029(3)	-.001(3)	.035(2)
F(7)	.110(4)	.044(2)	.103(3)	-.016(2)	.031(3)	.009(2)
F(8)	.128(4)	.053(2)	.103(3)	-.020(2)	.044(3)	-.030(2)
F(9)	.093(3)	.065(3)	.159(5)	.038(2)	.041(3)	.015(3)
F(10)	.067(2)	.074(2)	.079(3)	.012(2)	.031(2)	-.017(2)
F(11)	.073(3)	.110(3)	.060(2)	.003(2)	.003(2)	-.038(2)
F(12)	.136(4)	.068(2)	.059(2)	-.014(3)	.053(2)	-.014(2)
N(1)	.048(3)	.038(2)	.057(3)	.000(2)	.003(3)	-.006(2)
N(2)	.045(3)	.058(3)	.061(3)	-.004(3)	.016(3)	.010(3)
C(1)	.044(3)	.051(3)	.054(3)	.001(3)	-.007(3)	-.009(3)
C(2)	.031(3)	.061(4)	.049(3)	-.005(3)	.002(2)	.001(3)
C(3)	.036(3)	.049(3)	.052(3)	.010(3)	-.002(3)	-.008(3)
C(4)	.049(4)	.049(3)	.060(4)	.003(3)	-.006(3)	.020(3)
C(5)	.048(3)	.070(4)	.035(3)	.000(3)	-.003(3)	.008(3)
C(6)	.036(3)	.044(3)	.050(3)	-.007(2)	-.002(3)	.001(2)
C(7)	.081(5)	.056(4)	.054(4)	-.007(4)	-.010(4)	-.004(3)
C(8)	.042(3)	.067(4)	.086(5)	-.004(3)	.006(4)	.004(4)
C(9)	.034(3)	.049(3)	.033(2)	-.003(2)	.003(2)	.002(2)
C(10)	.060(4)	.058(3)	.043(3)	-.007(3)	.018(3)	-.005(3)
C(11)	.032(3)	.040(3)	.048(3)	-.004(2)	.005(3)	.008(2)
C(12)	.067(4)	.059(4)	.058(4)	.009(3)	.007(3)	.018(3)
C(13)	.038(3)	.039(3)	.049(3)	.001(2)	.002(3)	.008(2)
C(14)	.075(5)	.034(3)	.089(5)	.004(3)	.025(4)	0.000(3)
C(15)	.032(3)	.042(3)	.043(3)	-.003(2)	.009(2)	.003(2)
C(16)	.063(4)	.051(3)	.055(4)	.002(3)	.015(3)	-.014(3)
C(17)	.033(3)	.034(2)	.053(3)	-.003(2)	.013(2)	-.004(2)
C(18)	.041(3)	.040(3)	.046(3)	-.005(2)	.011(3)	0.000(2)
C(21)	.047(3)	.034(2)	.046(3)	-.001(2)	.002(3)	-.004(2)
C(22)	.068(4)	.053(4)	.049(3)	-.011(3)	.014(3)	-.006(3)
C(23)	.066(5)	.053(4)	.063(4)	-.017(3)	.008(4)	.000(3)
C(24)	.063(4)	.045(3)	.056(4)	-.001(3)	-.017(3)	-.008(3)
C(25)	.081(5)	.064(4)	.043(3)	.001(4)	.011(3)	-.007(3)
C(26)	.069(4)	.044(3)	.062(4)	-.009(3)	.017(4)	-.003(3)
C(27)	.099(7)	.095(6)	.089(6)	.004(5)	-.034(5)	-.046(5)
C(31)	.040(3)	.045(3)	.050(3)	0.000(3)	.015(3)	.006(3)
C(32)	.054(4)	.049(3)	.059(4)	-.012(3)	.004(3)	-.007(3)
C(33)	.079(5)	.057(4)	.047(3)	-.002(3)	.027(3)	-.004(3)
C(34)	.050(4)	.048(3)	.057(4)	.002(3)	.019(3)	.012(3)
C(35)	.046(3)	.062(4)	.052(3)	-.015(3)	.003(3)	.002(3)
C(36)	.056(4)	.066(4)	.042(3)	-.005(3)	.014(3)	-.002(3)
C(37)	.075(5)	.083(5)	.092(5)	-.008(4)	.045(5)	.010(4)

Table 3.13. Selected bond distances (Å) and angles (°) of complex (15).

W	- S	2.561(2)	
W	- C(2)	2.360(6)	
W	- C(4)	2.255(7)	
W	- C(9)	2.207(6)	
W	- C(17)	2.081(6)	
S	- C(6)	1.839(6)	
F(2)	- C(10)	1.344(8)	
F(4)	- C(12)	1.326(9)	
F(6)	- C(12)	1.350(9)	
F(8)	- C(14)	1.329(9)	
F(10)	- C(16)	1.325(8)	
F(12)	- C(16)	1.350(8)	
N(1)	- C(21)	1.404(8)	
N(2)	- C(31)	1.394(8)	
C(1)	- C(5)	1.397(9)	
C(3)	- C(4)	1.417(9)	
C(6)	- C(7)	1.521(9)	
C(9)	- C(10)	1.503(8)	
C(11)	- C(12)	1.516(9)	
C(13)	- C(14)	1.530(8)	
C(15)	- C(16)	1.504(8)	
C(21)	- C(26)	1.374(9)	
C(23)	- C(24)	1.372(10)	
C(24)	- C(27)	1.499(11)	
C(31)	- C(32)	1.376(9)	
C(32)	- C(33)	1.391(10)	
C(34)	- C(35)	1.396(9)	
C(35)	- C(36)	1.393(9)	

W	- C(1)	2.353(7)	
W	- C(3)	2.304(6)	
W	- C(5)	2.290(6)	
W	- C(15)	2.213(6)	
W	- C(18)	2.090(6)	
F(1)	- C(10)	1.334(8)	
F(3)	- C(10)	1.348(8)	
F(5)	- C(12)	1.331(8)	
F(7)	- C(14)	1.351(9)	
F(9)	- C(14)	1.322(9)	
F(11)	- C(16)	1.356(8)	
N(1)	- C(17)	1.147(7)	
N(2)	- C(18)	1.150(8)	
C(1)	- C(2)	1.401(9)	
C(2)	- C(3)	1.402(9)	
C(4)	- C(5)	1.398(9)	
C(6)	- C(8)	1.506(9)	
C(9)	- C(11)	1.354(8)	
C(11)	- C(13)	1.472(8)	
C(13)	- C(15)	1.359(8)	
C(21)	- C(22)	1.359(9)	
C(22)	- C(23)	1.380(10)	
C(24)	- C(25)	1.383(10)	
C(25)	- C(26)	1.383(9)	
C(31)	- C(36)	1.361(9)	
C(33)	- C(34)	1.369(10)	
C(34)	- C(37)	1.484(10)	

S	- W -	C(CP)	176.1
S	- W -	C(15)	73.4(2)
S	- W -	C(18)	72.4(2)
C(CP)	- W -	C(15)	104.7
C(CP)	- W -	C(18)	104.5
C(9)	- W -	C(17)	90.3(2)
C(15)	- W -	C(17)	148.7(2)
C(17)	- W -	C(18)	86.0(3)
C(17)	- N(1) -	C(21)	175.5(6)
S	- C(6) -	C(7)	110.3(5)
C(7)	- C(6) -	C(8)	111.3(6)
W	- C(9) -	C(11)	116.1(4)
F(1)	- C(10) -	F(2)	104.3(5)
F(1)	- C(10) -	C(9)	113.9(6)
F(2)	- C(10) -	C(9)	112.7(5)
C(9)	- C(11) -	C(12)	124.0(6)
C(12)	- C(11) -	C(13)	119.2(5)
F(4)	- C(12) -	F(6)	106.7(6)
F(5)	- C(12) -	F(6)	104.0(6)
F(6)	- C(12) -	C(11)	111.0(6)
C(11)	- C(13) -	C(15)	116.1(5)
F(7)	- C(14) -	F(8)	103.9(6)
F(7)	- C(14) -	C(13)	110.6(6)
F(8)	- C(14) -	C(13)	114.3(6)
W	- C(15) -	C(13)	116.2(4)
C(13)	- C(15) -	C(16)	121.5(5)
F(10)	- C(16) -	F(12)	104.2(6)
F(11)	- C(16) -	F(12)	103.7(5)
F(12)	- C(16) -	C(15)	113.2(5)
W	- C(18) -	N(2)	175.9(5)
N(1)	- C(21) -	C(26)	119.7(6)
C(21)	- C(22) -	C(23)	121.1(6)
C(23)	- C(24) -	C(25)	119.5(6)
C(25)	- C(24) -	C(27)	118.9(7)
C(21)	- C(26) -	C(25)	119.2(6)
N(2)	- C(31) -	C(36)	119.3(6)
C(31)	- C(32) -	C(33)	118.5(6)
C(33)	- C(34) -	C(35)	118.8(6)
C(35)	- C(34) -	C(37)	118.1(6)
C(31)	- C(36) -	C(35)	120.2(6)

S	- W -	C(9)	76.6(2)
S	- W -	C(17)	76.7(2)
C(CP)	- W -	C(9)	106.3
C(CP)	- W -	C(17)	105.7
C(9)	- W -	C(15)	74.4(2)
C(9)	- W -	C(18)	148.8(2)
C(15)	- W -	C(18)	93.2(2)
W	- S -	C(6)	115.2(2)
C(18)	- N(2) -	C(31)	172.3(6)
S	- C(6) -	C(8)	108.2(5)
W	- C(9) -	C(10)	122.0(4)
C(10)	- C(9) -	C(11)	121.4(5)
F(1)	- C(10) -	F(3)	107.0(5)
F(2)	- C(10) -	F(3)	103.2(5)
F(3)	- C(10) -	C(9)	114.8(6)
C(9)	- C(11) -	C(13)	116.2(5)
F(4)	- C(12) -	F(5)	106.1(6)
F(4)	- C(12) -	C(11)	115.5(6)
F(5)	- C(12) -	C(11)	112.7(6)
C(11)	- C(13) -	C(14)	121.3(5)
C(14)	- C(13) -	C(15)	122.3(6)
F(7)	- C(14) -	F(9)	107.0(6)
F(8)	- C(14) -	F(9)	108.3(6)
F(9)	- C(14) -	C(13)	112.1(6)
W	- C(15) -	C(16)	122.3(4)
F(10)	- C(16) -	F(11)	106.6(5)
F(10)	- C(16) -	C(15)	115.2(5)
F(11)	- C(16) -	C(15)	112.9(6)
W	- C(17) -	N(1)	178.1(5)
N(1)	- C(21) -	C(22)	120.0(6)
C(22)	- C(21) -	C(26)	120.2(6)
C(22)	- C(23) -	C(24)	119.4(7)
C(23)	- C(24) -	C(27)	121.6(7)
C(24)	- C(25) -	C(26)	120.6(6)
N(2)	- C(31) -	C(32)	119.6(6)
C(32)	- C(31) -	C(36)	121.1(6)
C(32)	- C(33) -	C(34)	121.7(6)
C(33)	- C(34) -	C(37)	123.2(6)
C(34)	- C(35) -	C(36)	119.6(6)

Table 3.14. Crystallographic and experimental details of the structure analyses of complexes (5), (7), (10), (11), (12) and (15).

Compound	[CpMo(SPr^i)$(hfb)_2$(PhCCMe)] (5)	[CpW(SPr^i)$(hfb)_2$(PhCCMe)] (7)
Formula	$C_{25}H_{20}F_{12}MoS$	$C_{25}H_{20}F_{12}SW$
Formula Wt.	676.4	764.3
Crystal habit	yellow needle	dark red needle
Crystal size, mm	0.64x0.20x0.20	0.64x0.20x0.12
Crystal system	monoclinic	monoclinic
Space group	P $2_1/c$	P $2_1/c$
a, Å	8.509(4)	8.086(1)
b, Å	14.120(1)	19.896(2)
c, Å	22.095(3)	15.614(2)
β, °	97.46(2)	90.33(1)
Obtained from	25 refln, 12<θ<18°	25 refln, 13<θ<18°
V, $Å^3$	2632(1)	2511.9(6)
Z	4	4
F(000)	1344	1472
d calc, gcm^{-3}	1.707	2.021
T, K	297	295
μ(Mo-Kα), cm^{-1}	6.6	48.8
Absorption factors on F^2	0.88-0.95	0.87-1.19
Scan width, °	0.75	0.70
Max count time, s	95	100
Total refln measured	8740	9426
Unique refln	6812	7309
R_{INT}	0.058	0.026
Miller indicies h	0→11	0→11
measured, k	-19→ 4	-28→22
l	-31→31	-22→22
2θ range, °	4-60	4-60
Unique refln ≥ 3σ(I)	3740	n/a
No. of parameters	352	432
R	0.039	0.054
R_w	0.050	0.031
$\|\Delta\rho\|_{max}$, $eÅ^{-3}$	0.75	0.89
Δ/σ_{max}	0.26	0.17

Table 3.14(cont).

Compound	[CpW(STol)(hfb)$_2$(dmad)] (10)	[CpMo(SPr^i)(hfb)$_2$(dmad)] (11)
Formula	$C_{25}H_{18}F_{12}O_4SW$	$C_{22}H_{18}F_{12}MoO_4S$
Formula Wt.	838.3	702.4
Crystal habit	black needle	dark red plate
Crystal size, mm	0.48x0.08x0.08	0.52x0.28x0.44
Crystal system	orthorhombic	triclinic
Space group	$P2_12_12_1$	P $\bar{1}$
a, Å	9.234(3)	10.898(3)
b, Å	15.185(3)	16.120(4)
c, Å	20.420(3)	17.482(4)
α, °	—	63.80(2)
β, °	—	73.11(2)
γ, °	—	71.44(2)
Obtained from	23 refln, 10<θ<15°	23 refln, 12<θ<14°
V, Å^3	2863(1)	2572(1)
Z	4	4
F(000)	1616	1392
d calc, gcm^{-3}	1.945	1.814
T, K	295	297
μ(Mo-Kα), cm^{-1}	43.0	6.9
Absorption factors on F^2	0.79-1.22	0.78-1.17
Scan width, °	0.80	1.00
Max count time, s	180	100
Total refln measured	3895	7171
Unique refln	3868	6268
R_{INT}	—	0.029
Miller indicies h	0→12	-11→11
measured, k	0→20	-17→17
l	0→26	-18→ 2
2θ range, °	4-56	4-44
Unique refln ≥ 3σ(I)	1676	4602
No. of parameters	188	721
R	0.041	0.044
R_w	0.047	0.060
$\|\Delta\rho\|_{max}$, eÅ^{-3}	0.72	0.64
Δ/σ_{max}	0.082	0.09

Table 3.14(cont).

Compound	[CpMo(SPr^i)(hfb)$_2$(dmad)] (12)	[CpW(SPr^i)(hfb)$_2$(CNTol)$_2$] (15)
Formula	$C_{22}H_{18}F_{12}MoO_4S$	$C_{32}H_{26}F_{12}N_2SW$
Formula Wt.	702.4	882.5
Crystal habit	red needle	orange plate
Crystal size, mm	0.56x0.24x0.20	0.60x0.25x0.70
Crystal system	monoclinic	monoclinic
Space group	P $2_1/c$	P $2_1/c$
a, Å	10.496(4)	10.163(1)
b, Å	15.881(3)	17.418(4)
c, Å	15.733(6)	18.577(2)
β, °	103.13(3)	98.934(7)
Obtained from	23 refln, 12<θ<15°	23 refln, 12<θ<14°
V, Å^3	2554(2)	3248.6(7)
Z	4	4
F(000)	1392	1720
d calc, gcm^{-3}	1.827	1.804
T, K	297	295
μ(Mo-Kα), cm^{-1}	6.9	37.9
Absorption factors on F^2	0.63-1.20	0.65-1.54
Scan width, °	0.80	0.80
Max count time, s	100	100
Total refln measured	6618	12075
Unique refln	4470	9490
R_{INT}	0.048	0.059
Miller indicies h	0→12	0→14
measured, k	-18→ 7	-24→ 4
l	-18→18	-26→26
2θ range, °	4-50	4-60
Unique refln ≥ 3σ(I)	2881	5735
No. of parameters	361	433
R	0.046	0.037
R_w	0.054	0.044
$\|\Delta\rho\|_{max}$, eÅ^{-3}	1.12	2.40
Δ/σ_{max}	0.051	0.154

CHAPTER 4: OTHER ORGANOMETALLIC COMPLEXES OF Mo AND W

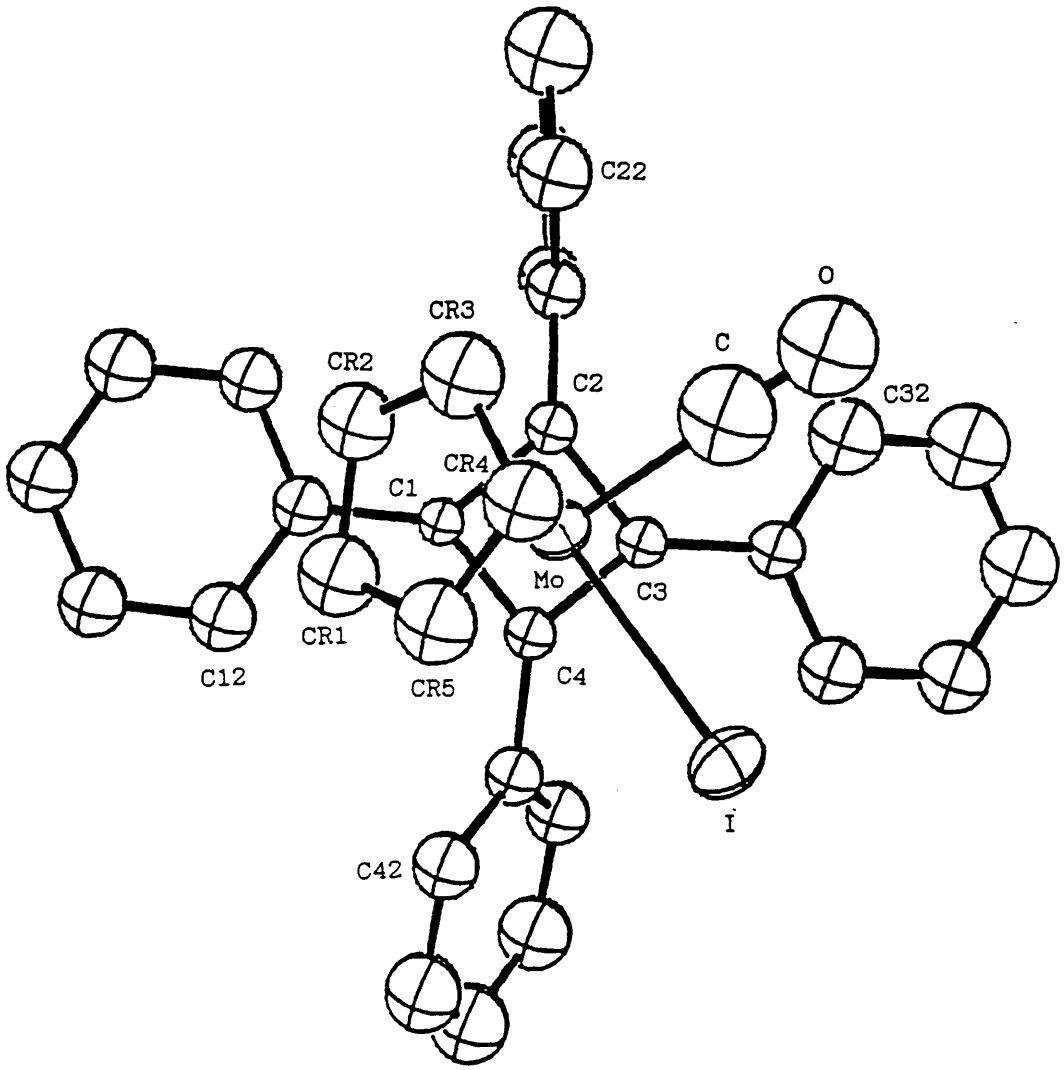
4.1 The Structure of $[CpMoI(CO)(C_4Ph_4)].CH_2Cl_2$ Black Isomer

The complex $[CpMoI(CO)(C_4Ph_4)].CH_2Cl_2$, (19) exists in two isomeric forms. Recrystallisation from hexane gives yellow crystals. On dissolving the yellow crystals in dichloromethane a yellow solution is obtained. This slowly turns black and deposits isomeric black crystals. To determine the nature of the isomerism it was decided to carry out crystal structure analyses of the yellow and black forms of (19). Unfortunately, Dr.J.L. Davidson was able to obtain diffraction quality crystals only of the black isomer whose structure is described below. Work on obtaining crystals of the yellow isomer is continuing at Heriot-Watt.

The black crystals of complex (19) contain well separated molecules of the type shown in Figure 4(a) and of dichloromethane, the solvent of crystallisation, in equal numbers (see Table 4.2 for bond distances and angles). The structure is of the form (18) shown in Scheme III in Chapter 3. The molybdenum atom has bonded to it in a tetrahedral arrangement a cyclopentadienyl ring, a cyclobutadienyl ring with phenyl substituents and disordered molecules of iodine and carbonyl.

In Figure 4(a) the site marked I is a superposition of $\alpha I + (1-\alpha)CO$ where $\alpha = 0.754(3)$. The second site I' contains $\alpha CO + (1-\alpha)I$. During the refinement the Mo-C-O and Mo-I vectors were constrained to coincide and the C-O distances was fixed at 1.15 Å. The Mo-I distances are

Figure 4(a). The structure of the major isomer of complex (19). For clarity hydrogen atoms are omitted. 50% probability ellipsoids are displayed for all atoms shown.



2.762(2) and 2.739(7) Å.

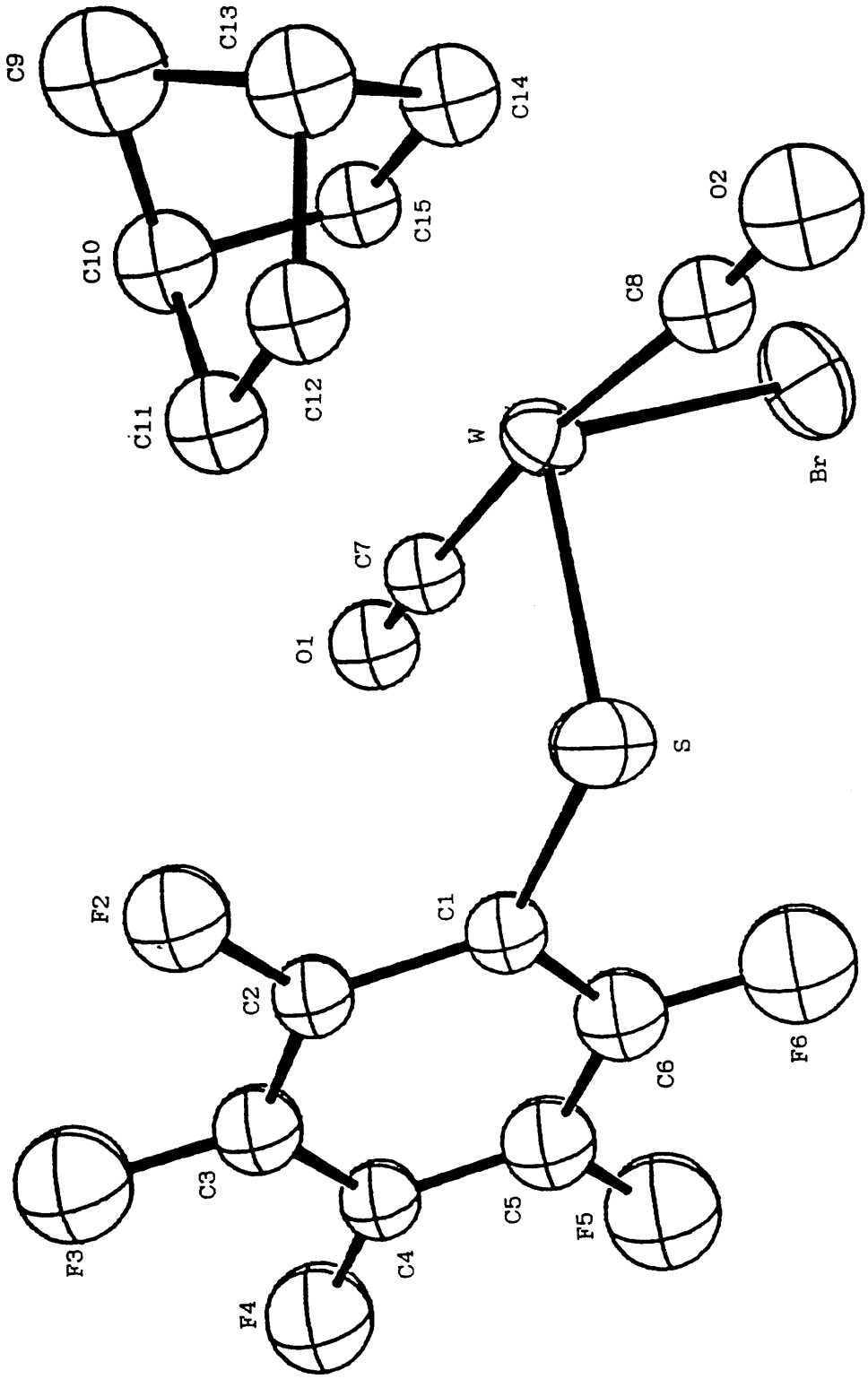
The cyclopentadienyl ring geometry is similar to those described in Chapter 3. Mo-C distances range from 2.307(17) to 2.339(18) Å and C-C distances from 1.36(3) to 1.42(3) Å. The Mo-C distances involving the cyclobutadienyl ligand are significantly shorter than those involving the five membered ring [2.231(14)-2.302(14) Å]. The ring C-C distances range from 1.450(20) to 1.478(20) Å and suggest that the π-bonding within the ring is delocalised over all four bonds. The phenyl substituents are staggered to reduce mutual steric interaction, resulting in two rings being roughly coplanar with the cyclobutadienyl ring [torsion angles C(2)-C(3)-C(31)-C(32) 4.5(15)° and C(4)-C(1)-C(11)-C(12) 11.6(15)°] and the other two clearly out of the plane [C(3)-C(4)-C(41)-C(42) 138.8(23)° and C(1)-C(2)-C(21)-C(22) 102.8(21)°].

It is difficult from the structure of the black form of (19) alone to suggest how the isomerism shown by (19) arises.

4.2 The Structure of $[WBr(CO)_2(SC_6F_5)(C_7H_8)]$

The complex $[WBr(CO)_2(SC_6F_5)(C_7H_8)]$, (20), shows unexpected fluxionality in that the six norbornadiene C-H groups are inequivalent at low temperature in the ^1H N.M.R. spectrum whereas at higher temperatures only three C-H resonances are observed. Restricted ratation about the W-S bond is one possible explanation for these observations. Alternatively, monomer-dimer equilibrium might explain them. A crystal structure analysis of (20) has accordingly

Figure 4(b). A view of complex (20). Hydrogen atoms are omitted and 50% ellipsoids are displayed for all other atoms.



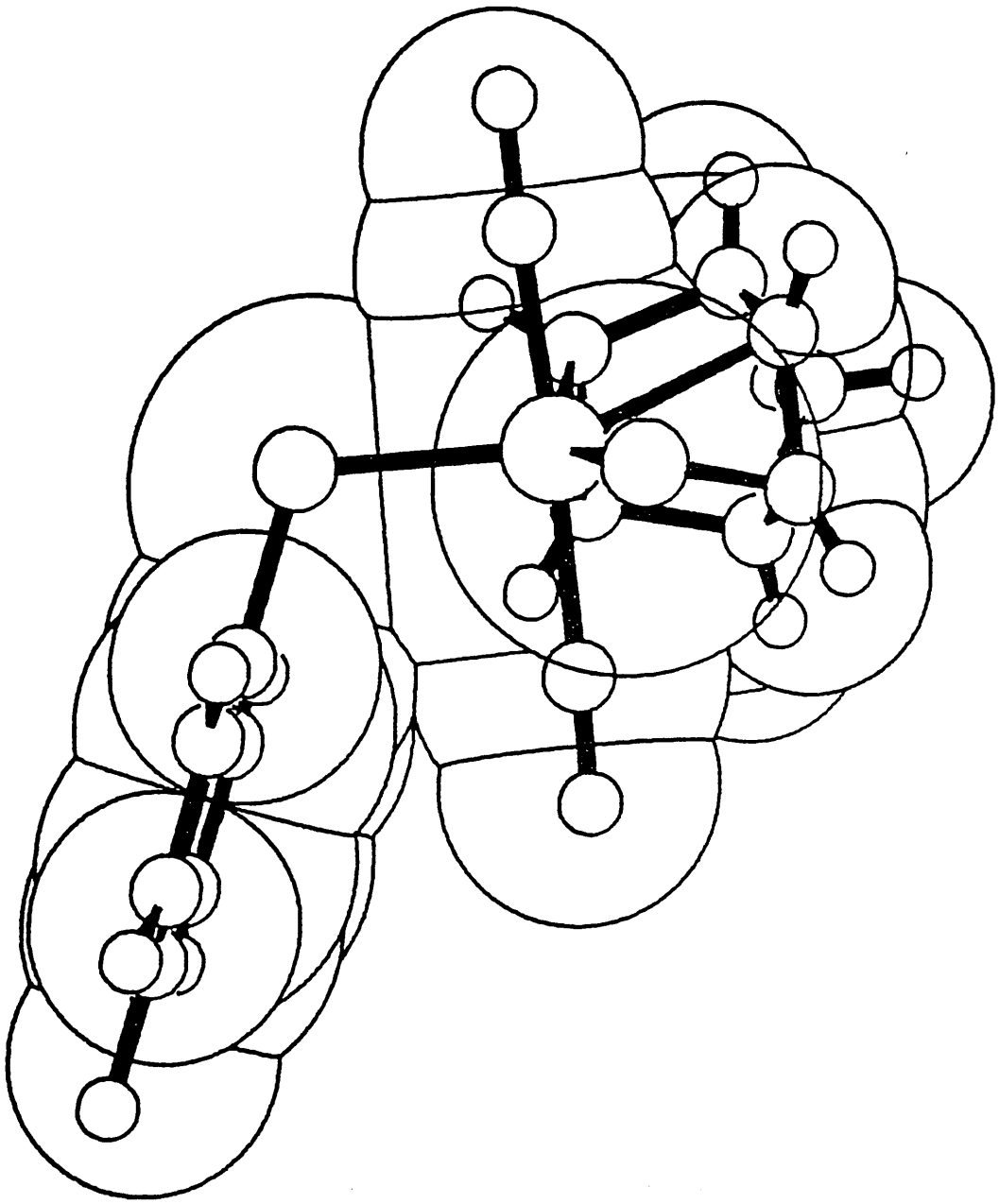
been carried out to see if the solid state structure at ambient temperature offers any explanation of the fluxionality.

Crystals of (20) are built of the well separated mononuclear molecules shown in Figure 4(b). The 16-electron divalent tungsten atom displays distorted octahedral coordination with mutually *trans* carbonyl ligands normal to a basal plane containing *cis* S and Br atoms respectively *trans* to the centroids of the C(14)-C(15) and C(11)-C(12) norbornadiene double bonds (see Table 4.4). The geometries of the penta-fluorophenylthiolato and norbornadiene ligands present no unusual features. Two features of the metal coordination merit comment: (i) the rather short W-S distance of 2.322(5) Å which lies at the lower end of the range of M(II)-S (M = Mo, W) distances observed in compounds discussed in this section of the thesis and (ii) the strong *trans*-influence exerted by the sulphur atom evident in the W-C(norbornadiene) distances of 2.38(2) and 2.40(2) Å *trans* to S compared with W-C distances of 2.23(3) and 2.28(2) Å *trans* to Br.

Inspection of interligand non-bonded distances confirms the conclusion, evident from Figure 4(c) which shows a space-filling view of the molecule, that steric effects leading to restricted rotation about the W-S bond do not provide a plausible explanation for the fluxionality.

However, the structural results are at least consistent with restricted rotation about the W-S bond arising from the electronic nature of the molecule. Only two of the t_{2g} orbitals can be filled and the strong π-acidity of carbonyl suggests that the vacant t_{2g} orbital will lie in the basal

Figure 4(c). Space filled view of complex (20) using van der Waal radii [52] to calculate shells.



plane containing the S and Br atoms. S→W π-donation is thereby favoured and is consistent with the short W-S bond length. On the assumption that the sulphur hybridisation is closer to sp^2 than sp^3 the multiple S-W bonding could thereby lead to locking of the thiolato conformation at low temperature. The flow of charge from S to W is also consistent with the high thiolato *trans*-influence.

4.3 Experimental

A fuller description of the experimental procedure is given in Chapter 2. Only deviations from the method described there are noted below.

$[CpMoI(CO)(PhCCPh)_2].CH_2Cl_2$ (19)

Data Collection. The cell dimensions and experimental parameters are listed in Table 4.5. A decomposition correction was applied which allowed for the 45% reduction in the mean intensity of the standard reflections.

Structure Analysis. The phenyl ring carbon atom positions were idealised [C-C distances 1.38 Å, C-C-C angles 120°] and refined as groups. All hydrogen atom positions were geometrically calculated. Phenyl hydrogens were included in the group refinement. Other hydrogen atoms were set to ride on their parent carbon atoms.

The disordered I and CO groups were treated thus: Mo-C distances were set at 1.97 Å and C-O distances at 1.15 Å along the Mo-I vectors. Atoms C' and O', and atoms C and O were set to ride on the I and I' atoms respectively. The

occupancy, α, of I was refined and those of C and O constrained to equal its value. Occupancies of C', O' and I' were constrained to $1-\alpha$.

Anisotropic displacement parameters were used for the Cl, Mo and I atoms. Atoms C, O, C' and O'had their displacement parameters set to and constrained to the I' isotropic displacement parameter. All other atoms were given isotropic displacement parameters and those of the hydrogen atoms were constrained to equal 1.2U(C). Final atomic positions and displacement parameters are listed in Table 4.1

$[WBr(CO)_2(SC_6F_5)(C_7H_8)]$ (20)

Data Collection. The cell dimensions and experimental parameters are given in Table 4.5. No decomposition correction was applied. Two scale factors were used because it was necessary to reallign the crystal after 1665 reflections.

The horizontal diffracted beam aperture was set at its minimum, 1.3mm, by mistake. The refinement, final individual ΔF values and the final difference synthesis do not suggest that major systematic errors in results have arisen in consequence.

Structure Analysis. Anisotropic displacement parameters were used for the W, Br, and S atoms. Isotropic parameters were used for all other atoms. The hydrogen atom positions were calculated geometrically and constrained to ride on their carbon atoms. U(H) were constrained to 1.2U(C). Final atomic positions and displacement parameters are given in

Table 4.3.

Table 4.1. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (19).

	X/A	Y/B	Z/C	U
I	.08717(13)	-.29229(8)	.04775(5)	.047
I'	-.2040(5)	-.2555(4)	.0965(2)	.091(2)
MO	-.02139(11)	-.17309(7)	.07579(5)	.034
CL(1)	-.4710(7)	-.0081(4)	.0839(4)	.201
CL(2)	-.2767(9)	.0671(5)	.0628(6)	.315
O'	.10121	-.30772	.04411	.091
O	-.22790	-.26623	.09919	.091
C'	.05602	-.25807	.05583	.091
C	-.15117	-.23162	.09050	.091
C(1)	.0602(11)	-.0997(7)	.1317(5)	.023(4)
C(2)	-.0370(12)	-.1358(7)	.1529(5)	.027(4)
C(3)	.0311(11)	-.1994(7)	.1542(5)	.027(4)
C(4)	.1238(11)	-.1632(8)	.1298(5)	.028(4)
C(11)	.0894(13)	-.0269(4)	.1273(5)	.035(4)
C(12)	.1960(13)	-.0079(5)	.1108(6)	.048(5)
C(13)	.2233(7)	.0605(6)	.1063(4)	.049(5)
C(14)	.1441(11)	.1100(4)	.1183(4)	.050(5)
C(15)	.0375(11)	.0910(5)	.1349(6)	.053(5)
C(16)	.0101(7)	.0226(6)	.1394(4)	.041(5)
C(21)	-.1303(15)	-.1081(4)	.1848(7)	.037(4)
C(22)	-.2379(16)	-.0942(8)	.1669(3)	.057(5)
C(23)	-.3183(9)	-.0639(9)	.1969(6)	.080(7)
C(24)	-.2911(13)	-.0475(4)	.2448(6)	.060(5)
C(25)	-.1834(14)	-.0613(8)	.2627(3)	.063(6)
C(26)	-.1031(6)	-.0917(9)	.2327(7)	.047(5)
C(31)	.0143(9)	-.2644(6)	.1802(5)	.034(4)
C(32)	-.0831(12)	-.2761(7)	.2074(7)	.061(5)
C(33)	-.0953(9)	-.3364(5)	.2333(5)	.079(6)
C(34)	-.0101(9)	-.3851(5)	.2320(4)	.071(6)
C(35)	.0873(11)	-.3734(7)	.2048(6)	.057(5)
C(36)	.0995(9)	-.3131(5)	.1789(4)	.047(5)
C(41)	.2485(7)	-.1790(8)	.1248(6)	.035(4)
C(42)	.3032(9)	-.1682(10)	.0806(5)	.046(4)
C(43)	.4194(10)	-.1779(5)	.0770(3)	.064(5)
C(44)	.4810(7)	-.1984(7)	.1176(5)	.070(6)
C(45)	.4262(9)	-.2093(8)	.1618(5)	.064(5)
C(46)	.3100(11)	-.1996(4)	.1654(4)	.045(5)
C(R1)	.0308(15)	-.0894(9)	.0186(6)	.059(5)
C(R2)	-.0746(15)	-.0700(9)	.0401(6)	.052(5)
C(R3)	-.1535(15)	-.1176(10)	.0265(6)	.061(6)
C(R4)	-.1004(14)	-.1699(9)	-.0017(6)	.053(5)
C(R5)	.0116(15)	-.1488(9)	-.0078(6)	.060(5)
C(S)	-.391(3)	.066(2)	.092(1)	.159(11)
H(12)	.25111	-.04230	.10238	.057
H(13)	.29748	.07376	.09473	.058
H(14)	.16309	.15759	.11518	.060
H(15)	-.01770	.12540	.14323	.063
H(16)	-.06408	.00934	.15089	.049
H(22)	-.25689	-.10566	.13356	.068
H(23)	-.39317	-.05426	.18441	.096
H(24)	-.34697	-.02637	.26563	.072
H(25)	-.16450	-.04993	.29605	.075
H(26)	-.02824	-.10130	.24520	.056
H(32)	-.14238	-.24218	.20836	.073
H(33)	-.16301	-.34444	.25228	.095
H(34)	-.01854	-.42703	.25003	.085
H(35)	.14660	-.40731	.20392	.068
H(36)	.16725	-.30504	.16001	.056
H(42)	.26038	-.15384	.05232	.056
H(43)	.45745	-.17029	.04620	.077
H(44)	.56185	-.20512	.11511	.084
H(45)	.46904	-.22363	.19009	.077
H(46)	.27197	-.20708	.19620	.054
H(R1)	.10220	-.06567	.02122	.070
H(R2)	-.08718	-.03086	.06081	.062
H(R3)	-.23305	-.11624	.03476	.073
H(R4)	-.13534	-.21073	-.01434	.063
H(R5)	.06742	-.17280	-.02710	.072
H(S1)	-.37310	.06974	.12657	.191
H(S2)	-.43607	.10469	.08265	.191

Table 4.1(cont).

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
I	.0505(10)	.0441(11)	.0466(10)	.0081(10)	-.0070(9)	-.0097(10)
MO	.0331(8)	.0352(9)	.0333(8)	.0039(9)	-.0043(8)	-.0015(9)
CL(1)	.140(7)	.161(8)	.302(12)	-.005(6)	-.074(8)	.022(9)
CL(2)	.197(10)	.168(9)	.579(22)	.080(8)	.234(13)	.124(12)

Table 4.2. Selected bond distances ($Å$) and angles (°) of complex (19).

I	- MO	2.762(3)	I'	- MO	2.739(7)
MO	- C'	1.969	MO	- C	1.946
MO	- C(1)	2.302(14)	MO	- C(2)	2.231(14)
MO	- C(3)	2.282(13)	MO	- C(4)	2.259(13)
MO	- C(R1)	2.339(18)	MO	- C(R2)	2.322(17)
MO	- C(R3)	2.319(18)	MO	- C(R4)	2.307(17)
MO	- C(R5)	2.359(17)	MO	- C(BU)	2.020
MO	- C(CP)	2.004	CL(1)	- C(S)	1.74(4)
CL(2)	- C(S)	1.57(4)	C(1)	- C(2)	1.461(19)
C(1)	- C(4)	1.450(20)	C(1)	- C(11)	1.467(17)
C(2)	- C(3)	1.478(20)	C(2)	- C(21)	1.499(22)
C(3)	- C(4)	1.458(19)	C(3)	- C(31)	1.468(19)
C(4)	- C(41)	1.502(16)	C(R1)	- C(R2)	1.42(3)
C(R1)	- C(R5)	1.38(3)	C(R2)	- C(R3)	1.36(3)
C(R3)	- C(R4)	1.42(3)	C(R4)	- C(R5)	1.39(3)

I	- MO	- I'	85.6(2)	I	- MO	- C(BU)	105.2
I	- MO	- C(CP)	108.2	I'	- MO	- C(BU)	104.4
I'	- MO	- C(CP)	108.3	C(BU)	- MO	- C(CP)	134.3
C(2)	- C(1)	- C(4)	90.1(11)	C(2)	- C(1)	- C(11)	133.1(13)
C(4)	- C(1)	- C(11)	135.0(12)	C(1)	- C(2)	- C(3)	89.6(11)
C(1)	- C(2)	- C(21)	128.6(12)	C(3)	- C(2)	- C(21)	133.3(12)
C(2)	- C(3)	- C(4)	89.2(11)	C(2)	- C(3)	- C(31)	131.8(12)
C(4)	- C(3)	- C(31)	137.7(13)	C(1)	- C(4)	- C(3)	90.8(11)
C(1)	- C(4)	- C(41)	132.9(13)	C(3)	- C(4)	- C(41)	132.0(13)
C(1)	- C(11)	- C(12)	119.9(11)	C(1)	- C(11)	- C(16)	120.1(13)
C(2)	- C(21)	- C(22)	122.3(15)	C(2)	- C(21)	- C(26)	117.5(14)
C(3)	- C(31)	- C(32)	120.8(12)	C(3)	- C(31)	- C(36)	119.1(11)
C(4)	- C(41)	- C(42)	120.0(13)	C(4)	- C(41)	- C(46)	119.8(13)
C(R2)	- C(R1)	- C(R5)	107.3(16)	C(R1)	- C(R2)	- C(R3)	107.3(16)
C(R2)	- C(R3)	- C(R4)	109.9(16)	C(R3)	- C(R4)	- C(R5)	105.5(16)
C(R1)	- C(R5)	- C(R4)	109.9(16)	CL(1)	- C(S)	- CL(2)	114.1(19)

Table 4.3. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (20).

	X/A	Y/B	Z/C	U
W	-.19348(7)	.23035(6)	-.24149(5)	.031
BR	-.0174(2)	.3613(2)	-.2044(2)	.057
S	-.3496(4)	.2407(4)	-.1098(3)	.042
F(2)	-.3934(9)	.0198(8)	-.0730(8)	.050(3)
F(3)	-.3180(11)	-.0885(10)	.0966(9)	.070(3)
F(4)	-.1881(11)	-.0041(9)	.2623(9)	.069(3)
F(5)	-.1298(12)	.1933(10)	.2568(9)	.079(4)
F(6)	-.2000(12)	.3027(10)	.0873(9)	.074(4)
O(1)	-.0055(12)	.0928(10)	-.0955(9)	.047(3)
O(2)	-.3714(13)	.3863(11)	-.3672(10)	.060(4)
C(1)	-.3004(16)	.1662(14)	.0014(12)	.032(4)
C(2)	-.3275(16)	.0646(14)	.0077(12)	.033(4)
C(3)	-.2895(17)	.0103(15)	.0942(14)	.042(5)
C(4)	-.2243(16)	.0534(15)	.1776(13)	.035(4)
C(5)	-.1941(18)	.1474(16)	.1728(15)	.049(5)
C(6)	-.2323(17)	.2064(15)	.0866(13)	.044(5)
C(7)	-.0739(16)	.1394(14)	-.1498(13)	.035(4)
C(8)	-.3044(17)	.3317(15)	-.3166(13)	.038(4)
C(9)	-.1958(22)	.0571(18)	-.4821(17)	.071(7)
C(10)	-.1287(19)	.0515(16)	-.3674(15)	.052(5)
C(11)	-.2483(19)	.0768(16)	-.2971(13)	.047(5)
C(12)	-.3243(18)	.1418(15)	-.3592(14)	.044(5)
C(13)	-.2526(19)	.1596(16)	-.4621(14)	.053(5)
C(14)	-.1333(18)	.2171(15)	-.4238(14)	.048(5)
C(15)	-.0549(16)	.1485(14)	-.3644(13)	.037(4)
H(9A)	-.26245	.00674	-.49518	.085
H(9B)	-.13353	.05553	-.53843	.085
H(10)	-.09493	-.01413	-.35154	.062
H(11)	-.25495	.03157	-.23829	.057
H(12)	-.41891	.14256	-.35029	.053
H(13)	-.31410	.17987	-.51806	.063
H(14)	-.12667	.28113	-.45771	.057
H(15)	.03496	.14140	-.33698	.044

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
W	.0309(4)	.0311(5)	.0298(4)	.0032(5)	.0008(3)	.0059(4)
BR	.046(1)	.046(2)	.077(1)	-.011(1)	-.007(1)	.009(1)
S	.041(2)	.047(4)	.038(2)	.013(3)	.005(2)	.006(2)

Table 4.4. Selected bond distances (Å) and angles (°) of complex (20).

W	-	BR	2.521(3)	W	-	S	2.322(5)
W	-	C(7)	2.040(18)	W	-	C(8)	1.975(19)
W	-	C(11)	2.233(21)	W	-	C(12)	2.279(19)
W	-	C(14)	2.397(18)	W	-	C(15)	2.380(17)
W	-	C(A)	2.148	W	-	C(B)	2.282
S	-	C(1)	1.774(17)	F(2)	-	C(2)	1.34(2)
F(3)	-	C(3)	1.35(3)	F(4)	-	C(4)	1.35(3)
F(5)	-	C(5)	1.37(3)	F(6)	-	C(6)	1.33(3)
O(1)	-	C(7)	1.14(3)	O(2)	-	C(8)	1.17(3)
C(1)	-	C(2)	1.39(3)	C(1)	-	C(6)	1.36(3)
C(2)	-	C(3)	1.35(3)	C(3)	-	C(4)	1.35(3)
C(4)	-	C(5)	1.30(3)	C(5)	-	C(6)	1.38(3)
C(9)	-	C(10)	1.57(3)	C(9)	-	C(13)	1.51(4)
C(10)	-	C(11)	1.55(3)	C(10)	-	C(15)	1.49(3)
C(11)	-	C(12)	1.38(3)	C(12)	-	C(13)	1.52(3)
C(13)	-	C(14)	1.49(3)	C(14)	-	C(15)	1.41(3)

BR	-	W	-	S	108.2(2)	BR	-	W	-	C(7)	85.1(6)
BR	-	W	-	C(B)	89.6(6)	BR	-	W	-	C(A)	155.2
BR	-	W	-	C(B)	91.5	S	-	W	-	C(7)	91.8(5)
S	-	W	-	C(B)	85.2(5)	S	-	W	-	C(A)	96.6
S	-	W	-	C(B)	160.1	C(7)	-	W	-	C(B)	172.7(8)
C(7)	-	W	-	C(A)	94.3	C(7)	-	W	-	C(B)	92.5
C(8)	-	W	-	C(A)	92.7	C(8)	-	W	-	C(B)	92.6
C(A)	-	W	-	C(B)	63.7	W	-	S	-	C(1)	110.6(6)
S	-	C(1)	-	C(2)	123.0(12)	S	-	C(1)	-	C(6)	121.2(15)
C(2)	-	C(1)	-	C(6)	115.8(16)	F(2)	-	C(2)	-	C(1)	119.3(15)
F(2)	-	C(2)	-	C(3)	119.3(17)	C(1)	-	C(2)	-	C(3)	121.4(16)
F(3)	-	C(3)	-	C(2)	119.3(16)	F(3)	-	C(3)	-	C(4)	119.9(17)
C(2)	-	C(3)	-	C(4)	120.9(19)	F(4)	-	C(4)	-	C(3)	118.7(18)
F(4)	-	C(4)	-	C(5)	122.1(16)	C(3)	-	C(4)	-	C(5)	119.1(18)
F(5)	-	C(5)	-	C(4)	120.3(18)	F(5)	-	C(5)	-	C(6)	117.5(19)
C(4)	-	C(5)	-	C(6)	122.0(18)	F(6)	-	C(6)	-	C(1)	120.3(16)
F(6)	-	C(6)	-	C(5)	119.1(16)	C(1)	-	C(6)	-	C(5)	120.7(19)
W	-	C(7)	-	O(1)	176.5(16)	W	-	C(8)	-	O(2)	174.8(16)
C(10)	-	C(9)	-	C(13)	92.5(16)	C(9)	-	C(10)	-	C(11)	101.3(15)
C(9)	-	C(10)	-	C(15)	100.3(16)	C(11)	-	C(10)	-	C(15)	100.9(16)
C(10)	-	C(11)	-	C(12)	103.8(15)	C(11)	-	C(12)	-	C(13)	108.1(16)
C(9)	-	C(13)	-	C(12)	101.0(17)	C(9)	-	C(13)	-	C(14)	102.6(17)
C(12)	-	C(13)	-	C(14)	101.8(15)	C(13)	-	C(14)	-	C(15)	105.3(17)
C(10)	-	C(15)	-	C(14)	106.5(15)						

Table 4.5. Crystallographic and experimental details of the structure analyses of complexes (19) and (20).

Compound	[CpMoI(CO)(PhCCPh)$_2$].CH_2Cl_2	[WBr(CO)$_2$(SC_6F_5)(C_7H_8)]
Formula	$C_{35}H_{27}Cl_2MoOI$	$C_{15}H_8BrF_5O_2SW$
Formula Wt.	757.4	611.0
Crystal habit	dark purple plate	purple plate
Crystal size, mm	0.30x0.20x0.32	0.36x0.16x0.02
Crystal system	orthorhombic	monoclinic
Space group	Pbca (No.61)	P $2_1/n$
a, Å	11.736(4)	10.040(4)
b, Å	19.538(4)	13.379(4)
c, Å	27.238(4)	12.575(3)
β, °	—	91.88(3)
Obtained from	23 refln, 9<θ<14°	23 refln, 11<θ<15°
V, Å^3	6246(3)	1688.2(8)
Z	8	4
F(000)	2992	1136
d calc, gcm^{-3}	1.611	2.404
T, K	296	293
μ(Mo-Kα), cm^{-1}	15.9	95.1
Absorption factors on F^2	0.91-1.10	0.80-1.32
Scan width, °	0.80	0.80
Max count time, s	100	90
Total refln measured	4284	3936
Unique refln	3806	2640
R_{INT}	—	0.063
Miller indicies h	0→12	0→11
measured, k	0→20	-15→ 4
l	0→29	-14→14
2θ range, °	4-44	4-48
Unique refln ≥ 3σ(I)	1385	1587
No. of parameters	130	116
R	0.047	0.052
R_w	0.053	0.056
$\|\Delta\rho\|_{max}$, eÅ^{-3}	0.70	2.3
Δ/σ_{max}	0.04	0.026

SECTION III: MISCELLANEOUS STRUCTURES

CHAPTER 1: A SULPHIMIDE COMPLEX OF PALLADIUM

The succesful clinical exploitation of the complex Cisplatin, *cis*-$[PtCl_2(NH_3)_2]$,[113] has led to an expansion in research to find structural analogues of the complex which would have similar chemotherapeutic properties but reduced toxicity.[114] One such group of complexes is comprised of $[PtCl_2L_2]$ species where L is a heterocyclic ligand.

A number of palladium and platinum complexes containing heterocyclic sulphimide ligands were synthesised by Dr J.L. Davidson and his group but were found to form dimers, with bridging chlorine atoms. These compounds were insoluble in most solvents and therefore could not be purified. However, it was possible to split these dimers, particularly the palladium complexes, by reaction with phosphines such as L = PEt_3, PMe_2Ph, $PMePh_2$ and PPh_3, to produce complexes of the form $[PdCl_2L(Me_2SNR)]$.

When R = 2-pyridyl or 2-pyrimidinyl, so that there is at least one heteroaromatic ring nitrogen as well as the ylide nitrogen present in the ligand, four possible isomers of $[PdCl_2L(Me_2SNR)]$ can exist. The chloride ligands can be either *cis* or *trans* and the sulphimide ligand can bond either through the ylide nitrogen or the ring nitrogen atom.

Since N.M.R. could not conclusively distinguish which structures were formed, X-ray diffraction analysis was used to determine the precise nature of the metal coordination. When L = PEt_3 and R = 2-pyridyl, (1), it was found that the complex was *trans*-square planar and that the sulphimide ligand bonded via the ylide nitrogen with the R-N-S plane

approximately normal to the square plane of the metal.[115]

The N.M.R. data for the complex with L = PPh_3 and R = 2-pyrimidinyl, (2), differed from (1). The most notable difference was that in complex (1) the methyl groups attached to the sulphur atom were equivalent whereas in (2) they clearly differ. Consequently an X-ray analysis was carried out to determine its structure.

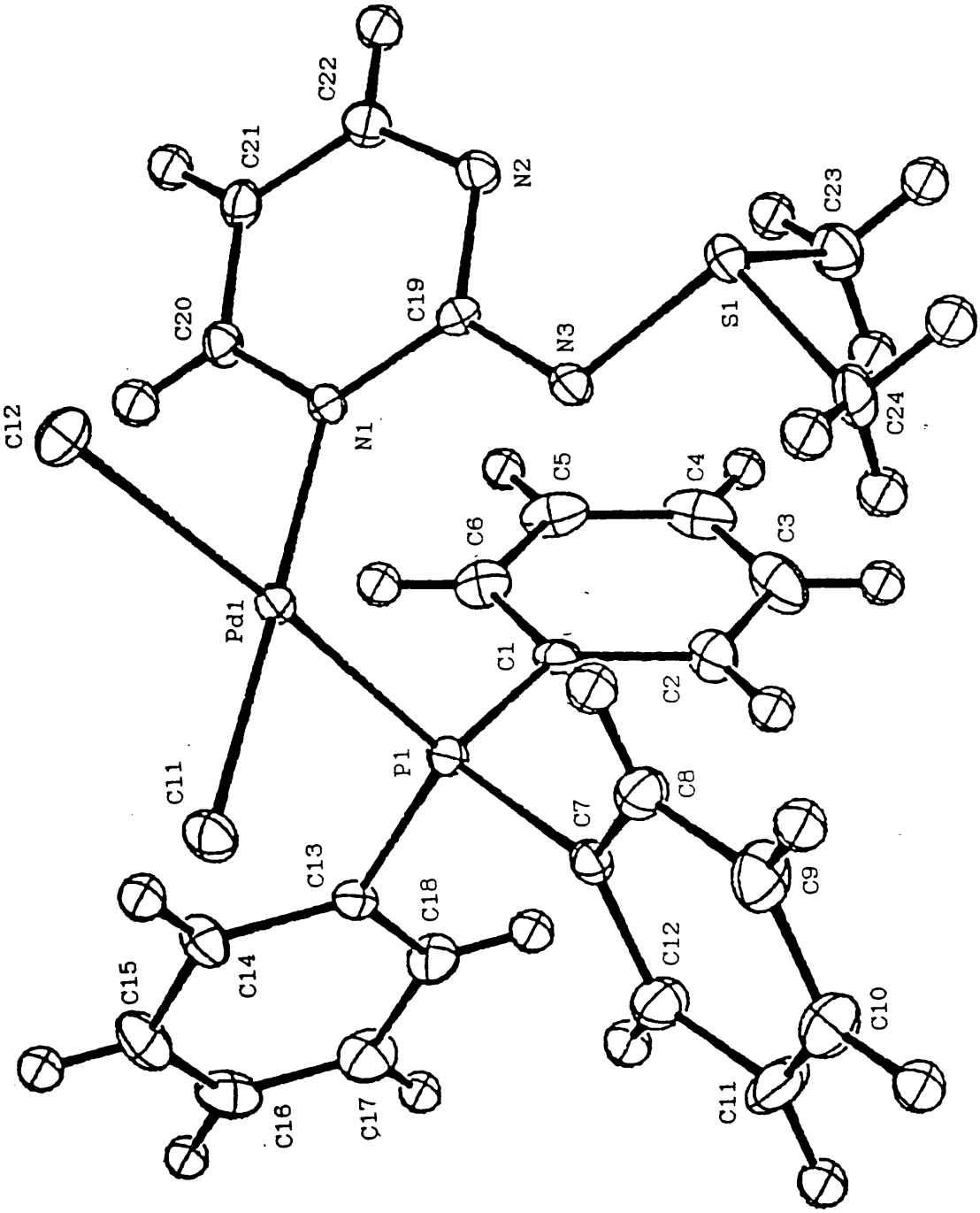
The crystals were shown to contain distinct molecules of complex (2) and of dichloromethane in equal numbers. Intermolecular contacts were consistent with appropriate van der Waals radii.[52]

Complex (2) (see Figure 1(a) and Tables 1.1 and 1.2)[116] consists of a central palladium atom with two chlorine atoms, a triphenylphosphine, and the $Me_2SNC_4H_3N_2$ sulphimide ligand attached to it in a square planar arrangement with the chloro ligands mutually *cis*. The sulphimide ligand is bonded to the palladium via a nitrogen atom of the pyrimidine ring. The Pd-N bond length of 2.022(5) Å is considerably shorter than that in *cis*-$[PdCl_2$-$(Bu^tPCH_2C_{10}H_8N)]$, of 2.078(4) Å, the only other *cis*-$PdCl_2PN$ sp^2 structure characterized.[117] However this could be due to intramolecular overcrowding in the latter complex.

A comparison of the geometry of the sulphimide ligand of (2) with free sulphimides show no major differences.[115,118] The short N(3)-C(19) bond length in (2) [1.332(7) Å compared to 1.366(6)-1.395(6) Å] and the C-N-S-Me torsion angles [-77.4(5) and -179.6(5)° compared to 92-100 and 157-164°] are the most obvious differences.

The PPh_3 ligand is attached to the palladium atom by a Pd-P single bond, length 2.246(2) Å, which is consistent

Figure 1(a). A view of complex (2). 50% probability ellipsoids are displayed for all atoms shown.



with other *cis*-$PdCl_2PN$ species.[117,119] The internal geometry of the PPh_3 ligand appears unaffected by coordination to the palladium atom, with the Pd-P-C-C torsion angles [16.0(5), 28.1(5) and 59.0(5)°] similar to those for solid PPh_3 [l.p.-P-C-C 21.7, 32.7 and 56.2°, l.p. = lone pair].[120]

The Pd-Cl(1) bond distance is 0.085(3) Å shorter than that for Pd-Cl(2). This is probably due to the higher *trans*-influence of the phosphine compared with the nitrogen atom. This effect is confirmed in other *cis*-$PdCl_2PN$ structures characterised.[117,119]

The bonding of the sulphimide ligand to the palladium atom through atom N(1) differs from *trans*-[$PdCl_2(PEt_3)$-($Me_2SNC_5H_4N$)], (1), where bonding is via the sulphimide nitrogen atom rather than that of the pyridine ring.[115] This does not appear to be due to steric effects. A plot of the conformation energy [121] of complex (2) as a function of the torsion angles ω_1 = N(1)-Pd(1)-P(1)-C(1) and ω_2 = P(1)-Pd(1)-N(1)-C(19) had its lowest local minimum close to the conformation found in the crystal structure of complex (2). When a similar calculation was carried out on the hypothetical molecule with the metal atom attached to atom N(3), rather than atom N(1), a local minimum of comparable energy to that above was found. An inspection of this conformation showed there to be no abnormally short non-bonded distances.

This suggests that electronic factors probably determine the mode of attachment of the sulphimide ligand in structures (1) and (2). However, the effect of a change in *trans* ligand together with a possible change in the

donor properties of the sulphimide nitrogen relative to the differing heteroaromatic ring nitrogens makes the exact reason difficult to predict. It should be noted however that the pyridine nitrogen atom is considerably more basic than the pyrimidine nitrogen atom [pK_a = 5.6, pK_{a1} = 1.3 respectively].[122]

Experimental

The experimental procedure used for this structure is broadly similar to that described more fully in Chapter 2 of Section II. Only differences between the two methods are mentioned below.

Data Collection. The cell dimensions and experimental parameters are listed in Table 1.3. No decomposition correction was applied.

Structure Analysis. Anisotropic displacement parameters were used for all non-hydrogen atoms. All the hydrogen atoms were calculated geometrically (C-H Ø.96 Å) and constrained to ride on their parent carbon atom. Isotropic displacement parameters were used for the hydrogen atoms and set at $1.2U_{ISO}(C)$ but not refined. Conformational energy calculations were made on a Uman computer using the Chemmod package.[121]

Table 1.1. Fractional atomic coordinates and displacement parameters ($Å^2$) of the crystal structure of complex (2).

	X/A	Y/B	Z/C	U
PD(1)	.13484(2)	-.02586(5)	.06308(2)	.028
CL(1)	.16331(9)	-.26864(16)	.05638(9)	.044
CL(2)	.02778(9)	-.07232(18)	.13044(8)	.047
CL(3)	.55382(15)	-.88938(31)	.22358(19)	.135
CL(4)	.53335(18)	-.60839(33)	.15375(15)	.127
S(1)	.26966(9)	.31325(17)	.22255(8)	.037
P(1)	.23098(8)	.01252(17)	-.00784(7)	.032
N(1)	.1086(3)	.1862(5)	.0768(2)	.031
N(2)	.1303(3)	.4006(5)	.1516(3)	.036
N(3)	.2228(3)	.2130(5)	.1548(2)	.033
C(1)	.2538(3)	.2025(6)	-.0237(3)	.036
C(2)	.3274(4)	.2610(7)	-.0035(4)	.050
C(3)	.3411(5)	.4072(9)	-.0174(4)	.074
C(4)	.2826(6)	.4941(8)	-.0497(4)	.076
C(5)	.2097(5)	.4365(8)	-.0702(4)	.063
C(6)	.1960(4)	.2919(7)	-.0580(4)	.052
C(7)	.3218(3)	-.0721(6)	.0315(3)	.036
C(8)	.3353(3)	-.0908(7)	.1091(3)	.047
C(9)	.4023(4)	-.1555(9)	.1412(4)	.062
C(10)	.4572(4)	-.2003(9)	.0986(5)	.073
C(11)	.4461(4)	-.1807(10)	.0225(4)	.074
C(12)	.3778(4)	-.1194(8)	-.0101(3)	.056
C(13)	.2095(3)	-.0543(6)	-.1045(3)	.036
C(14)	.1494(4)	-.1514(7)	-.1238(3)	.049
C(15)	.1335(4)	-.1982(8)	-.1972(4)	.063
C(16)	.1768(5)	-.1485(9)	-.2512(4)	.066
C(17)	.2360(4)	-.0541(9)	-.2329(4)	.065
C(18)	.2522(3)	-.0048(7)	-.1592(3)	.052
C(19)	.1537(3)	.2692(6)	.1288(3)	.029
C(20)	.0401(3)	.2404(7)	.0473(3)	.035
C(21)	.0140(3)	.3736(7)	.0677(3)	.040
C(22)	.0610(4)	.4482(6)	.1204(3)	.043
C(23)	.3104(4)	.4680(7)	.1816(3)	.054
C(24)	.3544(3)	.2050(7)	.2393(3)	.048
C(25)	.5805(5)	-.7084(11)	.2282(5)	.096
H(2)	.36847	.19985	.01972	.059
H(3)	.39207	.44703	-.00316	.087
H(4)	.29245	.59510	-.05868	.088
H(5)	.16857	.49768	-.09341	.076
H(6)	.14508	.25207	-.07228	.062
H(8)	.29650	-.05890	.13934	.057
H(9)	.41057	-.16823	.19468	.075
H(10)	.50429	-.24493	.12184	.087
H(11)	.48494	-.21263	-.00771	.084
H(12)	.36948	-.10675	-.06360	.064
H(14)	.11896	-.18590	-.08624	.055
H(15)	.09171	-.26567	-.21050	.076
H(16)	.16546	-.18155	-.30205	.077
H(17)	.26637	-.01964	-.27048	.075
H(18)	.29401	.06272	-.14589	.059
H(20)	.00836	.18359	.01039	.041
H(21)	-.03508	.41221	.04547	.048
H(22)	.04361	.54100	.13645	.049
H(23A)	.33781	.52588	.22083	.067
H(23B)	.26959	.52476	.15443	.067
H(23C)	.34568	.43674	.14754	.067
H(24A)	.38187	.26281	.27855	.055
H(24B)	.38192	.19801	.19614	.055
H(24C)	.34352	.10859	.25586	.055
H(25A)	.63571	-.70174	.22697	.113
H(25B)	.56812	-.66742	.27445	.113

Table 1.1(cont).

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
PD(1)	.0281(2)	.0282(2)	.0274(2)	-.0015(3)	.0028(2)	-.0017(2)
CL(1)	.0479(10)	.0289(9)	.0530(10)	-.0011(7)	.0046(8)	-.0003(7)
CL(2)	.0406(9)	.0559(11)	.0457(9)	.0006(8)	.0143(7)	.0093(8)
CL(3)	.083(2)	.101(2)	.223(3)	-.005(2)	.061(2)	-.007(2)
CL(4)	.142(2)	.141(3)	.095(2)	-.030(2)	.020(2)	-.001(2)
S(1)	.0359(9)	.0416(10)	.0326(8)	-.0018(7)	-.0027(7)	-.0065(7)
P(1)	.0327(8)	.0298(9)	.0317(8)	.0001(7)	.0053(6)	-.0021(7)
N(1)	.027(3)	.037(3)	.027(3)	.000(2)	0.000(2)	-.006(2)
N(2)	.035(3)	.029(3)	.043(3)	.004(2)	-.001(2)	-.005(2)
N(3)	.033(3)	.034(3)	.030(3)	0.000(2)	-.001(2)	-.006(2)
C(1)	.043(4)	.033(4)	.033(3)	.000(3)	.016(3)	-.005(3)
C(2)	.054(5)	.044(4)	.051(4)	-.011(4)	.014(3)	.005(3)
C(3)	.098(6)	.058(5)	.066(5)	-.037(5)	.025(5)	-.006(4)
C(4)	.125(7)	.040(5)	.064(5)	-.009(5)	.045(5)	.004(4)
C(5)	.085(6)	.044(5)	.062(5)	.019(4)	.033(4)	.017(4)
C(6)	.062(5)	.048(5)	.047(4)	.006(4)	.019(4)	.009(4)
C(7)	.036(3)	.033(4)	.038(3)	-.008(3)	.008(3)	-.006(3)
C(8)	.040(4)	.053(4)	.047(4)	.007(3)	.003(3)	-.003(3)
C(9)	.052(5)	.077(5)	.054(4)	.005(4)	-.011(4)	.005(4)
C(10)	.048(5)	.072(6)	.095(7)	.023(4)	-.016(5)	-.007(5)
C(11)	.042(5)	.104(7)	.076(6)	.025(4)	.015(4)	-.015(5)
C(12)	.049(4)	.074(5)	.045(4)	.012(4)	.001(4)	-.012(4)
C(13)	.039(3)	.032(4)	.035(3)	.005(3)	.004(3)	-.003(3)
C(14)	.059(5)	.048(4)	.039(4)	-.012(4)	.002(3)	-.006(3)
C(15)	.077(5)	.060(5)	.049(5)	-.009(4)	-.014(4)	-.011(4)
C(16)	.089(6)	.072(5)	.035(4)	.012(5)	.003(4)	-.016(4)
C(17)	.069(5)	.088(6)	.039(4)	.006(5)	.012(3)	-.004(4)
C(18)	.051(4)	.066(5)	.038(4)	-.003(4)	.016(3)	-.001(4)
C(19)	.029(3)	.031(4)	.028(3)	.004(3)	.007(3)	.003(3)
C(20)	.029(4)	.045(4)	.030(3)	-.002(3)	-.003(3)	-.002(3)
C(21)	.027(3)	.043(4)	.049(4)	0.000(3)	.000(3)	.001(3)
C(22)	.042(4)	.027(4)	.058(4)	.005(3)	.006(3)	-.001(3)
C(23)	.054(4)	.044(4)	.063(4)	-.003(4)	.001(3)	-.003(4)
C(24)	.040(4)	.047(4)	.053(4)	-.003(3)	-.019(3)	-.002(3)
C(25)	.090(7)	.106(8)	.090(6)	-.013(6)	.022(5)	-.021(6)

Table 1.2. Selected bond distances (Å) and angles (°) of complex (2).

PD(1) - CL(1)	2.289(2)	PD(1) - CL(2)	2.374(2)
PD(1) - P(1)	2.246(2)	PD(1) - N(1)	2.022(5)
CL(3) - C(25)	1.724(10)	CL(4) - C(25)	1.740(10)
S(1) - N(3)	1.656(5)	S(1) - C(23)	1.786(7)
S(1) - C(24)	1.767(7)	P(1) - C(1)	1.819(6)
P(1) - C(7)	1.815(6)	P(1) - C(13)	1.836(6)
N(1) - C(19)	1.372(7)	N(1) - C(20)	1.332(8)
N(2) - C(19)	1.352(8)	N(2) - C(22)	1.333(8)
N(3) - C(19)	1.332(7)	C(1) - C(2)	1.387(9)
C(1) - C(6)	1.379(9)	C(2) - C(3)	1.391(11)
C(3) - C(4)	1.361(13)	C(4) - C(5)	1.375(13)
C(5) - C(6)	1.371(10)	C(7) - C(8)	1.396(9)
C(7) - C(12)	1.367(9)	C(8) - C(9)	1.365(10)
C(9) - C(10)	1.356(11)	C(10) - C(11)	1.368(12)
C(11) - C(12)	1.374(11)	C(13) - C(14)	1.382(9)
C(13) - C(18)	1.377(8)	C(14) - C(15)	1.381(10)
C(15) - C(16)	1.375(11)	C(16) - C(17)	1.350(12)
C(17) - C(18)	1.394(9)	C(20) - C(21)	1.370(9)
C(21) - C(22)	1.355(9)		

CL(1) - PD(1) - CL(2)	92.2(1)	CL(1) - PD(1) - P(1)	86.8(1)
CL(1) - PD(1) - N(1)	175.9(2)	CL(2) - PD(1) - P(1)	176.0(1)
CL(2) - PD(1) - N(1)	84.8(2)	P(1) - PD(1) - N(1)	96.4(2)
N(3) - S(1) - C(23)	108.8(3)	N(3) - S(1) - C(24)	97.6(3)
C(23) - S(1) - C(24)	99.0(3)	PD(1) - P(1) - C(1)	115.5(2)
PD(1) - P(1) - C(7)	112.3(2)	PD(1) - P(1) - C(13)	114.0(2)
C(1) - P(1) - C(7)	106.1(3)	C(1) - P(1) - C(13)	101.2(3)
C(7) - P(1) - C(13)	106.8(3)	PD(1) - N(1) - C(19)	120.0(4)
PD(1) - N(1) - C(20)	120.9(4)	C(19) - N(1) - C(20)	117.8(5)
C(19) - N(2) - C(22)	116.9(5)	S(1) - N(3) - C(19)	112.2(4)
P(1) - C(1) - C(2)	122.8(5)	P(1) - C(1) - C(6)	118.8(5)
C(2) - C(1) - C(6)	118.5(6)	C(1) - C(2) - C(3)	119.9(7)
C(2) - C(3) - C(4)	120.5(8)	C(3) - C(4) - C(5)	119.8(8)
C(4) - C(5) - C(6)	120.0(7)	C(1) - C(6) - C(5)	121.2(7)
P(1) - C(7) - C(8)	118.1(5)	P(1) - C(7) - C(12)	124.2(5)
C(8) - C(7) - C(12)	117.7(6)	C(7) - C(8) - C(9)	120.2(6)
C(8) - C(9) - C(10)	120.8(7)	C(9) - C(10) - C(11)	120.2(8)
C(10) - C(11) - C(12)	119.1(7)	C(7) - C(12) - C(11)	121.9(6)
P(1) - C(13) - C(14)	120.7(5)	P(1) - C(13) - C(18)	120.0(5)
C(14) - C(13) - C(18)	119.2(6)	C(13) - C(14) - C(15)	119.6(6)
C(14) - C(15) - C(16)	120.6(7)	C(15) - C(16) - C(17)	120.3(7)
C(16) - C(17) - C(18)	119.8(7)	C(13) - C(18) - C(17)	120.4(6)
N(1) - C(19) - N(2)	122.3(5)	N(1) - C(19) - N(3)	115.7(5)
N(2) - C(19) - N(3)	122.0(5)	N(1) - C(20) - C(21)	122.2(6)
C(20) - C(21) - C(22)	116.7(6)	N(2) - C(22) - C(21)	124.0(6)
CL(3) - C(25) - CL(4)	112.0(6)		

Table 1.3. Crystallographic and experimental details of the structure analysis of complex (2).

Compound	*cis*-$[PdCl_2(PPh_3)(Me_2SNC_4H_3N_2)].CH_2Cl_2$
Formula	$C_{25}H_{26}Cl_4N_3PPdS$
Formula Wt.	679.8
Crystal habit	yellow plate
Crystal size, mm	0.28x0.10x0.05
Crystal system	monoclinic
Space group	P $2_1/n$
a, Å	17.307(6)
b, Å	9.182(2)
c, Å	17.960(2)
β, °	97.15(2)
Obtained from	21 refln, $10<\theta<15°$
V, $Å^3$	2832(1)
Z	4
F(000)	1368
d calc, gcm^{-3}	1.594
T, K	295
μ(Mo-Kα), cm^{-1}	11.74
Absorption factors on F	0.95-1.05
Scan width, °	0.70
Max count time, s	150
Total refln measured	4414
Unique refln	3463
R_{INT}	0.024
Miller indicies h	0→18
measured, k	-9→ 9
l	-18→18
2θ range, °	4-44
Unique refln ≥ 3σ(I)	1999
No. of parameters	316
R	0.024
R_w	0.028
$\|\Delta\rho\|_{max}$, $eÅ^{-3}$	0.30
Δ/σ_{max}	0.016

CHAPTER 2: STRUCTURE OF HEXAKIS(THIOUREA)RUTHENIUM(II) TRIFLUOROMETHYLSULPHONATE.

During kinetic studies of the replacement of coordinated water in $[Ru(H_2O)_6]^{2+}$, purple crystals of $[Ru(SC(NH_2)_2)_6][CF_3SO_3]_2$ were isolated by Dr.D. Richens of St. Andrews University. The new compound was the first thiourea complex of ruthenium(II) to be isolated and the mode of attachment (through N or S) of thiourea to the metal atom could not be unambiguously determined from spectroscopic data. Moreover, oxidation of the complex in solution gave a species, $[Ru(SC(NH)NH_2)_3]$, in which deprotonated thiourea appears to behave as a N,S-bonded chelate ligand.

X-ray diffraction analysis showed the crystal structure to contain layers of discrete cations of $[Ru(SC(NH_2)_2)_6]^{2+}$ (Figure 2(a)), the metal atoms lying exactly on the 00l planes, with $[CF_3SO_3]^-$ anions (Figure 2(b)) lying between these layers. Each anion is hydrogen-bonded to four cations, three in the same layer and one in an adjacent layer (Figure 2(c)). Two N-H...S hydrogen bonds also connect adjacent cations (see Table 2.2 for bond distances and angles).

The centrosymmetric cations contain planar thiourea ligands coordinated to the metal atom through sulphur as is usual for homoleptic $M(SC(NH_2)_2)_6$ species.[123-125] The RuS_6 coordination is D_{3d} trigonal antiprismatic rather than octahedral, with elongation along an axis through the metal atom and the centroid of the triangle defined by the three unique sulphur atoms so that the S-Ru-S angles are in the

Figure 2(a). Structure of the $[Ru(SC(NH_2)_2)_6]^{2+}$ cation. Hydrogen atoms are presented as spheres of arbitrary size and 50% probability ellipsoids are displayed for all other atoms.

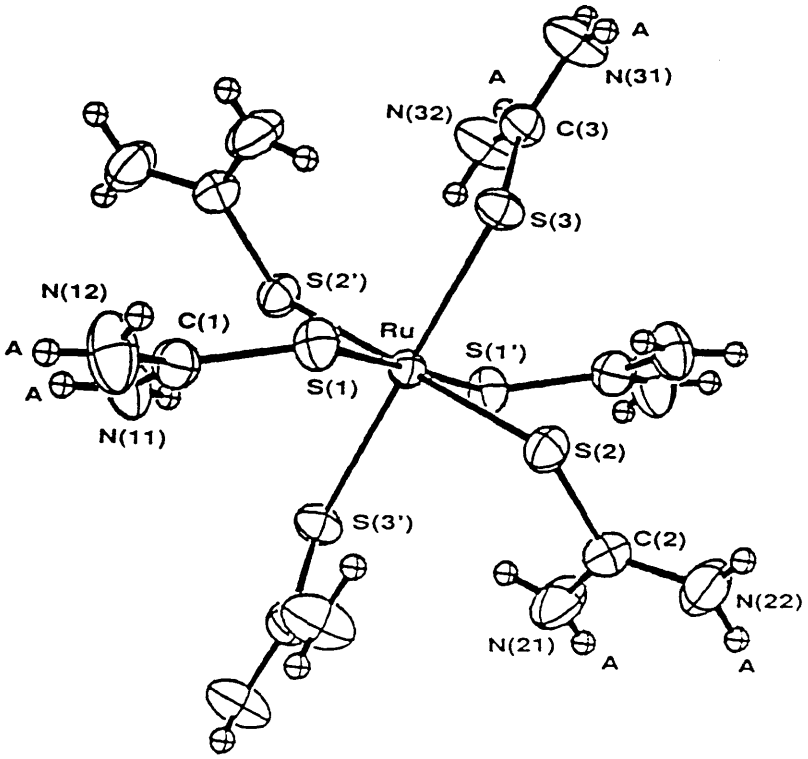
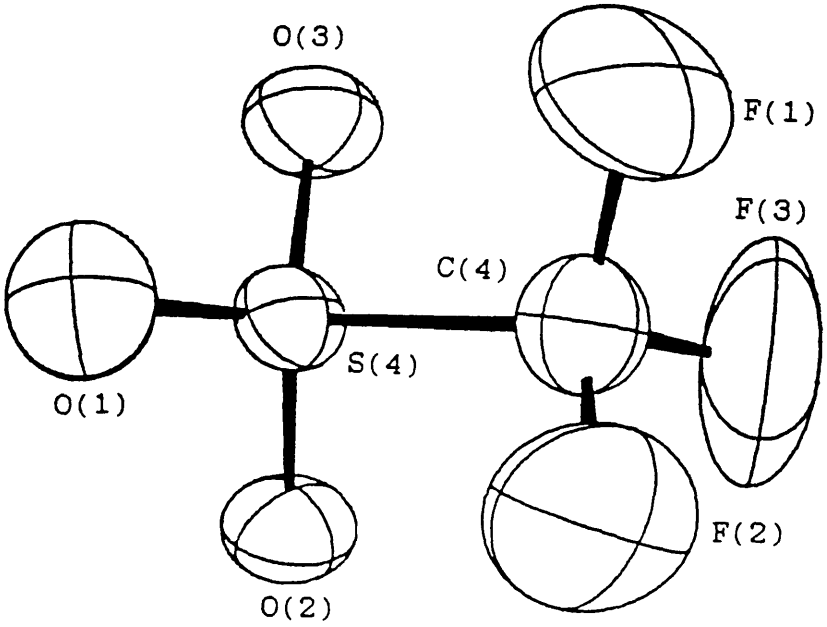


Figure 2(b). Structure of the $[CF_3SO_3]^-$ anion. 50% probability ellipsoids are displayed for all atoms.



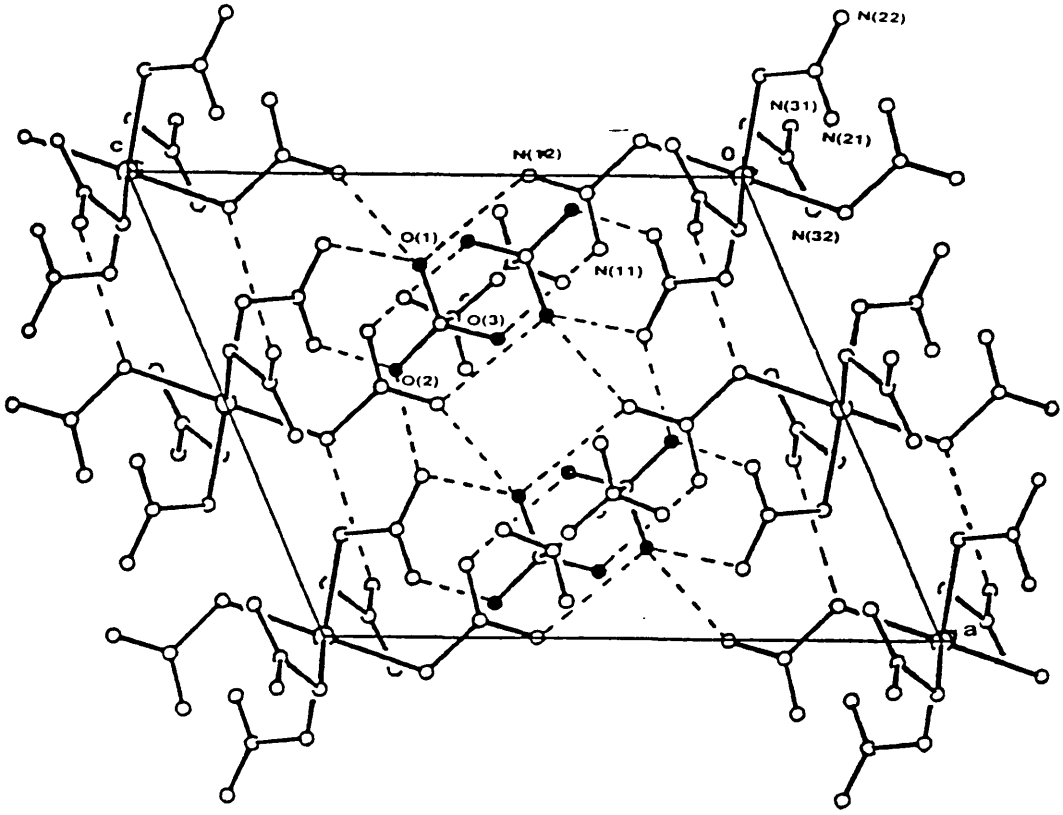


Figure 2(c). Crystal packing diagram showing the hydrogen bonding between adjacent ions.

range 81.4(1)-82.9(1)°. Similar distortions occur in several other metal ion complexes of thiourea. This suggests that it is unlikely to be due to electronic factors such as the Jahn-Teller effect.

The mean Ru-S bond distance [2.421(3) Å] is longer than values reported for other Ru(II)-S bonds [126] but comparable with that for the Tc^{3+} complex of thiourea [124] [2.428(16) Å]. The mean S-C bond length is similar to values for X-ray studies of free thiourea [127,128] but the mean N-C distance is slightly shorter than those in the free ligand [1.316(2) compared to 1.340(6) and 1.333(3) Å]. The Ru-S-C-N torsion angles show the ruthenium atom to be close to the plane of the thiourea ligands as previously noted in the

Tc^{3+} complex.[124] The S-Ru-S-C tilt angles [129] indicate that these Ru-thiourea planes bisect S-Ru-S angles. This probably minimises thiourea-thiourea ligand repulsion.

The $[CF_3SO_3]^-$ anions adopt a staggered C_{3v} conformation and their bond distances and angles are unexceptional.[130]

Experimental

The procedure used for this crystal structure analysis was similar to that described in Section 2, Chapter 2. Only differences in the methods are mentioned below.

Data Collection. The cell dimensions and experimental parameters are listed in Table 2.3. No decomposition correction was required.

Application of the transformation ($0\bar{1}0/100/102$) gave an A-centered cell with a = 11.06, b = 11.17 and c = 25.06 Å and $\alpha = \beta = \gamma = 90°$ to within experimental error. However, transformation of the intensity data and subsequent merging assuming Laue symmetry mmm gave R_{INT} = 0.39 confiming the monoclinic symmetry.

Structure Analysis. All hydrogen atom positions were found in difference syntheses. The positional and the isotropic displacement parameters of the hydrogen atoms were refined.

The ruthenium atom lies on a centre of symmetry. Consequently, each asymmetric unit comprises half a cation and one anion in each asymmetric unit.

Final atomic positions and displacement parameters are given in Table 2.1.

Table 2.1. Fractional atomic coordinates and displacement parameters ($Å^2$) of $[Ru(SC(NH_2)_2)_6][CF_3SO_3]_2$.

	X/A	Y/B	Z/C	U
RU	.00000	.00000	.00000	.026
S(1)	-.07517(5)	-.00101(5)	.14201(4)	.037
S(2)	-.22020(4)	.07580(5)	-.09936(4)	.034
S(3)	-.11327(4)	-.19199(5)	-.04361(4)	.035
S(4)	-.17574(6)	-.53665(6)	-.40784(4)	.043
N(11)	.1588(2)	.0688(2)	.2833(2)	.048
N(12)	.0016(3)	.0432(3)	.3459(2)	.063
N(21)	-.1286(2)	.2461(2)	-.1865(2)	.058
N(22)	-.3459(2)	.2061(2)	-.2714(2)	.054
N(31)	-.1111(2)	-.4112(2)	-.1140(2)	.058
N(32)	.0689(2)	-.2994(3)	-.0925(2)	.064
O(1)	-.3038(2)	-.5707(2)	-.4149(2)	.065
O(2)	-.0753(2)	-.5497(2)	-.3020(1)	.057
O(3)	-.1446(2)	-.5847(2)	-.4908(1)	.065
F(1)	-.2734(3)	-.3523(2)	-.5312(2)	.136
F(2)	-.2319(3)	-.3215(2)	-.3667(2)	.136
F(3)	-.0800(3)	-.3273(3)	-.4177(3)	.163
C(1)	.0382(2)	.0404(2)	.2660(2)	.041
C(2)	-.2313(2)	.1834(2)	-.1929(2)	.040
C(3)	-.0458(2)	-.3087(2)	-.0866(2)	.037
C(4)	-.1891(4)	-.3759(3)	-.4315(2)	.085
H(11A)	.217(2)	.075(3)	.344(2)	.049(7)
H(11B)	.178(2)	.070(3)	.231(2)	.052(7)
H(12A)	.055(3)	.052(3)	.403(2)	.049(7)
H(12B)	-.062(3)	.005(3)	.340(3)	.064(10)
H(21A)	-.134(3)	.290(3)	-.225(2)	.049(8)
H(21B)	-.051(3)	.220(3)	-.145(2)	.054(8)
H(22A)	-.354(3)	.260(3)	-.320(3)	.078(10)
H(22B)	-.407(3)	.171(3)	-.283(3)	.073(11)
H(31A)	-.188(3)	-.415(3)	-.116(2)	.073(9)
H(31B)	-.078(4)	-.452(4)	-.139(3)	.080(12)
H(32A)	.087(3)	-.350(3)	-.117(3)	.080(12)
H(32B)	.111(3)	-.234(3)	-.075(3)	.075(10)

Anisotropic displacement parameters ($Å^2$).

	U11	U22	U33	U12	U13	U23
RU	.0234(1)	.0251(1)	.0241(1)	-.0018(1)	.0097(1)	.0002(1)
S(1)	.0332(2)	.0426(3)	.0299(2)	-.0038(2)	.0153(2)	-.0015(2)
S(2)	.0282(2)	.0353(3)	.0331(2)	.0015(2)	.0108(2)	.0045(2)
S(3)	.0289(2)	.0291(2)	.0425(2)	-.0044(2)	.0170(2)	-.0033(2)
S(4)	.0522(3)	.0325(3)	.0354(2)	.0041(3)	.0158(2)	.0047(2)
N(11)	.0454(9)	.0600(14)	.0314(8)	-.0107(10)	.0158(7)	-.0093(9)
N(12)	.0552(12)	.0943(21)	.0342(9)	-.0165(14)	.0231(9)	-.0133(12)
N(21)	.0512(11)	.0534(14)	.0552(12)	-.0024(11)	.0139(10)	.0259(11)
N(22)	.0451(10)	.0543(14)	.0477(11)	.0042(11)	.0054(9)	.0177(10)
N(31)	.0510(11)	.0363(12)	.0782(15)	-.0108(10)	.0350(11)	-.0207(11)
N(32)	.0451(10)	.0437(14)	.0947(18)	-.0070(10)	.0405(12)	-.0191(13)
O(1)	.0533(9)	.0615(13)	.0684(11)	.0035(10)	.0221(8)	.0059(10)
O(2)	.0571(9)	.0591(12)	.0393(8)	.0052(9)	.0088(7)	.0043(8)
O(3)	.0783(11)	.0570(13)	.0477(9)	.0049(11)	.0290(8)	-.0071(9)
F(1)	.231(3)	.056(1)	.073(1)	.030(2)	.027(2)	.026(1)
F(2)	.226(3)	.049(1)	.103(2)	.037(2)	.073(2)	-.003(1)
F(3)	.183(3)	.070(2)	.207(3)	-.053(2)	.097(2)	.001(2)
C(1)	.0454(10)	.0375(11)	.0325(8)	-.0015(10)	.0185(8)	-.0009(9)
C(2)	.0401(9)	.0330(11)	.0374(9)	.0040(9)	.0121(8)	.0028(8)
C(3)	.0334(8)	.0332(10)	.0374(9)	-.0019(8)	.0137(7)	-.0020(8)
C(4)	.137(3)	.037(2)	.059(2)	-.007(2)	.036(2)	.001(1)

Table 2.2. Selected bond distances (Å) and angles (°) of $[Ru(SC(NH_2)_2)_6][CF_3SO_3]_2$.

RU	S(1)	2.415(1)	RU	S(2)	2.427(1)
RU	S(3)	2.420(1)	S(1)	C(1)	1.720(3)
S(2)	C(2)	1.717(3)	S(3)	C(3)	1.716(3)
S(4)	O(1)	1.445(2)	S(4)	O(2)	1.437(2)
S(4)	O(3)	1.422(2)	S(4)	C(4)	1.804(4)
N(11)	C(1)	1.307(3)	N(12)	C(1)	1.317(3)
N(21)	C(2)	1.312(4)	N(22)	C(2)	1.320(3)
N(31)	C(3)	1.317(4)	N(32)	C(3)	1.321(3)
F(1)	C(4)	1.335(5)	F(2)	C(4)	1.313(5)
F(3)	C(4)	1.275(6)	N	H	0.70(3)-0.87(4)

S(1)	RU	S(2)	81.3(1)	S(1)	RU	S(3)	82.9(1)
S(2)	RU	S(3)	81.7(1)	RU	S(1)	C(1)	116.0(1)
RU	S(2)	C(2)	114.1(1)	RU	S(3)	C(3)	119.1(1)
O(1)	S(4)	O(2)	112.8(2)	O(1)	S(4)	O(3)	114.0(2)
O(1)	S(4)	C(4)	103.8(2)	O(2)	S(4)	O(3)	115.3(2)
O(2)	S(4)	C(4)	104.7(2)	O(3)	S(4)	C(4)	104.7(2)
S(1)	C(1)	N(11)	122.3(2)	S(1)	C(1)	N(12)	118.4(2)
N(11)	C(1)	N(12)	119.3(2)	S(2)	C(2)	N(21)	121.4(2)
S(2)	C(2)	N(22)	119.6(2)	N(21)	C(2)	N(22)	119.0(3)
S(3)	C(3)	N(31)	118.5(2)	S(3)	C(3)	N(32)	122.3(2)
N(31)	C(3)	N(32)	119.2(3)	S(4)	C(4)	F(1)	110.4(3)
S(4)	C(4)	F(2)	110.9(3)	S(4)	C(4)	F(3)	112.6(3)
F(1)	C(4)	F(2)	107.8(4)	F(1)	C(4)	F(3)	107.7(4)
F(2)	C(4)	F(3)	107.2(3)				

Torsion Angles

S(3)-Ru-S(1)-C(1)	135.3(1)	Ru-S(1)-C(1)-N(11)	-1.2(2)
S(1)-Ru-S(2)-C(2)	143.4(1)	Ru-S(2)-C(2)-N(21)	-21.3(2)
S(2)-Ru-S(3)-C(3)	136.2(1)	Ru-S(3)-C(3)-N(32)	2.9(2)

Hydrogen Bonds

A-H---B	A-H	H...B	A...B	A-H---B
N(11)-H(11A)...O(3^{i})	0.83(3)	2.16(3)	2.989(3)	174(2)
N(12)-H(12A)...O(1^{i})	0.77(3)	2.36(3)	3.131(3)	172(3)
N(12)-H(12B)...O(1^{ii})	0.80(3)	2.29(3)	3.012(3)	150(3)
N(21)-H(21A)...O(2^{iii})	0.70(3)	2.30(3)	2.958(3)	158(3)
N(22)-H(22A)...O(1^{iii})	0.87(3)	2.47(3)	3.308(3)	161(3)
N(22)-H(22B)...O(2^{iv})	0.74(3)	2.24(3)	2.978(3)	172(3)
N(31)-H(31A)...S(1^{v})	0.85(3)	2.70(3)	3.512(2)	161(3)

Symmetry Code

i	½+x, -½-y, 1+z
ii	-½-x, ½+y, -z
iii	x, 1+y z
iv	-½+x,-½-y z
v	-½-x,-½+y, -z

Table 2.3. Crystallographic and experimental details of the structure analysis of $[Ru(SC(NH_2)_2)_6][CF_3SO_3]_2$.

Compound		$[Ru(SC(NH_2)_2)_6][CF_3SO_3]_2$
Formula		$C_8H_{24}F_6N_{12}O_6RuS_8$
Formula Wt.		855.9
Crystal habit		purple plate
Crystal size, mm		0.48x0.40x0.36
Crystal system		monoclinic
Space group		P $2_1/a$
a, Å		11.173(1)
b, Å		11.064(1)
c, Å		13.722(1)
β, °		113.96(1)
Obtained from		22 refln, $11<\theta<15°$
V, $Å^3$		1550.1(3)
Z		2
F(000)		860
d calc, gcm^{-3}		1.834
T, K		295
μ(Mo-Kα), cm^{-1}		11.0
Absorption factors on F		0.86-1.10
Scan width, °		0.80
Max count time, s		90
Total refln measured		6292
Unique refln		4506
R_{INT}		0.025
Miller indicies	h	0→15
measured,	k	-15→ 4
	l	-19→19
2θ range, °		4-60
Unique refln $\geq 3\sigma(I)$		3609
No. of parameters		236
R		0.026
R_w		0.037
$\lvert\Delta\rho\rvert_{max}$, $eÅ^{-3}$		0.43
Δ/σ_{max}		0.034

CHAPTER 3: THE STRUCTURE OF TETRACHLOROTHIOPHENE 1,1-DIOXIDE AT 295 AND 150K

3.1 Introduction

The main objectives of most modern single crystal X-ray diffraction studies are the identification of the chemical nature of each atom in the asymmetric unit and the derivation of reasonably accurate atomic positions. The analyses described in earlier parts of this thesis are typical of this approach. The objectives can be met by employing relatively standard experimental and computational techniques which incorporate the assumption that the individual atomic electron densities are spherically symmetric before allowance is made for thermal smearing.

During the last decade great progress has been made in developing methods of X-ray analysis which lead to accurate determination of the true molecular electron density. These methods allow deformation of the valence electron density from spherical symmetry to be studied and thus reveal the effects of bond formation and lone pair localisation. They also permit atomic charges to be determined experimentally.[131-133]

To achieve experimental electron density determinations which show these features it is necessary to work at low temperature so that thermal smearing is lessened and the intensities of high angle ($\sin\theta/\lambda$ up to 1.2 $\mathring{A}^{-1}$) reflections can be measured. Careful attention to

processing the raw intensity measurements is required and least-squares refinement must allow for the asphericity of the atomic electron densities. The recent study of an iron(II)-porphyrin illustrates this approach.[134]

The work described below was carried out as a preliminary exploration of the experimental and computational procedures required in studies of accurate electron densities. Specifically (i) an attempt was made to collect high-angle low temperature data, (ii) Blessing's data processing package[135] was installed on the Gould 3227 computer by the present author and used to process the data and (iii) the resulting structure was refined by Hansen's LSMOL multipole charge density refinement program as modified by Dr.P.R. Mallinson.[136]

3.2 Structure Analysis Of Tetrachlorothiophene 1,1-Dioxide At 295K

The chlorinated thiophene 1,1-dioxide, (1) was prepared in the du Pont Laboratories in 1980 and is useful as a Diels-Alder reagent since it is stable, yet reacts readily with double bonds with loss of SO_2 to add a tetrachloro-butadienediyl unit.[137] The small size and symmetry of the molecule and the stability of its crystals make it a suitable choice of test crystal. The details of the data collection at 295K are given in Table 3.5. The structure was readily solved by direct methods and refined by full-matrix least-squares with all atoms anisotropic. Final coordinates and temperature factors are given in Table 3.1. The refinement gave normal bond lengths and angles (Table

3.3) and the structure proved to be free of disorder, although the chlorine atoms showed fairly large thermal anisotropy (U_{ii} 0.04-0.14 $Å^2$).

3.3 Structure Analysis At 150K

Accordingly an attempt was made to collect a high resolution data set at 150K (Table 3.5). Initially it was intended to collect to higher angle and alsoto collect several asymmetric units of data but the crystal was lost during replenishement of the liquid nitrogen supply after an asymmetric unit of data to $\theta = 35°$ had been measured. For the data set thus collected reflection profiles were recorded and the data were processed using Blessing's program.[135] This determines the variable reflection width as a function of a unit vector normal to the incident and diffracted beam and also makes a careful allowance for all factors in deriving $\sigma(F)$. (It also has a very flexible procedure for scaling data according to the intensity standards but the small variation in the standards during this experiment made this feature superfluous.) A Gaussian absorption correction was also applied to the 150K data.

The data so obtained were used to refine the structure in the same way as for the 295K data set. Coordinates and temperature factors are presented in Table 3.2 and bond lengths and angles for both refinements in Table 3.3. A drawing of the molecule bsed on the 150K refinement is given in Figure 3(a).

As expected the transition from 295 to 150K greatly lowers the thermal motion (U_{ii} 0.02-0.07 $Å^2$ for Cl, see

Figure 3(a). Structure of $C_4Cl_4O_2S$ at 150K. 50% probability ellipsoids are displayed for all atoms.

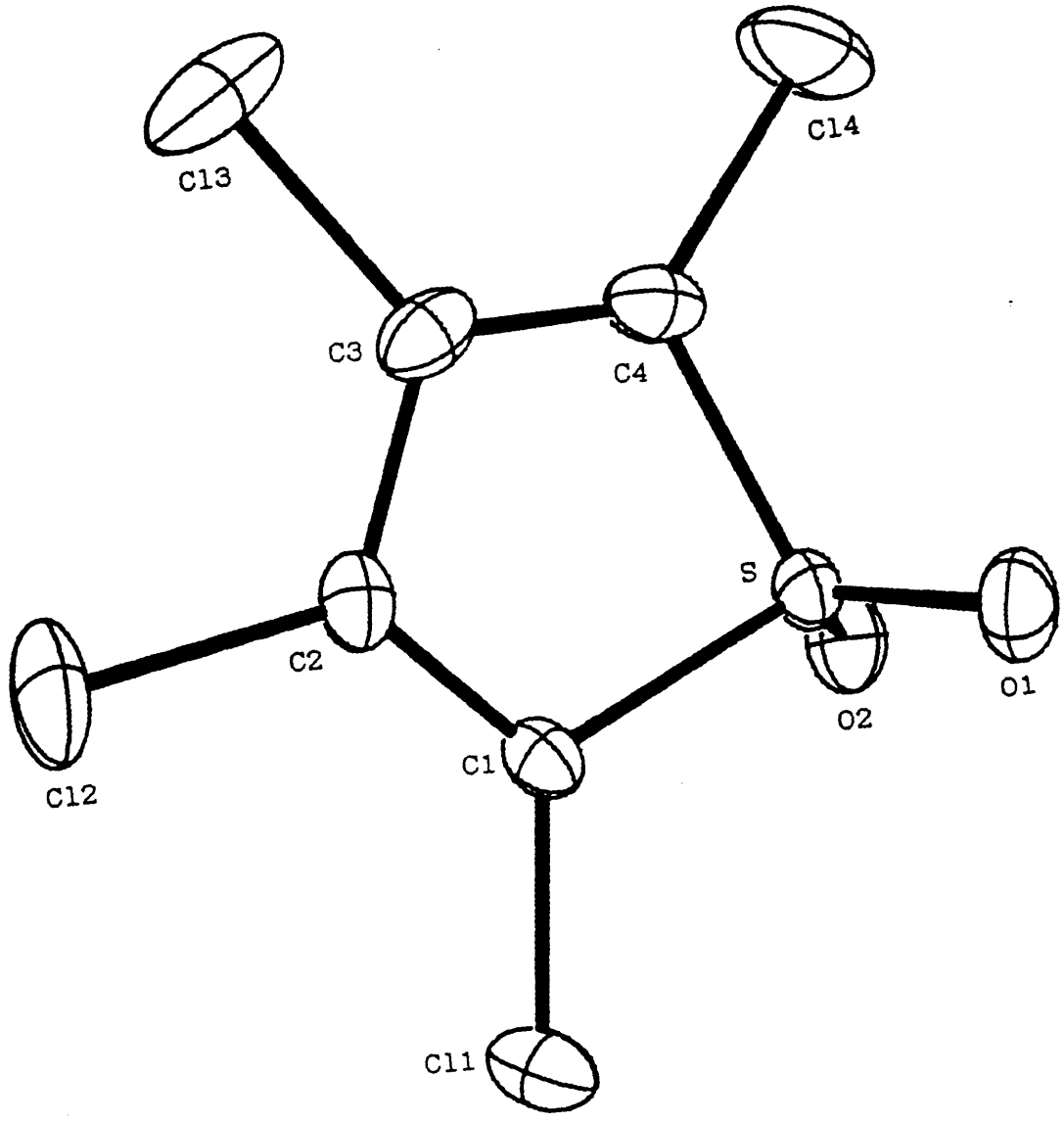


Table 3.2) and bond lengths tend to be slightly longer at 150K (see Table 3.3). The molecular structure at the two temperatures is, however, basically the same and approximates to C_{2v} symmetry. Since they are more accurate only the results for the 150K structure will be discussed. The butadiene unit, C(1)-C(4), is coplanar to ±0.06 Å with S displaced 0.09 Å from this plane. Atoms Cl(1) and Cl(2) are displaced in the same direction by 0.13 and 0.08 Å from this plane whereas Cl(3) and Cl(4) show smaller displacements of 0.07 and 0.04 Å in the opposite direction. The C-Cl bond lengths show significant variation, from 1.682(3) to 1.696(3) Å, for reasons which are not obvious.

As a check on the profile analysis (and of Blessing's program in general) the 150K data were processed normally (i.e. assuming that the peak was centred in the middle 2/3rds of the scan). This yielded fewer unique reflections with $I \geq 3\sigma(I)$ (2674 compared with 2721) showing the improved $\sigma(I)/I$ ratios for weaker reflections obtained by profile analysis. Refinement of this data set gave R = 0.043, R_w = 0.067 and distances and angles little different from those in Table 3.3. The maximum change in a bond length between the two low temperature refinements was 0.003 Å, for example.

3.4 Multipole Refinement

As previously noted, the 150K data collection was prematurely terminated. Nevertheless, it was considered worthwhile to attempt a multipole refinement using Dr.P.R. Mallinson's adaption of LSMOL. this expands the rest atomic

density, $\rho(\underline{r})$, in spherical harmonic functions of up to order 4:

$$\rho(\underline{r}) = P_c\rho_c(r) + P_v k'^3 \rho_v(k'r) + \sum_{l=0}^{4} k''^3 R_l(k''r) \sum_{m=-l}^{+l} P_{lm} y_{lm}$$

where $\rho_c(\underline{r})$ is a spherical core electron density normalised to unity, $\rho_v(k'r)$ is a spherical valence electron density normalised to unity, $R_l(k''r)$ defines the radial dependence of the multipole density function and y_{lm} defines its angular dependance.

P_c, P_v, P_{lm} are refinable population coefficients and the total number of valence electrons associated with the atom, Z, can be obtained from P_v+P_{00} since the $l \neq 0$ functions integrate to zero. k' and k" are refinable radial parameters. Analytical forms for R_l and y_{lm} are given in reference 136: l = 0, 1 and 2 correspond to s, p and d type electron densities. For first row atoms l = 0 to 3 is considered a sufficient multipole expansion, whereas l = 4 functions are required for second and higher row elements.

The multipole refinement of the 150K data set by LSMOL was based on the 2792 reflections with $I \geq 3\sigma(I)$ from the total of 3152 for which intensity measurements were made. Inclusion of the multipole expansion increased the number of refined parameters from 101 to 330. This refinement converged with R = 0.028 and R_w = 0.044 indicating a highly significant improvement in structure factor agreement. However, the derived atomic charges (Table 3.4) are poorly determined and some are implausible, notably the value for the sulphur atom and the differences between the equivalent pairs C(1) and C(4), C(2) and C(3). In addition, although the deformation density in the mean ring plane

(Figure 3(b)) contains maxima which could be attributed to bonding electron density, notably at the C-C bond centroids, it is dominated by features around Cl(2) and Cl(3) rising to nearly $2e\mathring{A}^{-3}$ which can only be attributed to the effects of uncorrected absorption or extinction.

3.5 Conclusions

The work just described led to succesful structure analyses of (1) at 295 and 150K in that the atomic positions were accurately located. In addition Blessing's data reduction program was succesfully installed and experience was gained using LSMOL. However, the quality of the 150K data is insufficient for accurate determination of the features of the bonding electron density.

Figure 3(b). Deformation density in plane of C_4S ring.

The coefficients used to compute the difference density function were of the form F^m-F^s where F^m is the calculated structure factor from the multipole refinement and F^s is the structure factor calculated assuming spherical atomic densities centred on the positions derived from the multipole refinement. Contour levels are at $0.1eÅ^{-3}$ intervals starting at $-0.7eÅ^{-3}$ and are numbered $1(-0.7eÅ^{-3})$ to $18(+1.0eÅ^{-3})$.

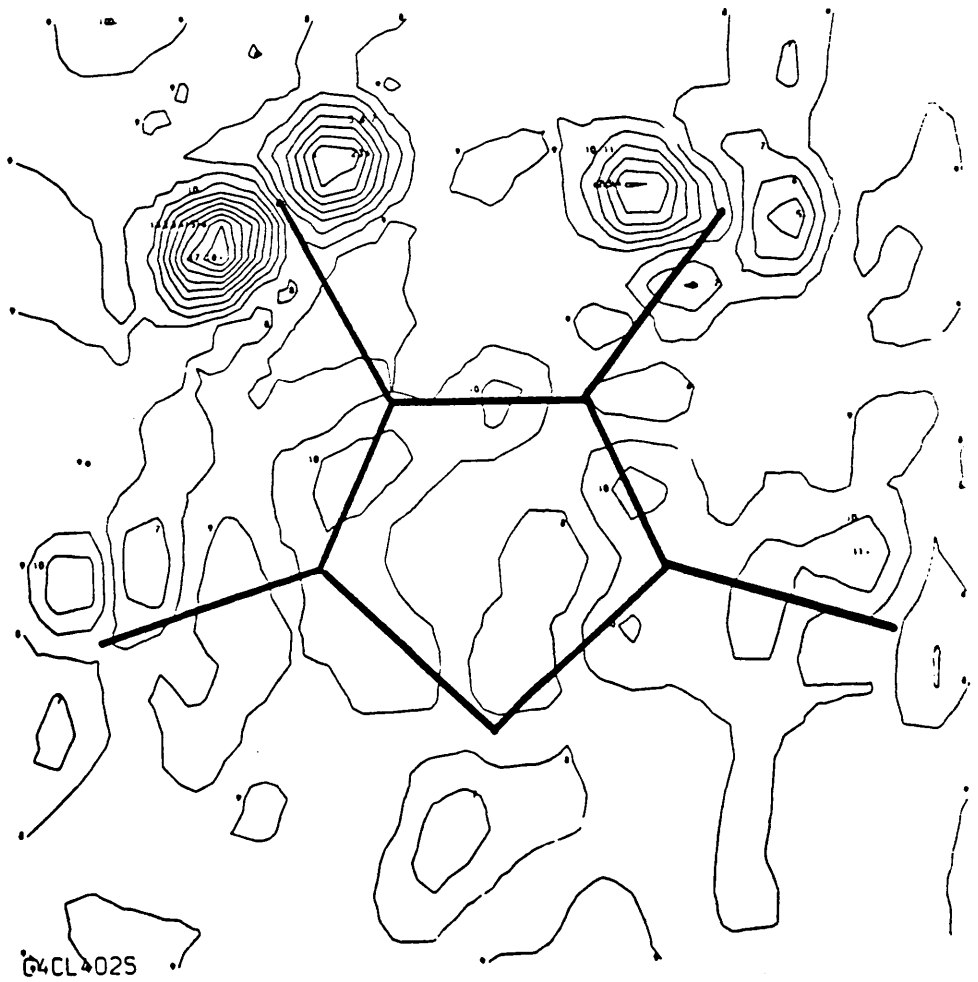


Table 3.1 Atomic positional and anisotropic displacement parameters ($Å^2$) of (1) at 295K

	X/A	Y/B	Z/C	U
CL(1)	.27352(6)	.43155(14)	.72829(9)	.077
CL(2)	.34478(8)	.72255(13)	.55626(13)	.094
CL(3)	.44515(7)	.55630(20)	.36593(10)	.095
CL(4)	.44699(8)	.12632(19)	.38339(11)	.106
S	.35739(5)	.19408(10)	.58474(7)	.048
O(1)	.40873(16)	.13019(36)	.66518(22)	.072
O(2)	.29582(16)	.09288(29)	.55500(25)	.068
C(1)	.33004(18)	.40217(37)	.62011(28)	.048
C(2)	.35825(18)	.51195(42)	.55072(31)	.052
C(3)	.40163(19)	.43363(48)	.46092(28)	.055
C(4)	.40450(20)	.26743(51)	.46513(26)	.054

	U11	U22	U33	U12	U13	U23
CL(1)	.0724(7)	.0806(7)	.0776(7)	.0071(5)	.0309(5)	-.0145(5)
CL(2)	.1029(10)	.0359(5)	.1439(11)	-.0009(5)	.0090(8)	.0069(5)
CL(3)	.0730(7)	.1364(12)	.0767(7)	-.0256(7)	.0065(5)	.0489(7)
CL(4)	.1165(11)	.1216(12)	.0792(8)	.0349(9)	.0348(7)	-.0267(7)
S	.0580(5)	.0357(4)	.0512(4)	.0047(3)	.0078(3)	.0006(3)
O(1)	.087(2)	.062(2)	.066(2)	.019(1)	-.004(1)	.013(1)
O(2)	.074(2)	.041(1)	.090(2)	-.011(1)	.005(1)	.000(1)
C(1)	.049(2)	.039(1)	.057(2)	.001(1)	.010(1)	-.005(1)
C(2)	.048(2)	.040(2)	.069(2)	-.001(1)	-.004(2)	.004(1)
C(3)	.044(2)	.071(2)	.051(2)	-.005(2)	-.002(1)	.014(2)
C(4)	.052(2)	.067(2)	.044(2)	.005(2)	.010(1)	-.002(1)

Table 3.2 Atomic positional and anisotropic displacement parameters ($Å^2$) of (1) at 150K

	X/A	Y/B	Z/C	U
CL(1)	.27236(3)	.43417(7)	.72966(4)	.031
CL(2)	.34378(4)	.72891(7)	.55617(7)	.041
CL(3)	.44528(3)	.56237(11)	.36506(5)	.044
CL(4)	.44822(4)	.12835(10)	.38269(5)	.048
S	.35837(2)	.19584(6)	.58590(3)	.019
O(1)	.41166(9)	.13183(21)	.66767(13)	.030
O(2)	.29570(9)	.09306(19)	.55521(14)	.029
C(1)	.33035(10)	.40449(23)	.62179(15)	.021
C(2)	.35816(10)	.51668(25)	.55064(16)	.023
C(3)	.40177(10)	.43896(29)	.46038(15)	.026
C(4)	.40437(11)	.26929(29)	.46424(16)	.026

	U11	U22	U33	U12	U13	U23
CL(1)	.0274(3)	.0354(3)	.0317(3)	.0039(2)	.0089(2)	-.0065(2)
CL(2)	.0424(3)	.0152(3)	.0659(4)	-.0014(2)	-.0021(3)	.0046(2)
CL(3)	.0297(3)	.0698(5)	.0335(3)	-.0159(3)	-.0023(2)	.0262(3)
CL(4)	.0493(4)	.0602(5)	.0346(3)	.0157(3)	.0124(3)	-.0156(3)
S	.0228(2)	.0153(3)	.0203(2)	.0021(2)	.0008(2)	-.0001(1)
O(1)	.0351(8)	.0262(7)	.0280(7)	.0070(6)	-.0055(6)	.0044(5)
O(2)	.0323(7)	.0178(7)	.0359(7)	-.0041(6)	-.0019(6)	-.0003(5)
C(1)	.0205(7)	.0186(8)	.0232(7)	.0008(6)	.0018(6)	-.0040(6)
C(2)	.0217(7)	.0168(8)	.0293(8)	-.0012(6)	-.0016(6)	.0022(7)
C(3)	.0199(7)	.0361(11)	.0214(7)	-.0041(7)	-.0011(6)	.0081(7)
C(4)	.0230(8)	.0365(11)	.0196(7)	.0045(7)	.0007(6)	-.0022(7)

Table 3.3 Bond lengths (Å) and angles (°) in (1) at 295 and 150K

Cl(1)	- C(1)	1.683(4)	1.691(2)	Cl(2)	- C(2)	1.687(4)	1.689(3)
Cl(3)	- C(3)	1.699(4)	1.696(3)	Cl(4)	- C(4)	1.681(4)	1.682(3)
S	- O(1)	1.432(3)	1.435(2)	S	- O(2)	1.430(3)	1.435(2)
S	- C(1)	1.775(4)	1.771(2)	S	- C(4)	1.775(4)	1.775(2)
C(1)	- C(2)	1.311(5)	1.326(3)	C(2)	- C(3)	1.479(5)	1.477(3)
C(3)	- C(4)	1.318(6)	1.334(4)				

O(1)	- S	- O(2)	119.0(2)	119.1(1)	O(1)	- S	- C(1)	110.8(2)	111.0(1)
O(1)	- S	- C(4)	109.2(2)	109.1(1)	O(2)	- S	- C(1)	110.7(2)	110.4(1)
O(2)	- S	- C(4)	112.1(2)	111.8(1)	C(1)	- S	- C(4)	91.7(2)	92.1(1)
Cl(1)	- C(1)	- S	119.3(2)	119.8(2)	Cl(1)	- C(1)	- C(2)	130.2(3)	129.8(2)
S	- C(1)	- C(2)	110.5(3)	110.3(2)	Cl(2)	- C(2)	- C(1)	124.8(3)	124.7(2)
Cl(2)	- C(2)	- C(3)	121.6(3)	121.5(2)	C(1)	- C(2)	- C(3)	113.6(4)	113.7(2)
Cl(3)	- C(3)	- C(2)	120.4(3)	120.7(2)	Cl(3)	- C(3)	- C(4)	125.2(3)	125.2(2)
C(2)	- C(3)	- C(4)	114.4(4)	114.1(2)	Cl(4)	- C(4)	- S	118.9(3)	119.3(2)
Cl(4)	- C(4)	- C(3)	131.3(3)	130.9(2)	S	- C(4)	- C(3)	109.7(3)	109.6(2)

Table 3.4 Refined number of valence electrons, Z, and atomic charge, A-Z, where A is the number of valence electrons of the isolated atom

	Z	A-Z		Z	A-Z
Cl(1)	6.9(1)	+0.1(1)	O(1)	6.2(1)	-0.2(1)
Cl(2)	7.0(1)	0.0(1)	O(2)	6.3(1)	-0.3(1)
Cl(3)	7.1(1)	-0.1(1)	C(1)	4.6(2)	-0.6(2)
Cl(4)	7.1(1)	-0.1(1)	C(2)	3.7(2)	+0.3(2)
S	4.8(3)	+1.2(3)	C(3)	4.2(2)	-0.2(2)
			C(4)	4.1(2)	-0.1(2)

Table 3.5: Summary Of Experimental Measurements On Tetrachlorothiophene 1,1-Dioxide

Formula $C_4Cl_4O_2S$, F.Wt. = 253.9, monoclinic, space group C 2/c, Z = 8, F(000) = 992.

T, K	295	150
Crystal size, mm	0.52x1.04x1.04	0.76x0.68x0.34
a, Å	18.424(4)	18.204(5)
b, Å	7.915(1)	7.855(2)
c, Å	11.927(5)	11.751(3)
β, °	90.48(3)	91.77(2)
V, $Å^3$	1379.2(8)	1679.6(6)
d(calc), gcm^{-3}	1.939	2.008
Refln for cell determination	21	23
Their θ range, °	14-18	12-17
μ(Mo-Kα), cm^{-1}	15.5	16.0
Transmission factors on F^2	-	0.37-0.58
Scan width in ω, °	1.2	1.2+0.53tanθ
Max. counting time, s	90	100
2θ range	4-60	4-70
Range of h	0-25	0-29
k	$\bar{1}\bar{1}$-11	0-12
l	$\bar{1}\bar{6}$-16	$\bar{1}\bar{9}$-19
Total refln measured	3370	3152
Unique refln	2073	3078
R_{int}	0.058	0.040
Unique refln > 3σ(I)	1843	2721
Refined parameters*	101	101
R	0.054	0.043
R_w	0.081	0.080
(Δ/σ)max	0.04	0.01
|Δρ|max, $eÅ^{-3}$	0.76	1.22

* 99 positional and U_{ij} parameters plus the scale and the isotropic extinction parameters.

Appendix 1: Single Crystal X-Ray Diffraction Analysis

The main experimental techniques and equations used for the structure analyses discussed earlier are briefly summarised.

Crystal Structure

A crystal is built by translational repetition in three dimensions of the structural motif contained in the unit cell. The geometry of the unit cell is defined by three lengths a, b, and c, which are the axes of the cell, and the three interaxial angles α, β, and γ. A unit cell belongs to one of the seven different crystal systems. This classification is based on the symmetry displayed both by the six cell parameters and by the contents of the cell.

The contents of the unit cell can be generated from the asymmetric unit by applying a series of symmetry operations. This set of symmetry operations defines the space group. The operations are most conveniently specified in terms of the equivalent positions: the fractional coordinates of points symmetrically equivalent to an arbitary general position, x, y, z, within the cell.

Bragg's Law

The conditions under which all unit cells in a crystal scatter in phase when the crystal is bathed in a uniform beam of monochromatic X-rays were first derived by Laue. Bragg suggested an alternative and conceptually simpler

approach in which the scattering is regarded as arising from stacks of symmetrically equivalent planes defined by integral Miller indices, h, k, l, where the intercepts of any plane on the axes of a reference unit cell are a/h, b/k, and c/l. It can be easily shown that for symmetrical scattering from such a stack of planes the interference condition is

$$2d\sin\theta = \lambda$$

where d is the interplanar spacing, θ the angle of incidence and λ the wavelength of the X-ray beam. Higher orders of diffraction are conventionally regarded as first order diffraction from planes of spacing d/n where n is the order of diffraction for planes of spacing d.

Measurements on Diffractometers

All the structure analyses described in this thesis were performed on an Enraf-Nonius CAD4 diffractometer. This, like other modern diffractometers, allows the crystal to be oriented by rotation about three independant axes and the counter to be swung about the crystal specimen so that a high proportion of all accesible Bragg reflections can be observed.

In a typical experiment 20-25 Bragg reflections were located and their setting angles carefully measured. The unit cell and its orientation were then deduced from the setting angles. If necessary, the reduced cell was derived and then the conventional cell by methods of International Tables for Crystallography, Volume A, Section 9.

A preliminary survey of intensities, out to $\theta = 8°$

typically with molybdenum radiation, was then made. Usually this would cover at least a hemisphere of reciprocal space, include lattice absences and sometimes might be based on doubled unit cell axes. Sorting and averaging these measurements would allow final decisions to be made concerning the Laue group and lattice type.

Final intensity measurements would then be made out to as high an angle as possible using the $\omega/2\theta$ scan method and an ω scan width of 0.8-1.0°, increased by 25% at each end to allow for background. This set of measurements would normally comprise more than an asymmetric unit of data.

Data Processing

Structure amplitudes were derived from the expression

$$I(hkl) = kLpAF^2(hkl)$$

where k is a scale factor for the experiment, L and p are the Lorentz and polarisation factors allowing respectively for the rapidity with which each reflection passes through the Bragg condition and for angle-dependant polarisation on scattering from the crystal monochromator and specimen. A allows for X-ray absorption and was estimated either by Gaussian quadrature[87] or by the empirical method of Stuart and Walker.[59] In cases where crystal decomposition was a problem the mean of the intensity standards was used to apply a linear decay correction to segments of data.

The scale factor, k, and any allowance for extinction were derived by least-squares refinement (see below).

The final structure amplitudes were then sorted and averaged according to the point (rather than Laue) group to

give a unique data set. Unobserved reflections with $I<K\sigma(I)$, with K = 2-3, were not subsequently used.

Structure Analysis

The wave scattered from a single unit cell during Bragg reflection from the hkl planes is defined by the structure factor

$$F(hkl) = \sum_{j=1}^{N} f_j \exp 2\pi i(hx_j+ky_j+lz_j) = |F(hkl)| \exp(i\alpha_{hkl})$$

where the summation is over the N atoms in the unit cell, f_j, x_j, y_j, z_j, are respectively the scattering factor and fractional coordinates of the jth atom and α_{hkl} is the phase of the reflection.

For atoms or ions at rest the scattering factor, f_j, can be calculated from suitable electronic wave functions which assume a spherical distribution of electron density. The scattering factor is therefore real and a function of $\sin\theta/\lambda$ only.

Such calculations ignore the peturbing effect of the atomic nucleus on the scattering process. For heavier atoms this approximation is not acceptable and, when allowance is made for anomalous dispersion, the scattering factor is of the form f + f' + if" where f' and f" correct the scattering factor, f, calculated for a spherical distribution of classical electrons. In non-centrosymmetric space groups anomalous dispersion leads to inequivalence of F(hkl) and $F(\bar{h}\bar{k}\bar{l})$ and thus implies that the chirality of the crystal structure can be determined.

The scattering factor also contains an allowance for

thermal vibration of the form $\exp(-8\pi^2 U\sin^2\theta/\lambda^2)$ where U is the mean-square amplitude of vibration normal to the Bragg planes. For anisotropic vibration this temperature factor is defined by six independent U_{ij} parameters in the expression:

$$\exp -2\pi^2(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+.....2hka^*b^*U_{12}....)$$

where a*, b* and c* are the reciprocal cell parameters.

The electron density at the point with fractional coordinates x, y and z is given by

$$\rho(xyz) = 1/V \sum_{hkl} F(hkl)\exp -2\pi i(hx+ky+lz)$$

where V is the cell volume. The summation, in principle triply infinite, is over all the Bragg reflections.

Phase Problem

In order to calculate the electron density function both the structure amplitude and the phase angle are required. However, only the structure amplitude is experimentally available. Without phase information it is impossible to work out the relative phases of the individual component waves from each atom. However, if atomic positions are known it is possible to work back and calculate phase angles.

There are two main methods used to overcome the phase problem:

(1) the heavy atom method

and (2) direct methods

(1) Heavy Atom Method

The Patterson function is defined by

$$P(uvw) = \sum_{hkl} |F_{hkl}|^2 \cos 2\pi(hu+kv+lw)$$

where P(uvw) is the value of the function at the position with fractional coordinates u, v and w, the summation is over all Bragg reflections and $|F_{hkl}|$ is the measurable structure amplitude. Atoms at positions (x_1,y_1,z_1) and (x_2,y_2,z_2) give rise to a peak in P(uvw) at $u = x_2-x_1$, $v = y_2-y_1$, $w = z_2-z_1$, and the height of the peak is roughly proportional to $\rho(x_1y_1z_1)$ x $\rho(x_2y_2z_2)$. Accordingly, heavy atom positions are easily calculated if the equivalent positions of the unit cell are known. These atomic positions can then be used to calculate approximate phase angles to be used with the observed structure amplitudes, thereby allowing an approximate electron density distribution to be obtained.

(2) Direct Methods

These methods use probalistic calculations to derive a set of phases from the structure amplitudes using criteria such as the non-negative nature of electron density. Usually it is sufficient to obtain phases for only a few hundred critically selected reflections to obtain an interpretable electron density.

In general, Patterson rather than direct methods were used in the structure analyses described earlier. Sometimes Patterson methods were used to assess solutions suggested by Direct Methods.

Refinement

Once an approximate electron density had been derived the positions of at least some atoms were known. Approximate phases for all structure amplitudes would then be calculated and an improved electron density distribution. This process was repeated till all atoms had been located.

Final parameters (scale, atomic coordinates and U_{ij} values) were obtained by minimising

$$M = \sum_{hkl} \omega(|F^o| - |F^c|)^2$$

by the method of least-squares using weights $\omega = 1/\sigma^2(F^o)$. When allowance for extinction was deemed necessary $|F^c|$ was modified by the factor $[1 + gF^{c2}f(\theta)]^{-1/2}$ where g is the refined extinction parameter and $f(\theta)$ a modified Lp factor.[138] Refinement was continued till the maximum shift/e.s.d. ratio was typically 0.5 or less. Structure factor agreement was assessed from

$$R = (\Sigma||F^o| - |F^c||)/\Sigma|F^o|$$

and

$$R_w = \{\Sigma\omega(|F^o| - |F^c|)^2/\Sigma\omega F^{o2}\}^{1/2}$$

REFERENCES

1. Lj. Manojlović-Muir, K.W. Muir, B.R.Lloyd, and R.J. Puddephatt, J. Chem. Soc., Chem. Comm., 1983, 1336.

2. A.M. Bradford, G. Douglas, Lj. Manojlović-Muir, K.W. Muir, and R.J. Puddephatt, Organometallics, 1990, 9, 409.

3. G. Douglas, Lj. Manojlović-Muir, K.W. Muir, M. Rashidi, C.M. Anderson, and R.J. Puddephatt, J. Amer. Chem. Soc., 1987, 109, 6527.

4. G. Douglas, Lj. Manojlović-Muir, K.W. Muir, M.C. Jennings, B.R. Lloyd, M. Rashidi, and R.J. Puddephatt, J. Chem. Soc., Chem. Comm., 1988, 149.

5. G. Douglas, M.C. Jennings, Lj. Manojlović-Muir, K.W. Muir, and R.J. Puddephatt, Inorg. Chem., 1988, 27, 4516.

6. G. Douglas, M.C. Jennings, Lj. Manojlović-Muir, K.W. Muir, and R.J. Puddephatt, J. Chem. Soc., Chem. Comm., 1989, 159.

7. C.A. McAuliffe and W. Levason, "Phosphine, Arsine and Stibine Complexes of Transition Elements", Elsevier, Amsterdam, 1979.

8. C.A. Tolman, Chem. Rev., 1977, 77, 313.

9. M. Cowie and S.K. Dwight, Inorg. Chem., 1979, 18, 1209.

10. Lj. Manojlović-Muir, K.W. Muir, and T. Solomun, Acta Cryst., 1979, B35, 1237.

11. A.R. Sanger, J. Chem. Soc., Dalton Trans., 1981, 228.

12. M.M. Olmstead, C.L. Lee, and A.L. Balch, Inorg. Chem., 1982, 21, 2712.

13. R.J. Puddephatt, Chem. Soc. Rev., 1983, 12, 99.

14. M.P. Brown, S.P. Cooper, A.A. Frew, Lj. Manolović-Muir, K.W. Muir, R.J. Puddephatt, and M.A. Thomson, J. Chem.

Soc., Dalton Trans., 1982, 299.
15. Lj. Manojlović-Muir and K.W. Muir, International Union of Crystallography, Abstracts of XIIIth International Congress, Hamburg, W. Germany, Acta Cryst., 1984, A40, C292.
16. Lj. Manojlović-Muir, K.W. Muir, M.C. Grossel, M.P. Brown, C.D. Nelson, A. Yvari, E. Kallas, R.P. Moulding, and K.R. Seddon, J. Chem. Soc., Dalton Trans., 1986, 1955 and references therein.
17. M.P. Brown, S.J. Cooper, A.A. Frew, Lj. Manojlović-Muir, K.W. Muir, R.J. Puddephatt, K.R. Seddon, and M.A. Thomson, Inorg. Chem., 1981, 20, 1500.
18. E.W. Stern and P.K. Maples, J. Catal., 1972, 27, 120.
19. R.J. Puddephatt, M.A. Thomson, Lj. Manojlović-Muir, K.W. Muir, A.A. Frew, and M.P. Brown, J. Chem. Soc., Chem. Comm., 1981, 805.
20. P.J. Pringle and B.L. Shaw, J. Chem. Soc., Chem. Comm., 1982, 581.
21. S.S.M. Ling, R.J. Puddephatt, Lj. Manojlović-Muir, and K.W. Muir, Inorg. Chim. Acta, 1983, 77, L95.
22. S.S.M. Ling, R.J. Puddephatt, Lj. Manojlović-Muir, and K.W. Muir, J. Organomet. Chem., 1983, 255, C11.
23. S.S.M. Ling, I.R. Jobe, Lj. Manojlović-Muir, K.W. Muir, and R.J. Puddephatt, Organometallics, 1985, 4, 1198.
24. R. Poilblanc, Inorg. Chim. Acta, 1982, 62, 75.
25. C.L. Lee, C.J. Hunt, and A.L. Balch, Inorg. Chem., 1981, 20, 2498.
26. L.L. Kesmodel, L.H. Dubois, and G.A. Somorjai, J. Chem. Phys., 1979, 70, 2180; J.C. Bertolini and J. Massardier, "The Chemical Physics of Solid Surfaces and

Heterogeneous Catalysis", D.A. King and D.P. Woodruff Eds., Elsevier, Amsterdam, 1984, Vol. 3, Chapter 3; H. Steininger, H. Ibach, and S. Lehwald, Surf. Sci., 1982, 117, 685; C.E. Megiris, P. Berlowitz, J.B. Butt, and H.H. King, Surf. Sci., 1985, 159, 184; K.M. Ogle and J.M. White, Surf. Sci., 1986, 165, 234; P.-K. Wang, C.P. Slichter, and J.H. Sinfelt, Phys. Rev. Lett., 1984, 53, 82.

27. R.J. Koestner, M. Salmeron, E.B. Kollin, and J.L. Gland, Surf. Sci., 1986, 172, 668; E. Protopopoff and P. Marcus, Surf. Sci., 1986, 169, L237; S.R. Keleman, T.E. Fischer, and J.A. Schwarz, Surf. Sci., 1979, 81, 440; J. Billy and M. Abon, Surf. Sci., 1984, 146, L525.

28. K. Hayek, H. Glassl, A. Gutmann, H. Leonhard, M. Prutton, S.P. Tear, and M.R. Welton-Cook, Surf. Sci., 1985, 152/153, 419.

29. D.M.P. Mingos and R.W.M. Wardle, Transition Metal Chem., 1985, 10, 441.

30. K.M. Thomas, R. Mason, and D.M.P. Mingos, J. Amer. Chem. Soc., 1973, 95, 3802; D.M.P. Mingos and M.I. Forsyth, J. Chem. Soc., Dalton Trans., 1977, 610.

31. K.M. Thomas, "Transition Metal Clusters", B.F.G. Johnson Ed., J. Wiley, Chichister, 1980, 193; D.M.P. Mingos, Acc. Chem. Res., 1984, 17, 311.

32. R. Hoffman, Angew. Chem., Int. Ed. Engl., 1982, 21, 711.

33. M. Elian, M.M.L. Chen, R. Hoffman, and D.M.P. Mingos, Inorg. Chem., 1976, 15, 1148; D.M.P. Mingos, Adv. Organomet. Chem., 1977, 15, 1.

34. D.G. Evans and D.M.P. Mingos, J. Organomet. Chem., 1982, 240, 321.

35. C. Mealli, J. Amer. Chem. Soc., 1985, 107, 2245.
36. G. Longoni and P. Chini, J. Amer. Chem. Soc., 1976, 98, 7225.
37. C.E. Briant, D.I. Gilmour, D.M.P. Mingos, and R.W.M. Wardle, J. Chem. Soc., Dalton Trans., 1985, 1693.
38. D.G. Evans, G.R. Hughes, D.M.P. Mingos, J.-M. Basset, and A.J. Welch, J. Chem. Soc., Chem. Comm., 1980, 1255.
39. C.E. Briant, R.W.M. Wardle, and D.M.P. Mingos, J. Organomet. Chem., 1984, 267, C49.
40. O.J. Ezomo, D.M.P. Mingos, and I.D. Williams, J. Chem. Soc., Chem. Comm., 1987, 924.
41. A. Albinati, G. Carturan, and A. Musio, Inorg. Chim. Acta, 1976, 16, L3.
42. D.M.P. Mingos, P. Oster, and D.J. Sherman, J. Organomet. Chem., 1987, 320, 257.
43. J.J. Bour, R.P.F. Kanters, P.P.J. Schlebos, W. Bos, W.P. Bosman, H. Behm, P.T.B. Eurskens, and J.J. Steggeroa, J. Organomet. Chem., 1987, 329, 405.
44. A. Albinati, Inorg. Chim. Acta, 1977, 22, L31.
45. R. Bender, P. Braunstein, A. Tiripicchio, and M.T. Camellini, Angew. Chem., Int. Ed. Engl., 1985, 24, 861.
46. P.W. Frost, J.A.K. Howard, J.L. Spencer, D.G. Turner, and D. Gregson, J. Chem. Soc., Chem. Comm., 1981, 1104.
47. L.J. Guggenberger, J. Chem. Soc., Chem. Comm., 1968, 512.
48. Lj. Manojlović-Muir, K.W. Muir, B.R. Lloyd, and R.J. Puddephatt, J. Chem. Soc., Chem. Comm., 1985, 536.
49. Lj. Manojlović-Muir, K.W. Muir, and R.J. Puddephatt, unpublished results.
50. G. Ferguson, B.R. Lloyd, and R.J. Puddephatt,

Organometallics, 1986, 5, 344.

51. G. Ferguson, B.R. Lloyd, Lj. Manojlović-Muir, K.W. Muir, and R.J Puddephatt, Inorg. Chem., 1986, 25, 4190.

52. L. Pauling, "The Nature of the Chemical Bond", Cornell University Press, Ithaca, New York, 1960.

53. J. Wisner, T. J. Bartczak, and J.A. Ibers, Organometallics, 1986, 5, 2044.

54. M.D. Alvey and J.T. Yates, J. Amer. Chem. Soc., 1988, 110, 1782.

55. Q.-B. Bao, S.J. Geib, A.L. Reingold, and T.B. Brill, Inorg. Chem., 1987, 26, 3453.

56. A.N. Caldwell, Lj. Manojlović-Muir, and K.W. Muir, J. Chem. Soc., Dalton Trans., 1977, 35, 3087.

57. D.G. Evans, J. Organomet. Chem., 1988, 352, 397.

58. B.R. Lloyd, A. Bradford, and R.J. Puddephatt, Organometallics, 1987, 6, 424.

59. N. Walker and D. Stuart, Acta Cryst., 1983, A39, 158.

60. P.R. Mallinson and K.W. Muir, J. Appl. Cryst., 1985, 18, 51.

61. "International Tables for X-ray Crystallography", Kynoch Press, Birmingham, 1974, Vol. 4.

62. M.C. Jennings, N.C. Payne, and R.J. Puddephatt, Inorg. Chem., 1987, 26, 3776; M.C. Jennings, N.C. Payne, and R.J. Puddephatt, J. Chem. Soc., Chem. Comm., 1986, 1809.

63. S.S.M. Ling, N. Hadj-Bagheri, Lj. Manojlović-Muir, K.W. Muir, and R.J. Puddephatt, Inorg. Chem., 1987, 26, 231.

64. M. Rashidi and R.J. Puddephatt, J. Amer. Chem. Soc., 1986, 108, 7111.

65. J. Silvestre and R. Hoffman, Langmuir, 1985, 1, 621.

66. A. Moor, P.S. Pregosin, L.M. Venanzi, and A.J. Welch, Inorg. Chim. Acta, 1984, 85, 103; R.G. Vranka, L.F. Dahl, P. Chini, and J. Chatt, J. Amer. Chem. Soc., 1969, 91, 1574.

67. N.K. Eremko, E.G. Mednikov, and S.S. Kurasov, Russ. Chem. Rev., 1985, 54, 394.

68. A.A. Frew, R.H. Hill, Lj. Manojlović-Muir, K.W. Muir, and R.J. Puddephatt, J. Chem. Soc., Chem. Comm., 1982, 198.

69. "International Tables For Crystallography", Vol. A, Reidel, Dordrecht, 1983, Chapter 9.

70. R. Usón, J. Fornies, M. Tomes, J.M. Casas, F.A. Cotton, and L.R. Falvello, Inorg. Chem., 1987, 26, 3482; S. Bhaduri, K. Sharma, P.G. Jones, and C.F. Erdbrugger, J. Organomet. Chem., 1987, 326, C46.

71. R. Usón, J. Fournies, M. Thomas, J.M. Casas, F.A. Cotton, and L.R. Falvello, J. Amer. Chem. Soc., 1985, 107, 2556; R. Usón, J. Fournies, B. Mejon, F.A. Cotton, L.R. Falvello, and M. Thomas, Inorg. Chem., 1985, 24, 4651.

72. P. Braunstein, H. Lehner, D. Matt, A. Tiripicchio, and M. Tiripicchio-Camellini, Angew. Chem., Int. Ed. Engl., 1984, 23, 304.

73. P. Braunstein and J. Rose, J. Gold Bull., 1985, 18, 17; P.D. Boyle, B.J. Johnson, B.D. Alexander, J.A. Casalnuovo, P.R. Gannon, S.M. Johnson, E.A. Larka, A.M. Mueting, and L.H. Pignolet, Inorg. Chem., 1987, 26, 1346; J.J. Bour, R.P.F. Kanters, P.P.J. Schlebos, W.P. Bosman, H. Behm, P.T. Beurskens, and J.J. Steggerda, Recl., J. R. Neth. Chem. Soc., 1987, 106, 157.

74. H.H. Murray, D.A. Briggs, G. Garzon, R.G. Raptis, L.C. Porter, and J.P. Fackler Jr., Organometallics, 1987, 6,

1992.

75. D.E. Smith, A.J. Welch, I. Treurnicht, and R.J. Puddephatt, Inorg. Chem., 1986, 25, 4616; G.J. Arsenault, Lj. Manolović-Muir, K.W. Muir, R.J. Puddephatt, and I. Treurnicht, Angew. Chem., Int. Ed. Engl., 1987, 26, 86; Lj. Manojlović-Muir, K.W. Muir, I. Treurnicht, and R.J. Puddephatt, Inorg. Chem., 1987, 26, 2418.

76. C.E. Briant, D.I. Gilmour, and D.M.P. Mingos, J. Chem. Soc., Dalton Trans., 1986, 835.

77. C.E. Briant, D.I. Gilmour, and D.M.P. Mingos, J. Organomet. Chem., 1984, 267, C52; C.E. Briant, R.W.M. Wardle, and D.M.P. Mingos, J. Organomet. Chem., 1984, 267, C49; D.M.P. Mingos and R.W.M. Wardle, J. Chem. Soc., Dalton Trans., 1986, 73.

78. R. Usón, Pure Appl. Chem., 1986, 58, 647.

79. R. Pruett and J. Bradley, Eur. Pat. 37700, 1982; Chem. Abstr., 1982, 96, 35540k; W.E. Walker, E.S. Brown and R.L. Pruett, U.S. Pat. 3878292, 1975; Chem. Abstr., 1975, 83, 45426y; J. Schwank, J. Gold Bull., 1985, 18, 1.

80. W. Bos, J.J. Bour, P.P.J. Schlebos, P. Hageman, W.P. Bosman, J.M.M. Smits, J.A.C. van Wietermaschen, and P.T. Beurskens, Inorg. Chim. Acta, 1986, 119, 141.

81. G.K. Anderson, H.C. Clark, and J.A. Davies, Inorg. Chem., 1983, 22, 427 and 434.

82. A. Roberti, V. Ponec, and W.M.H. Sachtler, J. Catal., 1973, 28, 381.

83. S.R. Adkins and B.H. Davis, J. Catal., 1984, 89, 371; B.A. Sexton, A.E. Hughes, and K. Foger, J. Catal., 1984, 88, 466; Yu.I. Yermakov and B.N. Kuznetsov, J. Mol. Catal., 1980, 9, 13; R. Srinavasan, R.J. de Angelis, and B.H.

Davis, J. Catal., 1987, 106, 449.

84. G.K. Campbell, P.B. Hitchcock, M.F. Lappert, and M.C. Misra, J. Organomet. Chem., 1985, 289, C1.

85. C.J. Gilmore, J. Appl. Cryst., 1984, 17, 42.

86. D. Rogers, Acta Cryst., 1981, A37, 734.

87. P. Coppens, "Crystallographic Computing", F.R. Ahmed Ed., Munksgaard, Copenhagen, 1970, 187.

88. J.D. Dunitz, "X-ray Analysis and the Structure of Organic Molecules", Cornell University Press, Ithaca, New York, 1979, Chapter 10.

89. "Advanced Inorganic Chemistry", F.A. Cotton and G. Wilkinson Eds., J. Wiley and Sons, New York, 1980, Chapters 29 and 30.

90. "The Organometallic Chemistry of the Transition Metals", R.H. Crabtree Ed., J. Wiley and Sons, New York, 1988, Chapters 9 and 11.

91. P. Cossee, J. Catal., 1964, 3, 80; E.J. Arlman, J. Catal., 1964, 3, 89; E.J. Arlman and P. Cossee, J. Catal., 1964, 3, 99.

92. T.C. Clarke, C.S. Yannoni, and T.J. Kate, J. Amer. Chem. Soc., 1983, 105, 7787 and references therein.

93. J.L. Davidson, M. Shiralian, Lj. Manojlović-Muir, and K.W. Muir, J. Chem. Soc., Chem. Comm., 1979, 30.

94. J.L. Davidson, I.E.P. Murray, P.N. Preston, M.V. Russo, Lj. Manojlović-Muir, and K.W. Muir, J. Chem. Soc., Chem. Comm., 1981, 1059.

95. J.L. Davidson, G. Vasapollo, Lj. Manojlović-Muir, and K.W. Muir, J. Chem. Soc., Chem. Comm., 1982, 1025.

96. J.L. Davidson, W.F. Wilson, and K.W. Muir, J. Chem. Soc., Chem. Comm., 1985, 460.

97. P.S. Braterman, J.L. Davidson, and D.W.A. Sharp, J. Chem. Soc., Dalton Trans., 1976, 241.

98. J.L. Davidson, J. Chem. Soc., Chem. Comm., 1980, 113.

99. L. Carlton, J.L. Davidson, J.C. Miller, and K.W. Muir, J. Chem. Soc., Chem. Comm., 1984, 11.

100. L. Carlton, J.L. Davidson, P. Ewing, Lj. Manojlović-Muir, and K.W. Muir, J. Chem. Soc., Chem. Comm., 1985, 1474.

101. N.M. Agh-Atabay, J.L. Davidson, G. Douglas, and K.W. Muir, J. Chem. Soc., Chem. Comm., 1987, 1526.

102. N.M. Agh-Atabay, J.L. Davidson, G. Douglas, and K.W. Muir, J. Chem. Soc., Chem. Comm., 1989, 549.

103. L.J. Canoira, J.L. Davidson, G. Douglas, and K.W. Muir, J. Organomet. Chem., 1989, 362, 135.

104. J.L. Davidson, W.F. Wilson, Lj. Manojlović-Muir, and K.W. Muir, J. Organomet. Chem., 1983, 254, C6.

105. S.H. Taylor and P.M. Maitlis, J. Amer. Chem. Soc., 1978, 100, 4700.

106. L. Brammer, M. Crocker, B.J. Dunne, M. Green, C.E. Morton, K.R. Nagle, and A.G. Orpen, J. Chem. Soc., Chem. Comm., 1986, 1226.

107. A. Davison and W.C. Rode, Inorg. Chem., 1967, 6, 2124; R. Davis and L.A. Kane-Maguire in "Comprehensive Organometallic Chemistry", G. Wilkinson, F.G.A. Stone, and E.W. Abel Eds., Pergamon, Oxford, 1982, Vol. 3, pp. 1159 and 1327 and references therein.

108. "Molecular Structures and Dimensions", O. Kennard, D.G. Watson, F.H. Allen, N.W. Issacs, W.D.S. Motherwell, R.C. Pettersen, and W.G. Town, Oosthoek, Utrecht, 1972, Vol. A1, S1-S3.

109. J. Browning, M. Green, J.L. Spencer, and F.G.A. Stone, J. Chem. Soc., 1974, 97; J. Browning, M. Green, B.R. Penfold, J.L. Spencer, and F.G.A. Stone, J. Chem. Soc., Chem. Comm., 1973, 31; H.C. Clark and A. Shaver, Canad. J. Chem., 1975, 53, 3462.

110. J.L. Davidson, W.F. Wilson, and K.W. Muir, J. Chem. Soc., Chem. Comm., 1985, 460.

111. J.L. Davidson, Lj. Manojlović-Muir, K.W. Muir, and A.N. Keith, J. Chem. Soc., Chem. Comm., 1980, 749.

112. J.L. Davidson and W.F. Wilson, J. Chem. Soc., Dalton Trans., 1988, 27.

113. B. Rosenberg, "Metal Ions in Biological Systems", Vol. 11, E. Sigel Ed., Marcel Dekker, New York, 1981, 127.

114. A. Pasini and F. Zunino, Angew. Chem., Int. Ed. Engl., 1987, 26, 615.

115. K.W. Muir and Lj. Manojlovic-Muir, Acta Cryst. 1986, C42, 1294.

116. J.L. Davidson, P.N. Preston, S.A.R. Spankie, G. Douglas, and K.W. Muir, J. Chem. Soc., Dalton Trans., 1989, 497.

117. A.J. Deeming, I.P. Rothwell, M.P. Hursthouse, and K.M.A. Malik, J. Chem. Soc., Dalton Trans., 1980, 1974.

118. A.F. Cameron, A.A. Freer, and A. Maltz, Acta Cryst., 1981, B37, 1608.

119. A. Takenaka, Y. Sasada, K. Yamamoto, and J. Tsuji, Bull. Chem. Soc. Jpn., 1977, 50, 3177.

120. C.P. Brock and J.A. Ibers, Acta Cryst., 1973, A29, 2426; J.J. Daly, J. Chem. Soc., 1964, 3799.

121. D.N.J. White, J.K. Tyler, and M.R. Lindley, Comput. Chem., 1986, 10, 193.

122. "Dictionary of Organic Compounds", 5th Edn., Chapman and Hall, New York, 1982, Vol. 5, 4845 and 4860.

123. I. Goldberg and F.H. Herbstein, Acta Cryst., 1972, B28, 400.

124. M.J. Abrams, A. Davison, R. Faggiani, A.G. Jones, and C.J.L. Lock, Inorg. Chem., 1984, 23, 3284.

125. M.S. Weininger, J.E. O'Connor, and E.L. Amma, Inorg. Chem., 1969, 8, 424.

126. S.C. Rawle and S.R. Cooper, J. Chem. Soc., Chem. Comm., 1987, 308.

127. M.R. Truter, Acta Cryst., 1967, 22, 556.

128. M.M. Elcombe and J.C. Taylor, Acta Cryst., 1968, A24, 410.

129. D.A. Berta, W.A. Spofford, P. Boldrini, and E.L. Amma, Inorg. Chem., 1970, 9, 136.

130. J.-O. Lundgren, Acta Cryst., 1978, B34, 2428.

131. P. Coppens, J. Chem. Ed., 1984, 61, 761.

132. P. Coppens, Angew. Chem., Int. Ed. Engl., 1977, 16, 32.

133. K. Angermund, K.H. Claus, R. Goddard, and C. Kruger, Angew. Chem., Int. Ed. Engl., 1985, 24, 237.

134. N. Li, P. Coppens, and J. Landrum, Inorg. Chem., 1988, 27, 482.

135. R.H. Blessing, Crystallography Reviews, 1987, 1, 1.

136. N.K. Hansen and P. Coppens, Acta Cryst., 1978, A34, 909; A.H. Holliday, P. Leung, and P. Coppens, Acta Cryst., 1983, A39, 377.

137. M.S. Raasch, J. Org. Chem., 1980, 45, 856.

138. A.C. Larsen, "Crystallographic Computing", F.R. Ahmed Ed., Munksgaard, Copenhagen, 1970, 291.

X-RAY DIFFRACTION ANALYSIS OF ORGANOMETALLIC COMPOUNDS WITH CATALYTIC PROPERTIES

VOLUME II

Submitted to the University of Glasgow in partial fulfilment of the requirements for the degree of Doctor of Philosophy in the Faculty of Science

by

Graeme Douglas

Chemistry Department

September 1990

APPENDIX 2

CONTENTS

CALCULATED AND OBSERVED STRUCTURE FACTORS OF $[Pt_3(CO)(CNC_6H_{11})(dppm)_3][PF_6]_2$

0, 0, L			14 919 603			17 942 869			-18 444 612			0, 5, L			0, 6, L		
4	2047	3151	15	738	959	0, 3, L			-15	560	614	-23	774	837	-22	659	686
5	2152	1714	16	779	587	-25	908	994	-14	637	583	-22	882	992	-21	761	767
6	2121	1902	17	1259	1157	-23	814	959	-13	1184	1123	-21	995	992	-20	785	830
10	548	799	19	1358	1262	-16	1265	1160	-12	1068	1130	-20	790	825	-19	643	676
12	1619	1617	20	864	901	-15	1108	1175	-11	1382	1351	-19	619	801	-18	621	648
14	1531	1615	21	613	537	-14	1668	1483	-10	1263	1478	-18	701	741	-17	636	620
16	2392	2268	0, 2, L			-13	1747	1641	-9	1177	1411	-17	790	772	-16	560	519
17	661	1001	-19	776	878	-12	1601	1462	-8	1692	1538	-12	649	667	-15	502	552
18	1488	1586	-17	1566	1495	-11	2033	2099	-7	1125	1086	-11	1003	995	-14	475	329
19	931	1041	-16	1303	1290	-10	731	826	-6	1884	1973	-10	811	852	-13	399	262
20	840	900	-15	1833	1767	-9	2404	2552	-5	639	468	-9	1468	1472	-12	569	454
21	864	806	-14	2435	2107	-7	2870	2703	-4	810	978	-8	940	907	-10	510	549
0, 1, L			-13	1448	1565	-6	810	460	-3	659	705	-7	1086	1329	-8	904	836
-20	1065	1213	-12	2488	2647	-5	1838	1679	-2	1096	1029	-6	1354	1333	-7	560	481
-19	643	947	-10	2994	2908	-4	639	581	-1	719	727	-5	2100	2324	-6	1308	1339
-18	1111	1439	-9	540	713	-2	1546	1134	0	1084	284	-4	784	712	-5	635	727
-17	1572	1578	-8	2203	2168	-1	319	577	1	1600	1155	-3	938	852	-4	1484	1602
-16	845	1430	-7	1090	1202	0	340	200	2	603	404	-2	1180	1241	-3	364	242
-15	2547	2477	-6	1082	1391	1	1525	1505	3	729	773	-1	730	878	-1	991	863
-13	2329	2093	-5	1788	1741	4	589	457	4	802	552	0	1251	1018	0	468	515
-11	2686	2834	-4	767	643	5	2005	1711	5	536	735	1	611	335	1	1083	1305
-9	1957	1978	-3	1364	1148	7	2001	2011	6	1044	1081	2	1162	1367	3	1400	1445
-8	1071	1131	-2	638	381	9	1335	1242	7	907	746	3	544	611	4	921	902
-6	845	610	-1	1057	932	10	353	376	8	398	392	4	1295	1348	5	1524	1668
-5	343	273	0	1515	1967	11	547	703	10	996	893	5	347	450	6	1453	1340
-4	1557	1785	1	823	547	12	625	551	12	513	797	6	1393	1233	7	1610	1567
-3	1359	1621	2	1512	1856	13	704	707	14	723	746	8	1099	1070	8	863	766
-2	354	749	3	898	1186	14	886	990	15	660	670	10	394	377	9	1353	1340
2	581	468	4	3756	4102	15	530	560	16	452	530	14	664	559	11	1001	944
3	3930	4197	5	1426	978	16	806	983	17	1297	1325	16	1156	994	12	591	486
4	1549	1422	6	2915	2630	18	758	815	18	1194	1035	17	550	584	14	494	602
5	3862	3664	8	2004	1956	20	679	576	19	917	992	18	1070	951	15	638	503
7	1876	2233	9	296	240	0, 4, L			21	1268	1120	19	739	673	17	1085	1036
8	442	496	10	572	551	-23	825	931	23	719	710	20	1173	996	19	1072	1014
10	457	414	13	649	708	-22	1026	1066				22	1320	1167	21	1279	1285
11	286	57	15	578	445	-21	583	676				24	881	999	23	1386	1267
13	805	798	16	777	709	-20	891	989				25	806	694	24	533	454

0, 6, L		
25 1090	1088	
0, 7, L		
-21 515	605	
-14 602	479	
-13 468	57	
-11 422	346	
-8 430	469	
-7 539	707	
-5 1118	1141	
-4 974	980	
-3 312	181	
-2 496	302	
0 1066	664	
2 1801	1767	
3 467	542	
4 1800	1983	
5 497	581	
6 2162	2231	
7 628	730	
8 2332	2183	
10 2032	2103	
12 1612	1609	
13 657	766	
14 797	778	
15 1042	1060	
17 1092	1066	
18 823	863	
20 1004	1048	
22 1137	1158	
24 1262	1204	
0, 8, L		
-11 759	755	
-9 692	728	
-7 1286	1264	
-6 838	832	
-5 1314	1344	
-4 852	923	
-3 1684	1748	
-2 330	101	
-1 1606	1578	
0 508	381	
1 655	370	
2 809	876	
3 1024	847	
4 970	979	
5 1547	1591	
6 792	801	
7 2190	2313	
9 2596	2399	
11 2174	2104	
13 1777	1782	
15 1318	1259	
16 938	957	
17 505	424	
18 903	999	
20 557	588	
21 504	712	
23 847	844	
0, 9, L		
-13 602	320	
-11 577	568	
-10 639	617	
-8 1052	993	
-7 586	793	
-6 1233	1234	
-5 852	873	
-4 1647	1620	
-3 846	791	
-2 1947	1993	
-1 684	459	
0 2370	2262	
1 321	254	
2 1002	1061	
3 543	708	
5 910	919	
6 943	1001	
8 1884	1884	
10 2059	1976	
12 1989	2004	
13 554	83	
14 1647	1711	
16 1438	1323	
18 619	595	
19 525	586	
0, 10, L		
-16 545	612	
-14 412	339	
-13 451	324	
-10 719	753	
-8 1087	1114	
-7 1050	1062	
-6 567	809	
-5 1054	1089	
-3 1634	1550	
-2 783	534	
-1 1646	1847	
1 1937	1873	
3 1556	1558	
4 631	628	
5 565	521	
6 492	573	
9 1378	1350	
11 1451	1528	
13 1467	1491	
14 566	37	
15 1251	1088	
17 1158	1235	
19 795	830	
0, 11, L		
-14 560	507	
-7 1060	1051	
-5 1123	1091	
-4 771	913	
-3 662	1052	
-2 1124	1139	
-1 1233	899	
0 1427	1382	
1 1003	679	
2 1278	1365	
3 490	490	
4 1150	1178	
6 785	768	
8 408	284	
9 513	546	
10 609	648	
12 1012	1065	
14 701	784	
16 748	858	
18 607	799	
0, 12, L		
-11 647	681	
-9 644	683	
-6 648	591	
-4 841	824	
-2 873	868	
-1 831	765	
0 986	894	
1 1072	1058	
2 839	760	
3 1048	1063	
4 616	538	
5 987	967	
7 734	876	
13 402	434	
0, 13, L		
-3 558	482	
-1 551	528	
0 583	542	
2 761	820	
3 580	502	
4 866	905	
6 625	735	
0, 14, L		
3 625	604	
5 655	693	
1, -13, L		
0 782	686	
2 703	533	
5 745	619	
1, -12, L		
-8 959	922	
-6 1175	1107	
-5 644	509	
-4 1274	1156	
-3 1031	848	
-2 1122	984	
-1 912	829	
0 943	841	
1 1006	938	
3 795	809	
1, -11, L		
-17 956	927	
-15 1095	1020	
-9 539	363	
-7 1251	1021	
-6 564	377	
-5 1210	1154	
-4 754	678	
-3 1302	1243	
-2 1020	984	
-1 1318	1211	
0 1159	970	
1 1223	1170	
2 1186	1177	
3 908	847	
4 1179	1122	
6 905	833	
1, -10, L		
-18 1273	1190	
-16 1355	1307	
-14 1238	1293	
-13 660	416	
-12 1401	1251	
-10 939	926	
-7 592	575	
-6 1010	907	
-4 1766	1556	
-2 1774	1634	
-1 906	675	
0 1527	1445	
1 1250	869	
2 1155	1217	
3 952	970	
4 1183	1212	
5 1136	1256	
6 671	711	
7 886	981	
13 738	558	
15 721	658	
1, -9, L		
-20 708	633	
-19 932	919	
-17 1354	1366	
-15 1632	1604	
-14 638	391	
-13 1791	1642	
-11 1924	1673	
-9 1472	1455	
-8 939	931	
-6 773	893	
-3 1654	1519	
-1 2002	1786	
0 819	680	
1 1557	1478	
2 1156	905	

1, -9, L		
3	962	971
4	722	871
7	871	827
8	681	591

1, -8, L		
-22	575	580
-19	744	761
-16	1134	1094
-14	1218	1267
-12	1697	1656
-11	843	625
-10	1615	1652
-9	1104	851
-8	1422	1488
-7	1009	988
-6	1136	1097
-5	543	788
-4	513	315
-2	491	463
0	1194	1183
1	1073	930
2	928	830
3	1002	903
4	960	776
5	842	898
7	521	630
8	706	617
10	664	567
12	766	690

1, -7, L		
-23	965	820
-18	803	687
-15	829	707
-13	1207	1161
-11	1555	1593
-10	700	791
-9	1537	1563
-8	828	870
-7	1622	1442
-5	1258	1450
-4	327	558
-3	635	610
-1	712	567
0	456	296
1	470	398
2	1158	1034
4	848	1008
6	705	809
8	793	841
13	746	728
14	834	631
15	1134	1107
17	1079	1121
18	768	641
19	987	998

1, -6, L		
-24	1150	1130
-22	1012	964
-20	635	761
-12	666	665
-10	1101	1154
-9	744	794
-8	1125	1152
-7	744	784
-6	1093	1112
-4	1197	1542
-3	492	349
-2	1206	1152
-1	654	625
0	828	749
1	805	946
2	1133	982
3	960	950
5	1311	1238
6	1079	938
7	714	741
8	755	580
9	644	469
14	858	725
15	1087	931
16	1020	920
17	1098	1008
18	1298	1221
19	932	787
20	1201	1180
22	997	1066

1, -5, L		
-25	824	783
-23	966	1069
-21	1005	1070
-19	844	872
-17	639	688
-12	546	480
-10	1113	986
-8	462	662
-7	378	477
-5	529	588
-4	356	437
-3	1035	939
-2	625	695
-1	1097	1271
0	1257	1260
1	704	673
2	1790	2009
3	1439	1106
4	2415	2507
5	1137	1291
6	1979	1986
7	1765	1460
8	1731	1589
9	1671	1423
10	751	556
11	700	753
15	883	493
17	805	662
18	1143	1037
19	1145	1008
20	957	1069
21	1338	1264
22	648	718
23	1221	1125

1, -4, L		
-22	828	747
-20	1078	1071
-18	804	891
-16	812	705
-15	651	647
-13	691	576
-12	401	292
-11	1313	1408
-9	1358	1380
-7	808	885
-5	582	363
-1	1080	1135
0	1032	747
1	1911	2004
3	1870	1781
5	3298	2942
6	1631	1606
7	2605	2443
8	1809	1723
9	1906	2055
10	1526	1840
11	958	948
12	1494	1462
14	710	572
18	536	503
20	707	754
21	1045	1038
22	1043	1165
24	1213	1191

1, -3, L		
-17	868	923
-14	911	791
-12	730	849
-10	1834	1870
-8	2429	2423
-6	2908	2663
-5	827	723
-4	1713	1806
-3	1365	1539
-2	675	405
-1	450	250
0	590	459
1	1047	1222
2	1954	1871
3	1619	1426
4	2822	2426
5	335	71
6	3429	3112
7	994	1005
8	3107	3197
9	1706	1668
10	2047	1989
11	1914	1896
12	1162	1386
13	2044	1930
14	790	773
15	1124	1173
20	614	681
22	1022	932
24	989	882
25	770	1045

1, -2, L		
-19	1059	1029
-11	1845	1743
-10	789	855
-9	2320	2306
-7	4074	4040
-6	796	582
-5	3950	4057
-4	950	763
-3	6473	5900
-2	2369	2917
-1	2109	2480
0	586	1212
1	1078	302
2	2432	1704
3	1659	1266
4	2977	3065
5	2486	2568
6	651	664
7	2882	2932
9	2524	2735
10	1038	892
11	2304	2132
12	1963	1850
13	2112	1996
14	2572	2155
15	1026	1129
16	1361	1353
18	603	567

1, -1, L		
-22	1058	1161
-21	596	811
-20	1845	1705
-18	1545	1608
-16	1582	1605
-15	945	591
-14	630	783
-12	589	678
-11	912	743
-10	1553	1661
-8	2279	2189
-7	515	714
-6	4040	4073
-4	5003	4564

1, -1, L		
-2	4388	4547
-1	495	949
0	2451	3298
1	1571	1375
2	710	699
3	1042	1143
4	2480	2150
5	1891	2015
6	2958	2632
8	2123	2283
9	619	521
10	2955	2679
11	619	877
12	2327	2426
13	501	1612
14	1815	1733
15	2062	1612
16	1026	1219
17	1381	1432

1, 0, L		
-22	904	1086
-21	1393	1234
-20	904	1229
-19	2071	2006
-17	1907	2132
-15	1901	2129
-14	925	665
-13	1214	1093
-12	1226	913
-11	968	1042
-8	856	1090
-7	1978	2111
-5	3481	3285
-3	5609	5449
-2	588	1619
2	1750	959
3	1786	350
6	1438	1169
9	1173	1086
11	2041	1836
13	1855	2016
15	1685	1654
17	1166	1266
18	1073	1065
19	924	748

1, 1, L		
-23	631	648
-20	974	1030
-19	1031	1204
-18	1518	1722
-16	2359	2335
-14	2181	2166
-12	2298	2426
-11	1490	1350
-10	1616	1255
-9	815	912
-7	1099	1035
-6	1091	1182
-5	1440	692
-4	3503	2686
-2	3462	3282
-1	522	206
2	2151	2482
4	2081	2579
5	1089	1344
6	477	208
8	339	386
11	894	869
13	963	963
15	1153	928
16	622	799
17	890	919
18	678	506
20	747	537
23	526	403

1, 2, L		
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-19	692	737
-18	1158	1186
-17	1151	1194
-16	1052	1208
-15	2511	2211
-13	2350	2307
-11	2031	1832
-10	826	685
-9	1384	1333
-8	630	753
-7	697	555
-3	670	384
-1	619	298
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1	1696	1650
2	966	1178
3	2133	2520
5	2237	2296
7	864	1106
8	557	421
10	627	744
14	1592	1382
16	856	476
16	695	942
18	708	624
22	699	455

1, 3, L		
-19	704	562
-17	917	1024
-16	1418	1404
-15	911	1085
-14	2022	1773
-13	1059	1080
-12	2173	2130
-10	2105	2088
-9	2144	2261
-6	1269	1344
-5	647	890
-4	702	1119
-3	823	107
-2	1815	1564
-1	1027	635
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1	1645	761
2	487	252
4	1935	1451
5	543	854
8	800	862
9	668	569
11	546	797
12	780	575
13	1009	1036
14	1762	1211
15	1101	1000
16	628	801
17	1124	1019
19	811	836
20	639	577

1, 4, L		
-23	851	946
-21	643	848
-15	1354	1281
-14	472	413
-13	1398	1220
-12	621	759
-11	1598	1563
-10	959	861
-9	1916	1859
-8	1143	1027
-7	1897	2001
-6	622	917
-5	1520	1469
-4	922	971
-3	1464	1408
-2	487	664
-1	1479	1099
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1	1636	1874
2	547	692
3	645	288
4	1297	908
5	468	359
6	903	875
10	887	991
11	853	622
12	1061	994
13	678	876
14	940	1216
15	1139	1198
16	1184	1233
17	935	933
18	1636	1573
19	1080	1036
20	1432	1358
21	1035	996
23	614	567

1, 5, L		
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-12	1229	1218
-10	1080	1285
-8	1160	1289
-6	1036	888
-5	1274	1184
-4	953	891
-3	1690	1662
-2	1788	1671
-1	1216	1317
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1	1968	1911
2	1186	1204
3	1902	1561
5	1689	1665
7	1529	1369
8	572	527
11	809	822
13	1022	1068
15	1499	1379
16	582	420
17	1921	1714
18	870	708
19	1526	1546
20	652	686
21	1691	1651
22	1014	1015
23	1110	1036

1, 6, L		
-16	469	353
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-10	661	507
-9	1124	1171
-8	360	346
-7	1189	1186
-5	563	529
-2	891	844
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3	852	703
4	2385	2417
6	2610	2426
8	1953	1782
9	596	623
10	1077	1077
11	1560	1511
13	1212	1198
14	1050	1011
16	1724	1597
18	1530	1458

1, 6, L		
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22	1521	1467
24	1061	1091
1, 7, L		
-17	532	443
-15	609	566
-14	682	464
-13	685	732
-12	1205	473
-11	947	988
-9	1222	1362
-8	799	701
-7	1411	1451
-6	927	1323
-3	973	1028
-2	857	764
-1	786	609
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1	2093	2302
2	455	656
3	1952	2152
5	2203	2374
6	789	688
7	2557	2604
9	2180	2099
11	1869	1845
12	1425	1465
13	646	618
14	1276	1384
15	674	693
16	750	784
17	1498	1476
19	1254	1315
21	1291	1273
23	1034	1029
25	936	876

1, 8, L		
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-12	872	851
-11	815	626
-10	1546	1566
-8	1523	1673
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-5	391	525
-4	2186	2251
-3	550	510
-2	1248	1261
-1	798	472
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1	1048	924
2	2124	1395
3	722	732
4	2372	2129
6	2677	2594
8	2574	2542
10	2262	2221
11	467	452
12	1877	1835
13	1020	1070
14	1229	1104
15	1174	1205
17	974	889
18	787	821
20	861	968
22	991	991
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1, 9, L		
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-10	695	831
-9	1383	1494
-7	1649	1751
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-3	2517	2405
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1	1014	1022
2	741	796
4	496	717
5	1449	1438
7	2159	2087
9	2197	2220
10	703	569
11	1797	1673
13	1615	1579
14	439	524
15	1250	1233
16	786	629
1, 10, L		
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-9	929	990
-8	1107	1194
-7	616	741
-6	1451	1473
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-3	770	466
-2	1969	1988
-1	419	230
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2	1148	1054
5	517	560
6	667	666
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10	1371	1422
12	1296	1231
14	1323	1241
16	990	1057

1, 11, L		
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-7	601	692
-6	787	857
-5	1015	970
-3	1384	1367
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1	1449	1536
3	806	926
11	817	827
13	843	763
1, 12, L		
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-3	686	838
-2	766	820
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0	1246	1208
1	964	563
2	1189	1178
4	967	968
6	673	739
1, 13, L		
-4	533	310
-1	659	649
1	860	828
2	487	381
3	746	800
5	682	681
7	478	466
2, -13, L		
-5	713	788
-3	861	809
-1	884	764

2, -12, L		
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-9	1089	1016
-8	657	692
-7	1119	1032
-6	863	888
-5	857	857
-4	1052	941
-3	800	726
-2	984	1000
-1	589	546
0	1030	999
2	931	824
3, -11, L		
-16	1000	887
-14	630	603
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-6	1310	1215
-5	764	787
-4	1288	1217
-3	889	1001
-2	1144	1105
-1	1132	1088
0	998	970
1	1165	1135
2	843	608
3	949	960
5	539	578
11	778	727
2, -10, L		
-17	1096	1065
-16	589	579
-15	1173	1105
-14	649	670
-13	904	913
-12	801	743
-7	677	674
-5	1406	1247
-4	605	554
-3	1365	1272
-2	1071	879
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2	895	953
3	866	783
4	871	879
5	448	417
2, -9, L		
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-18	1148	1148
-16	1260	1224
-15	820	643
-14	1284	1206
-13	810	668
-12	1285	1177
-11	844	773
-10	853	774
-7	585	717
-6	762	593
-4	1158	1086
-3	713	658
-2	875	864
-1	891	836
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3	607	650
4	748	720
5	612	638
6	736	729
8	734	701
2, -8, L		
-19	659	689
-17	878	969
-15	1247	1232
-14	790	763

2, -8, L		
-13	1122	1087
-12	592	568
-11	1245	1213
-10	720	661
-9	1057	1055
-8	837	731
-7	586	696
-2	835	790
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2	1071	1059
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9	816	775
10	670	406
11	970	969
15	985	891

2, -7, L		
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-15	512	494
-14	764	893
-13	707	761
-12	899	1055
-11	789	754
-10	892	1029
-8	939	946
-6	881	998
-4	1121	1108
-3	482	405
-2	797	854
-1	903	899
0	878	854
1	849	849
2	817	692
3	509	482
5	819	827
6	527	566
11	786	672
12	1107	956
13	1022	921
14	1559	1419
15	867	771
16	1425	1427
18	1138	1186
20	789	744

2, -6, L		
-21	649	603
-11	886	902
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-7	469	691
-5	1076	1048
-4	929	821
-3	1167	1094
-2	1450	1541
-1	1663	1519
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1	1764	1279
2	1666	1324
3	1824	1899
4	740	863
5	1098	1264
7	1021	871
9	591	529
12	515	733
13	1299	1051
14	1400	1230
15	1783	1554
16	1181	1056
17	1098	1506
19	1681	1475
21	1132	1065

2, -5, L		
-15	614	815
-13	955	980
-11	757	870
-8	396	568
-6	501	482
-5	499	708
-3	1205	1149
-1	2204	2171
0	671	438
1	2481	2443
2	1643	1794
3	1966	1924
4	2101	2050
5	477	1575
6	1717	1797
7	730	713
8	1249	1183
10	1203	1083
14	850	614
15	1284	911
16	1226	961
17	1362	1265
18	1453	1453
19	978	903
20	1637	1500
22	1368	1347

2, -4, L		
-19	625	643
-14	1608	1572
-13	823	596
-12	1534	1546
-10	1631	1590
-8	884	942
-7	827	666
-4	420	325
-2	1084	1163
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1	638	732
2	3224	3481
3	1644	1606
4	2341	2268
5	1727	1776
6	1885	2178
7	2043	2000
8	1596	1543
9	2090	2201
11	1377	1473
13	727	828
18	1218	1143
20	935	955
21	1261	1192
23	1207	1207

2, -3, L		
-15	652	618
-13	1834	1673
-11	2011	2230
-9	3337	3151
-8	1257	1074
-7	3838	3513
-6	1707	1722
-5	1775	1889
-4	957	791
-3	1015	857
-2	999	997
-1	408	569
0	318	575
1	805	771
2	1465	1454
3	2718	2693
4	419	421
5	2921	3262
6	2051	2025
7	2948	2635
8	2511	2272
9	2009	1904
10	2125	2365
11	617	750
12	1626	1637
14	960	916
19	581	504

2, -2, L		
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-14	848	697
-12	1087	1300
-10	3547	3293
-8	4489	3696
-7	686	935
-6	4241	4226
-5	1556	1551
-4	3040	3039
-3	1398	1648
-2	1146	1272
-1	582	453
0	521	208
4	1090	759
5	1124	980
6	2490	2440
8	2779	2694
9	2338	2234
10	1845	2094
11	2861	2625
12	1176	1226
13	2380	2145
15	1198	1095
17	453	403

2, -1, L		
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-23	1200	1209
-21	1713	1671
-19	1641	1800
-18	881	670
-17	844	968
-15	698	937
-14	919	850
-12	688	817
-11	2017	1668
-9	3372	2953
-8	576	431
-7	4191	4341
-6	895	857
-5	5127	4575
-4	868	1068
-3	3080	3773
-2	2865	2605
-1	2624	2107
0	825	647
1	1392	1768
2	807	1118
4	855	266
5	644	824
6	782	798
7	2080	2109
8	1224	1056
9	1940	2203
10	1848	1840
11	1930	2008
12	2160	2026
14	2055	1672
16	961	890

2, 0, L		
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-22	1438	1487
-20	1788	1887
-18	1920	1874
-16	1416	1503
-15	1052	992
-14	528	809
-13	1017	1038
-11	1050	981
-10	931	999
-8	1933	1869
-6	3896	3999
-5	411	468
-4	3316	3318
-3	1459	1288

2, 0, L		
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-1	1575	1661
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1	776	460
2	484	664
4	825	426
5	431	168
7	823	858
9	1661	1520
11	1076	1199
13	1335	1508
15	1321	1150
18	636	741
20	612	637

2, 1, L		
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-19	1754	1884
-17	1899	2038
-15	2217	2201
-14	1116	1078
-13	1225	1283
-12	1364	1263
-11	923	1061
-10	1109	992
-8	793	773
-7	1562	1415
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-3	4011	4399
-2	2387	1366
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1	3437	1731
2	533	1125
3	865	1162
4	1635	1841
6	936	792
7	873	887
8	560	553
9	503	545
10	594	707
11	708	489
12	1068	918
14	1279	1162
22	576	609
23	684	750
25	797	765
27	684	800

2, 2, L		
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-18	1569	1470
-16	1792	1865
-14	1919	1940
-12	1973	1774
-10	558	634
-9	377	179
-8	519	437
-7	396	255
-2	1632	1774
-1	988	854
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1	529	449
2	675	625
4	2039	2191
5	461	680
6	893	757
7	1191	992
8	779	828
9	1283	1098
10	832	916
11	920	1178
12	1456	1444
13	1315	1387
14	1378	1275
15	942	912
16	533	600
21	656	627
23	748	686
24	580	718
25	801	664
26	807	830

2, 3, L		
-19	846	787
-17	1179	1076
-16	654	670
-15	1786	1600
-13	1600	1630
-11	1782	1669
-9	1303	1132
-8	720	657
-7	913	866
-6	766	613
-3	373	68
-2	1494	1402
-1	2014	1642
0	900	375
1	2720	3268
4	1837	1136
5	1506	1343
6	736	694
7	1106	1006
8	1426	1183
9	1006	1066
10	1336	1283
11	1391	1499
12	999	972
13	1846	1713
14	1859	1731
15	1958	1773
16	1136	1252
17	965	1139
18	898	878
19	1229	1102
24	782	690
27	695	742

2, 4, L		
-24	740	777
-16	979	1024
-14	1303	1200
-12	1508	1463
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-9	878	772
-8	1401	1307
-7	693	658
-6	646	721
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-3	1019	1258
-1	2473	2273
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1	553	941
2	735	444
3	739	683
4	796	537
5	1207	1023
9	1407	1389
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11	1753	1670
12	1557	1512
13	1475	1351
14	1381	1380
15	1586	1773
16	1482	1560
17	1709	1759
18	1605	1624
19	1342	1355
20	1372	1326
22	831	835

2, 5, L		
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-11	1112	932
-9	530	639
-6	897	1036
-4	1816	2120
-3	821	560
-2	2341	2301
-1	1096	414
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2	2770	2482
3	574	98
4	2397	2305
5	800	802
6	1319	1278
7	686	741
8	573	438
9	633	764
10	914	869
12	968	1441
14	1879	1776
15	886	836
16	1665	1661
17	940	849
18	1889	1873
19	1373	1299
20	1418	1396
21	1471	1445
22	689	632
23	1029	1084

2, 6, L		
-13	879	766
-12	795	820
-11	1310	1400
-10	616	596
-9	1465	1560
-7	810	779
-5	494	679
-3	1626	1701
-2	440	67
-1	2361	2378
0	613	196
1	3004	2971
2	500	79
3	3267	2879
5	2880	2847
6	542	654
7	1996	1875
8	1262	1321
10	1575	1467
11	736	663
12	1247	1013
13	1627	1632
15	2333	1939
16	647	623
17	1732	1664
18	620	714
19	1688	1611
20	832	973
21	1478	1379
22	1015	1098
23	780	786
24	733	761

2, 7, L		
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-13	1321	321
-12	1150	1159
-11	723	410
-10	1877	1928
-8	2191	2147
-7	602	655
-6	1710	1579

2, 7, L		
-5	1260	1564
-3	1146	1242
-2	1150	924
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1	596	388
2	2776	2922
4	2669	2797
6	2681	2658
8	2638	2542
9	1513	1491
10	1514	1549
11	1765	1794
12	576	213
13	1162	1192
14	1448	989
16	1293	1240
18	1223	1294
20	1279	1099
22	898	826

2, 8, L		
-15	829	837
-14	884	782
-13	1416	1469
-12	1275	419
-11	1631	1984
-9	2002	2203
-7	2364	2463
-5	1770	1941
-4	705	987
-3	761	731
-2	953	919
-1	1095	308
0	776	719
1	1971	1705
2	762	727
3	2617	2557
5	2248	2632
6	529	559
7	2501	2496
8	813	738
9	2234	2246
11	1851	1741
12	1149	1219
13	863	985
14	1262	1118
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-9	950	811
-8	465	869
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-4	713	546
-3	725	648
-2	494	689
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1	337	401
2	1413	1125
3	1135	1171
4	1482	1791
5	2557	2572
6	1286	1306
7	2520	2366
8	1206	1234
9	1240	1252
10	1169	1250
11	1323	1379
12	924	906
13	862	927
14	569	523
15	756	727
17	1146	1122
18	938	899
19	1117	1122
20	650	749
21	1316	1395
23	1329	1349
25	1153	1246
4, 2, L		
-20	1028	1088
-18	1332	1227
-16	1331	1299
-14	1345	1305
-12	965	845
-9	821	865
-7	1583	1430
-6	495	264
-5	634	667
-1	640	360
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2	2304	2067
3	815	375
4	3226	3019
6	3046	2697
7	1181	963
8	2045	2128
9	1518	1421
10	1855	1820
11	1488	1452
12	2160	2212
14	1765	1747
17	958	997
19	1026	1036
20	875	1077
22	1141	1315
24	1183	1322
26	1066	1102
4, 3, L		
-19	942	926
-17	988	1020
-15	1061	1012
-13	881	789
-12	966	979
-11	1192	1096
-10	1235	1107
-8	1442	1570
-6	2373	2093
-4	2360	2135
-3	990	994
-2	2112	1887
-1	1559	1483
1	318	492
2	1529	1865
3	329	573
4	2400	1925
5	2098	2077
6	1694	1162
7	2666	2639
8	2048	2005
9	2302	2391
10	1962	1895
11	2115	2237
12	1814	1904
13	2208	2465
14	1106	1277
15	2049	2132
17	915	1077
20	774	777
23	887	1016
25	1008	1107
27	838	961
4, 4, L		
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-10	1170	963
-9	2056	1964
-8	904	870
-7	1862	1705
-5	2475	2310
-3	3303	3013
-2	1346	932
-1	2014	2111
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1	613	317
2	1622	1809
3	1127	829
4	2479	2377
5	1798	1780
7	2487	2402
8	1604	1703
9	2128	2086
10	1917	1848
11	1624	1740
12	2057	2174

4, 4, L			19 1328 1238			-14 1682 1748			-7 837 942			12 812 833			17 1090 1048		
13	1713	1795	4, 6, L			-13 772 383			-6 710 751			13 758 790			18 813 773		
14	1865	1727	-21 696 766			-12 1871 1855			-3 665 1153			14 1043 1034			19 960 918		
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16	1800	1863	-17 1222 1346			-10 1330 1346			0 723 657			16 778 715			22 890 775		
17	720	738	-15 1439 1514			-9 1078 998			1 1579 1576			17 692 695			4, 12, L		
18	1174	1258	-13 1979 1794			-8 582 749			2 694 719			19 708 739			-12 602 190		
4, 5, L			-12 1114 900			-7 1003 1017			3 1588 1558			4, 10, L			-10 478 304		
-18	812	942	-11 1006 1213			-5 409 376			4 816 914			-13 746 828			-7 668 782		
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-2	2847	3103	2 2609 2334			6 1410 1297			4, 9, L			14 652 704			8 801 781		
-1	1186	1168	3 2312 2320			7 1082 1288			-16 831 796			15 933 839			10 580 558		
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2	1900	2014	6 1555 1534			13 734 740			-11 859 244			18 712 633			20 977 938		
3	1585	1716	8 1069 1063			14 835 746			-10 1506 1640			19 784 701			4, 13, L		
5	2131	1779	9 1236 1137			15 1230 1134			-8 1509 1545			21 844 673			-9 788 772		
6	1118	1101	11 846 1230			16 629 519			-6 1134 1127			4, 11, L			0 538 15		
7	1153	1173	13 967 1396			17 902 921			-5 507 576			-10 845 1030			2 1200 284		
8	2293	2462	14 1251 1195			19 838 725			0 1020 950			-8 1265 1362			3 956 1002		
9	883	784	15 1461 1249			4, 8, L			1 329 338			-6 991 1107			4 828 152		
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11	1423	1212	17 833 788			-17 1059 1134			3 554 681			-2 734 587			7 1426 1523		
12	1377	1979	18 908 902			-15 1358 1462			4 826 1014			1 743 710			8 586 656		
13	1926	1691	19 611 626			-14 1137 385			5 719 774			3 406 508			9 1135 1242		
14	1752	1811	20 956 927			-13 1966 1948			6 862 1013			4 378 346			10 794 795		
15	1577	1646	4, 7, L			-12 872 115			7 871 736			5 489 458			11 799 784		
16	1287	1373	-20 805 799			-11 1878 1981			8 957 891			6 345 396			12 852 772		
17	1408	1509	-18 1102 1242			-9 1531 1555			9 402 290			15 830 643					
18	703	737	-16 1493 1559			-8 880 723			10 723 776			16 435 306					

4, 14, L		
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-4	857	889
3	705	415
4	908	907
6	1279	1390
8	1463	1602
10	1189	1272
11	737	828
12	849	857
13	695	728
14	642	537

5, -10, L		
4	960	893
6	826	885
8	603	738

5, -9, L		
-7	691	620
3	740	785
5	1246	1279
7	1358	1433
9	955	1142

5, -8, L		
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-11	514	532
-10	857	807
-9	1109	1117
-8	1341	1245
-4	1271	1329
-2	710	779
-1	674	144
1	411	228
4	809	875
6	1532	1572
8	1633	1824
10	1101	1580
12	1300	1248
14	598	665

5, -7, L		
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-8	1064	1070
-7	1517	1479
-6	886	914
-5	1672	1707
-3	1687	1801
-1	1109	1052
1	568	410
4	397	447
5	623	696
6	617	644
7	1157	1245
8	600	682
9	1743	1840
11	1571	1839
13	1982	1549
15	1427	1021

5, -6, L		
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-9	951	881
-7	1331	1315
-6	1016	1158
-5	1296	1392
-4	1851	1965
-3	581	552
-2	2009	2173
-1	508	89
0	1840	1996
1	753	468
2	935	896
7	455	568
8	822	843
10	1275	1331
12	1727	1573
14	1939	1461
16	1429	1059

5, -5, L		
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-19	802	733
-18	935	1001
-17	950	1026
-15	848	963
-10	465	334
-8	951	933
-6	1257	1210
-5	1028	936
-4	1511	1486
-3	1598	1679
-2	1149	1139
-1	2240	2357
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1	2408	2610
2	792	108
3	1913	1930
5	706	733
12	719	497
13	1068	977
15	1197	1057
19	818	874

5, -4, L		
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-19	1182	1137
-17	1485	1574
-16	1094	1218
-15	1423	1432
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-13	937	1051
-12	1271	1264
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-7	702	634
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-3	1345	1233
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2	2659	2236
3	1129	704
4	1936	2101
6	998	1206
14	556	541
16	825	740

5, -3, L		
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-18	1107	1063
-17	625	529
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-15	1169	1040
-14	1958	1981
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-12	1601	1780
-11	1683	1626
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-9	1624	1569
-7	1017	963
-4	891	844
-2	883	896
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1	1995	2097
2	1448	1289
3	2210	2317
4	939	954
5	1913	2062
6	729	1047
7	1678	1789
9	481	458
10	424	584

5, -2, L		
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-19	753	658
-17	939	987
-15	1511	1501
-14	904	828
-13	1940	2025
-12	1658	1517
-11	1674	1683
-10	1738	1582
-9	1841	1680
-8	1637	1602
-7	593	807
-6	984	1122
-4	536	569
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1	536	662
2	1606	1897
3	723	590
4	1958	2003
5	457	576
6	1211	1280
7	1065	1167
8	1115	1152
11	1138	1065
13	1124	1155
15	724	887
16	584	522
17	973	1002
19	916	844

5, -1, L		
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-16	1124	1102
-14	1164	1262
-13	583	399
-12	1746	1592
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-10	1644	1435
-9	841	1083
-8	899	1113
-7	1072	778
-6	768	863
-5	625	609
-4	1093	878
-2	591	568
-1	549	634
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5	1537	1669
7	597	826
12	1390	1299
14	1313	1323
15	717	624
16	1182	1221
18	1154	1329
20	1308	1178

5, 0, L		
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-12	494	545
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-9	404	705
-8	1064	926
-7	765	725
-6	479	423
-5	1100	944
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-1	1632	1518
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1	1287	1313
2	1156	920
3	1230	1298
4	1555	1392
5	1600	1826
6	1596	1605

5, 0, L		
7	1206	1316
10	814	965
12	1037	1021
13	1439	1451
15	1833	1515
17	1615	1558
19	1464	1618
21	1537	1567
23	902	1059
5, 1, L		
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-20	735	703
-18	872	960
-16	900	807
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-7	925	774
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3	1537	1202
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5	1225	1377
6	3149	3233
7	1097	1242
8	2186	2056
9	495	621
10	1996	1817
14	863	751
15	678	824
16	1615	1302
18	1492	1421
20	1459	1573
22	1411	1607
24	1223	1377

5, 2, L		
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3	1919	2164
4	1877	1851
5	3190	3349
6	1161	1463
7	2937	2644
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9	2876	2823
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13	1069	1237
16	830	1015
17	740	811
19	1032	1199
21	1376	1451
23	1191	1312
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5, 3, L		
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2	1376	1320
3	1809	1742
4	1602	1289
5	1993	2122
6	2992	2462
7	2365	2092
8	2271	2279
9	2047	1879
10	2217	2387
11	1391	1427
12	2341	2344
14	1696	1666
16	935	786
17	749	665
22	989	985
24	883	1034
5, 4, L		
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-12	1605	1485
-10	2097	1979
-8	2502	2327
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-6	2553	2354
-5	521	509
-4	2659	2589
-3	571	896
-2	2235	2018
-1	1941	2185
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3	762	898
4	1903	1880
5	812	837
6	1810	1581
7	2267	2421
8	1657	1694
9	2192	2252
10	1439	1500
11	2121	1901
12	1841	1807
13	1687	2021
14	903	773
15	1455	1431
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5, 5, L		
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-19	1159	1176
-17	1156	1333
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-9	1699	1709
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2	1491	1688
3	612	146
4	1586	1503
5	1897	1919

6	599	390
7	1774	1667
8	1139	1247
9	1220	1458
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11	1259	1478
12	1775	1756
5, 6, L		
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-3	1022	1108
-2	2312	2496
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2	1643	1619
3	2136	2076
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7	577	489
8	721	685

11	803	797
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16	668	652
17	786	831
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5, 7, L		
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-17	1398	1406
-15	1431	1444
-14	663	637
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-12	960	831
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3	1375	1308
4	1833	1695
5	1045	918
6	597	519
7	784	635
10	419	455
12	1037	978
14	1181	1161
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5, 8, L		
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-16	1370	1429
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5, 8, L			7 648 729			6 432 462			6 1557 1608			6, -8, L			-1 1266 1383		
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12	740	787	2	327	364	3	1440	1473	9	1075	1157	-4	1605	1633	-2	1829	2033
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14	687	602	11	584	649	5	1177	1249	11	755	819	0	669	473	0	1739	1929
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5, 9, L			14	1314	1201	8	877	902	5, 15, L			4	691	661	4	782	738
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1	780	585	-1	465	252	0	721	684	6, -9, L			-9	775	743	-15	1324	1423
2	492	458	0	909	931	1	1070	284	-10	984	928	-8	1065	1078	-13	1030	1114
3	835	662	2	914	973	2	1365	1299	2	1240	1191	-7	1448	1356	-11	678	865
4	635	678	3	812	749	3	898	112	4	1427	1455	-6	744	747	-8	543	426
5	538	689	4	786	686	4	1821	1822	6	1360	1436	-5	1455	1614	-6	742	673
6	396	554	5	802	753	5	963	835	8	900	1087	-3	1736	1905	-5	806	740

6, -4, L		
-4	1111	1035
-3	1625	1726
-2	824	871
-1	1890	2047
0	852	770
1	1914	1965
2	643	187
3	1226	1321
5	786	946

6, -3, L		
-19	1342	1230
-18	567	645
-17	1331	1417
-16	852	1008
-15	1409	1498
-14	1223	1218
-13	1092	1183
-12	1429	1357
-10	1029	1005
-8	576	601
-4	704	832
-2	1558	1622
-1	1049	808
0	1790	1840
1	1151	695
2	1600	1570
3	830	659
4	1294	1260
5	725	851
7	686	777
11	934	964
13	754	916
15	809	761
17	541	546

6, -2, L		
-18	958	850
-16	960	1040
-15	1018	972
-14	932	1077
-13	908	1014
-12	1049	1134
-11	1327	1256
-9	1076	1026
-7	707	630
-3	963	863
-2	501	432
-1	1476	1598
0	612	417
1	1477	1759
2	601	136
3	1337	1548
5	703	678
6	914	960
8	864	1059
10	1327	1314
12	1374	1387
14	1435	1443
15	773	82
16	1103	1172
18	1021	949

6, -1, L		
-17	838	708
-16	627	541
-14	994	711
-12	674	721
-11	551	407
-10	510	545
-9	819	608
-7	788	750
-5	567	717
-3	1388	1423
-1	1133	1215
0	818	810
1	1160	1092
2	951	1088
3	1361	1244
4	881	816
8	648	563
9	1058	972
10	616	565
11	1760	1726
12	555	524
13	1693	1766
15	1690	1693
17	1480	1625
19	1236	1350
21	841	868

6, 0, L		
-6	765	766
-5	659	584
-4	1305	1023
-2	1733	1621
-1	709	544
0	2304	2310
1	2284	907
2	2452	2373
3	1072	688
4	2379	2483
5	460	191
6	1638	1695
7	473	618
9	1485	1664
10	1013	890
11	1014	1163
12	1746	1732
14	1889	1807
16	2003	1807
18	1768	1813
20	1509	1590
22	910	1134

6, 1, L		
-17	1119	1070
-15	614	718
-10	730	810
-8	464	616
-5	506	388
-4	1150	1002
-3	1041	1011
-2	673	812
-1	2028	2078
0	1095	914
1	2611	2539
2	1206	1098
3	2914	2793
4	1001	880
5	3115	3156
6	792	590
7	2328	2503
9	1563	1522
10	1007	889
12	926	941
13	1038	933
15	1918	1552
17	1583	1523
19	1470	1371
21	1545	1508
23	1030	1177
25	768	745

6, 2, L		
-16	1015	796
-15	1008	1218
-14	1074	906
-13	994	1149
-11	1316	1423
-10	997	962
-9	1185	1210
-8	1064	1021
-7	783	1011
-6	1342	1146
-4	430	586
-3	1093	1033
-1	980	839
0	1167	1515
1	869	934
2	2350	2367
3	1137	1029
4	2732	2751
5	1227	1153
6	2864	2920
7	914	1016
8	2819	2646
10	2717	2484
12	1080	1045
13	815	1015
16	1218	887
18	1047	1010
20	1239	1262
22	1183	1276
24	1077	1075

6, 3, L		
-14	1452	1438
-13	1078	837
-12	1452	1402
-11	609	817
-10	1553	1417
-9	933	987
-8	1308	1424
-7	1279	1272
-6	845	743
-5	1497	1304
-3	1233	1474
-2	1148	1127
-1	577	605
0	1026	1080
1	1261	1412
2	1671	1939
3	1339	1134
4	1951	2090
5	2126	1904
6	1657	1508
7	2211	2069
8	1400	1469
9	2407	2361
10	619	511
11	2099	1977
13	1113	1128
15	513	381
19	637	825
21	908	951
23	888	989
25	1020	994

6, 4, L		
-18	611	563
-13	1428	1355
-11	2014	1913
-9	2183	2056
-8	1371	1302
-7	1901	1853
-6	1501	1257
-5	1767	1636
-4	1867	1842
-3	885	1104
-2	2039	2208
-1	564	211
0	1156	1102
1	1095	1165
2	706	328
3	1487	1557
4	541	230
5	2465	2331
6	2263	2274
7	1829	1681
8	1697	1665
9	1561	1586

6, 4, L		
10	1749	1615
11	987	927
12	1501	1557
13	396	487
14	1001	1195
16	724	730
26	690	622

6, 5, L		
-20	1099	1107
-15	853	762
-12	1295	1168
-10	1835	1697
-8	2212	2110
-7	1292	1326
-6	2535	2247
-5	1927	1875
-4	1621	1703
-3	2066	2224
-2	955	995
-1	1963	2029
0	1084	700
1	1625	1865
3	469	401
4	689	544
5	959	966
6	1138	1011
7	1506	1511
8	1376	1379
9	2067	2105
10	812	691
11	1519	1507
12	740	807
13	1338	1279
15	843	800
16	501	178

6, 6, L		
-19	1215	1262
-17	1023	1097
-15	785	649
-14	742	665
-12	783	621
-11	811	802
-9	1364	1304
-8	535	445
-7	1694	1766
-6	1224	1200
-5	2119	2117
-4	1575	1701
-3	1825	1915
-2	2090	2178
-1	1532	1624
0	2059	2251
1	735	719
2	1602	1843
3	294	288
4	909	915
6	916	1071
8	957	920
10	1561	1635
12	1479	1561
13	564	272
14	1078	1032
21	550	409
23	824	772
25	735	663

6, 7, L		
-20	1160	1242
-18	1250	1315
-16	1265	1285
-14	877	869
-12	446	435
-11	570	529
-8	818	945
-6	1062	1161
-5	764	763
-4	1313	1234
-3	1048	945
-2	1377	1488
-1	1662	1644
0	1728	1454
1	1725	1758
2	1181	976
3	1506	1317
4	914	1107
5	818	643
6	851	781
7	351	568
8	770	631
9	332	497
10	817	684
11	887	879
13	1175	1168
22	985	1005
24	855	982
26	1043	1010

6, 8, L		
-19	853	1044
-17	1163	1258
-15	1317	1296
-14	533	568
-13	927	871
-11	467	468
-3	407	567
-2	531	434
-1	674	720
0	923	785
1	786	724
2	729	754
3	732	654
4	658	625
5	787	746
7	1437	1312
8	834	851
9	1313	1283
10	1030	1025
11	1490	1355
12	1005	951
13	1110	1061
15	670	643
16	418	335
23	972	989
25	1066	1136

6, 9, L		
-16	962	1002
-14	1188	1151
-12	1007	925
-10	568	528
-7	517	475
-5	572	619
1	582	447
3	448	407
7	595	580
8	867	917
9	1176	1153
10	1389	1440
11	987	996
12	1585	1665
13	860	718
14	1646	1572
16	973	991

6, 10, L		
-15	503	656
-13	923	817
-11	722	722
-9	694	649
-7	385	387
-6	569	526
-4	670	762
-3	614	698
-2	702	643
-1	768	788
0	545	614
1	608	623
2	337	451
10	876	1014
11	790	1039
12	968	1081
13	1236	1526
14	849	776
15	1471	1572
17	1285	1306
19	1000	910

6, 11, L		
-5	559	609
-3	1092	1150
-2	529	628
-1	1184	1312
0	1116	1048
1	1230	1225
2	1523	1365
3	569	595
4	1062	989
6	778	781
8	478	531
11	750	798
12	416	297
13	1125	1203
14	918	923
15	1194	1107
16	1171	1233
17	824	740
18	1421	1414
20	1148	1084
22	822	658

6, 12, L		
-12	731	617
-10	550	440
-2	1168	1194
-1	598	237
0	1507	1547
1	1003	747
2	1606	1689
3	1388	1225
4	1296	1275
5	1256	1242
6	787	849
7	902	1015
8	507	538
9	792	802
14	1125	1015
16	1271	1196
17	955	894
18	933	912
19	1170	1093

6, 13, L		
-9	571	710
-1	898	886
0	527	69
1	1579	1466
2	1045	550
3	1694	1619
4	1094	1025
5	1531	1534
6	1314	1277
7	996	1051
8	961	1043
9	600	534
10	672	740
17	773	812

6, 14, L		
0	755	623
1	750	248
2	1135	1088
3	753	308
4	1297	1255
5	785	724
6	1248	1300
7	898	982
8	939	991
9	971	999
11	655	723
13	505	480

6, 15, L		
0	529	510
5	650	673
9	749	726

7, -9, L		
-1	806	710
1	1269	1295
3	1511	1533
5	1245	1347
6	633	719

7, -8, L		
-10	1174	1266
-8	1133	1117
-6	741	752
0	583	671
2	1112	1183
4	1337	1398
6	1262	1321
8	886	1042

7, -7, L		
-11	1011	1013
-9	1428	1423
-7	1394	1493
-5	933	1045
-3	658	601
-1	450	55
0	575	344
3	861	876
5	1028	1213
7	1040	1258
9	652	1240

7, -6, L		
-11	746	689
-10	930	956
-9	544	503
-8	1104	1173
-6	1676	1638
-4	1184	1440
-2	1024	1039
0	703	673
1	492	272
2	393	170
8	652	918
10	891	1056
14	817	533
16	605	391

7, -5, L		
-17	866	950
-15	661	754
-9	655	630
-8	559	640
-7	1086	1122
-6	586	629
-5	1605	1616
-3	1552	1670
-1	1222	1299
0	487	257
1	1034	1035
3	473	474
13	541	522

7, -4, L		
-19	669	827
-18	1045	1233
-16	1218	1220
-14	1040	1001
-6	1137	1148
-4	1453	1441
-2	1484	1665
0	1257	1399
1	474	430
2	873	844
3	492	517
4	511	505

7, -3, L		
-17	1125	966
-16	640	761
-15	991	1075
-13	966	1048
-11	782	769
-5	869	861
-3	1200	1322
-1	1259	1392
0	557	302
1	1204	840
2	618	584
3	623	359
4	1002	1008
6	1045	1205
8	1100	1201
10	1070	1166
12	1046	1202
14	988	1073

7, -2, L		
-16	581	674
-14	657	671
-13	587	563
-12	916	864
-10	590	650
-7	568	606
-5	610	558
-4	804	852
-3	1046	1115
-2	799	1015
-1	1088	1066
0	862	835
1	551	486
3	607	560
5	961	1002
7	1594	1668
9	1518	1570
11	1682	1731
13	1492	1651
15	1364	1453
16	1026	616
17	793	1014

7, -1, L		
-15	721	676
-8	908	797
-6	796	853
-4	954	1140
-3	509	462
-2	1753	1847
-1	944	957
0	1696	1847
1	748	560
2	1390	1331
3	549	247
7	884	929
8	1276	1172
10	1693	1749
12	1733	1897
14	1889	1889
15	1042	513
16	1527	1556
18	1056	1171

7, 0, L		
-7	1092	948
-5	1408	1470
-3	1638	1775
-1	2134	2068
0	694	590
1	2317	2336
2	1105	209
3	1988	2014
4	550	185
5	1313	1316
8	716	890
9	813	727
10	764	889
11	1548	1560
13	1585	1632
15	1920	1822
17	1674	1705
19	1204	1324
21	587	744
22	805	731

7, 1, L		
-17	636	856
-16	620	620
-15	1053	1036
-14	547	497
-10	780	909
-7	840	893
-6	551	627
-5	871	1018
-4	1708	1589
-2	2185	2124
-1	692	501
0	2561	2416
1	1410	598
2	2920	2629
3	836	255
4	2414	2521
6	2006	2071
7	667	623
8	879	831
9	830	909
12	1216	1113
14	1568	1619
16	1989	1754
18	1719	1718
20	1462	1474
22	1083	1156

7, 2, L		
-17	674	821
-16	772	971
-15	796	863
-14	1106	1145
-13	847	837
-10	785	1008
-9	1400	1235
-7	1009	1004
-6	706	760
-4	1807	1484
-3	1031	1149
-2	1201	1303
-1	1537	1685
0	923	999
1	1886	1958
2	1197	1110
3	2827	2928
4	870	738
5	2355	2296
6	721	747
7	2071	1875
9	1939	1916
10	512	507
11	851	867
12	936	952
13	447	372
15	1378	941

7, 2, L			-11	1020	1273	4	635	493	24	884	1027	7	783	874	2	696	674
17	1115	987	-10	1250	1470	5	1447	1511	7, 7, L			8	1835	1707	7	908	834
19	1182	1132	-9	1625	1523	6	1690	1601	-19	920	1033	9	893	929	9	822	979
21	1224	1190	-8	1498	1455	7	1215	1036	-17	732	798	10	1872	1660	10	785	1147
23	846	907	-7	2026	1930	8	1244	1148	-15	718	530	11	537	516	11	918	985
25	838	681	-6	1094	1084	9	900	912	-7	593	520	12	1251	1339	12	1465	1646
7, 3, L			-5	2118	2003	10	1483	1550	-6	789	682	14	845	876	13	680	643
-17	867	758	-3	2030	2024	12	614	744	-5	638	683	20	858	698	14	1570	1695
-15	892	1118	-1	945	744	13	433	235	-4	1102	1044	22	1074	1143	16	1212	1218
-14	1097	922	0	1658	1462	19	693	834	-3	560	565	24	1358	1406	18	1098	1068
-13	1201	1315	1	644	312	21	504	781	-2	1167	1291	7, 9, L			7, 11, L		
-12	1200	1116	2	2186	1874	7, 6, L			-1	583	596	-15	945	759	-6	871	1028
-11	1396	1355	3	1693	1508	-20	917	1079	0	790	830	-13	650	587	-4	1262	1428
-10	1441	1438	4	1287	1245	-18	731	766	1	751	937	-10	552	389	-2	1393	1406
-9	1251	1092	5	1825	1645	-15	554	677	3	880	870	-8	749	790	-1	1549	1440
-8	1872	1632	6	1510	1673	-12	762	762	4	604	311	-6	816	773	0	914	890
-6	1554	1763	7	2546	2300	-10	1153	1153	5	1540	1632	-5	806	789	1	1322	1252
-4	1202	1114	8	739	672	-9	795	836	6	1047	1157	-3	633	738	2	661	604
-3	1067	988	9	2096	2020	-8	1206	1212	7	2087	2035	-1	631	608	3	1145	1097
-1	1299	1325	11	1375	1231	-7	1531	1463	8	570	754	5	573	404	5	737	661
0	1033	1140	13	910	881	-6	1327	1477	9	1295	1219	6	754	849	8	477	509
1	1770	1806	7, 5, L			-5	1876	1909	10	834	823	7	1258	1238	10	817	972
2	1972	1946	-20	710	741	-4	1105	1136	11	1186	1080	8	995	1120	12	902	1078
3	1544	1413	-18	879	934	-3	2135	2241	12	451	477	9	1604	1653	13	937	1130
4	1996	1882	-15	625	665	-2	483	341	19	1090	1022	10	993	962	14	789	846
5	1525	1510	-13	1280	1255	-1	1203	1283	21	1310	1378	11	1868	1878	15	1366	1395
6	2374	2218	-11	1552	1543	0	936	919	23	1332	1385	13	1595	1640	16	529	328
7	679	691	-10	1057	1184	2	755	824	25	1153	1117	15	1194	1135	17	1318	1312
8	2172	2045	-9	1418	1502	3	530	388	7, 8, L			7, 10, L			19	1238	1198
10	2056	1812	-8	1567	1608	4	1124	1169	-16	887	952	-14	587	417	21	859	770
12	906	787	-7	1509	1565	5	774	958	-11	461	96	-12	614	444	7, 12, L		
20	749	860	-6	2209	2107	6	668	647	-1	561	563	-7	552	664	-11	452	417
22	839	975	-5	1247	1246	7	1223	1343	0	414	336	-6	440	605	-5	1072	1011
7, 4, L			-4	2417	2253	9	966	1089	1	551	298	-5	915	958	-3	1138	1221
-19	689	648	-2	2071	2133	11	977	1062	2	436	476	-4	785	948	-1	1399	1614
-14	1272	1397	-1	596	275	13	645	688	3	643	193	-3	785	764	0	1006	1112
-13	1079	843	0	1196	1132	20	1264	1338	4	904	784	-2	1258	1312	1	1613	1577
-12	1425	1388	1	350	479	22	1076	1198	6	1323	1298	0	912	976	2	1733	1541

7, 12, L		
3	1109	1069
4	1429	1266
5	714	716
6	1023	992
8	396	494
11	851	861
13	986	1167
14	818	787
15	953	1057
16	1005	1024
17	757	672
18	1157	1074
20	999	939
7, 13, L		
-9	651	653
-2	912	977
0	1330	1322
1	1023	758
2	1616	1460
3	1313	1199
4	1279	1275
5	1263	1284
6	895	948
7	1023	1093
9	430	591
14	755	757
15	748	698
17	604	699
7, 14, L		
-1	706	636
1	889	786
2	677	550
3	937	873
4	792	808
5	939	939
6	915	945
7	562	718

8	766	792
10	692	606
7, 15, L		
5	610	602
8, -8, L		
1	943	965
3	1116	1105
5	979	983
8, -7, L		
-10	1254	1282
-8	1188	1207
-6	733	801
2	527	530
4	640	685
8, -6, L		
-11	825	921
-9	1204	1321
-7	1208	1335
-5	956	985
8, -5, L		
-10	755	794
-8	1023	1112
-6	1362	1403
-4	1205	1258
-2	937	1062
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8, -4, L		
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-7	1088	1085
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-3	1014	1060
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8	864	911
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8, -3, L		
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-8	774	613
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-4	843	773
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7	1256	1420
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11	1306	1357
13	766	999
14	727	547
19	618	717
8, -2, L		
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8	1633	1714
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8, -1, L		
-9	1024	1018
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-3	1942	2049
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13	1535	1670
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16	1502	1121
17	1022	885
18	825	862
8, 0, L		
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-9	690	879
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-6	1720	1795
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3	990	724
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5	755	938
7	936	999
8	958	947
10	1297	1336
12	1466	1491
14	1437	1459
15	1058	687
16	1503	1500

16	1090	1173
8, 1, L		
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-8	946	956
-7	900	848
-6	1010	975
-5	1417	1586
-4	703	848
-3	2242	2188
-2	659	586
-1	2412	2307
0	1928	710
1	2974	2768
2	2048	254
3	2594	2258
4	668	310
5	1618	1518
6	847	874
8	638	819
11	1096	1057
13	1062	1049
15	1601	1465
17	1466	1571
19	1339	1350
8, 2, L		
-19	694	771
-18	856	689
-16	874	875
-15	897	1013
-14	905	1097
-10	1010	1291
-8	577	736
-7	894	845
-5	1084	1206
-4	1043	1096
-3	1058	1097
-2	1918	1871
-1	1088	973

0	2167	2240
1	820	633
2	2492	2476
3	685	580
4	2287	2266
5	528	134
6	1877	1763
7	679	546
8	929	993
10	595	598
12	517	402
16	1298	855
18	1170	1031
20	1127	1049
8, 3, L		
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-16	1095	1053
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-14	965	1202
-13	1257	1429
-11	1348	1492
-9	1826	1932
-7	1471	1336
-5	569	572
-4	856	911
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2	1383	1467
3	2332	2137
4	879	835
5	1865	1701
6	595	444
7	1497	1473
9	1260	1291
11	620	683
12	432	548

8, 4, L		
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-15	1057	1123
-14	970	829
-13	954	1067
-12	1487	1428
-11	1000	1106
-10	1826	1965
-9	673	875
-8	1902	1931
-6	1732	1806
-4	875	943
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1	914	1016
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3	477	397
4	1946	1677
6	1719	1717
8	1242	1274
10	1269	1163
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19	632	647
8, 5, L		
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-12	955	982
-11	1183	1122
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-9	1856	1763
-7	1948	1764
-6	577	763
-5	1717	1830
-3	1050	1155
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-1	507	381
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2	540	280
3	1522	1423
4	878	665
5	1102	1042
7	1519	1343
9	1154	974
14	631	628
16	958	1064
18	1061	1194
20	985	1112
22	648	882
8, 6, L		
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-8	1444	1342
-6	1663	1613
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3	1669	1533
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6	837	814
7	420	445
10	637	584
15	577	647
16	845	337
17	1375	1391
19	1650	1698
21	1353	1504
23	1059	1129
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8, 7, L		
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3	977	785
4	2291	2395
6	1850	1973
7	493	561
8	1484	1482
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16	825	600
18	1116	1171
20	1802	1767
22	1418	1522
24	1029	1058
8, 8, L		
1	693	614
2	945	675
3	1227	1154
4	1467	979
5	1816	1903
6	718	732
7	2262	2360
9	1884	1816
11	1478	1482
13	654	678
19	994	880
21	1190	1202
23	1362	1344
8, 9, L		
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-4	921	893
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2	441	44
3	830	713
4	854	760
5	866	926
6	980	1077
7	1128	1089
8	1744	1790
9	417	506
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12	1636	1488
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16	525	721
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8, 10, L		
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-5	1010	1084
-4	846	900
-3	1312	1388
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3	349	294
4	381	441
6	924	1009
7	635	687
8	1079	1109
9	1279	1409
10	668	689
11	1678	1770
13	1558	1518
15	1363	1313
17	1091	989
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8, 11, L		
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-3	1233	1322
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7	724	747
9	823	1023
10	531	856
11	802	1015
12	1077	1371
13	587	627
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16	1218	1304
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8, 12, L		
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-3	942	964
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3	1268	1194
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11	663	591
12	734	850
13	906	961
15	1042	1020
17	1025	952
8, 13, L		
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-1	882	1045
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1	1015	1059
2	1236	1288
3	729	779
4	1207	1190
6	856	819
14	687	734
8, 14, L		
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2	674	598
3	1052	1022
5	768	879
6	455	486
7	689	679
8, 15, L		
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9, -6, L		
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-8	969	982
-6	651	765
9, -5, L		
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-9	914	1003
-7	968	968
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9, -4, L		
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3	818	868

9, -4, L			14 969 943			9 1252 1394			0 1257 543			12 887 903			13 426 351		
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9, -3, L			-8	1418	1529	13	1170	1262	5	1084	1181	9, 5, L			18	1704	1817
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9, -2, L			10	1381	1471	2	1713	1535	1	539	403	7	488	351	9	599	522
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9, 8, L		
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8	1463	1574
9	855	863
10	706	723
11	559	675
12	653	516
13	786	809
15	579	602
18	898	907
20	1349	1274
22	1191	1256

9, 9, L		
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3	993	743
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6	745	701
7	1698	1844
9	1575	1696
11	1414	1327
12	616	570
13	977	942
14	729	589
15	761	672
23	839	973

9, 10, L		
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3	660	650
4	672	542
5	773	1028
6	1023	1028
7	795	992
8	1401	1433
10	1507	1579
12	1612	1547
14	1247	1215
16	951	887

9, 11, L		
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-3	1522	1608
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8	704	865
9	1108	1034
10	580	652
11	1095	1290
13	1182	1248
15	1127	1141
17	955	879

9, 12, L		
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2	1133	1196
8	535	622
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14	558	817
16	695	758

9, 13, L		
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1	1177	1098
2	532	502
3	1042	997
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9, 14, L		
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2	649	656
4	579	571
6	522	357
13	525	596

10, -5, L		
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1	717	707
2	627	544
3	646	540
6	504	379

10, -4, L		
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1	423	424
2	941	1098
4	1024	1157
6	763	930
7	911	889
9	699	775

10, -3, L		
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-7	714	715
-6	428	512
-3	435	511
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3	1143	1228
5	1234	1357
6	896	890
7	1240	1260
8	869	945
9	871	887
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10, -2, L		
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-8	1191	1236
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10	1018	1119
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10, -1, L		
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3	812	717
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6	814	709
7	1090	1215
8	811	937
9	1177	1273
10	1027	1063
11	1060	1281
12	1016	1086
13	882	969
14	727	704
15	644	542

10, 0, L		
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-8	1540	1498
-6	1642	1666
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8	993	1073
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11	671	761
12	1192	1246
14	823	860
15	717	366

10, 1, L		
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-7	1506	1501
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-3	1831	1823
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13	778	842
14	845	548
15	845	840

10, 2, L		
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-6	1264	1113
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2	1058	939
3	636	308
4	669	676
13	507	617

10, 3, L		
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6	402	133
10	703	693

10, 3, L		
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10, 4, L		
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14	988	946
15	935	1031
16	663	575
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10, 5, L		
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14	1645	1647
15	1033	919
16	1496	1500
17	800	933
18	824	941
19	660	680
21	535	474

10, 6, L		
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5	955	806
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13	1563	1575
15	1470	1728
16	651	647
17	1685	1762
18	860	866
19	1253	1205
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10, 7, L		
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2	1852	1897
3	679	418
4	1693	1606
5	855	827
6	1132	1206
7	620	701
8	813	855
9	700	773
14	1024	1101
16	1575	1500
17	1149	529
18	1578	1491
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10, 8, L		
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-9	852	814
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2	680	545
3	1562	1543
5	1710	1711
6	760	756
7	1059	1150
8	629	731
9	1033	1067
10	667	689
11	798	884
12	773	697
14	653	353
16	533	35
17	902	915
19	1031	1101
21	972	999
10, 9, L		
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-8	1204	1253
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6	1577	1657
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9	584	514
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11	695	664
12	962	938
13	812	679
10, 10, L		
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-11	997	893
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-8	745	775
-7	1435	1489
-5	1318	1377
-3	1083	1033
-1	679	607
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2	901	819
3	1118	831
4	1178	1003
5	1494	1478
6	641	609
7	1563	1599
9	1515	1481
11	1403	1360
13	1105	1001
15	817	769
10, 11, L		
-10	627	664
-8	1066	1136
-6	1390	1421
-5	488	648
-4	1519	1572
-2	1205	1300
0	869	846
4	469	425
5	702	808
6	1064	1012
8	1123	1191

10	1113	1073
12	1056	1101
14	770	840
10, 12, L		
-8	553	656
-7	766	818
-5	1046	1089
-3	1246	1304
-1	1027	1066
1	797	808
7	603	684
10, 13, L		
-2	668	844
0	864	806
2	739	638
11	478	629
10, 14, L		
3	436	164
4	427	438
6	459	491
8	607	575
10	735	781
12	789	922
11, -4, L		
-1	773	857
1	851	965
2	755	767
4	861	832
6	734	843
11, -3, L		
-7	673	615
-2	844	810
0	1042	982
2	1051	1098
3	844	831
4	1047	1132
5	1013	1041
6	824	953

7	1048	1065
8	532	474
9	872	878
11, -2, L		
-11	1087	1074
-9	1041	1047
-8	701	500
-7	814	857
-4	546	610
-1	685	669
1	911	1015
3	941	1058
4	892	879
5	1060	1230
6	1036	1052
7	946	1043
8	775	933
10	851	814
11, -1, L		
-12	1093	1069
-10	1296	1337
-8	1440	1409
-6	947	1131
-3	812	818
-1	592	556
2	583	668
4	824	764
6	973	989
7	885	856
9	984	985
11	873	710
11, 0, L		
-11	1219	1149
-9	1352	1285
-7	1431	1384
-5	1141	1161
-3	1003	1042
-2	745	705

11, 0, L			12 988 1236			11, 7, L			17 952 462			7 724 728			12, 0, L		
5 573 478			13 945 925			-6 482 477			18 857 844			9 671 717			-10 1177 1097		
9 922 899			14 996 1100			-5 803 719			19 582 480			18 565 519			-8 1037 951		
10 752 824			15 955 886			-3 1240 1312			11, 9, L			11, 12, L			-6 836 759		
11 782 811			11, 5, L			-1 1667 1732			-11 1601 1301			-6 754 908			9 619 557		
11, 1, L			-7 805 810			0 451 91			-9 1325 1209			-4 938 921			12, 1, L		
-10 864 917			-5 1416 1325			1 1924 1705			-7 910 882			-2 716 702			-7 904 774		
-8 1266 1256			-3 1365 1302			2 1171 953			-1 793 812			7 619 538			12, 2, L		
-6 1417 1392			-1 1088 1069			3 1382 1248			1 1202 1250			11, 13, L			4 681 675		
-4 1413 1317			0 430 344			4 1352 1264			2 640 512			6 656 576			5 693 681		
-2 1019 950			1 739 804			5 933 939			3 1361 1331			8 660 877			12, 3, L		
12 565 636			7 784 725			6 982 968			4 648 263			10 692 834			-6 615 463		
11, 2, L			9 1417 1430			7 413 562			5 1625 1617			11, 14, L			4 826 766		
-7 906 937			10 625 476			8 746 728			6 512 347			5 642 516			5 833 777		
-5 1284 1200			11 1676 1789			11 788 722			7 1438 1515			7 775 779			6 1159 1145		
-3 1327 1257			12 959 976			13 1116 1080			8 574 553			9 812 947			7 1011 1024		
-1 796 915			13 1565 1717			15 1347 1318			9 1414 1478			12, -3, L			8 872 1066		
11, 3, L			14 1245 1199			16 770 554			10 884 874			-3 658 695			9 886 1007		
-14 830 868			15 1285 1190			17 1338 1317			11 812 910			-1 775 757			10 706 871		
-4 754 624			16 1192 987			18 746 740			11, 10, L			0 648 670			13 591 610		
0 749 794			17 543 549			11, 8, L			-10 1474 1384			1 727 869			12, 4, L		
1 590 341			18 644 618			-12 1128 903			-8 1353 1396			2 829 878			-7 1058 909		
2 392 384			11, 6, L			-10 837 776			-6 1225 1150			4 951 950			-5 868 797		
7 886 809			-6 949 915			-5 476 390			1 819 691			5 643 708			-3 532 546		
8 510 643			-4 1353 1281			-3 483 530			2 1087 1049			12, -2, L			-1 401 309		
9 897 924			-2 1663 1745			-2 932 997			3 868 407			-2 650 634			5 1085 983		
10 707 847			0 1592 1512			0 1248 1288			4 1186 1184			0 662 691			6 746 498		
12 681 521			1 947 808			2 1599 1579			5 635 102			1 711 689			7 1599 1608		
13 636 906			2 1135 916			3 604 275			6 1064 1167			2 781 831			8 1128 1106		
11, 4, L			3 893 865			4 1623 1636			8 1083 1108			3 1008 1084			9 1368 1474		
-6 1038 1045			5 676 646			5 906 925			10 961 1002			5 1121 961			10 1243 1201		
-4 814 829			10 1248 1141			6 1353 1362			11, 11, L			6 796 764			11 1098 1265		
-2 657 612			12 1445 1560			7 892 943			-7 1347 1271			7 909 814			12 1144 1058		
1 464 385			13 564 632			8 1068 1203			-5 1275 1263			12, -1, L			13 943 973		
6 683 622			14 1633 1693			9 1033 1058			-3 1060 994			3 593 600			14 1114 929		
8 1265 1311			15 1181 939			11 701 515			-1 487 466			4 800 821			16 592 636		
10 1393 1521			16 1374 1459			15 776 186			3 620 561			6 979 970					
11 1077 1120			18 1001 958			16 855 894			5 599 761								

12, 5, L		
-10	593	702
-8	973	1038
-6	1200	1191
-4	1156	1122
-2	976	819
-1	728	781
6	1122	1051
7	532	252
8	1537	1562
9	908	780
10	1634	1661
11	1200	1063
12	1417	1469
13	1120	1073
14	1101	1057
15	1199	948

12, 6, L		
-7	982	954
-5	1344	1346
-3	1391	1410
-2	670	667
-1	1145	1150
0	936	859
1	841	799
2	970	1060
3	527	283
4	804	764
6	490	444
7	743	559
9	1118	1114
10	708	522
11	1326	1392
12	824	798
13	1388	1461
14	1172	1018
15	1126	1071
16	1059	886

12, 7, L		
-6	864	883
-4	1123	1249
-2	1514	1564
0	1397	1297
1	942	894
2	1333	1100
3	1318	1254
4	982	870
5	1027	921
6	476	614
12	810	872
14	1029	1175
15	805	797
16	564	865

12, 8, L		
-5	519	593
-3	798	948
-1	1245	1287
1	1259	1239
2	619	475
3	1297	1276
4	765	735
5	1192	1334
6	832	887
7	726	781
16	687	612

12, 9, L		
-8	798	712
-5	480	424
-2	713	793
0	1002	933
2	981	944
4	1017	982
6	1098	1232
8	826	978

12, 10, L		
-7	1007	859
1	907	916
2	528	85
3	912	897
4	525	369
5	765	697
7	792	845
9	775	915
16	658	658
18	618	644

12, 11, L		
-4	632	641
3	486	389
5	577	573
15	573	559

12, 12, L		
2	414	336
4	520	560
6	577	710

12, 13, L		
1	466	499
5	740	721
7	798	875

13, -1, L		
1	475	478

13, 2, L		
1	680	679
2	763	770
3	906	929
4	810	780
5	997	988

13, 3, L		
2	610	582
3	1136	1095
4	1241	1118
5	1273	1194
6	1265	1170
7	988	967
8	1117	1069

13, 4, L		
-8	749	910
2	692	675
4	1187	1176
5	1128	938
6	1455	1481
7	1254	1212
8	1192	1299
9	1255	1233
10	982	896
11	1068	1024

13, 5, L		
-9	1007	988
-7	959	970
-5	851	899
-4	922	886
-3	629	603
-2	799	852
0	669	837
2	536	597
5	945	982
6	712	463
7	1384	1544
8	1134	1012
9	1337	1411
10	1163	1139
11	1063	1138
12	1191	1042
14	824	758

13, 6, L		
-8	1176	1143
-6	1141	1165
-5	598	526
-4	1049	1046
-2	842	893
-1	848	950
0	569	592
1	749	873
3	718	746
6	573	456
8	777	790
9	652	612
10	963	994
11	966	853
12	957	937
13	902	855
14	787	604
15	714	661

13, 7, L		
-8	1084	1219
-3	1080	1170
-1	980	995
0	737	786
1	775	768
2	832	834
3	675	687
4	753	720
12	750	676
13	570	608

13, 8, L		
-6	539	637
-4	920	984
-2	1027	1088
0	1142	1063
1	779	662
2	1094	1072
3	862	746
4	958	942
5	686	543

13, 9, L		
-3	669	701
-1	834	740
1	882	756
3	918	791
5	851	863
9	418	348

13, 10, L		
2	503	471
4	518	453
6	517	593

13, 11, L		
0	467	461

13, 12, L		
1	586	628
2	545	259
3	657	842
4	528	504

14, 1, L		
1	651	798

14, 2, L		
1	803	895
2	1149	1032
4	1047	934
6	810	721

14, 3, L		
0	761	833
1	747	793
2	1009	1038
3	1183	1094
4	1131	1125
5	1244	1151
6	898	855
7	1102	1035
9	788	767

14, 4, L		
-4	652	733
1	632	677
2	647	602
3	971	970
4	1152	943
5	1112	1141
6	1245	1043

14,	4,	L
7	1040	992
8	1172	1049
10	891	802
14,	5,	L
-5	866	932
-3	784	939
-1	451	739
4	800	842
5	978	837
6	881	963
7	1082	932
8	866	903
9	1007	925
10	610	555
11	842	730
14,	6,	L
-4	739	853
-2	836	895
0	776	877
5	494	493
6	666	580
7	559	569
8	947	724
9	577	613
10	779	749
14,	7,	L
-4	796	821
-2	708	771
-1	707	734
1	791	766
3	617	505
9	498	580
14,	8,	L
-1	792	779
0	621	526
1	825	775
2	672	452
3	705	711
12	484	386
14,	9,	L
2	654	631
4	609	606
11	499	484

CALCULATED AND OBSERVED STRUCTURE FACTORS OF $[Pt_3(CO)(S_2CNMe_2)(dppm)_3][PF_6]$

0, 0, L

4	5374	5676
6	4490	4591
8	2032	1991
10	1905	1894
12	4676	4601
14	455	453
16	5589	5440
18	989	837
20	3373	3198
22	1578	1548
24	1537	1492
28	3460	3049

0, 1, L

2	7956	8304
3	4064	3916
4	1837	1725
5	469	434
6	3976	3904
7	991	936
8	325	338
10	3380	3449
11	742	756
12	488	462
13	762	860
14	4444	4520
15	786	955
16	381	364
18	4464	4698
19	2045	2172
20	1028	1065
22	1875	1804
26	2536	2353

0, 2, L

0	4837	5192
1	4054	3922
2	568	541
4	4821	4705
5	1967	1827
6	1511	1523
7	1478	1480
8	5023	5094
9	2568	2570
10	2084	2040
11	2338	2433
12	3886	4069
14	1298	1315
15	1373	1433
16	4164	4243
17	2661	2612
20	2660	2655
21	1298	1259
24	2479	2407
25	880	879
26	743	800
27	1413	1436
28	1851	1986

0, 3, L

1	3190	3141
2	5612	5574
3	5226	5131
4	406	306
6	6364	6440
7	2210	2101
8	2488	2514
9	1670	1645
10	5548	5548
11	642	727
12	1228	1291
13	2649	2747
14	2393	2536
15	1630	1620
17	892	977
18	2340	2321
19	1839	1858
20	1155	1153
22	3126	3022
24	1218	1156
25	843	931
26	2485	2335
28	1291	1266
29	898	915

0, 4, L

0	806	678
1	1831	1857
2	1532	1560
3	1552	1504
4	3032	3042
5	4061	4058
6	1663	1575
7	1313	1263
8	5616	5624
9	2421	2369
10	1675	1760
11	1774	1921
12	2563	2653
13	1241	1195
14	1064	1080
15	1648	1695
16	352	406
17	1574	1673
18	1461	1448
19	651	767
20	2630	2621
21	914	936
22	671	625
23	1013	1105
24	3319	3218
25	807	971
26	1621	1601
28	1102	1048

0, 5, L

1	1015	1042
2	2982	2945
3	1704	1641
4	1564	1549
5	2518	2613
6	3837	3904
7	3258	3274
9	2092	2166
10	3054	3054
11	1882	1928
12	2237	2224
13	1100	1183
14	981	932
15	522	507
17	1022	1049
18	1746	1781
19	626	605
20	560	585
21	2354	2280
22	2805	2794
23	1760	1699
24	752	757
25	975	945
26	1483	1463
27	1372	1314

0, 6, L

0	3077	3034
1	1390	1366
2	294	216
3	1697	1826
4	2171	2179
5	1822	1863
6	418	390
7	3846	3985
8	2768	2719
9	3666	3754
12	1876	1901
13	2228	2166
14	691	717
16	1379	1365
18	420	442
19	2432	2405
20	2280	2353
21	1794	1806
22	570	654
23	1933	1950
24	1476	1464
25	1975	1915

0, 7, L

1	2021	2075
2	1523	1538
3	442	533
4	1621	1572
5	4008	4086
6	821	782
7	2875	2966
9	2848	2945
10	501	643
11	2746	2764
12	1391	1409
14	1716	1774
15	913	980
17	1330	1308
18	1552	1594
19	1666	1700
20	1167	1202
21	2132	2104
23	1808	1829
25	1010	927

0, 8, L

0	2111	2151
1	1663	1650
2	1842	1826
3	2053	2185
4	865	832
5	1381	1432
6	1648	1705
7	2802	2825
8	701	585
9	2050	2130
10	1633	1625
11	1520	1481
12	1374	1353
13	1467	1515
14	1128	1070
15	1405	1352
16	2292	2264
17	1771	1621
18	1430	1389
19	1360	1313
21	1406	1427
23	1312	1298
24	522	512

0, 9, L

1	2047	2078
2	976	911
3	2571	2596
4	1576	1535
5	784	772
6	406	328
7	1368	1371
8	664	618
9	1870	1889
11	2014	1947
12	1362	1279
13	1962	1851
14	1576	1502
15	2415	2351
16	519	605
17	1397	1347
18	772	699
19	1509	1446
20	983	943

0, 9, L
23 528 577
0, 10, L
1 3027 3015
2 618 497
3 764 769
5 1842 1864
6 344 309
7 520 481
8 758 691
9 771 694
10 434 459
11 2383 2427
12 475 459
13 1533 1545
15 2255 2211
17 2396 2407
21 800 799
0, 11, L
1 1694 1687
2 919 911
3 1842 1866
4 903 882
5 472 452
7 592 547
9 1022 1066
12 711 700
13 2287 2272
14 995 933
15 1897 1903
17 930 904
19 1466 1530
0, 12, L
0 1794 1795
1 1024 1049
2 677 672
3 1159 1188
5 833 807
6 625 672
7 1067 1025
9 620 614
10 979 914
11 1326 1344
12 1043 990
13 1160 1187
14 551 636
15 969 865
16 1174 1189
0, 13, L
1 743 740
2 1201 1214
4 613 629
5 1160 1154
7 1075 1095
9 845 877
11 869 909
12 1115 1100
0, 14, L
3 1006 1018
4 697 623
1, 0, L
-28 1082 1006
-26 2040 1889
-22 1703 1708
-20 1348 1298
-18 4906 4694
-16 621 509
-14 4457 4551
-12 2203 2252
-10 2270 2228
-8 1491 1533
-6 3251 3224
-4 1633 1517
4 679 676
6 1151 1152
8 804 778
10 1986 1932
12 367 200
14 3947 3980
16 1163 1067
18 4513 4273
20 1405 1346
22 1112 1041
24 753 759
26 2331 2055
28 886 769
1, 1, L
-28 2647 2515
-27 941 1066
-26 569 661
-25 841 765
-24 1539 1371
-22 980 989
-20 2815 2694
-18 832 783
-17 1400 1418
-16 4906 4883
-15 524 613
-14 794 852
-12 4359 4418
-11 1368 1334
-10 1458 1457
-9 1829 1873
-8 2223 2413
-7 833 829
-6 757 762
-5 940 1043
-4 4468 4434
-3 2266 2196
-2 642 608
2 1625 1533
3 2724 2713
4 5393 5472
6 2606 2605
7 998 1125
8 1144 1108
9 1904 1945
10 457 449
11 932 1061
12 4455 4485
13 702 682
16 5060 4960
17 1805 2068
18 1341 1414
20 2909 2745
21 949 1320
22 1268 1245
24 1210 1377
25 1080 1059
28 2768 2670
1, 2, L
-29 1220 1303
-26 2428 2362
-25 871 987
-22 1813 1944
-21 819 817
-19 2373 2488
-18 2755 2725
-17 828 839
-16 385 424
-15 1751 1813
-14 4114 4247
-13 1812 1927
-11 907 925
-10 3456 3573
-9 1985 1980
-8 1152 1134
-7 621 606
-6 4898 4875
-5 1848 1810
-4 1469 1460
-3 3745 3616
-2 6289 6280
-1 3248 3109
0 1207 1214
1 1656 1600
2 3980 3823
3 4873 4667
4 1453 1384
5 2328 2203
6 5134 5205
7 1913 1904
8 2150 2185
9 733 776
10 3605 3670
11 534 553
12 1207 1238
13 1944 1980
14 4159 4271
15 2050 2152
16 373 391
18 2746 2782
19 2824 2794
21 765 934
22 2689 2500
24 642 685
26 2345 2201
29 1124 1075
1, 3, L
-24 2848 2725
-21 638 771
-20 2128 2169
-18 1103 1214
-17 2089 2156
-16 1480 1580
-15 2351 2467
-13 534 471
-12 3550 3641
-11 992 1119
-10 364 314
-8 6013 6043
-7 1266 1367
-6 1090 1067
-5 4705 4727
-4 1208 1175
-3 1110 1036
-2 3403 3284
-1 1257 1185
0 1282 1280
1 3442 3433
2 3124 2988
3 395 313
4 4892 4846
5 2217 2256
6 424 355
8 5817 5959
10 2521 2503
11 2199 2189
12 2288 2428
13 760 853
15 1087 1076
16 1506 1657
17 2707 2701
18 1219 1299
20 2215 2241
21 1464 1437
22 569 533
24 2762 2704
26 1404 1355
27 646 790
28 1657 1632
1, 4, L
-28 982 1064
-26 1763 1745
-25 1295 1255
-24 1221 1167
-22 3265 3201
-21 1214 1280

1, 4, L			22	3246	3293	8	4875	4863	-1	2178	2274	-6	1541	1566	-12	1913	1796
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9	3104	3101
10	372	364
11	2102	2138
12	3326	3337
13	997	1125
14	374	414
15	1161	1149
16	2860	3001
17	2675	2602
19	841	871
20	1712	1787
21	1175	1134
23	628	676
24	1511	1576
25	927	957
27	793	956
28	1572	1533

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14	1352	1394
15	2844	2937
18	1522	1522
19	2354	2395
20	499	567
22	2240	2154
24	770	672
26	1875	1804
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-24	2357	2387
-20	1852	1748
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-18	1434	1407
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-12	1932	2042
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9	1624	1902
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12	1168	1105
13	2194	2227
14	479	495
15	572	468
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22	748	673
24	2450	2398
25	733	870
26	1142	1061
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-24	825	816
-23	697	790
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19	1476	1566
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21	698	718
22	2167	2085
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13	1795	1817
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15	911	932
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22	862	720

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3, 6, L		
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-12	722	662
-11	948	900
-10	1133	1209
-9	1175	1184
-8	1485	1487
-7	799	737
-6	1743	1749
-5	3350	3330
-4	945	956
-3	2330	2287
-1	752	647
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1	2319	2239
2	1283	1312
3	568	479
4	914	949
5	1969	1916
6	1154	1116
7	2094	2186
8	1690	1634
10	890	958
11	2333	2382
12	909	961
13	1892	1899
14	543	573
15	634	564
16	382	412
18	1070	1042
20	1169	1240
22	1117	1145
23	1838	1783
24	492	505

3, 7, L		
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-23	1295	1224
-22	1559	1629
-19	1385	1455
-18	2313	2282
-17	1087	1213
-16	1309	1296
-14	426	367
-12	621	600
-10	708	711
-9	645	635
-8	835	860
-7	2173	2241
-6	2245	2289
-5	504	425
-4	876	796
-3	2276	2251
-2	2739	2691
-1	906	968
0	1972	2016
1	669	576
2	412	404
3	371	299
4	1127	1010
5	860	879
8	1081	1087
9	2343	2414
10	2242	2234
11	1009	923
12	1644	1615
13	711	793
14	518	563
15	1131	1114
16	1483	1476
20	635	642
21	821	795
25	1688	1675

3, 8, L		
-24	844	856
-22	646	711
-21	488	581
-20	2351	2324
-18	1305	1288
-17	1097	1133
-16	1147	1098
-14	1494	1502
-13	479	458
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-9	856	831
-8	1399	1385
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-2	2470	2503
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1	590	615
2	1869	1868
3	1074	1072
5	633	698
6	881	853
7	1223	1217
8	2282	2216
9	612	729
11	1540	1543
12	2941	2955
13	357	354
14	1960	1919
15	656	673
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23	1346	1454
24	1232	1254

3, 9, L		
-22	1407	1325
-18	1907	1853
-16	1589	1552
-15	1461	1437
-14	1536	1445
-12	898	851
-9	1049	1081
-8	1685	1684
-7	534	543
-6	3030	3021
-5	793	756
-4	540	536
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2	425	417
3	590	579
5	1022	1006
6	1792	1727
7	2141	2065
10	2223	2199
11	883	816
12	744	758
13	769	716
14	2408	2420
15	1314	1301
16	1248	1265
17	905	1013
21	693	694
22	687	693

3, 10, L		
-20	1058	1023
-19	896	916
-17	727	703
-16	1837	1844
-15	956	1007
-14	877	898
-13	1852	1729
-12	2074	2052
-11	1290	1317
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-3	2395	2458
-2	931	901
-1	1759	1760
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1	787	627
3	1770	1781
4	1602	1602
5	1204	1228
6	635	596
8	1305	1371
10	616	538
11	814	715
12	2040	2108
13	1470	1563
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15	856	930
16	1250	1304
19	952	1015

3, 11, L		
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-15	962	933
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-9	707	711
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6	1990	2026
8	1122	1119
9	675	640
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11	1022	1012
13	467	499
14	1017	1086
15	1381	1391
16	522	503
17	761	884
18	1340	1381

3, 12, L		
-15	631	710
-14	765	779
-12	2437	2436
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-8	1130	1174
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-3	1262	1257
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2	886	840
3	761	771
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6	921	914
8	979	971
10	860	859
13	843	888

3, 13, L		
-10 1878	1922	
-9 1395	1428	
-8 1011	1007	
-7 657	603	
-5 664	634	
-2 1194	1123	
0 907	842	
1 634	626	
2 2748	2778	
3 988	972	
6 1669	1654	
7 761	794	
8 882	918	
3, 14, L		
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-4 772	772	
-1 858	845	
0 1562	1567	
1 1098	972	
3 856	790	
4 1758	1795	
5 1322	1414	
4, 0, L		
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-24 1878	1791	
-20 1383	1455	
-18 2763	2755	
-16 2103	2144	
-14 1922	1740	
-12 855	830	
-10 987	1037	
-8 2835	2815	
-6 2887	2838	
-4 3264	3288	
-2 1378	1323	
0 667	609	
2 3043	3117	
4 3639	3517	
6 3191	3168	
8 3107	3072	
10 1614	1564	
14 700	588	
16 1282	1246	
18 2109	2146	
20 1555	1541	
24 1252	1283	
26 1103	1054	
4, 1, L		
-27 424	410	
-26 1257	1214	
-22 1308	1324	
-21 1350	1327	
-20 1645	1669	
-19 525	487	
-16 1140	1074	
-15 1036	953	
-14 521	521	
-13 2353	2342	
-12 1599	1713	
-11 1584	1572	
-10 1543	1636	
-9 440	462	
-8 554	545	
-7 2067	1994	
-6 500	492	
-5 2988	2808	
-4 1996	1911	
-3 1119	1162	
-2 1739	1641	
-1 2237	2134	
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1 1456	1405	
2 1342	1244	
3 2551	2522	
4 2029	1997	
5 739	728	
6 1637	1670	
7 409	366	
9 459	495	
10 818	829	
11 990	970	
12 999	956	
13 1468	1409	
14 969	1004	
15 1292	1275	
16 1248	1325	
17 407	452	
18 453	558	
19 557	581	
20 590	677	
21 1397	1435	
22 1073	1159	
23 1048	971	
24 728	762	
26 420	377	
27 442	317	
4, 2, L		
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-16 787	816	
-15 2488	2483	
-14 876	857	
-13 1415	1375	
-12 447	416	
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-10 460	523	
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-8 297	319	
-7 2378	2337	
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-5 1000	1059	
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-3 1656	1635	
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-1 1863	1830	
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1 644	588	
3 1364	1382	
5 500	485	
6 492	449	
7 2620	2624	
8 669	603	
9 1089	1134	
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12 652	578	
13 309	380	
14 433	477	
17 1771	1656	
19 1592	1558	
21 786	781	
23 1046	942	
25 691	716	
4, 3, L		
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-19 657	736	
-18 1138	1068	
-17 840	827	
-16 854	843	
-14 1338	1396	
-13 2429	2393	
-12 1641	1654	
-11 2020	2032	
-10 1688	1695	
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-8 770	710	
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-6 299	377	
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1 904	885	
2 1528	1347	
3 2086	2059	
4 2490	2415	
5 2686	2668	
6 1656	1642	
7 894	875	
8 396	411	
9 1391	1398	
10 583	644	
11 1117	1120	
12 1382	1351	
14 1866	1966	
15 1704	1938	
17 957	927	
19 351	483	
20 598	653	
21 1298	1412	
23 836	910	
4, 4, L		
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-24 475	660	
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-14 2189	2083	
-13 381	569	
-12 502	525	
-11 726	822	
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-9 1514	1482	
-8 1578	1528	
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-2 511	506	
-1 431	418	
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1 537	593	
2 2447	2327	
3 396	300	
4 1148	1130	
5 861	797	
6 2627	2567	
8 2744	2762	
9 948	888	
10 1392	1384	
11 1000	961	
12 1030	1050	
13 362	443	
15 1213	1244	
16 1470	1488	
18 1998	1970	
19 766	972	
20 974	962	
22 842	841	
24 1087	1021	
26 791	771	
4, 5, L		
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-18 1056	1067	
-16 900	951	
-15 1347	1334	
-14 997	1022	
-13 921	1012	
-12 2668	2648	
-10 1667	1651	
-8 1474	1465	

4, 5, L		
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3	940	933
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6	1913	1936
7	1310	1267
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13	2215	2292
14	841	795
15	999	1010
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18	472	533
19	485	553
20	1597	1549
22	871	880
4, 6, L		
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-21	1011	1009
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3	893	814
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14	809	711
15	1173	1129
16	661	611
17	1407	1381
18	610	481
22	767	802
25	1202	1115
4, 7, L		
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-22	735	685
-21	1034	1039
-20	2147	2206
-19	1679	1668
-16	965	899
-15	773	795
-13	864	871
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-9	442	394
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3	1264	1261
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7	2036	1963
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9	796	812
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12	2647	2604
13	1492	1549
14	1851	1891
15	685	687
18	1062	1038
19	984	951
20	634	687
23	1078	1092
24	879	961
25	664	610
4, 8, L		
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-22	1593	1655
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-18	1920	1878
-17	805	775
-16	986	940
-14	570	582
-13	1109	1122

-11	701	701
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6	1367	1369
7	1603	1700
8	1823	1810
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11	392	404
12	1315	1341
13	561	520
14	1412	1392
16	1868	1968
17	841	827
22	478	510
4, 9, L		
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-21	566	737
-20	1765	1716
-18	874	896
-16	1609	1714
-14	1544	1489
-12	889	891
-11	1469	1370
-10	704	671
-9	1160	1203
-8	1616	1645
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2	1240	1225
3	558	537
4	866	867
5	1795	1861
6	538	454
7	600	583
8	2366	2256
9	1384	1349
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12	2263	2265
13	869	827
14	1791	1728
16	1109	1097
18	975	967
21	529	543
22	667	599
4, 10, L		
-19	625	607
-18	1437	1393
-17	1149	1111
-16	718	646
-14	1872	1961
-12	728	704
-10	2021	1928
-9	1639	1639
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6	1834	1881

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11	520	435
12	915	915
13	667	604
14	2251	2287
15	908	938
16	864	1000
17	772	769
18	1036	1097
19	878	878
4, 11, L		
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-15	716	621
-12	2314	2447
-11	494	514
-10	1140	1176
-9	1300	1388
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6	1038	1060
7	1065	1064
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11	1313	1355
12	1023	1020
13	1331	1336
16	1641	1664

4, 12, L		
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-8	1919	1882
-7	908	953
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-4	678	663
-3	745	677
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11	558	615
12	946	979
14	552	530
15	846	802

4, 13, L		
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-8	1036	1077
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-6	1388	1396
-3	594	613
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3	557	575
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5	737	671
6	1008	1099
8	743	774
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4, 14, L		
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2	1760	1756
3	1480	1494

5, 0, L		
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-24	636	758
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-20	1016	914
-16	1116	1041
-12	2547	2580
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-8	2902	2929
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-2	1934	1875
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4	1885	1909
6	4808	4984
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18	1546	1639
22	2284	2284
24	1822	1793
26	994	962
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5, 1, L		
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-25	812	897
-24	2283	2203
-23	764	676
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-18	1305	1272
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-16	687	715
-15	2021	2009
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-13	486	523
-12	2667	2767
-11	746	733
-10	692	731
-9	1587	1584
-8	3164	3165
-7	1592	1622
-6	2913	2891
-4	1807	1776
-3	1248	1248
-2	2318	2259
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4	2347	2275
6	460	481
7	1985	2031
8	3683	3679
9	874	944
10	2775	2856
11	589	692
12	1094	1135
14	2326	2381
15	808	887
17	810	793
18	530	507
19	1044	1015
20	1901	1873
21	1214	1273
22	491	555
24	1613	1589
25	578	684
26	1459	1401

5, 2, L		
-27	893	920
-26	1070	998
-25	775	701
-23	1046	1006
-22	1028	1104
-21	1900	1899
-20	693	740
-19	489	359
-18	1219	1222
-17	465	601
-16	1010	997
-14	3333	3361
-13	3282	3274
-12	1655	1660
-11	2586	2599
-10	1962	2071
-9	2147	2133
-7	2036	1920
-6	1242	1273
-5	3767	3735
-4	1840	1853
-3	2458	2335
-2	1055	1053
-1	977	986
0	1268	1285
1	586	594
2	2080	2001
3	1527	1477
4	1017	1055
5	3411	3354
6	2652	2690
7	1576	1540
8	1751	1754
9	1301	1291
10	1216	1263
11	2134	2143
12	1485	1454
13	1553	1547
14	2548	2514
15	1624	1622
16	500	610
18	1135	1100
19	410	388
20	517	560
21	1722	1713
23	1362	1266
24	632	594
26	1053	1062

5, 3, L		
-28	1041	928
-26	660	652
-25	958	993
-23	1140	1083
-20	470	475
-19	812	784
-16	3748	3734
-15	734	878
-14	2174	2355
-13	1447	1518
-12	1218	1306
-11	651	591
-10	1739	1750
-9	1898	2014
-8	623	623
-7	2097	2016
-6	1079	1035
-4	2667	2628
-3	1365	1359
-2	741	713
0	2539	2500
1	785	716
2	2945	2886
3	1344	1360
4	1561	1542
5	307	331
6	3232	3123
7	2363	2360
9	2502	2473
10	525	414
11	932	993
12	2422	2483
14	363	368
16	2345	2326
18	2001	1900
19	1022	1117
21	930	1008
22	687	750
23	812	809
25	882	869
28	1005	922

5, 4, L		
-25	561	484
-23	624	606
-21	699	696
-20	1104	1020
-18	2132	2113
-16	1100	1101
-15	1562	1610
-14	2594	2531
-13	392	410
-12	3329	3409
-11	1251	1216
-10	1096	1082
-9	1081	1100
-8	612	513
-7	2629	2734
-6	898	835
-5	995	1041
-4	1327	1366
-2	3413	3295
-1	662	556
0	1268	1241
1	715	593

5, 4, L		
2	3215	3027
3	561	493
4	4326	4145
5	458	460
6	1158	1199
7	977	1109
8	1125	1026
9	1562	1614
12	663	756
13	1577	1599
14	2770	2748
16	1554	1586
17	427	677
18	451	574
20	1639	1731
22	440	809
26	574	665

5, 5, L		
-26	1174	1179
-20	1105	1064
-17	1984	1967
-16	2214	2166
-15	1298	1314
-14	2158	2113
-13	587	629
-12	1073	1044
-11	1407	1422
-10	3021	2976
-8	823	729
-7	1319	1322
-6	992	948
-5	2629	2644
-4	919	983
-3	285	367
-1	1216	1264
0	3608	3501
1	1013	1201
2	3328	3111
3	453	246
5	1695	1712
6	1660	1684
8	1018	1027
11	2355	2379
12	1490	1412
14	1034	1039
15	2318	2284
16	967	1009
17	1511	1510
18	2004	2001
22	849	832

5, 6, L		
-24	764	782
-22	747	780
-19	2368	2263
-18	1350	1402
-17	754	813
-16	1018	1045
-15	1729	1710
-14	797	804
-13	2080	2045
-12	1228	1230
-11	341	373
-8	2027	2027
-7	1158	1191
-4	1585	1468
-3	3963	3971
-2	1136	1125
-1	1211	1317
0	1062	998
1	1728	1724
2	1175	1099
3	2670	2619
4	1687	1572
5	1758	1638
6	366	361
7	909	885
8	1914	1926
9	1512	1568
10	529	511
12	1958	1996
13	2501	2494
14	504	557
15	1934	1948
16	1069	1114
17	479	388
19	1830	1877
20	1130	1135
25	819	816

5, 7, L		
-24	603	636
-22	1565	1615
-21	1427	1418
-18	1360	1452
-17	2067	1978
-15	1409	1454
-11	1182	1075
-10	1213	1247
-9	330	449
-8	732	745
-6	2250	2216
-5	2277	2280
-3	806	753
-2	1756	1743
-1	2250	2400
0	977	967
1	3305	3314
2	743	607
4	1080	1037
5	1124	1046
6	1333	1259
7	419	364
8	1159	1112
9	645	665
10	2864	2797
11	2036	2100
12	942	973
13	1078	1120
14	805	733
15	835	746
16	1197	1200
17	1954	2028
21	624	564
22	686	684
24	613	652

5, 8, L		
-22	838	877
-21	676	805
-20	2261	2224
-19	838	987
-18	758	726
-17	884	865
-16	1148	1193
-15	1245	1164
-14	611	578
-13	930	924
-10	734	818
-9	758	714
-8	1810	1929
-7	961	980
-6	719	768
-5	723	586
-4	2841	2843
-3	929	984
-2	2047	2014
-1	1573	1575
0	608	568
1	458	319
2	956	990
3	1978	2014
4	458	446
5	1147	1089
6	1893	1887
7	479	402
8	3105	3046
9	1055	1009
12	2710	2588
13	855	873
14	2009	2085
15	949	946
17	744	831
18	1070	1021
19	1430	1434
22	805	767

5, 9, L		
-22	1320	1282
-21	644	600
-19	1174	1165
-18	1772	1794
-16	1220	1141
-15	674	788
-14	930	940
-13	1190	1162
-12	732	680
-11	877	805
-10	947	999
-9	1972	1962
-8	1277	1231
-7	1459	1445
-6	2111	2130
-5	387	445
-3	1299	1289
-2	1849	1823
0	2018	1947
1	531	519
2	487	448
3	999	927
5	1189	1171
6	1756	1746
7	1345	1231
8	774	681
9	1719	1651
10	2615	2598
12	1138	1165
14	1610	1549
16	1953	1936
19	1093	1067

5, 10, L		
-20	1030	986
-16	1193	1243
-14	684	705
-12	1653	1587
-11	1589	1566
-10	658	640
-9	1954	1968
-8	1425	1415
-7	1570	1554
-5	1809	1880
-4	1338	1331
-3	858	895
-2	1252	1198
0	1050	1059
2	946	937
3	660	587
4	897	825
5	1244	1286
6	519	493
7	1510	1520
8	1432	1415
10	935	945
11	1682	1648
12	1437	1371
13	812	784
14	1212	1235
16	1159	1166

5, 11, L			7 1038 1001			18 593 594			9 885 920			-6 1897 1823			-21 1656 1648		
-17	884	890	9	567	613	20	2695	2665	10	2935	3056	-5	926	983	-18	2596	2645
-14	1560	1556	10	1496	1494	22	742	777	11	1391	1437	-4	2722	2645	-16	1503	1479
-12	756	814	13	625	640	24	2228	2222	12	4668	4706	-3	1809	1798	-15	702	785
-11	829	774	5, 13, L			26	1885	1980	13	2593	2621	-2	1846	1815	-14	4128	4265
-10	1923	1992	-10	1521	1580	28	632	506	14	1277	1236	-1	976	994	-12	3618	3646
-9	828	895	-9	741	714	6, 1, L			15	982	970	0	2390	2355	-11	2273	2182
-8	1252	1231	-8	1548	1570	-26	2164	2126	16	1336	1352	1	422	398	-10	1455	1455
-7	1734	1710	-4	1142	1146	-24	618	647	17	391	335	2	331	236	-9	2225	2205
-6	752	727	-3	892	967	-23	711	771	18	1330	1350	3	2007	2037	-7	1886	1838
-4	481	480	-2	715	731	-22	2671	2590	19	515	542	4	3270	3246	-6	2119	2060
-3	952	988	1	1290	1263	-21	1447	1451	21	975	928	5	375	354	-5	4446	4346
-2	1194	1234	2	2001	1966	-20	1040	1098	22	1906	1896	6	2127	2081	-4	552	516
-1	674	630	3	503	567	-18	1360	1347	23	1531	1515	7	2405	2537	-3	670	659
2	1892	1894	4	932	952	-16	1228	1251	24	1729	1704	8	2730	2859	-2	3769	3656
3	871	768	5	925	925	-14	2801	2826	26	1200	1119	9	3035	3123	-1	345	237
4	867	786	6	1062	1030	-13	1090	1141	28	961	1009	10	2273	2321	0	2225	2084
5	788	785	7	902	854	-12	540	547	6, 2, L			12	2481	2584	1	576	582
6	1376	1387	8	1135	1150	-11	1105	1117	-28	1350	1282	13	357	354	2	2922	2821
7	581	504	6, 0, L			-10	5449	5618	-26	588	537	14	1847	1883	3	463	436
8	1619	1534	-28	1435	1399	-9	2245	2280	-25	1055	1004	15	1344	1444	4	3956	3864
9	1510	1492	-24	3230	3050	-8	2963	3007	-24	1661	1631	16	2430	2416	5	1467	1549
11	845	903	-20	2076	2127	-7	277	358	-23	1681	1652	17	758	671	6	1985	1951
13	751	648	-18	1999	2060	-6	4051	4076	-22	646	607	18	1734	1743	7	3154	3092
14	1051	1087	-16	1006	1021	-5	1629	1599	-20	1249	1219	19	1413	1370	8	1975	2015
5, 12, L			-12	4311	4347	-4	5646	5728	-19	1612	1649	20	539	540	9	1163	1118
-13	648	607	-8	6054	6297	-3	339	430	-18	662	651	21	1820	1713	10	1719	1738
-12	2260	2295	-6	5982	6062	-2	1546	1546	-17	534	620	22	798	733	11	1938	1945
-10	1425	1381	-4	775	770	-1	940	940	-16	3342	3316	23	831	759	14	4290	4348
-9	814	853	-2	3025	2881	0	1779	1803	-15	1625	1654	24	1127	1123	15	380	405
-8	816	863	0	2902	3109	1	1386	1357	-14	1996	2026	25	1016	1002	16	1702	1704
-6	1810	1775	4	5726	6078	2	2702	2761	-13	1016	1033	26	1154	1158	18	1358	1297
-5	1433	1470	6	645	755	3	2764	2838	-12	4174	4168	28	1081	1084	19	442	386
-3	469	530	8	4683	4783	4	1859	1867	-11	488	462	6, 3, L			20	1371	1340
-1	900	869	10	4289	4427	5	1230	1236	-10	894	902	-27	868	818	21	1743	1659
0	1832	1874	12	1190	1195	6	5263	5312	-9	1872	1940	-26	785	754	23	1352	1419
4	2153	2258	14	3590	3611	7	1488	1477	-8	2517	2503	-25	889	812	24	774	700
6	1452	1441	16	389	332	8	1484	1614	-7	4964	5037	-23	560	567	26	1056	995

6, 3, L			18 2845 2841			14 1699 1714			14 1374 1326			11 786 727			9 1432 1394		
27 993 962			22 775 923			15 2101 2099			15 1388 1385			12 2250 2213			10 3060 3019		
6, 4, L			25 806 877			16 2245 2121			17 2631 2588			13 1650 1650			11 865 812		
-26 1326 1272			6, 5, L			18 1180 1202			18 1323 1241			14 805 861			12 640 610		
-23 989 964			-26 501 565			19 1701 1851			20 565 632			15 2242 2230			13 1387 1434		
-20 1362 1362			-25 495 628			20 2133 2103			21 1478 1458			16 667 769			15 813 741		
-19 864 780			-24 1066 1084			26 642 663			22 710 771			19 2410 2314			16 1394 1444		
-17 1380 1319			-22 726 735			6, 6, L			24 803 733			22 1021 1005			17 1873 1873		
-16 3709 3679			-19 1555 1506			-22 785 837			6, 7, L			24 985 1048			20 592 587		
-15 1476 1487			-18 1894 1967			-21 1347 1409			-24 1081 1078			6, 8, L			21 1290 1210		
-14 2464 2507			-17 1527 1430			-20 1301 1330			-22 627 719			-23 1207 1225			6, 9, L		
-13 780 770			-16 880 855			-19 647 715			-20 1551 1567			-22 1615 1549			-21 1710 1817		
-12 2562 2663			-15 2096 2143			-17 2375 2364			-19 1943 1942			-21 712 749			-20 1786 1767		
-11 2056 2068			-14 2004 1979			-16 895 958			-17 1804 1929			-19 1476 1426			-18 734 711		
-10 2599 2550			-13 2579 2529			-15 2295 2195			-16 912 890			-18 1707 1756			-17 1305 1351		
-9 1671 1659			-12 2513 2552			-14 880 921			-15 1636 1646			-17 1242 1346			-16 812 857		
-7 2180 2151			-10 335 318			-11 2509 2547			-13 1969 1987			-16 855 814			-14 961 981		
-6 730 656			-9 2053 1985			-10 1457 1453			-11 824 809			-15 2019 2045			-13 1120 1110		
-5 2207 2043			-8 1491 1486			-8 976 946			-10 1339 1312			-13 625 582			-11 1971 1904		
-4 2921 2906			-7 1663 1709			-7 1287 1231			-9 1561 1499			-11 1274 1341			-10 838 812		
-3 1279 1296			-6 470 431			-6 2337 2321			-8 1510 1476			-10 653 625			-9 1423 1526		
-1 778 697			-5 1320 1230			-5 2137 2078			-7 476 421			-9 836 848			-8 1435 1396		
0 4087 4015			-4 418 248			-4 966 932			-6 1862 1877			-8 1859 1863			-7 1357 1312		
1 1520 1429			-3 3382 3202			-3 2221 2116			-5 1167 1214			-7 1857 1713			-5 2156 2127		
2 3636 3599			-2 3920 3857			-2 627 600			-4 2479 2431			-6 2117 2142			-4 1756 1811		
3 1699 1570			-1 1486 1479			-1 3231 3258			-3 3246 3273			-5 1382 1344			-2 1653 1586		
4 1866 1824			0 2161 2108			0 2313 2240			-2 734 730			-4 337 329			-1 1283 1255		
5 3107 3006			1 627 517			1 4180 4067			-1 3542 3593			-3 2304 2286			0 618 559		
6 2328 2306			2 2977 2885			2 2200 2050			0 610 528			-2 1959 1833			1 586 646		
7 737 745			3 2873 2867			4 1198 1100			1 1832 1879			-1 1160 1262			2 1511 1502		
9 2560 2580			4 2971 2974			5 1966 1963			2 467 376			0 2289 2205			3 1809 1870		
11 1634 1674			7 2278 2291			6 1646 1650			3 3539 3503			1 3002 2967			5 994 1033		
12 3320 3298			8 381 396			7 349 338			4 785 671			3 726 742			6 918 916		
13 1154 1181			9 1509 1480			9 620 514			6 1409 1375			4 721 759			7 2128 2197		
14 845 944			10 821 857			10 1150 1183			7 797 768			5 2229 2242			8 1827 1853		
15 1151 1275			11 1302 1328			11 2711 2696			8 2063 2111			6 1055 1106			10 459 515		
16 2449 2463			12 435 418			12 777 763			9 1502 1460			7 692 619			11 1814 1732		
17 1226 1342			13 2182 2187			13 1595 1566			10 719 690			8 1966 1940			12 1524 1658		

6, 9, L		
14	1446	1471
15	1062	984
19	1002	1057
21	1130	1114

6, 10, L		
-19	1698	1667
-18	705	839
-17	829	921
-16	531	561
-15	385	387
-11	1135	1131
-10	1111	1197
-9	2019	1982
-7	2497	2425
-6	974	935
-3	1689	1780
-2	928	919
0	767	737
1	736	605
2	939	975
3	912	871
4	423	403
5	1765	1729
6	1069	1058
7	908	844
8	601	623
9	2561	2513
10	1036	1083
11	507	560
12	734	750
13	885	903
14	714	805
16	483	616
18	734	771
19	1392	1377

6, 11, L		
-17	831	769
-13	409	466
-12	1253	1306
-11	868	949
-10	1311	1374
-9	1558	1622
-8	864	848
-7	990	951
-6	784	797
-5	2215	2339
-1	940	992
0	1106	1118
3	744	826
4	1075	1090
5	1543	1513
6	1331	1269
7	2447	2360
10	1305	1201
11	1711	1743
13	823	875
16	1071	1097

6, 12, L		
-12	827	874
-11	708	727
-10	1351	1349
-8	1767	1787
-7	1026	1036
-4	963	880
-3	1505	1542
1	777	823
2	1328	1351
4	982	1035
5	1120	1237
6	792	835
8	1351	1401
9	1062	1105
13	914	883

6, 13, L		
-6	1594	1569
-5	679	650
-1	1357	1358
0	762	839
3	1597	1618
4	1417	1452
5	808	783
6	1498	1498

7, 0, L		
-26	2609	2680
-24	650	689
-22	3608	3628
-20	2261	2409
-18	1645	1691
-16	1714	1741
-14	1516	1542
-10	5586	5762
-8	3221	3200
-6	3729	3724
-4	6430	6533
-2	966	880
0	1538	1559
2	5155	5330
4	922	1007
6	6767	6934
8	1788	1817
10	3421	3461
12	5189	5375
14	706	718
16	1085	1017
18	2060	1975
22	3253	3329
24	2231	2190
26	1129	1178

7, 1, L		
-26	615	763
-24	3081	3099
-23	1321	1326
-22	1618	1627
-20	2154	2140
-19	1089	1113
-18	2116	2074
-17	448	471
-16	1502	1536
-15	1558	1575
-14	1117	1138
-13	585	570
-12	4404	4460
-11	599	479
-10	570	702
-9	387	469
-8	4842	4955
-7	3026	2959
-6	4802	4897
-5	1333	1323
-4	3053	3000
-3	1159	1187
-2	4014	3987
-1	811	870
0	1379	1419
1	552	595
2	303	184
3	768	700
4	5881	5946
5	812	322
6	519	588
7	1694	1749
8	3882	4023
9	1917	1877
10	4079	4167
11	1091	1098
12	2744	2739
14	3174	3244
15	1576	1474
16	1663	1696
17	840	805
18	498	522
19	1223	1245
20	2715	2694
21	1369	1464
22	1523	1435
24	1925	1911
25	1019	1092
26	1823	1760

7, 2, L		
-27	898	934
-26	1686	1703
-25	877	961
-24	1120	1096
-23	743	711
-22	1942	1841
-21	1840	1918
-20	1006	1039
-18	2167	2124
-16	2075	2120
-14	3722	3818
-13	1191	1204
-12	2350	2381
-11	2110	2147
-10	3770	3866
-9	2508	2555
-8	1244	1316
-6	3307	3415
-5	3795	3750
-4	3148	3124
-3	740	717
-2	3428	3429
-1	336	290
0	2527	2504
1	717	712
2	3354	3400
3	551	497
4	2167	2097
5	2706	2722
6	3421	3485
7	2976	2938
8	2388	2438
9	708	697
10	3214	3279
11	2317	2366
12	2382	2476
13	1790	1861
14	3626	3689
15	1194	1224
16	2430	2428
18	1707	1709
19	577	589
20	876	958
21	1806	1824
22	1364	1372
23	1824	1794
24	1235	1279
26	1450	1399

7, 3, L		
-26	1098	1082
-25	774	802
-24	891	879
-23	1910	1931
-22	420	416
-20	1737	1635
-19	2024	2019
-18	676	692
-16	3865	3772
-14	2622	2712
-12	3377	3439
-11	847	882
-10	2477	2402
-9	1729	1773

7, 3, L		
-8	1802	1825
-7	3410	3490
-6	368	325
-4	3524	3525
-3	1283	1292
-2	1624	1656
-1	298	302
0	3255	3322
1	398	31
2	3292	3322
3	2009	2000
4	2390	2448
5	2799	2805
6	2699	2729
7	575	614
8	1763	1783
9	4071	4068
10	813	832
12	3891	3922
13	706	768
14	1651	1718
16	3312	3327
18	2425	2393
19	964	1034
21	1220	1263
22	1396	1381
23	827	863
24	575	634
25	1644	1585
26	601	661
27	443	500

7, 4, L		
-26	962	857
-25	684	713
-24	1058	1028
-22	765	818
-21	1659	1601
-19	662	691
-18	2151	2128
-17	1921	1931
-16	1098	1120
-15	936	901
-14	3381	3458
-13	2013	1931
-12	3085	3113
-11	1057	1080
-10	1087	1147
-9	2566	2556
-8	1419	1391
-7	1162	1124
-6	1143	1116
-5	2179	2206
-3	770	709
-2	4463	4400
-1	1229	1183
0	3306	3258
2	3215	3192
3	2385	2342
4	4096	4098
5	425	416
6	855	808
7	4280	4262
8	908	904
10	1612	1594
11	1974	1924
14	3724	3777
15	1482	1487
16	2394	2440
18	1921	1907
19	965	968
20	2784	2710
23	1108	1109

7, 5, L		
-26	1671	1636
-23	777	769
-21	742	686
-20	1649	1578
-19	1535	1530
-17	1775	1770
-16	1990	1915
-15	2552	2497
-14	1652	1578
-12	1509	1510
-11	2665	2783
-10	1786	1724
-9	532	558
-8	1037	1089
-7	980	1007
-6	1154	1159
-5	3093	2965
-4	2735	2745
-3	2404	2328
-2	1371	1359
-1	1247	1261
0	3644	3677
1	3488	3490
2	3777	3698
3	614	546
4	1040	974
5	2899	2845
6	1287	1248
8	471	430
9	2459	2570
11	1853	1830
12	2168	2254
13	1615	1580
14	1395	1416
15	1015	886
16	2154	2124
17	2425	2290
18	2735	2676
20	790	814
21	1139	1244
22	1292	1346
25	749	772

7, 6, L		
-25	831	920
-24	1327	1274
-22	636	660
-21	1180	1083
-19	2067	1876
-18	1476	1417
-17	2286	2233
-15	1362	1325
-14	739	692
-13	3278	3196
-12	905	877
-11	1276	1233
-10	1483	1475
-9	1940	1886
-8	1664	1640
-6	1499	1441
-5	920	941
-4	1461	1382
-3	3312	3311
-2	1797	1733
-1	4110	4101
0	813	728
1	1172	1134
2	1324	1346
3	3662	3685
4	1696	1671
5	1655	1583
6	780	852
7	1797	1842
9	486	506
10	1536	1558
11	1184	1241
12	1424	1394
13	1931	1828
14	949	964
15	2707	2667
16	1765	1800
18	1153	1066
19	2995	2820
20	1240	1239
21	612	672
22	837	894
23	859	870
24	592	690

7, 7, L		
-24	977	918
-23	702	731
-22	1231	1236
-21	738	753
-19	1516	1455
-18	964	912
-17	2305	2309
-15	2507	2432
-11	2626	2629
-9	977	885
-8	2922	2903
-7	1430	1429
-6	2379	2425
-5	1111	1037
-4	750	732
-3	2885	2784
-2	1746	1728
-1	2306	2285
0	650	571
1	4476	4403
2	994	1015
3	2514	2552
6	686	750
8	1426	1466
9	1246	1262
10	1288	1230
11	1286	1294
12	889	912
13	2338	2348
14	1097	1012
17	2721	2774
20	1044	1028
21	1674	1687
22	762	715

7, 8, L		
-22	695	725
-21	1216	1150
-20	1627	1630
-19	799	866
-18	554	485
-17	2219	2226
-15	567	582
-14	701	680
-13	1532	1554
-12	1014	984
-10	1930	1967
-9	1392	1358
-8	1091	962
-7	713	727
-6	2250	2121
-5	2723	2733
-4	2205	2170
-3	1086	970
-2	1244	1185
-1	2591	2645
0	487	361
1	1104	1107
2	885	961
3	2731	2700
6	1471	1404
7	1803	1785
8	1363	1321
9	373	376

7, 8, L		
10	1642	1607
11	2123	2128
12	1315	1330
13	1170	1163
14	823	776
15	2334	2351
19	1663	1670
22	1137	1134
7, 9, L		
-19	1921	1902
-18	1043	1025
-16	1162	1133
-15	1455	1469
-14	1011	1018
-13	577	573
-12	835	880
-11	1564	1564
-9	1805	1869
-8	1474	1455
-7	2456	2617
-6	1307	1273
-3	2667	2620
-2	1364	1272
0	1573	1503
1	1500	1539
3	804	714
5	2678	2661
8	1660	1664
9	2621	2648
10	1603	1668
13	2283	2276
16	854	830
17	1030	1069
19	1053	968

7, 10, L		
-17	1044	1004
-13	689	748
-11	1729	1787
-9	2429	2404
-7	949	812
-5	2834	2929
-4	690	643
-3	674	699
-1	1337	1360
2	662	675
3	1006	1063
5	1743	1671
7	3257	3278
8	443	562
11	2573	2569
14	575	662
15	616	638
17	558	558
7, 11, L		
-15	495	372
-13	1001	923
-12	818	767
-11	1235	1210
-10	605	590
-9	775	869
-8	937	933
-7	2128	2155
-3	1820	1844
-1	489	523
1	914	909
3	954	912
4	385	509
5	1711	1677
7	1084	1049
8	1296	1369
9	2532	2449
10	678	711

13	1059	1061
7, 12, L		
-12	978	911
-11	824	779
-10	1269	1309
-9	1082	1091
-6	1002	1016
-5	1719	1812
-4	689	643
-1	1517	1524
3	1283	1278
4	1087	1129
6	2019	2016
7	1469	1497
10	706	758
11	1333	1334
7, 13, L		
-7	480	583
-6	550	554
-4	719	641
-3	1113	1091
-2	891	780
-1	624	612
1	1444	1522
2	635	640
4	1158	1212
5	1178	1194
7	456	460
8, 0, L		
-24	3367	3343
-22	2254	2231
-20	2231	2213
-18	2603	2577
-16	1029	1046
-14	999	1021
-12	2984	3072
-10	1096	1187
-8	3819	3963

-6	3883	4054
-4	2274	2358
-2	2854	2989
0	1909	2174
2	592	688
4	5433	5456
8	4173	4266
10	4959	5051
12	1156	1198
14	3581	3664
16	1462	1544
20	3502	3469
22	2120	2067
24	2242	2221
26	2570	2473
8, 1, L		
-26	2388	2466
-25	427	550
-24	1113	1212
-23	698	861
-22	2969	2949
-21	1564	1613
-20	2089	2053
-19	455	455
-18	1500	1522
-17	332	381
-16	1866	1769
-14	1486	1491
-13	1548	1495
-12	663	658
-11	1389	1336
-10	4137	4213
-9	1712	1744
-8	1842	1956
-6	3594	3687
-5	1434	1431
-4	4191	4326
-3	1296	1249

-2	1827	1865
-1	1040	1054
0	2156	2253
1	388	350
2	3212	3262
3	932	935
4	803	897
5	1934	1912
6	4098	4341
7	1619	1616
8	2469	2626
10	2963	2961
11	832	872
12	3848	3990
13	2097	2214
14	1524	1601
15	978	933
16	1707	1651
17	402	482
18	2285	2334
20	1197	1261
21	944	999
22	2650	2551
23	1674	1750
24	2069	2198
26	1288	1251
8, 2, L		
-26	860	825
-25	1114	1129
-24	2017	2110
-23	2123	2038
-22	1138	1077
-20	2214	2226
-19	1446	1433
-18	1962	2020
-17	890	920
-16	1927	1924
-15	665	693

-14	1842	1878
-12	3123	3127
-11	432	414
-10	938	950
-9	887	882
-8	3090	3114
-7	3321	3475
-6	2331	2308
-5	881	907
-4	2945	2917
-3	1930	1970
-2	2139	2194
-1	887	951
0	2567	2581
1	787	679
2	2921	2889
3	2251	2264
4	3220	3225
5	1590	1642
6	1929	1935
7	726	757
8	1818	1925
9	2635	2811
10	2289	2282
11	1067	1050
12	2560	2627
13	306	403
14	2024	2033
15	1148	1163
16	2821	2771
18	1451	1449
19	895	894
20	1907	1899
21	1933	1846
22	1852	1853
23	633	711
24	1339	1350
25	1599	1595

8, 2, L			13 1237 1292		12 3071 3027		9 502 399		7 718 642		6 1561 1559	
26 1750	1778		14 3992 3952		13 1611 1494		10 1358 1343		8 1652 1528		7 1099 1086	
8, 3, L			16 2274 2213		14 1447 1358		11 1443 1470		9 1346 1290		8 871 882	
-26 1054	1089		18 2210 2147		16 3324 3322		13 1125 1170		11 1413 1391		9 413 365	
-25 1019	1013		19 467 474		17 1129 1156		14 2660 2675		12 1482 1506		10 1385 1407	
-24 852	831		20 2381 2260		18 3039 3034		15 1779 1793		13 1458 1478		11 1731 1736	
-23 408	472		21 1258 1198		21 1117 1163		16 2075 2069		14 1434 1417		12 1214 1130	
-22 1011	1070		23 2038 1958		22 1420 1461		18 1882 1944		16 1411 1430		13 1268 1270	
-21 2163	2170		24 988 927		25 1416 1380		19 2194 2158		17 3088 3022		15 2735 2736	
-20 927	978		26 1171 1163		8, 5, L		20 2341 2373		18 1160 1228		16 806 785	
-18 2202	2223		8, 4, L		-25 841 833		21 948 997		19 1117 1177		19 2250 2167	
-17 1141	1232		-26 1691 1645		-24 1002 958		23 1013 919		20 1110 1133		21 772 708	
-16 1690	1794		-23 1151 1134		-22 1032 1043		25 502 586		21 1592 1532		22 1362 1325	
-14 3050	3011		-20 1702 1693		-21 1619 1523		8, 6, L		22 980 930		23 1084 1080	
-12 3014	3093		-19 2494 2443		-19 952 993		-23 754 722		24 660 795		8, 8, L	
-11 818	804		-16 3051 3017		-18 1897 1845		-20 1059 1042		8, 7, L		-19 1884 1882	
-10 2373	2408		-15 1442 1363		-17 2763 2643		-19 1842 1901		-22 769 754		-18 825 776	
-9 2150	2103		-14 2572 2597		-16 505 511		-17 1756 1725		-21 974 974		-17 732 763	
-8 1376	1375		-12 2276 2288		-15 660 647		-16 1041 939		-20 515 573		-16 1005 915	
-7 695	694		-11 2090 2142		-14 2378 2352		-15 3079 2970		-19 1183 1222		-15 2697 2627	
-6 2130	2198		-10 2568 2549		-13 3310 3356		-12 961 993		-17 2452 2419		-14 1198 1137	
-5 2654	2609		-8 548 499		-12 1859 1869		-11 3070 3004		-15 753 726		-12 1037 1037	
-3 798	711		-7 1721 1788		-11 1360 1279		-10 854 888		-13 2751 2896		-11 1843 1865	
-2 4277	4343		-6 1118 1083		-10 1226 1178		-9 2154 2074		-12 738 721		-10 761 714	
-1 394	308		-5 616 614		-9 1732 1771		-8 2194 2200		-11 1169 1118		-8 2979 2906	
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1 535	426		-3 1581 1657		-6 1277 1219		-5 1590 1583		-9 1634 1616		-6 1783 1767	
2 2416	2476		-2 1243 1250		-5 970 1014		-4 2509 2534		-8 991 928		-4 716 650	
3 543	560		-1 300 159		-3 2193 2158		-3 2618 2671		-7 500 467		-3 2755 2647	
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5 1284	1290		1 1349 1283		-1 3003 3091		-1 2130 2085		-5 1682 1716		-1 949 879	
6 1723	1692		2 4553 4565		0 3169 3120		0 2022 1952		-4 1871 1820		0 648 580	
7 3578	3593		4 1461 1576		1 460 387		1 4324 4433		-3 1559 1570		1 2835 2689	
8 1257	1230		5 2891 2919		2 2509 2528		2 1591 1539		-1 3976 3970		2 634 594	
9 615	674		6 1769 1801		3 2843 2983		3 1195 1170		1 1020 1039		4 688 747	
10 2525	2496		8 1113 1127		4 2766 2813		4 948 842		2 604 559		5 2357 2349	
11 2146	2207		9 2458 2599		5 1120 1152		5 2511 2452		3 3135 3183		7 1045 1022	
12 995	993		11 355 340		7 2745 2682		6 1087 1038		5 1127 1205		8 2233 2296	

8, 8, L		
9	1785	1801
10	1266	1226
13	3081	3036
17	1901	1882
18	578	638
20	1247	1293
21	1366	1366

8, 9, L		
-20	1014	1066
-18	608	595
-17	1749	1753
-13	1541	1471
-12	1503	1427
-11	1285	1155
-10	1973	1914
-9	1908	1904
-7	563	510
-6	836	814
-5	2961	2942
-4	1123	1148
-1	1372	1407
1	570	556
2	999	1037
3	1239	1192
4	1132	1056
5	884	795
6	1572	1494
7	2555	2525
10	1211	1199
11	2977	3005
12	521	563
14	667	692
15	1579	1498
16	730	735
19	926	979

8, 10, L		
-14	807	815
-13	1178	1242
-11	1700	1661
-10	599	573
-9	938	1023
-7	3072	3060
-5	607	516
-3	2200	2118
-1	914	909
3	1243	1237
5	1964	1856
6	508	480
7	1245	1216
8	616	625
9	3372	3358
12	478	485
13	1358	1395

8, 11, L		
-13	852	855
-11	1163	1190
-10	641	658
-9	1985	2065
-5	2238	2288
-4	718	699
-3	648	738
-2	960	971
-1	1512	1564
2	496	535
3	1016	985
5	1463	1472
6	1189	1061
7	2350	2371
8	797	710
11	1846	1919
12	1045	1042

8, 12, L		
-11	1076	1062
-8	860	854
-7	1274	1352
-6	892	835
-3	1353	1304
-2	1140	1132
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1	937	927
3	628	557
4	953	947
5	1218	1258
8	1348	1320
9	1320	1259
10	1341	1358

8, 13, L		
-5	791	809
-4	1239	1210
-3	432	501
-1	1104	1115
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1	640	646
3	1280	1321

9, 0, L		
-26	2231	2157
-22	2438	2462
-20	2765	2828
-18	642	651
-16	1148	1178
-14	1369	1265
-12	820	742
-10	3487	3507
-8	2172	2097
-6	4128	4247
-4	4694	4736
-2	2380	2296
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2	2643	2660
4	1086	999
6	4034	4188
8	3289	3400
10	1255	1290
12	3169	3067
16	803	806
18	2146	2196
20	1074	1163
22	2350	2242
24	2304	2363
26	831	788

9, 1, L		
-25	644	760
-24	2594	2536
-23	1514	1502
-22	1920	1964
-20	1639	1603
-19	511	443
-18	2095	2009
-17	617	564
-16	618	627
-15	678	681
-14	664	735
-12	2258	2266
-10	1012	1002
-9	776	734
-8	3577	3574
-7	1818	1846
-6	2960	3011
-4	2750	2777
-3	1979	1992
-2	2713	2773
-1	1980	2000
0	878	868
1	345	292
2	1065	1028
4	3419	3474
5	1459	1463
6	1891	1917
7	895	896
8	2960	3023
9	1478	1600
10	3350	3452
11	1277	1261
12	713	744
14	2181	2133
15	575	622
16	1729	1687
18	325	286
19	495	541
20	2617	2577
21	1003	992
22	1839	1864
24	1793	1703
25	794	888
26	2308	2306

9, 2, L		
-26	1302	1318
-25	1008	1037
-24	845	805
-22	1829	1892
-21	1772	1680
-20	1332	1376
-19	1618	1569
-18	1363	1346
-16	1917	1865
-15	682	742
-14	1467	1478
-13	1001	1010
-12	1049	1107
-11	1198	1168
-10	2087	2090
-9	2295	2208
-8	1447	1536
-7	599	652
-6	2406	2477
-5	2701	2699
-4	1546	1594
-3	2202	2241
-2	2635	2645
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2	3087	3132
4	3270	3256
5	1580	1574
6	1912	1932
7	1938	1977
8	2276	2277
9	1019	1012
10	1917	1856
11	1712	1630
12	1932	1941
13	1750	1786
14	2046	2012
15	702	607
16	1311	1284
18	2267	2214
20	1386	1330
21	1393	1291
22	1498	1477
23	1953	1912
24	1580	1580
26	797	798

9, 3, L		
-26	996	984
-25	802	749
-24	618	636
-23	1500	1482
-21	635	660
-20	1696	1742
-19	1458	1449
-18	939	958
-17	1427	1439

9, 3, L		
-16	2007	2043
-14	1755	1776
-12	2226	2133
-11	1317	1269
-10	2245	2128
-9	1165	1228
-8	1387	1370
-7	3275	3367
-5	1184	1280
-4	3246	3143
-3	2088	2088
-2	1679	1735
-1	942	900
0	3814	3821
1	632	546
2	4325	4376
4	1013	1050
5	1936	1908
6	1844	1941
8	1003	1016
9	2586	2616
11	1249	1278
12	2193	2224
13	652	673
14	1472	1424
15	650	622
16	2554	2556
18	2081	2100
19	916	849
20	493	536
21	1645	1653
22	1244	1313
24	583	553
25	1389	1372

9, 4, L		
-25	643	627
-24	510	442
-22	806	875
-21	1421	1487
-18	2187	2295
-17	1470	1369
-16	794	813
-14	2285	2246
-13	1129	1150
-12	2427	2446
-10	412	517
-9	1931	1830
-6	1627	1591
-5	1824	1747
-4	929	937
-3	513	457
-2	3715	3712
-1	1743	1629
0	3414	3336
1	905	849
2	2469	2342
3	1725	1802
4	3014	3052
5	569	601
6	834	822
7	2202	2275
10	1229	1253
11	1912	1890
13	811	761
14	2923	2876
15	1209	1179
16	1555	1610
18	1790	1815
19	1120	1169
20	2218	2200
23	1402	1391

9, 5, L		
-20	1280	1258
-19	1266	1210
-18	548	512
-16	2457	2460
-15	2089	2149
-14	1841	1813
-13	648	651
-12	1448	1490
-11	1844	1792
-10	1468	1568
-9	2002	1973
-6	1225	1136
-5	487	404
-4	2981	2973
-3	2030	2002
-2	846	779
-1	686	652
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1	3395	3396
2	2933	2888
3	1641	1684
4	1162	1219
5	2358	2306
6	1217	1265
7	980	956
8	906	825
9	1340	1206
10	773	695
11	785	764
12	1824	1790
13	987	918
14	515	528
15	651	741
16	2247	2232
17	2162	2220
18	2359	2279
19	1052	1034

20	502	581
21	1270	1271
22	821	809
9, 6, L		
-22	1052	1036
-21	666	623
-19	752	754
-18	1403	1360
-17	1951	1812
-15	581	638
-14	1301	1249
-13	3136	3131
-12	1145	1065
-11	1882	1847
-10	1496	1459
-9	857	829
-8	809	763
-7	765	744
-6	1793	1762
-5	611	606
-4	497	441
-3	1506	1569
-2	1539	1520
-1	4173	4202
1	943	859
2	1482	1565
3	3160	3241
4	1258	1269
5	2207	2229
6	1190	1267
7	1190	1209
10	1132	1104
11	665	636
12	358	369
13	1095	1084
14	1239	1256
15	2363	2346
16	1175	1127

17	623	604
18	879	901
19	2076	2137
21	1585	1583
22	914	918
9, 7, L		
-20	829	822
-19	1376	1300
-17	795	893
-15	2846	2875
-13	613	573
-12	1128	1163
-11	1819	1794
-9	1552	1482
-8	2854	2794
-7	736	689
-6	1474	1468
-4	1141	1106
-3	2703	2709
-1	805	830
1	3440	3448
2	976	904
3	884	812
4	1880	1793
5	1753	1635
7	1208	1202
8	1672	1712
9	1145	1162
10	407	470
11	659	630
12	1018	946
13	2085	2109
14	931	944
17	2189	2145
18	566	540
19	1049	1046
20	1446	1409
21	757	806

9, 8, L		
-21	661	724
-17	1790	1764
-13	1919	1936
-12	1202	1155
-10	2283	2167
-9	1631	1680
-7	538	538
-6	2191	2152
-5	2191	2181
-4	984	917
-1	1486	1512
0	772	761
1	915	886
3	1877	1857
4	1475	1494
5	650	652
6	2269	2229
7	949	919
8	988	994
10	1254	1193
11	2273	2127
15	2350	2276
16	854	847
19	802	833
20	819	765
9, 9, L		
-19	1445	1444
-16	444	484
-15	1156	1195
-14	1503	1461
-13	608	593
-12	1632	1633
-11	1495	1509
-10	842	896
-8	1361	1343
-7	2814	2879
-5	1085	1058

9, 9, L		
-3	2104	2031
-1	404	366
2	1556	1467
3	808	799
4	1048	976
5	1446	1496
8	2130	2139
9	2843	2815
10	657	720
11	674	741
13	2029	1977
15	485	434
17	618	665
18	1050	1012

9, 10, L		
-17	890	814
-16	836	818
-13	838	861
-12	1321	1313
-11	992	1038
-10	582	595
-9	2272	2232
-8	913	786
-5	2413	2373
-3	1353	1395
-2	594	584
-1	807	849
2	434	408
4	1103	1076
5	1692	1678
6	1166	1063
7	2599	2582
11	2438	2536
12	679	629
13	951	1042
16	833	766

9, 11, L		
-14	467	415
-13	1111	1137
-11	1093	1062
-8	442	467
-7	1822	1840
-6	1088	1144
-5	689	674
-4	783	749
-3	1086	1075
-2	632	655
-1	591	631
0	1314	1279
2	382	381
3	1356	1353
5	1233	1189
6	479	491
7	1302	1242
9	2408	2461
10	1155	1122
11	611	678
12	814	778
13	618	509

9, 12, L		
-10	657	672
-9	1132	1177
-8	1153	1219
-5	935	932
-4	1538	1498
-2	1628	1582
-1	777	785
0	801	758
1	662	601
2	752	784
3	804	871
5	747	683
6	1321	1350
7	1240	1245

8	1037	1015

10, 0, L		
-24	1922	1922
-22	2364	2346
-18	1477	1376
-14	380	292
-12	1227	1225
-10	563	606
-8	3564	3673
-6	2353	2393
-4	1354	1310
-2	2790	2933
2	854	805
4	1537	1454
6	1566	1560
8	2719	2622
10	3056	3164
12	717	735
14	729	654
16	937	859
20	1777	1739
22	1406	1376
24	1551	1497

10, 1, L		
-26	1183	1228
-25	573	641
-24	778	809
-22	1364	1311
-21	877	957
-20	1651	1677
-19	923	934
-17	652	671
-16	975	997
-15	566	553
-14	745	760
-13	603	527
-11	660	721
-10	1652	1690

-8	2064	1995
-7	1012	953
-6	2558	2570
-5	1014	1045
-4	2881	3028
-3	1353	1163
-1	1066	1157
0	1126	1069
1	1018	938
2	809	778
4	1342	1352
5	1061	1104
6	3200	3177
7	1648	1597
8	3085	3032
10	1260	1247
11	620	661
12	2263	2186
13	532	553
18	1217	1235
19	335	404
21	475	547
22	1539	1559
23	700	719
24	1580	1539

10, 2, L		
-25	909	938
-24	881	943
-23	1648	1674
-22	575	593
-21	1074	1030
-20	1569	1536
-19	383	306
-18	1083	1116
-17	1781	1780
-16	583	532
-15	919	897
-14	730	697

-13	544	514
-12	965	907
-11	561	558
-10	559	527
-9	1297	1349
-8	1898	1917
-7	2822	2871
-6	1905	1859
-5	1711	1674
-4	1011	1039
-3	1187	1120
-2	685	615
-1	3189	3208
0	2483	2486
1	1216	1242
2	2316	2333
3	1339	1391
4	1297	1408
5	981	967
6	2166	2099
8	1164	1157
9	2276	2286
10	1251	1302
11	1643	1651
12	822	835
14	1274	1265
15	1121	1094
16	1004	970
17	557	561
18	795	761
19	797	796
20	1079	1065
21	585	618
22	716	684
24	724	760
25	936	977

10, 3, L		
-25	630	619
-21	1090	1112
-19	1470	1516
-18	1577	1567
-16	808	804
-15	985	988
-14	828	874
-13	723	702
-12	1409	1488
-11	1101	1117
-10	451	430
-9	1969	1920
-8	458	603
-6	955	899
-5	2360	2311
-4	715	755
-3	2029	2023
-2	3051	3073
-1	483	436
0	2160	2056
1	670	669
2	1782	1918
4	1864	1845
7	1645	1624
9	916	940
10	1062	1086
11	1100	1124
12	296	225
13	1582	1572
14	1685	1624
16	1230	1239
18	1581	1515
19	359	453
20	1618	1584
21	503	464
23	1434	1401
25	1043	977

10, 4, L		
-21	391	471
-20	1460	1394
-19	431	521
-17	894	915
-16	2479	2365
-14	2011	1997
-12	673	637
-11	794	877
-10	1711	1673
-8	660	643
-7	1255	1352
-6	1689	1632
-5	1314	1301
-4	2220	2209
-3	1202	1168
-1	412	338
0	2971	3059
1	1374	1248
2	3539	3543
3	1281	1221
4	420	413
5	679	618
6	1159	1220
7	577	575
9	944	925
10	694	788
11	730	796
12	1182	1224
13	999	999
14	526	628
16	1871	1864
17	647	699
18	2413	2360
21	950	927
22	407	391

10, 5, L		
-22	461	438
-20	752	793
-18	1889	1874
-17	1059	1008
-14	1769	1735
-13	1699	1628
-12	1766	1688
-11	998	985
-9	645	594
-8	901	895
-7	857	794
-6	896	951
-4	810	838
-2	2664	2576
-1	2503	2517
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1	1432	1458
2	1500	1425
3	2014	2057
4	1701	1724
5	1631	1679
6	295	395
7	425	456
9	609	534
10	755	740
11	375	371
12	799	779
14	1847	1882
15	1278	1229
16	1286	1302
17	844	847
18	656	648
19	1165	1254
20	838	839
21	1434	1480

10, 6, L		
-20	735	728
-18	508	624
-17	619	657
-16	1050	984
-15	2165	2189
-14	578	553
-13	742	777
-12	763	766
-11	875	953
-9	1696	1739
-8	749	705
-7	982	970
-6	642	666
-4	1412	1409
-3	1780	1748
-2	518	528
0	1216	1180
1	3250	3227
3	2246	2262
4	1478	1545
5	834	861
6	567	594
7	1397	1385
8	1134	1098
11	681	667
12	893	921
13	967	931
16	1114	1148
17	2021	2070
19	1869	1901
20	906	906
10, 7, L		
-17	1274	1252
-14	686	619
-13	1801	1767
-11	1239	1223
-10	1701	1660
-7	725	716
-6	1751	1785
-5	356	362
-1	1882	1879
0	1219	1244
2	1084	1097
3	1723	1695
4	604	612
5	1806	1848
6	1988	2058
8	651	617
9	509	484
10	830	786
11	586	586
12	850	833
15	2177	2201
16	510	465
17	787	792
18	791	814
19	816	821
20	908	944
21	1322	1297
10, 8, L		
-20	617	651
-19	614	464
-16	486	404
-15	1323	1299
-14	1138	1168
-13	471	475
-12	1197	1263
-11	813	762
-10	1113	1047
-8	2339	2351
-7	1505	1341
-5	807	683
-3	1310	1352
-2	755	743
1	1159	1186
2	2321	2280
3	487	454
4	2504	2411
7	1308	1282
8	2007	2030
9	1041	1015
10	995	926
13	2062	2044
17	794	723
18	1449	1462
10, 9, L		
-17	596	528
-16	763	752
-12	1498	1488
-10	1500	1431
-9	1113	1161
-8	817	802
-7	480	483
-6	912	903
-5	1698	1656
-3	1086	1029
-1	640	594
0	1273	1240
2	951	933
4	1895	1924
6	2603	2587
7	1477	1459
9	483	499
10	989	951
11	1886	1913
13	1052	981
15	551	543
16	1300	1308
10, 10, L		
-14	1109	1063
-13	1009	988
-12	824	804
-11	818	748
-10	1300	1390
-8	736	711
-7	1779	1786
-6	831	867
-5	1224	1257
-4	975	1001
-3	872	890
-1	815	842
0	893	915
1	497	515
2	840	853
3	1253	1221
4	1086	1056
5	641	560
6	934	909
7	835	876
8	1248	1262
9	2439	2536
11	902	917
14	1031	977
10, 11, L		
-12	849	783
-11	1150	1206
-9	1138	1191
-8	1400	1338
-5	1191	1188
-4	1527	1464
-3	912	950
-2	1580	1565
0	762	757
2	1414	1401
4	605	644
5	1353	1328
7	1869	1852
8	1037	1040
10	778	861
11	1114	1166
12	1165	1239

10, 12, L			-13	429	414	-7	603	602	3	596	577	12	1564	1532	11, 6, L		
-7	547	536	-12	516	394	-5	1232	1238	5	522	539	13	1390	1349	-22	513	617
-6	1624	1709	-9	1267	1305	-3	2652	2715	8	334	266	14	1727	1674	-21	810	878
-4	1217	1256	-8	1294	1248	-2	435	527	9	842	873	16	1285	1282	-20	592	694
-2	1467	1437	-7	1159	1174	-1	2126	2143	10	978	972	20	701	692	-18	553	576
0	1986	2003	-6	1501	1519	0	494	438	11	1496	1528	11, 5, L			-17	866	884
2	638	418	-5	896	925	3	1265	1300	12	619	631	-22	794	753	-14	941	1005
3	907	956	-4	449	492	5	1643	1673	14	636	600	-18	784	729	-13	1338	1287
5	567	510	-3	384	442	6	659	639	15	1403	1358	-16	1723	1649	-11	1349	1324
7	720	714	-1	3256	3383	7	1346	1392	16	674	655	-15	875	904	-10	577	533
11, 0, L			0	2023	1991	9	359	480	17	621	593	-14	1178	1150	-9	659	750
-20	1904	1909	1	1734	1837	10	719	706	18	1270	1239	-13	822	840	-8	1095	1079
-18	987	969	2	2520	2510	12	570	623	23	507	552	-9	1108	1092	-7	612	546
-14	323	208	4	919	871	13	999	984	11, 4, L			-8	377	397	-6	1140	1123
-12	1053	1032	5	852	879	15	707	753	-20	1461	1468	-7	513	501	-5	944	900
-10	1345	1425	6	534	616	21	737	727	-19	506	581	-6	2556	2519	-4	1036	992
-8	1143	1181	7	474	537	22	545	554	-18	1604	1532	-5	651	561	-2	766	787
-6	1182	1142	8	1803	1785	23	750	728	-14	970	1013	-4	1500	1414	-1	1655	1651
-4	1652	1589	9	1046	1044	11, 3, L			-12	1356	1329	-2	514	542	0	520	403
-2	1017	1072	10	1537	1547	-23	770	761	-10	1224	1234	-1	444	443	1	1288	1380
4	1197	1269	11	1216	1160	-22	623	651	-9	1011	987	0	1854	1875	2	1285	1276
6	2478	2477	16	734	751	-21	696	771	-8	794	745	1	1797	1836	3	888	883
8	2271	2398	17	737	685	-20	1223	1271	-7	1389	1419	2	762	729	5	2052	1990
12	949	915	19	485	329	-17	1761	1754	-5	406	403	3	1221	1214	6	1275	1252
14	793	878	20	665	644	-16	1038	1004	-4	2355	2336	5	421	318	7	986	1058
16	440	386	21	344	134	-15	1141	1115	-3	1304	1258	6	690	683	10	501	474
18	521	341	24	672	739	-14	847	830	-2	2569	2480	7	725	722	12	403	326
22	914	925	11, 2, L			-10	1080	1020	-1	712	684	9	1170	1080	13	691	685
24	1347	1399	-21	756	730	-9	895	898	0	704	625	10	1468	1437	14	746	797
11, 1, L			-19	1547	1439	-7	1880	1902	1	664	686	12	1225	1212	15	1275	1258
-25	651	710	-18	652	564	-6	597	556	2	1335	1320	13	570	499	17	1359	1310
-24	454	387	-17	902	878	-5	1688	1727	4	1708	1653	16	1270	1271	20	572	561
-23	1024	1045	-15	815	812	-4	825	840	5	718	683	17	793	791	21	1503	1471
-22	803	732	-14	345	311	-2	372	197	6	960	972	18	751	753	11, 7, L		
-21	864	840	-13	549	516	-1	1826	1797	7	856	883	19	1199	1187	-17	428	276
-17	723	748	-11	1496	1343	0	2404	2304	8	1392	1411	22	528	510	-15	1454	1552
-15	637	648	-9	839	871	1	839	791	9	728	616				-14	1096	1095
-14	988	938	-8	747	768	2	1762	1829	10	694	750				-13	1096	1113

11, 7, L		
-12	753	728
-11	548	538
-10	1087	1032
-9	1038	987
-8	1383	1450
-7	942	1038
-6	399	358
-4	578	443
-3	615	565
-2	1316	1292
1	1204	1257
2	1654	1702
3	1474	1483
4	2200	2237
6	371	407
7	1379	1382
8	1633	1554
9	835	811
10	577	453
12	517	461
13	858	849
17	806	880
18	1335	1350
19	1345	1407
20	1499	1553
11, 8, L		
-16	857	849
-12	1374	1384
-10	2026	1890
-6	1312	1333
-1	645	667
0	1568	1534
2	1543	1551
4	1776	1754
5	752	710
6	2416	2363
9	600	532

16	1260	1238
18	1070	1081
11, 9, L		
-17	804	768
-15	630	711
-14	1511	1438
-12	1145	1194
-10	1315	1339
-8	1897	1824
-7	708	613
-5	793	787
-4	687	563
2	1805	1835
4	2412	2482
6	733	713
7	512	441
8	1856	1821
9	979	867
11	845	836
14	781	764
11, 10, L		
-14	748	748
-13	874	864
-12	1638	1565
-11	1083	1021
-10	895	843
-9	579	540
-8	1319	1291
-6	913	915
-5	946	893
-4	756	765
-3	1000	1025
-2	1024	933
0	856	854
2	1544	1581
4	1024	1005
5	878	877
6	1531	1551

7	1336	1338
8	611	618
10	936	965
11	552	613
13	802	804
14	874	958
11, 11, L		
-9	1051	1097
-7	711	727
-6	1536	1571
-5	554	485
-4	1193	1263
-2	930	952
0	1899	1920
1	606	493
3	1263	1248
4	779	730
6	713	722
7	765	729
9	1171	1184
10	851	973
11, 12, L		
-4	1392	1444
-2	2093	2129
0	687	618
1	441	616
2	1152	1201
12, 0, L		
-22	701	660
-20	794	848
-16	1245	1272
-14	2219	2191
-10	1252	1259
-8	888	816
-4	1433	1493
-2	1727	1659
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2	4520	4707

4	1186	1046
6	663	668
8	1677	1743
10	1320	1307
12	673	637
14	1091	1065
16	1925	1911
18	1626	1648
22	378	414
12, 1, L		
-24	497	535
-19	1334	1338
-18	798	776
-17	928	888
-16	1222	1173
-14	471	488
-12	1376	1375
-11	973	970
-9	463	449
-7	823	769
-6	375	371
-4	427	459
-3	1624	1486
-2	2174	2270
-1	2226	2261
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2	776	825
3	701	588
4	1741	1696
5	1472	1486
6	1135	1184
7	1517	1531
8	685	659
9	456	478
10	359	356
14	1038	1013
15	355	332
16	1319	1346

17	412	408
18	835	796
20	934	907
21	399	393
22	455	513
12, 2, L		
-24	701	668
-23	504	519
-22	793	756
-21	875	841
-18	1032	984
-17	1407	1429
-15	1108	1171
-14	1091	1062
-13	570	621
-12	529	558
-9	1233	1222
-8	898	966
-7	1478	1416
-5	1728	1799
-3	561	589
-2	1391	1482
-1	2579	2645
1	2061	2095
2	1305	1307
3	593	603
4	630	615
6	900	918
9	1007	1093
10	640	680
11	1966	1906
13	683	638
15	880	856
16	752	660
17	1426	1406
19	708	733

12, 3, L		
-20	1737	1724
-19	1238	1220
-18	924	882
-17	1051	1025
-16	723	737
-15	964	935
-14	566	578
-13	1046	1099
-11	619	641
-10	1669	1653
-9	373	325
-8	741	816
-7	667	554
-6	886	984
-4	2472	2411
-3	2014	1936
-2	833	809
-1	1227	1241
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3	1525	1541
4	460	424
5	1265	1253
6	1017	1034
8	2449	2473
9	745	675
12	1093	1049
13	1854	1774
14	472	358
15	1379	1314
22	494	428
12, 4, L		
-22	1632	1687
-19	701	701
-18	1337	1303
-17	791	771
-16	1336	1346
-15	1056	1002

12, 4, L			-4 2182 2103			-8 2285 2267			3 1199 1166			13, 1, L		
-14 498 456			-3 772 761			-7 1035 1032			4 1677 1686			-22 520 605		
-13 507 453			-2 800 756			-3 675 660			6 622 644			-21 559 538		
-12 864 859			0 381 477			2 2007 2013			8 1053 1078			-20 1027 1005		
-11 713 683			1 392 599			3 671 612			11 651 639			-18 972 937		
-9 764 783			2 691 597			4 2049 2068			12 1056 976			-17 1047 1097		
-8 1385 1375			5 1456 1421			5 1041 1070			12, 11, L			-16 1485 1512		
-7 482 401			7 2381 2462			6 1281 1218			-8 881 923			-15 847 802		
-6 2156 2104			8 1264 1209			7 758 732			-6 768 780			-14 2651 2639		
-5 1249 1200			9 436 435			8 1656 1680			-4 1256 1230			-10 1842 1861		
-4 346 395			10 547 545			9 907 927			-3 667 716			-9 1084 1097		
-3 1039 1052			11 934 917			14 448 391			-2 1522 1574			-8 512 545		
-2 1782 1697			12 1643 1637			12, 9, L			-1 776 835			-7 822 787		
-1 599 622			14 1422 1349			-13 1350 1282			0 448 440			-6 562 546		
0 1900 1890			17 927 896			-12 1723 1710			2 1251 1232			-5 831 788		
2 1047 1089			21 745 686			-10 1619 1638			3 711 653			-4 1822 1796		
4 907 899			12, 6, L			-9 529 431			5 777 813			-3 896 1001		
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8 1185 1221			-18 635 724			-6 1379 1282			-18 1317 1302			-1 1914 1992		
9 1229 1242			-15 736 732			-1 527 492			-16 1736 1805			0 2363 2325		
10 2394 2448			-14 390 427			0 1354 1389			-14 890 822			1 1702 1811		
11 990 1000			-13 1487 1415			2 1546 1518			-12 2531 2552			2 3887 3922		
12 1080 1106			-11 810 755			3 997 958			-8 442 425			3 538 589		
15 584 603			-10 910 957			4 1583 1597			-6 726 661			5 942 927		
20 629 595			-9 1019 1070			6 2118 2041			-4 349 404			6 1329 1363		
22 648 600			-8 446 349			10 858 808			-2 3745 3564			8 861 841		
12, 5, L			-7 2556 2539			15 968 934			0 3595 3519			9 679 682		
-21 1312 1345			-6 1960 1938			12, 10, L			2 2043 2067			11 1192 1228		
-20 1646 1628			-4 658 647			-12 992 908			4 2606 2526			12 1100 1137		
-18 605 726			-3 1318 1282			-11 912 906			6 891 843			13 733 795		
-15 850 811			-2 978 949			-10 1103 1140			8 688 650			14 1680 1672		
-14 911 912			-1 419 421			-9 866 893			12 932 913			16 1608 1606		
-11 1147 1127			1 708 768			-8 1341 1392			14 1536 1569			17 1064 1032		
-10 767 746			2 397 483			-5 669 683			16 2777 2651			18 2251 2207		
-9 1138 1037			3 1475 1414			-4 744 788			18 1217 1271			22 1022 983		
-8 1724 1704			4 658 687			0 1151 1118			20 1793 1718					
-7 1025 1060			5 770 703			1 1471 1404								
-5 1758 1777			6 848 941			2 483 543								
			7 1074 1093											
			8 827 836											
			9 2226 2147											
			10 940 809											
			11 1042 1031											
			12 818 751											
			14 922 908											
			16 823 772											
			18 807 767											
			19 1139 1139											
			12, 7, L											
			-16 755 814											
			-12 1286 1322											
			-11 1298 1316											
			-10 1819 1798											
			-9 1841 1760											
			-7 494 394											
			-6 891 883											
			-5 1584 1579											
			-4 496 521											
			0 1024 1026											
			1 998 983											
			2 1109 1181											
			3 610 557											
			4 1160 1182											
			5 1375 1418											
			6 1467 1448											
			7 1880 1855											
			11 823 776											
			13 951 1000											
			16 1211 1201											
			18 825 814											
			12, 8, L											
			-14 1608 1646											
			-12 1077 1043											
			-11 493 470											
			-10 969 1037											
			-9 862 819											

13, 2, L		
-22	642	596
-20	1250	1234
-19	1622	1588
-18	542	576
-17	1429	1400
-16	1882	1858
-14	833	880
-13	1046	1043
-12	1720	1767
-11	1505	1516
-10	1383	1403
-8	1036	1029
-7	373	469
-6	1194	1163
-5	929	889
-4	1782	1732
-3	1592	1615
-2	481	387
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3	1409	1427
4	2134	2199
5	1827	1801
6	524	536
7	1156	1151
8	1975	1986
9	790	759
12	948	985
13	1267	1289
14	821	826
15	1796	1759
16	1389	1401
17	1032	991
18	574	545
19	739	762
20	911	936
21	1056	1036
13, 3, L		
-22	1587	1635
-19	830	759
-18	1910	1868
-17	873	878
-16	692	675
-15	1653	1615
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-11	685	645
-10	877	905
-8	1750	1821
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1	1953	1836
2	782	755
3	1046	1097
4	1604	1601
5	800	806
6	1977	1959
7	729	682
8	1434	1411
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11	1714	1641
13	1114	1093
14	925	895
15	596	592
16	351	389
17	1429	1410
19	839	841
20	690	656
22	949	961
13, 4, L		
-21	851	863
-20	2237	2254
-18	609	608
-17	994	1010
-16	981	955
-13	1433	1371
-12	713	615
-10	1468	1514
-9	1304	1268
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-7	523	467
-6	758	685
-5	1737	1623
-4	2496	2476
-3	540	485
-2	597	621
-1	939	886
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1	430	451
3	652	605
6	1575	1465
7	2075	2034
8	3015	2965
9	739	738
11	957	1066
12	2076	2023
13	1174	1083
14	1186	1132
15	1145	1132
19	766	725
13, 5, L		
-19	1305	1291
-18	1306	1347
-16	804	721
-15	516	498
-13	1090	1111
-11	1707	1709
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-8	873	938
-7	2581	2527
-6	2116	2157
-3	2138	2095
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6	1319	1334
8	772	818
9	2652	2722
10	2606	2584
12	1458	1427
13	745	609
14	1076	1060
16	610	592
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13, 6, L		
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-18	394	319
-16	761	838
-14	819	686
-12	659	771
-11	1209	1245
-10	494	467
-9	2500	2402
-8	1398	1475
-5	2711	2651
-4	1338	1376
-3	660	573
-1	889	935
1	390	337
2	539	525
3	534	523
4	910	971
5	1428	1420
7	2693	2767
8	1175	1227
11	1677	1652
12	899	942
13	944	941
16	856	846
17	628	602
19	936	975
13, 7, L		
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-14	1742	1752
-13	730	725
-12	1189	1227
-11	1174	1204
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-7	2719	2710
-5	1278	1282
-3	1711	1662
2	1389	1447
3	1056	1067
4	840	839
5	1494	1553
6	2011	2083
7	723	761
8	1078	1121
9	2080	2175
11	707	679
13	1101	1126
14	877	802
15	574	558
13, 8, L		
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-13	1025	1103
-12	1977	1956
-10	2132	2142
-9	1066	1581
-6	1036	983
-5	1866	1901
-4	763	683
-3	862	776
-1	1081	1054
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3	1432	1378
4	2168	2232
6	1635	1655
7	1651	1718
11	1012	976
14	436	474
15	1071	1026
13, 9, L		
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-11	1322	1274
-10	1038	983
-8	1925	1909
-7	553	525
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2	1271	1270
3	521	591
4	1565	1583
5	1269	1294
6	819	897
8	1164	1192
9	749	707
13	1408	1403
13, 10, L		
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-6	880	882
-3	759	723
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3	1264	1256
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5	989	1100

13, 10, L			-12	3132	3096	-13	1157	1074	-8	2472	2516	1	633	658	12	1816	1795
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13, 11, L			-6	892	922	-6	1528	1556	-2	584	601	6	2012	1969	-17	772	842
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14, 0, L			0	3559	3569	1	2026	1963	5	1684	1685	14	1318	1318	-6	1752	1751
-22	756	715	2	1887	1958	2	2426	2394	6	1752	1825	17	1030	1015	-5	1366	1371
-20	1203	1228	3	704	643	3	1016	973	7	476	507	19	627	717	-3	1758	1783
-18	1072	1115	4	2818	2755	4	1486	1470	8	3196	3158	14, 5, L			-2	1333	1344
-16	1991	2004	5	1590	1597	6	2729	2678	9	445	364	-19	1035	1053	-1	1075	1108
-14	3272	3336	7	790	776	7	502	425	10	427	502	-17	688	615	2	928	950
-12	369	357	8	1294	1287	8	698	709	11	1199	1176	-16	888	927	3	731	743
-10	3352	3381	9	486	456	9	742	764	12	2327	2305	-13	753	806	5	1725	1729
-6	1247	1229	10	797	832	10	2074	2053	13	749	740	-12	836	835	6	1942	1958
-4	2083	2064	12	1885	1854	11	1441	1455	15	1748	1710	-11	763	724	9	2938	2965
-2	3366	3335	13	533	560	12	916	967	16	909	842	-10	741	725	10	1381	1381
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6	1977	1995	16	3184	3139	16	777	804	19	866	871	-7	692	771	13	788	737
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12	1132	1115	18	714	763	18	1780	1798	14, 4, L			-5	1789	1808	15	509	566
14	2971	2909	19	596	531	19	1192	1166	-19	1163	1243	-4	2007	2031	16	633	643
16	1143	1124	20	2041	1926	20	557	582	-18	1889	1884	-3	943	886	14, 7, L		
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14, 1, L			14, 2, L			-20	2019	2034	-12	1261	1242	-1	955	879	-13	656	653
-20	750	724	-21	521	584	-19	784	735	-11	1595	1615	0	858	862	-12	1479	1483
-19	1021	1005	-20	1102	1114	-17	1651	1645	-10	1655	1726	2	969	912	-11	767	808
-18	1859	1843	-18	1829	1844	-16	1709	1713	-8	1312	1366	4	1010	984	-10	1097	1051
-17	728	772	-17	1111	1096	-13	1609	1637	-7	1592	1558	6	1404	1436	-9	2286	2389
-16	2316	2325	-16	1055	1073	-12	1413	1382	-6	2370	2386	7	2546	2547	-8	657	640
-14	1246	1204	-15	1741	1763	-11	1405	1409	-3	1335	1378	8	2597	2590	-7	893	959
-13	875	877	-14	2496	2417	-10	2060	2172	-2	2040	2116	11	2153	2184	-5	2652	2748

14, 7, L		
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-2	649	630
-1	951	959
0	808	787
2	525	576
3	957	972
4	2125	2122
6	965	1002
7	2120	2214
8	898	982
9	774	804
11	1903	1866
13	1230	1225
15	657	684
16	1116	1122

14, 8, L		
-14	1740	1758
-13	500	491
-12	811	881
-11	1126	1119
-10	1099	1022
-8	1343	1276
-7	1859	1862
-5	794	822
-3	1388	1385
0	654	643
1	1548	1549
2	2011	1961
4	815	824
5	1705	1744
6	1450	1451
7	857	864
8	1155	1176
9	1259	1323
12	536	574
13	1587	1627

14, 9, L		
-11	899	943
-10	1176	1228
-9	906	925
-7	381	387
-6	795	776
-5	912	899
-4	433	427
-2	749	737
-1	2136	2177
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1	614	551
2	643	624
3	1767	1803
4	1094	1110
5	1503	1559
6	1153	1192
7	725	775
11	1184	1178

14, 10, L		
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2	507	375
3	1437	1439
4	643	694
5	863	831

15, 0, L		
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-18	1848	1922
-16	2423	2430
-14	1491	1467
-12	3816	3801
-10	652	739
-8	2308	2164
-4	1501	1517
-2	1832	1843
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2	1926	1982
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8	1335	1288
10	817	861
12	2051	2082
14	1932	1776
16	3800	3678
20	2102	2110

15, 1, L		
-20	924	947
-18	1390	1337
-17	812	798
-16	1882	1861
-15	1060	1050
-14	3011	2995
-13	782	850
-12	576	646
-10	3320	3324
-9	883	868
-7	792	810
-6	1765	1766
-5	697	638
-4	736	776
-3	1005	1080
-2	3100	3075
-1	702	738
0	1339	1388
1	804	816
2	3281	3320
3	1019	1091
6	2542	2556
7	494	522
10	1883	1911
11	552	591
12	1297	1205
13	926	882
14	2965	2931
17	1017	1053
18	2804	2697
19	929	931

15, 2, L		
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-19	1135	1172
-18	1252	1281
-17	1383	1365
-16	2178	2152
-14	972	965
-13	1490	1481
-12	2678	2704
-11	2132	2028
-10	1124	1059
-8	2683	2563
-6	810	849
-4	1954	1974
-3	662	692
-1	1593	1580
0	2653	2680
1	602	694
2	1002	967
3	1447	1541
4	2810	2905
5	1564	1547
6	825	828
7	418	466
8	2496	2457
10	855	897
11	372	315
12	2829	2830
13	679	639
15	1754	1698
16	2075	2071
17	1195	1198
19	560	524

15, 3, L		
-19	745	784
-18	2096	2010
-15	2047	2042
-14	1263	1267
-13	1123	1087
-12	1423	1439
-11	841	859
-10	2248	2203
-9	1278	1263
-8	1585	1556
-7	440	415
-6	3107	2970
-3	835	787
-2	1735	1708
-1	643	634
1	1707	1792
2	1837	1880
3	1498	1481
4	1448	1497
5	716	688
6	2271	2253
7	674	712
8	1851	1814
10	2767	2802
11	587	572
13	1816	1786
14	1841	1786
17	1158	1122
18	1036	1007
19	1312	1274

15, 4, L		
-17	1310	1245
-16	988	993
-13	1311	1295
-12	1074	963
-10	2055	2057
-9	1358	1349
-8	3227	3249
-7	610	611
-6	723	749
-5	1058	1000
-4	2861	2912
-2	1093	1143
-1	1250	1252
0	1167	1169
1	474	409
2	838	804
3	1169	1137
4	1248	1234
5	913	942
6	2231	2142
7	1359	1367
8	2943	3011
11	2047	1973
12	2425	2358
14	1166	1168
15	997	1061
16	526	490
18	590	621

15, 5, L		
-17	848	868
-15	844	837
-14	581	619
-12	620	623
-11	1606	1525
-10	1695	1664
-8	1038	1040
-7	2460	2456
-6	2523	2456
-5	1496	1439
-3	1212	1301
-2	1640	1616
-1	1137	1155
1	436	708
2	655	649

15, 5, L

4	1485	1460
5	1815	1827
6	1585	1619
8	1113	1137
9	2667	2682
10	2504	2563
11	1409	1371
12	629	655
13	966	979
14	1141	1112
15	778	707

15, 6, L

-16	819	896
-13	697	664
-12	1011	993
-11	637	652
-9	2302	2297
-8	1277	1275
-7	1295	1301
-6	799	862
-5	2560	2453
-4	1645	1585
-3	2117	2079
-1	701	743
0	727	759
3	965	990
4	1262	1279
5	770	756
7	2656	2669
8	1173	1240
9	1172	1228
11	2099	2136
12	1177	1214
13	1295	1301

15, 7, L

-14	1384	1493
-11	1406	1393
-10	946	974
-7	2600	2601
-6	675	608
-5	1450	1393
-3	1901	1851
-1	1210	1225
0	600	512
1	853	811
2	1565	1620
3	377	427
4	465	597
5	1678	1735
6	1290	1349
8	796	756
9	2096	2040
11	1470	1516
12	847	829
13	1065	1082
14	894	870

15, 8, L

-12	1287	1287
-10	849	894
-9	1564	1563
-7	460	515
-5	1969	2014
-4	673	620
-3	1094	1091
-2	1171	1244
-1	1477	1446
0	1047	1045
3	1671	1697
4	1553	1615
5	976	936
6	1149	1202
7	1130	1140
9	1170	1154
11	1341	1331

15, 9, L

-8	826	787
-7	764	854
-6	926	804
-4	657	635
-3	1471	1487
0	629	585
1	2106	2124
2	1160	1167
3	1063	1066
4	674	655
5	1013	1067
7	1354	1417

16, 0, L

-18	959	1033
-16	1846	1840
-14	3205	3231
-10	2549	2575
-8	616	681
-6	1515	1511
-4	1335	1315
-2	3339	3180
0	1325	1252
2	3396	3528
6	2135	2014
10	1192	1266
12	1277	1271
14	2271	2362
16	712	708
18	2818	2724

16, 1, L

-18	1334	1354
-17	641	652
-16	1875	1864
-14	1136	1108
-13	1025	1034
-12	2839	2812
-11	1331	1289
-10	369	434
-9	848	812
-8	2006	1913
-6	743	746
-4	1674	1635
-3	493	539
-2	1262	1345
-1	998	911
0	2931	2802
1	507	447
2	592	646
3	669	630
4	2746	2743
5	1140	1119
8	1617	1637
9	543	487
10	723	695
11	464	541
12	1862	1808
13	729	676
14	1141	1151
15	1008	1012
16	2810	2725
17	557	477

16, 2, L

-18	1499	1468
-17	638	594
-16	705	663
-15	1714	1678
-14	1786	1745
-13	1460	1454
-12	687	697
-10	2284	2274
-9	1399	1453
-8	858	928
-7	358	370
-6	2295	2266
-5	1012	1012
-3	868	839
-2	1691	1762
0	705	726
1	1705	1676
2	2457	2418
3	1270	1299
4	362	421
5	784	747
6	2166	2192
7	980	969
8	655	684
10	2234	2207
11	557	613
12	643	527
13	1055	1068
14	2117	2083
17	1092	1076
18	1593	1588

16, 3, L

-17	1301	1338
-16	1177	1170
-15	866	882
-13	1451	1455
-12	1051	1088
-11	1745	1786
-10	1575	1595
-8	2928	2996
-7	699	649
-4	2479	2367
-3	664	638
-1	1794	1805
0	1675	1683
1	1166	1150
3	1533	1490
4	1936	1892
5	1600	1578
6	1444	1423
8	2131	2122
10	458	549
11	986	986
12	2550	2548
14	785	772
15	1296	1266
16	901	872
17	1152	1099

16, 4, L

-17	859	868
-15	1086	1114
-13	757	715
-12	1094	1084
-11	1035	985
-10	1511	1452
-9	863	782
-8	1597	1550
-7	1170	1101
-6	3133	3047
-5	936	892
-3	868	924
-2	1423	1391
-1	542	502
1	1616	1649
2	515	496
3	1373	1398
4	1800	1796
5	989	968
6	1647	1701
7	834	894
8	1474	1493
9	980	989
10	2816	2791
11	932	929
12	465	546
13	917	919
14	947	977

16, 4, L		
15 891 916		
16, 5, L		
-15 783 739		
-13 455 445		
-12 385 504		
-10 1339 1364		
-9 1618 1613		
-8 2007 2021		
-7 1340 1295		
-6 805 872		
-5 1704 1607		
-4 2197 2246		
-3 1798 1785		
-2 676 746		
-1 688 615		
0 780 853		
1 747 683		
3 1126 1116		
6 1793 1799		
7 2088 2106		
8 1860 1928		
9 1193 1223		
11 1509 1515		
12 1515 1514		
13 1409 1449		
16, 6, L		
-14 626 609		
-12 676 684		
-11 1125 1125		
-10 1086 1124		
-8 769 773		
-7 2063 2023		
-6 1163 1154		
-5 2043 2046		
-3 1178 1132		
-2 753 844		
-1 1652 1601		
1 445 447		
2 882 935		
5 1614 1701		
6 1002 1016		
7 464 538		
9 2130 2109		
10 1126 1052		
11 2137 2150		
16, 7, L		
-12 860 906		
-9 1597 1682		
-7 914 950		
-6 843 831		
-5 1886 1978		
-3 1766 1808		
-2 1055 1118		
-1 734 733		
0 728 754		
3 1163 1239		
4 1042 1101		
7 1842 1949		
9 1605 1678		
10 924 934		
11 1141 1156		
16, 8, L		
-7 1399 1473		
-6 514 434		
-5 986 1002		
-4 1140 1074		
-3 1335 1358		
-1 678 734		
0 1014 979		
1 1114 1143		
2 1244 1270		
3 547 619		
5 1078 1150		
7 1053 1098		
16, 9, L		
-2 1240 1280		
-1 1807 1825		
0 989 991		
1 863 807		
17, 0, L		
-16 1628 1626		
-14 878 950		
-12 2426 2375		
-10 997 1036		
-6 702 708		
-4 1185 1198		
-2 2119 2111		
0 2486 2478		
4 2565 2611		
6 585 708		
8 1106 1003		
14 1623 1780		
16 2105 2098		
17, 1, L		
-16 996 1044		
-15 1016 1023		
-14 2011 1979		
-13 1103 1133		
-10 1401 1447		
-9 631 600		
-8 436 333		
-7 923 890		
-6 848 854		
-5 1019 946		
-4 1511 1452		
-3 587 601		
-2 1954 1965		
0 726 691		
1 624 469		
2 2423 2412		
3 867 933		
5 327 367		
6 1604 1673		
7 756 700		
10 864 899		
12 1060 1072		
14 1650 1654		
17, 2, L		
-16 1056 1026		
-15 634 624		
-13 1183 1158		
-12 1210 1229		
-11 1906 1912		
-9 930 915		
-8 1691 1695		
-4 1402 1410		
-3 981 914		
-2 801 751		
-1 1300 1271		
0 1506 1497		
1 1046 1007		
3 981 974		
4 1752 1751		
5 1579 1633		
7 539 554		
8 1266 1275		
10 412 445		
12 1486 1498		
13 655 629		
15 1086 1068		
16 1433 1389		
17, 3, L		
-15 912 917		
-13 1462 1436		
-12 657 711		
-10 1127 1108		
-9 964 937		
-8 1046 1133		
-6 2379 2307		
-5 520 534		
-3 564 574		
-2 1136 1135		
1 1797 1735		
2 883 848		
3 1640 1635		
4 743 800		
6 1243 1262		
7 955 952		
8 981 991		
9 494 501		
10 2005 1885		
13 597 604		
14 1027 992		
15 688 599		
17, 4, L		
-11 658 662		
-10 1471 1558		
-8 1929 1955		
-7 923 958		
-6 637 638		
-4 2211 2271		
-2 863 853		
-1 874 866		
1 802 785		
2 399 444		
3 854 890		
5 906 865		
6 1648 1704		
8 2061 2016		
9 598 619		
12 1559 1545		
13 1096 1086		
14 852 847		
17, 5, L		
-13 427 490		
-12 1072 1017		
-10 818 787		
-8 1379 1426		
-7 887 896		
-6 1676 1721		
-5 1498 1552		
-2 1170 1161		
-1 1034 1006		
0 685 653		
4 1383 1416		
5 852 883		
6 1057 1019		
7 750 805		
8 961 964		
9 835 829		
10 1492 1475		
11 1673 1640		
17, 6, L		
-10 918 935		
-9 947 1083		
-8 729 680		
-7 749 799		
-6 673 716		
-5 881 1042		
-4 585 583		
-3 2011 2080		
0 586 529		
1 511 607		
4 723 742		
6 908 936		
7 1772 1763		
8 811 845		
9 1660 1646		
10 793 783		
11 407 411		
17, 7, L		
-8 650 691		
-7 810 907		
-5 1416 1478		
-4 1104 1157		
-1 1005 1014		

17, 7, L
0 585 608
2 999 973
5 1292 1289
7 829 801
8 550 511
17, 8, L
-3 838 867
-2 1577 1621
0 1024 1005
1 671 674
18, 0, L
-14 1470 1426
-8 808 802
-6 425 353
-4 1585 1617
-2 1061 1058
2 1894 1902
4 1171 1145
6 1035 1072
8 991 1054
10 387 392
12 1275 1197
14 526 544
18, 1, L
-13 637 651
-12 1079 1027
-11 1073 1089
-10 707 707
-9 963 999
-7 363 450
-5 423 473
-4 453 523
-3 527 695
-2 1084 1097
-1 627 696
0 1399 1431
1 1063 1000
4 1221 1236
5 1054 1079
6 1097 1089
7 344 295
13 570 553
14 1170 1181
18, 2, L
-13 1270 1256
-10 621 603
-9 519 536
-7 1352 1324
-6 821 840
-5 1066 1120
-4 568 639
-2 732 723
1 707 779
2 889 895
3 1318 1259
6 524 551
7 676 651
9 817 815
10 570 575
11 851 808
18, 3, L
-11 1242 1217
-10 918 992
-8 1287 1274
-5 705 690
-4 1572 1546
-3 518 475
-1 849 889
1 965 1042
5 1188 1234
6 673 679
7 805 862
8 1031 1049
11 557 564
12 816 838
18, 4, L
-12 646 668
-9 436 407
-8 1183 1201
-6 1718 1711
-5 484 448
-2 656 638
1 372 402
4 1397 1352
6 824 837
8 867 896
10 1209 1260
11 728 698
18, 5, L
-10 1298 1321
-8 695 635
-7 591 593
-6 694 691
-4 1039 1084
-3 1317 1285
-1 408 471
2 600 558
6 1421 1421
7 528 493
8 1263 1239
9 656 650
18, 6, L
-7 812 762
-5 1521 1505
-1 1020 1016
1 712 742
3 496 490
4 693 747
5 909 927
6 526 581
18, 7, L
0 662 711
19, 0, L
-10 961 1054
-8 1278 1305
-4 832 839
-2 1160 1246
0 985 961
2 556 517
6 1506 1526
8 645 694
10 630 588
19, 1, L
-10 395 426
-7 983 1002
-6 846 810
-5 765 774
-4 740 822
1 407 278
2 643 561
3 1096 1118
4 1117 1069
9 523 496
10 772 823
11 900 911
19, 2, L
-11 930 973
-9 835 799
-7 587 584
-5 889 862
-3 631 583
-2 353 289
-1 672 624
1 1138 1098
5 1106 1072
6 437 383
7 989 1074
9 688 634
19, 3, L
-7 1197 1273
-6 809 785
-5 640 736
2 934 963
3 1007 996
4 494 492
5 774 807
9 813 835
19, 4, L
-4 480 663
-2 715 691
0 1058 1116
2 740 718
6 826 906
7 679 576
19, 5, L
-5 957 1021
-3 779 774
-1 608 651
1 820 841
2 671 664
4 1170 1173
20, 0, L
-6 1747 1802
-4 656 665
-2 914 946
0 678 630
4 1006 959
6 1037 1060
20, 1, L
-5 636 618
-4 1423 1424
-3 543 663
-2 929 930
1 694 727
4 613 617
5 706 748
6 739 751
20, 2, L
-6 806 764
-5 1082 1088
-2 668 729
0 612 599
2 808 777
3 1063 1100
5 838 962
20, 3, L
-3 635 503
0 1398 1345
1 616 600
2 692 715

CALCULATED AND OBSERVED STRUCTURE FACTORS OF
$[Pt_3(CO)(SnF_3)(dppm)_3]_{0.75}[Pt_3Cl(SnF_3)(dppm)_3]_{0.25}[PF_6]_{0.25}$

2, 2, L	5, 2, L	6, 3, L	7, 1, L	7, 7, L	8, 5, L
-210502 9217	-1 1467 1555	-3 2249 2406	0 2031 1907	-2 3755 3696	-3 2923 2930
020219 20959	0 1903 1619	-2 1797 1660	7, 2, L	0 2073 2242	-2 4848 4873
210876 9300	1 1825 2038	-1 2006 2038	-1 2450 2249	2 4216 4259	-1 754 825
3, 1, L	5, 3, L	0 1469 1314	1 2860 2722	4 4817 4699	0 4922 4780
0 1965 2815	-2 2834 2912	1 1824 1858	7, 3, L	6 6068 6224	1 788 868
3, 2, L	-1 2540 2578	2 1411 1294	-2 1952 2127	8, 0, L	2 5150 5193
-1 2103 1994	0 991 866	3 2159 2429	-1 899 782	0 858 927	3 3072 3147
1 1967 1839	1 2529 2579	6, 4, L	0 1740 1862	8, 1, L	4 5172 5381
3, 3, L	2 3311 3349	-4 1399 1348	1 838 788	-1 5156 5231	5 4621 4577
-2 608 1129	5, 4, L	-3 1844 1896	2 2693 2904	0 2437 2371	8, 6, L
0 4433 4137	-3 4893 4844	-2 2782 2973	7, 4, L	1 5261 5354	-2 3002 2925
4, 0, L	-2 3458 3062	-1 2928 2928	-3 4125 3842	8, 2, L	-1 1826 1766
0 9380 8832	-1 3406 3429	0 883 646	-2 1376 1572	-2 1635 1662	0 3113 3116
4, 1, L	0 1467 1296	1 2747 2817	-1 3095 3082	-1 1935 1875	1 1889 1843
-1 2458 2441	1 2968 2995	2 2803 3070	0 1614 1591	0 1497 1544	2 2945 2883
0 1150 1162	2 3671 3330	3 1924 1985	1 2976 2919	1 2113 2004	3 2641 2464
1 2150 2233	3 4531 4543	4 1281 1213	2 1350 1583	2 1574 1641	4 2590 2779
4, 2, L	5, 5, L	6, 5, L	3 4038 3845	8, 3, L	5 2143 2005
-210335 10792	-4 6209 6210	-5 6630 6674	7, 5, L	-3 6000 5598	6 5045 5133
-1 1245 1184	-2 3286 3223	-4 3346 3311	-4 5393 5323	-2 3338 3232	8, 7, L
0 8091 8091	0 3481 3444	-3 4137 4123	-2 3195 3146	-1 3723 3685	0 5469 5231
1 1340 1291	2 4212 4165	-2 3908 3961	-1 1078 1045	0 3239 3448	2 5552 5277
210741 11249	4 6033 6072	-1 1319 1437	0 1565 1499	1 3833 3754	3 3599 3849
4, 3, L	6, 0, L	0 3565 3836	1 1031 1023	2 3044 2897	4 3646 3656
-3 3737 3588	0 3979 3794	1 1778 1786	2 3849 3796	3 5835 5529	5 5579 5620
-2 1520 1609	6, 1, L	2 4324 4405	4 5382 5479	8, 4, L	7 5228 5272
-1 1389 1349	-1 2731 2515	3 4364 4397	7, 6, L	-4 1764 1574	8, 8, L
1 1586 1503	0 989 1086	4 3423 3511	-4 1781 1838	-3 2970 2973	0 4823 4261
2 1755 1831	1 2751 2551	5 6411 6465	-3 5686 5359	-2 2876 2832	2 3774 3863
3 3092 2998	6, 2, L	6, 6, L	-2 3429 3405	-1 2861 3025	4 5038 4962
4, 4, L	-2 1846 1598	-4 3082 3208	-1 2985 2880	0 2378 2593	6 3924 3599
-4 3412 3305	-1 1851 1797	-2 1257 1130	0 4379 4005	1 2824 2945	8 4934 5439
-2 4076 4233	0 3726 3704	0 3732 3534	1 2580 2487	2 2656 2603	9, 1, L
012506 11336	1 1660 1592	2 1051 862	2 3589 3599	3 2987 3083	0 792 393
2 4453 4732	2 2573 2394	4 2793 2930	3 5411 5133	4 1442 1494	
4 3839 3809		6 2391 2167	4 1744 1836		
			5 6049 6114		

9, 2, L	9, 9, L	5 2700 2780	11, 3, L	6 2565 2424	12, 6, L
-1 2721 2701	4 2501 2225	6 3885 3886	2 3097 3018	7 2383 2370	1 2997 2993
0 1242 1233	6 3005 3045	10, 7, L	11, 4, L	8 1579 1569	2 1396 1472
1 3019 3084	8 3328 3324	0 5381 5054	1 3996 4236	9 2489 2459	3 3630 3658
9, 3, L	10, 0, L	1 1647 1720	3 3324 3248	11, 11, L	4 2559 2470
-2 2313 2410	0 5491 5412	2 5582 5326	11, 5, L	0 3516 3303	5 3027 3203
2 2761 2843	10, 1, L	3 3818 3777	2 2419 2301	2 3487 3312	6 1879 1850
9, 4, L	-1 8789 8758	4 3699 3713	4 2593 2757	4 3624 3476	12, 7, L
-2 1690 1666	0 1778 1660	5 4356 4512	11, 6, L	6 2960 2870	0 5914 5633
-1 3708 3916	1 8667 8522	6 2458 2711	0 2506 2600	8 1945 1853	1 2317 2172
0 2226 2089	10, 2, L	7 4944 4899	1 4872 4428	10 2227 2336	2 5395 5225
1 3837 4153	0 1164 1087	10, 8, L	2 2540 2467	12, 1, L	3 5483 5430
2 1727 1643	1 2895 3016	0 3632 3691	3 2803 2838	0 1142 1041	4 3783 3879
3 3789 3832	2 3746 3780	2 3165 3061	4 1896 1938	1 8037 7939	5 4854 4701
9, 5, L	10, 3, L	3 1883 1753	5 2984 2936	12, 2, L	6 3290 3316
2 3337 3060	0 3213 3217	4 2933 3100	11, 7, L	0 3792 4034	7 3185 3492
4 4205 4414	1 6244 5923	6 3993 3950	1 1953 1944	1 2466 2542	12, 8, L
9, 6, L	2 4134 4161	7 1602 1703	6 2549 2471	2 1944 1856	1 1507 1469
0 3795 3383	3 5483 5574	10, 9, L	11, 8, L	12, 3, L	2 1573 1648
1 3844 3895	10, 4, L	0 4545 4408	1 2753 2840	0 2468 3041	4 1283 1453
2 3190 3073	0 3080 3786	1 1594 1565	2 2624 2294	1 7355 7120	5 1562 1594
3 3920 3887	1 3836 3644	2 4478 4418	3 2403 2462	2 4093 3827	7 2324 2331
4 1586 1625	2 2826 2609	3 3020 3061	4 2611 2604	3 6709 6884	12, 9, L
5 5612 5362	3 3862 3784	4 3120 3076	5 2639 2513	12, 4, L	0 4085 3758
9, 7, L	4 2372 2286	5 4009 4120	6 1075 1138	1 3515 3723	1 2400 2477
4 3035 3088	10, 5, L	6 3049 2849	7 2657 2712	2 3377 3449	2 3972 3879
6 4639 4676	0 4921 4783	7 3770 3924	11, 9, L	3 4313 4261	3 3913 3953
9, 8, L	1 3370 3221	8 1898 2097	2 1320 1447	4 1754 1598	4 3399 3432
0 3361 3207	2 5347 5154	9 3281 3373	4 2172 2343	12, 5, L	5 3233 3415
1 2400 2283	3 3536 3653	10, 10, L	6 1956 2125	0 4683 4983	6 3471 3486
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3 3441 3219	5 3832 3836	2 1904 1833	11, 10, L	2 5519 5174	8 3200 3090
4 2152 2227	10, 6, L	4 2667 2463	0 2167 2250	3 5067 5086	9 3253 3209
5 4293 4432	0 3573 3464	8 1576 1543	1 1128 1266	4 4557 4416	12, 10, L
6 1358 1393	1 2814 2645	11, 2, L	2 2727 2610	5 6304 6429	1 1200 1113
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	3 3238 3322		4 2959 2926		
	4 2989 3240		5 1898 2271		

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1 1794 1936
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6 1084 801
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5 2092 1995
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9 2789 2756
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7 1981 1959
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9 1952 2090
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3 2088 1923
4 2323 2120
6 2636 3011
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9 2370 2571
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13 3191 3078

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3 3856 3777
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3 1782 1413
4 1715 1510
7 1707 1582
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6 2709 2492
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6 2295 2525
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6 3466 3533
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4 3004 3022
6 3314 3281
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3 3951 3885
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3 2637 2606
4 2750 2389
16, 5, L
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3 3295 3302
4 2459 2641
5 3548 3584
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5 1736 2061
6 2308 2008
16, 7, L
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3 2826 2890
5 2487 2424
7 2072 1830
16, 8, L
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4 2187 1848
6 1899 2117
8 2549 2816
16, 9, L
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3 1995 2208
5 1699 1933
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7 1706 1812
9 1966 2009
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8 1734 2182
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10 2128 2061
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1 2244 2458
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4 2538 2587
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7 1806 1875
8 3113 3118
9 1928 1902
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11 1966 1929
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9 1929 1785
10 1620 1337
11 1573 1876
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8 3452 3396
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13 1880 2032
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0 2379 2058
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2 2250 2097
4 3203 3026
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8 2799 3010
9 1622 1430
10 2340 2400
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13 2031 2031
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8 1627 1761
14 1915 2104
16 2388 2543
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3 2041 2285
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3 2287 2117
5 1781 1659
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3 3917 3658
5 2140 1855
17, 8, L
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3 2003 1931
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1 4884 5123
3 4301 4178
5 3158 2992
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7 1511 1554
8 1352 1243
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3 1702 1821
4 1378 1667
7 1565 1513
9 1783 1780
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5 2878 2888
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4 2015 1951
6 2535 2365
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8 1854 1805
9 2015 1829
17, 13, L
1 3458 3462
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3 2935 2761
4 2540 2798
5 2124 2036
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4 2256 2315
6 2613 2480
8 1845 2070
9 1473 1503
17, 15, L
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4 3197 3217
6 3464 3201
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4 1963 1996
6 1999 2012
8 1794 1699
17, 17, L
0 1861 1510
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4 2967 2944
6 3075 3117
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2 2369 2506
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2 2438 2655
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2 3823 3734
4 2848 2563
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2 1362 1737
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18, 8, L
6 2100 2130
8 2161 2647
18, 9, L
7 1721 1642
8 2335 2267
18, 10, L
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9 2695 2472
10 2676 2479
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4 2467 2461
6 3216 3179
8 3556 3563
10 3265 3115
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7 1375 1319
9 1928 2109
10 1998 2161
11 2014 2304
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6 3337 3195
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10 3012 3082
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8 1574 1728
14 1807 1646
18, 15, L
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2 2837 2429
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6 2367 2611
8 2709 2604
10 2297 2298
12 1940 1825
18, 16, L
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14 2038 2113
16 3492 3723

18, 18, L
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2 1967 2024
14 2895 2983
16 3411 3460
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3 2906 2851
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1 1717 2698
3 1743 1925
19, 6, L
1 2717 2934
3 2364 2416
5 2255 1925
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1 3703 3912
3 3278 3321
5 1892 1990
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1 4845 5190
3 4116 4298
5 3298 2985
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3 1943 2092
4 2042 1742
6 1775 1868
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1 2450 2249
3 1591 1703
4 2193 2189
6 2106 2296
19, 13, L
1 3696 3614
3 2726 2702
19, 14, L
13 1373 800
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2 1846 1767
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6 2274 2621
19, 17, L
4 2728 2546
6 2763 2818
19, 19, L
2 1444 1441
4 2764 2333
6 2797 2827
8 2590 2644
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2 3262 3364
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0 3383 3420
1 2004 2360
2 1936 2366
3 2212 2315
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2 1820 1895
4 2739 2797
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0 3123 3231
2 2547 2681
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2 1535 1824
6 2121 2164
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6 1865 1491
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9 2369 2274
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12 1957 1614
20, 13, L
0 2140 1907
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12 1949 2144
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10 1356 1425
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2 2006 1723
4 1432 1761
6 2169 2055
8 1997 2161
10 1583 2018
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16 2810 2921
20, 18, L
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14 2194 2215
16 3572 3472
18 3208 3294
20, 20, L
14 2249 2174
16 2682 2656
18 3019 3066
20 2558 2642
21, 6, L
3 1659 1871
21, 7, L
1 3080 3580
3 2456 2645
21, 8, L
3 1372 2017
21, 9, L
1 4657 4654
3 3687 3708
5 2266 2226
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1 1758 2451
6 1692 1647
21, 11, L
1 4249 4172
3 3188 3235
21, 12, L
4 1851 1778
21, 13, L
1 2374 2443
21, 15, L
2 1589 1610
4 2098 2126
6 1997 1876
21, 16, L
0 1795 1810
21, 17, L
4 2360 2350
8 1545 1649
21, 18, L
2 1738 1582
21, 19, L
4 2388 2111
6 2530 2636
21, 20, L
11 1491 751
21, 21, L
6 2547 2515
8 1789 2115
22, 1, L
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22, 3, L
0 2461 2632
1 3221 3239
2 1634 2012
3 3133 3180
22, 5, L
0 3016 3059
2 2390 2507
22, 7, L
4 1561 1780
22, 8, L
8 2314 1908
22, 9, L
8 1788 1547
22, 10, L
2 1550 1404
8 1820 1784
22, 11, L
8 2347 2398
10 2417 2273
11 1504 1657
22, 12, L
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10 2520 2366
12 1842 1752
22, 13, L
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10 2177 2095
11 1566 1578
22, 14, L
2 1497 1838
22, 15, L
4 1645 1596
22, 16, L
0 2307 2269
16 2843 2429
22, 18, L
16 2299 2168
18 2293 2658
22, 20, L
20 2338 1994
23, 7, L
1 1984 3013
23, 9, L
1 2600 3014
3 2663 2561
23, 11, L
1 1707 2032
3 1667 1784
10 1635 1839

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11 1546 1615
23, 13, L
8 2091 1967
23, 14, L
4 1500 1430
6 1955 1677
8 1654 1663
23, 16, L
10 1632 1334
23, 17, L
5 1630 1051
23, 18, L
6 1736 1816
23, 19, L
6 2148 1938
23, 20, L
4 2245 2031
23, 21, L
4 1726 1541
6 2368 1909
23, 22, L
2 1519 1445
23, 23, L
6 1724 1522
24, 1, L
1 3158 2934
24, 3, L
0 2838 2551
1 2634 2809
3 2403 2640
24, 4, L
3 1634 2031
24, 5, L
0 3045 3029
2 2621 2701

24, 6, L
3 1996 2291
5 1715 2079
24, 7, L
2 1877 2275
4 2125 2173
24, 8, L
0 1565 1673
5 1658 1525
24, 10, L
2 1579 1523
24, 12, L
0 2150 2042
2 2201 1940
12 1989 2020
24, 13, L
11 1843 1635
13 1725 1925
24, 14, L
0 2088 2377
24, 15, L
4 1453 1318
25, 9, L
6 1675 1724
8 1508 1722
25, 13, L
10 1620 1551
25, 19, L
1 1894 1872
7 1520 1173
25, 21, L
5 1696 1237
26, 1, L
1 1730 1980
26, 3, L
0 1859 2002

26, 4, L
3 1874 2017
26, 5, L
0 2216 2442
2 2128 2496
4 2253 2335
26, 6, L
1 1474 1817
3 1807 2049
5 2218 2013
26, 7, L
0 2035 1918
2 1873 2060
26, 13, L
11 1826 1745
27, 8, L
7 1585 1430
27, 9, L
6 1677 1569
27, 10, L
9 1733 1657
27, 17, L
1 2523 2293
5 1770 1590
27, 19, L
1 2346 2262
28, 3, L
0 1460 1705
28, 9, L
7 1547 1473
28, 11, L
11 1918 1870
29, 8, L
0 1951 1790
29, 10, L
0 1956 1771

29, 19, L
1 1744 2036
3 1748 1698
30, 9, L
5 1509 1297
31, 7, L
0 1525 1853
31, 8, L
2 1713 1511
4 1767 1141
31, 10, L
2 1562 1656
33, 12, L
0 1701 1579
34, 0, L
0 1614 1234

CALCULATED AND OBSERVED STRUCTURE FACTORS OF $[Pt_3(SnF_3)_2(dppm)_3]$

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4	762	752
5	676	652
6	1742	1766
8	2828	2881
10	2338	2326
11	1135	1238
12	2011	2124
14	1602	1638
16	989	1035
21	719	741
22	784	839
0, 1, L		
-23	748	854
-22	1250	1226
-20	704	630
-17	573	563
-15	1012	1086
-14	999	979
-13	1698	1721
-12	1410	1493
-11	1866	1963
-10	2003	2104
-9	2220	2280
-8	1470	1529
-7	2443	2414
-6	1039	1052
-5	1088	1071
-4	1045	924
-3	1802	1735
-2	1199	1110
2	2637	2886
3	2110	2404
4	1254	1308
6	396	386
7	1382	1438
8	1513	1628
9	1563	1637
10	1192	1334
11	1381	1541
13	1440	1507
15	1115	1120
17	660	677
23	726	707
0, 2, L		
-21	1156	1177
-19	716	644
-15	955	1034
-14	510	524
-13	1679	1654
-12	1251	1276
-11	2181	2292
-10	1655	1691
-9	2954	2956
-8	1077	1114
-7	1765	1718
-6	651	654
-5	971	854
-4	1791	1587
-3	2521	2222
-2	2005	1833
-1	2886	2766
0	1843	1820
1	2781	2632
2	672	677
3	1529	1638
4	945	971
5	1512	1567
6	376	478
7	1788	1873
9	1927	1970
11	842	801
14	733	738
16	947	965
18	977	1018
20	481	499
0, 3, L		
-22	1267	1288
-21	594	647
-20	902	926
-18	498	586
-14	523	517
-12	1765	1762
-11	677	695
-10	2885	2895
-9	868	862
-8	2625	2519
-6	1020	989
-5	408	379
-4	294	210
-3	1986	1796
-2	2664	2589
-1	419	246
0	2663	2788
2	1039	1174
3	1261	1327
4	1509	1640
5	1277	1407
6	915	961
7	2172	2246
8	690	694
9	1365	1447
11	1029	1098
12	668	668
14	516	514
15	433	557
17	1475	1492
19	1128	1082
21	759	731
0, 4, L		
-22	1013	1014
-21	438	463
-20	616	654
-19	533	524
-17	869	837
-16	673	658
-15	700	724
-14	967	963
-12	1051	1016
-11	894	887
-9	2540	2406
-7	2592	2445
-6	1595	1406
-5	2047	1891
-4	2475	2349
-3	1754	1665
-2	2267	2328
-1	1970	2005
0	3688	3621
2	1077	1046
3	604	578
4	2068	2162
5	1315	1432
6	2720	2993
8	1533	1720
9	1720	1785
10	925	997
11	1186	1310
12	471	519
13	1656	1718
14	542	613
15	611	624
16	776	895
18	1234	1187
20	928	933
22	907	811
0, 5, L		
-18	948	950
-16	1954	1933
-15	541	597
-14	1744	1709
-13	1199	1125
-12	1651	1656
-11	429	455
-8	2112	2025
-7	585	560
-6	2486	2350
-5	2142	1988
-4	1638	1520
-3	2905	2806
-2	1170	1135
-1	1965	2021
0	2031	2025
1	1323	1263
2	1933	1877
3	931	945
5	2694	2731
6	609	675
7	2391	2629
8	1638	1795
9	1073	1142
10	2633	2820
12	2253	2311
13	608	599
14	1286	1310
15	524	569
20	827	833
0, 6, L		
-20	390	318
-19	1008	936
-17	1814	1861
-15	2444	2447
-13	2405	2352
-11	1627	1648
-10	502	564
-7	1348	1302
-6	514	449
-5	2472	2398
-4	1109	998
-3	2797	2784
-1	2541	2526
0	409	445
1	2751	2704
2	1528	1567
3	1249	1300
4	2445	2432
5	1479	1422
6	2539	2528
7	2366	2421
8	1218	1225
9	2694	2810
10	442	528
11	2122	2328
12	975	1030
13	1441	1415
14	793	835
15	600	583
16	543	597
21	593	653
0, 7, L		
-20	537	520
-18	1392	1363
-17	795	823
-16	1829	1786
-15	1218	1254
-14	1934	1892
-13	1222	1227
-12	1528	1516
-11	1004	1024
-10	627	629
-9	399	365
-8	689	644
-6	2261	2270
-5	422	408
-4	2248	2335
-2	1525	1587
-1	813	864
0	2222	2183

0, 7, L		
1	1645	1607
2	1608	1582
3	2378	2411
4	1100	1108
5	1763	1689
6	1701	1634
8	1946	1831
9	746	842
10	1500	1492
11	1232	1240
12	911	861
13	1017	1017
18	584	542
0, 8, L		
-19	625	606
-18	847	845
-17	891	835
-16	1398	1376
-15	977	958
-14	1515	1500
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13	901	780
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6	1353	1263
8	2430	2376
9	519	438
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11	935	949
12	1013	991
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14	701	766
15	671	611
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-11	900	930
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-7	508	396
-6	976	971
-5	991	986
-4	623	598
-3	2312	2186
-2	1446	1355
-1	2733	2713
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2	2339	2244
3	955	1024
4	1504	1490
5	1156	1028
6	501	475
7	2658	2636
8	1743	1625
9	2467	2372
10	2361	2144
11	1024	1038
12	1585	1427
13	506	546
14	1132	1023
16	847	800
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19	431	461
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-15	2231	2201
-13	2718	2613
-11	2365	2332
-9	1922	1993
-6	722	722
-5	946	1058
-3	1999	2011
-2	1356	1434
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3, -2, L			13 763 827			16 820 757			3, 2, L			-9 726 785			2 1074 1175		
18 1879	1785		14 1650	1519		19 1267	1203		-19 385	545		-8 387	434		3 1129	1206	
19 889	933		15 735	795		21 1266	1212		-18 568	626		-7 1149	1213		4 2131	2270	
20 1670	1589		17 921	880		23 832	847		-17 1459	1481		-6 1026	1000		5 1944	1964	
21 1144	1130		18 896	962		3, 1, L			-16 1191	1275		-4 595	592		6 1989	2174	
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-1 875	846		2 514	537		3 2104	2165		15 924	1013		-16 600	601		-15 562	609	
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3 3913	3810		6 3311	3180		10 2119	1931		20 842	827		-10 445	284		-9 473	462	
4 842	605		7 1954	1748		11 1174	1235		21 951	938		-9 1237	1348		-8 2103	2148	
5 2619	2419		8 1651	1557		12 1626	1582		23 659	626		-8 602	632		-7 906	966	
6 880	703		9 2954	2736		13 1325	1380		3, 3, L			-7 2020	2049		-6 2185	2214	
7 2939	2640		10 640	673		14 979	1009		-17 1108	1051		-5 1282	1393		-5 1742	1814	
8 1798	1531		11 3139	2985		15 631	649		-15 1724	1823		-4 1012	1038		-4 324	350	
9 1658	1412		12 901	872		17 379	305		-14 855	945		-2 2097	2064		-3 2383	2424	
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3, 5, L		
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2	1962	2062
3	2456	2516
4	615	530
5	2449	2549
6	1010	1103
7	2480	2458
9	2079	2228
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11	1954	2050
12	797	820
13	685	751
16	1208	1301
17	1451	1481
18	1158	1221
19	1817	1905
20	896	976
21	1420	1428
3, 6, L		
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-16	1216	1278
-14	1106	1190
-13	586	573
-12	484	509
-11	1235	1326
-10	636	696
-9	1420	1407
-8	1836	1894
-7	837	795
-6	2591	2631
-5	740	706
-4	2698	2785
-3	1822	1853
-2	2570	2612
-1	2013	2003
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1	1790	1821
2	1086	1093
3	640	614
4	2015	2092
6	2204	2258
7	703	711
8	2548	2777
10	2061	2251
12	1688	1623
14	477	429
16	867	943
18	1876	1955
20	1741	1846
22	1197	1110
3, 7, L		
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-16	402	492
-15	844	870
-14	602	671
-13	593	575
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-11	513	588
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-6	1346	1363
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-2	2874	2751
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2	604	572
4	777	678
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7	1210	1200
8	1053	1013
9	1250	1345
11	1713	1712
16	631	501
17	808	742
19	1031	1075
20	790	724
21	923	960
3, 8, L		
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4	1469	1398
5	1258	1286
7	901	929
10	975	1021
12	802	937
14	1006	908
15	655	624
19	714	725
3, 9, L		
-16	580	618
-14	804	853
-12	837	881
-10	484	492
-5	832	788
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-3	658	645
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1	1973	2029
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7	922	879
8	543	463
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11	1226	1285
13	1482	1423
15	1699	1711
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3, 10, L		
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2	2598	2492
3	1742	1578
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6	1508	1491
7	1270	1294
11	1085	1071
12	1111	1050
13	1156	1041
14	1896	1691
16	1730	1691
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3, 11, L		
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-8	1671	1773
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-6	1513	1536
-5	1041	951
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-2	710	661
1	1699	1659
2	1863	1775
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4	2764	2556
5	1375	1315
6	2260	2185
8	1005	963
9	784	766
12	741	850
13	916	874
14	1257	1248
15	1081	1078
16	1265	1108
17	1290	1193
18	1003	1030
3, 12, L		
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-5	2199	2304
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3	2392	2429
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7	1553	1454
13	867	738
15	1025	1061
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3, 13, L		
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2	1875	1870
3	1119	935
4	1897	1940
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6	1094	1191
7	794	618
8	817	861
3, 14, L		
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-6	1025	1060
-5	827	890
-4	976	1039
-3	665	665
-2	656	722
2	1089	1142
3	616	649
4	1352	1372
6	806	737
9	632	644
3, 15, L		
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-2	505	475
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3, 15, L			12	1176	1278	-1	531	450	-7	1533	1606	-2	1386	1356	9	555	563
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3, 16, L			-12	798	688	7	980	1021	-4	1917	1925	3	1128	1134	14	930	888
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6	704	727	1	1130	1181	4, -8, L			1	579	620	10	1190	1175	4, -4, L		
4,-14, L			2	584	480	-14	1157	1031	2	1194	1192	11	2958	2633	-17	680	579
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4,-12, L			8	973	891	14	620	641	-17	1086	1058	-5	1478	1560	3	2973	2894
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4, -4, L			-12	580	596	-9	773	736	-6	4558	4680	-2	1795	1870	3	812	804		
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4, -2, L			-14	841	780	-12	1897	1869	-6	1011	944	-1	711	759	5	2271	2334		
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4, 3, L			12 900 1070			10 1358 1370			21 1314 1434			-2 1512 1554			5 1794 1832		
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-18 667 694			4, 5, L			-15 656 673			-5 1170 1246			21 600 578			4, 11, L		
-16 558 628			-19 522 576			-14 377 410			-4 1885 1950			4, 9, L			-13 458 473		
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-13 1556 1580			-17 641 656			-11 1236 1288			-2 711 722			-8 390 487			-11 1032 1108		
-12 1070 1091			-16 696 718			-10 546 621			-1 2200 2183			-6 745 695			-9 1436 1520		
-11 760 840			-15 460 522			-9 1761 1855			0 821 779			-5 783 816			-7 1289 1434		
-10 1407 1452			-14 360 399			-8 1066 1022			1 934 907			-3 590 681			-5 656 761		
-8 1303 1430			-12 1301 1339			-7 2343 2439			2 1652 1606			0 873 852			-3 467 539		
-7 1337 1279			-11 852 880			-6 1057 1040			3 597 606			2 1547 1424			-1 542 541		
-6 2185 2338			-10 1021 1049			-5 2610 2658			4 1478 1535			4 1921 1998			0 902 903		
-5 1221 1283			-9 1578 1509			-3 2449 2496			5 1023 1064			6 1473 1415			1 666 605		
-4 583 677			-8 1078 1085			-2 2190 2190			6 675 647			8 891 985			2 1291 1270		
-3 673 742			-7 2101 2193			-1 794 716			7 1114 1160			10 672 627			3 2236 2072		
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-1 1345 1304			-5 2224 2262			1 948 934			14 785 692			14 2327 2417			5 2923 2776		
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2 3716 3896			-1 1906 2049			4 920 1000			20 1026 1010			4, 10, L			12 795 869		
3 2117 2046			0 319 332			5 2524 2666			22 988 977			-13 543 552			13 1833 1875		
4 2024 2122			1 3139 3136			6 564 506			4, 8, L			-11 798 809			14 990 1065		
5 1860 1988			2 2338 2233			7 1358 1516			-16 424 447			-10 968 1000			15 1680 1639		
6 2235 2397			3 2187 2200			8 466 306			-11 459 508			-8 859 875			16 870 782		
7 1946 2101			4 3092 3225			9 1422 1488			-9 857 878			-1 641 590			17 1323 1213		
8 643 751			5 1499 1531			10 769 764			-7 1120 1149			1 1350 1309			4, 12, L		
9 1683 1690			6 2222 2312			11 872 915			-6 1101 1146			2 790 696			-12 851 925		
10 789 815			7 635 636			17 1245 1192			-5 857 946			3 2060 1989			-10 1347 1393		
11 603 530			8 1717 1797			19 1449 1400			-4 1403 1443			4 1948 1801			-8 1379 1496		

4, 12, L		
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4	2639	2481
5	702	419
6	2604	2478
7	1221	1005
8	1308	1236
9	609	532
12	1154	1104
14	1539	1572
16	1182	1059

4, 13, L		
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-9	898	895
-8	836	859
-7	987	1061
-6	672	787
-5	1195	1293
-4	654	638
-3	586	553
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2	699	544
3	1921	1777
4	1351	1208
5	1729	1665
6	1105	955
7	1368	1355
8	863	797
12	569	563

4, 14, L		
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-7	784	773
-6	462	509
-5	770	838
-3	530	604
-2	502	564
1	555	665
3	1343	1289
5	1156	1118
8	585	736
11	853	860
12	685	422
13	960	855

4, 15, L		
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-1	606	610
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3	837	779
9	1161	1147
11	1423	1402
12	696	559

4, 16, L		
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2	896	948
3	630	559
4	881	823

5,-13, L		
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-3	1326	1231
-2	1520	1484
-1	1042	1010
0	793	773
2	560	556
7	852	1015

5,-12, L		
-6	528	473
-5	1403	1425
-3	1858	1814
-2	566	406
-1	1619	1656
1	865	860
3	534	586
9	691	813
10	587	695
11	1140	1267

5,-11, L		
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-11	670	735
-6	765	824
-4	1115	1212
-2	1161	1193
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10	666	780
12	759	750

5,-10, L		
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-13	1211	1132
-12	1054	1135
-11	920	850
-10	573	558
-4	548	629
3	470	467
5	939	1046
6	473	415

5, -9, L		
-15	1058	968
-13	1390	1292
-11	707	797
-8	967	1042
-7	575	547
-6	897	995
-4	683	733
-1	681	656
2	591	600
4	1021	1066
6	1299	1253
8	1243	1213
10	852	857
12	562	563
16	797	775

5, -8, L		
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-13	785	628
-9	1276	1277
-7	1843	1896
-5	2040	2051
-3	1326	1393
-2	1002	1037
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3	1226	1155
5	1186	1235
6	848	780
7	1081	1056
8	906	757
9	1406	1379
10	835	762
11	1103	1078
12	1184	1164
13	532	550
14	906	885
15	374	370
17	1084	1024

5, -7, L		
-17	731	729
-16	1138	981
-14	1189	1134
-13	777	697
-10	532	578
-8	1704	1759
-6	1993	2120
-5	1031	1031
-4	1620	1671
-3	1973	2007
-2	878	920
-1	2010	1989
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3	1141	1232
4	1365	1357
5	1003	932
6	776	848
7	1010	897
8	939	958
9	1078	1024
10	811	898
11	1663	1517
12	996	920
13	1905	1804
15	893	854
16	617	603
18	676	674
19	1096	1025

5, -6, L		
-18	1310	1248
-17	589	586
-16	1476	1318
-14	1297	1250
-12	1158	1073
-11	572	535
-9	1706	1667
-8	937	959
-7	1339	1360
-6	1456	1486
-5	687	748
-4	2036	2072
-2	2694	2722
-1	979	907
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1	1521	1574
3	1221	1298
4	1101	1045
6	1482	1343
8	1256	1104
10	1287	1136
12	1825	1640
14	1686	1490
18	669	620
20	1145	1079

5, -5, L		
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-15	1429	1332
-13	1401	1352
-12	878	870
-11	742	708
-10	1646	1626
-9	987	984
-8	889	884
-7	1334	1333
-5	1275	1345
-4	1209	1173
-3	1316	1392
-2	2160	2060
-1	1593	1543
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1	930	905
2	607	646
5	528	504
6	1078	926
7	696	588
8	587	527
9	934	717
11	1141	1011
13	1298	1251
15	737	639

5, -5, L		
18	896	826
19	383	317
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5, -4, L		
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-13	667	444
-12	839	888
-11	934	938
-9	846	748
-8	947	1006
-5	811	880
-3	1541	1549
-2	551	522
-1	1381	1392
2	1526	1541
4	2586	2381
6	1663	1507
7	734	673
8	1547	1304
9	581	341
12	954	802
14	1062	863
15	555	499
16	989	918
17	929	887
18	834	805
19	1162	1101
20	585	577
21	655	637
5, -3, L		
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-11	512	516
-10	862	797
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-3	1205	1261
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2	450	460
3	2867	2775
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5	4046	3697
6	1020	896
7	3484	2952
8	719	700
9	1442	1267
12	654	676
13	683	621
15	1718	1611
17	2358	2286
18	613	589
19	1804	1779
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5, -2, L		
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-7	956	940
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3	399	439
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5	2227	2347
6	2808	2709
7	3216	2907
8	2499	2112
9	1192	1156
10	921	711
13	860	818
14	862	877
15	853	785
16	2314	2227
17	692	726
18	2617	2386
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22	555	638
5, -1, L		
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-6	2558	2512
-5	1764	1757
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4	2055	2030
5	2095	1989
6	2881	2863
7	1550	1427
8	3031	2914
9	1648	1507
10	1269	1263
11	636	689
14	691	709
15	1039	950
16	1277	1311
17	1676	1573
18	1446	1408
19	1733	1657
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21	1093	1048
22	825	803
5, 0, L		
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-17	1219	1220
-16	805	862
-15	1101	1104
-14	941	925
-13	922	864
-12	839	799
-11	419	398
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-7	2929	2863
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5	3535	3664
6	963	938
7	3111	3330
8	549	453
9	2156	2006
10	499	432
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12	532	401
14	450	451
15	515	433
16	390	349
17	1028	1031
18	1065	1008
19	1328	1350
20	690	613
21	914	892
23	541	530
5, 1, L		
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-14	427	448
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3	1581	1654
4	1827	1875
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6	2432	2428
7	1573	1540
8	1606	1532
10	1340	1318
11	718	677
13	957	1006
15	507	475
16	690	677
18	799	733
21	401	271
5, 2, L		
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-7	753	760
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2	1646	1668
3	588	584
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5	912	833
6	2041	2174
8	733	859
9	1308	1385
10	1265	1235
11	2186	2178
12	2156	2118
13	1869	1775
14	1195	1201
15	710	692
16	741	679
5, 3, L		
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-17	556	659
-15	594	591
-14	433	483
-13	798	898
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5, 3, L			-5	1166	1219	0	2339	2344	9	1131	1099	-1	543	573	-2	1152	1200
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9	1191	1189	17	779	662	-12	1621	1626	2	646	758	1	1241	1277	-12	1133	1256
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5, 4, L			-10	660	632	-1	1445	1330	21	605	595	16	831	872	2	1022	966
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5, 11, L		
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5, 12, L		
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-7	812	924
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7	1815	1804
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9	776	723
10	740	576
13	1451	1436
15	1388	1379
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5, 13, L		
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6	1610	1454
7	1121	1014
8	1274	1196
9	911	736
12	697	615
13	941	800
15	825	794
5, 14, L		
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6	611	553
12	622	703
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5, 15, L		
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5, 16, L		
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6, -9, L		
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4	662	678
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13	468	570
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6, -8, L		
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-8	1345	1396
-6	1830	1924
-4	2098	2166
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6	1784	1809
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14	699	636
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6, -7, L		
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3	1782	1852
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12	1110	1002
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15	604	565
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6, -6, L		
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-8	852	805
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-3	2370	2390
-1	1555	1513
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3	1568	1591
4	963	1042
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6	670	680
7	1155	1098
9	745	695
11	1291	1079
13	1020	862
19	707	638
6, -5, L		
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-14	888	818
-8	1007	1032
-7	410	223
-6	1774	1687
-4	2375	2373
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-2	1767	1750
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2	1262	1223
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6	971	845
12	540	483
15	503	431
16	504	435
17	575	479
19	446	405
6, -4, L		
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-15	982	914
-13	861	767
-8	396	417
-7	830	797
-6	726	779
-5	1318	1301
-4	678	691
-3	1384	1383
-2	717	671
-1	471	440
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4	1068	1132
5	947	926
6	607	561
7	1196	1060
9	1069	998
10	572	486
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13	1232	1126
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6, -4, L			-1 322 280			1 1578 1528			6 3380 3388			12 1143 1202			6, 3, L		
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6, -3, L			4	1131	1101	6	632	533	13	803	689	23	686	663	-8	750	757
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6, 4, L		
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2	2323	2404
3	618	606
4	3011	3086
5	761	793
6	2788	2885
7	1202	1141
8	901	916
9	1340	1486
10	2050	2171
12	3232	3363
13	722	849
14	2949	3104
15	940	989
16	1428	1530
17	683	672
18	679	661
19	505	455
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6, 5, L		
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-13	1046	1008
-12	1147	1228
-11	827	896
-10	1912	2004
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-8	2137	2218
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-2	783	765
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2	1404	1409
3	2456	2532
4	1707	1683
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6	2289	2345
7	1065	1083
8	1814	1889
9	585	516
11	2049	2158
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13	1843	1910
14	1806	1850
15	997	1044
16	1394	1409
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6, 6, L		
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-16	776	779
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3	2700	2697
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5	2923	3036
6	801	868
7	1699	1819
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6, 7, L		
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6, 8, L		
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6, 9, L		
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6, 10, L		
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13	1891	1953
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16	1175	1164
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6, 11, L		
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8	776	697
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12	1261	1235
13	1289	1267
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15	1400	1399
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6, 12, L		
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7	767	728
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12	817	802
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6, 13, L		
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3	866	810
5	957	833
7	659	782
6, 14, L		
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-1	701	745
6	733	729
6, 15, L		
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7, -1, L

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7, 0, L

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9	1395	1429
10	901	924
11	512	508
12	846	820
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15	1079	1063
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7, 1, L

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22	815	828

7, 2, L

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2	546	571
3	371	350
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7	691	635
9	767	725
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12	936	937
13	1031	1081
14	1259	1328
15	1384	1416
16	866	896
17	1642	1663
21	795	788
22	670	626

7, 3, L

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3	408	455
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9	672	654
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11	562	546
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13	577	620
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19	901	881
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7, 4, L

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3	1575	1684
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6	758	757
7	804	876
8	515	514
9	612	636
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18	759	844
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7, 5, L

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-7	2347	2273
-6	985	997
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12	973	972
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17	1451	1506
18	573	616

7, 6, L

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-2	1045	1019
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4	1963	1983
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6	1966	1996
8	1130	1245
12	1135	1186
14	1887	1984
16	1984	2019
18	939	1046

7, 7, L

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12	485	428
13	850	908
15	1468	1396
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7, 8, L

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7, 8, L		
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13	801	844
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7, 9, L		
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1	1775	1761
5	676	659
7	1388	1366
9	2261	2236
11	2034	2004
13	1394	1378
15	535	478
18	587	664
19	610	552
20	1104	1104

7, 10, L		
-12	606	686
-10	861	867
-8	760	762
-4	1468	1458
-3	519	405
-2	2291	2271
-1	1351	1150
0	1941	1816
1	1523	1470
2	1174	1201
3	1071	923
6	866	853
8	1971	1980
10	2098	2119
11	873	747
12	1774	1853
13	744	685
14	1197	1243
18	579	484

7, 11, L		
-11	842	886
-10	1084	1111
-8	732	832
-5	479	545
-4	709	792
-3	1465	1560
-2	1640	1522
-1	1280	1274
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1	756	675
2	2145	1961
4	921	843
7	860	823
8	1195	1071
9	1003	1054
10	1282	1143
11	1099	1226

12	872	814
13	1179	1105
14	986	900
15	682	733

7, 12, L		
-9	1328	1369
-7	646	745
-3	1576	1620
-2	651	661
-1	2158	2063
1	2008	1952
3	1323	1263
9	594	569
11	841	714
13	912	776
15	736	778

7, 13, L		
-8	864	980
-7	505	482
-6	419	22
-4	1111	1175
-2	1455	1475
-1	641	568
0	1445	1429
1	489	432
2	907	936

7, 14, L		
-4	506	488
-2	1109	1139
0	1062	965
4	792	672
5	892	690
6	828	803
7	806	676

7, 15, L		
-2	865	893
0	691	630
5	672	641

6	1319	1166
8	1220	1103
10	767	740

8,-11, L		
-3	658	687
6	596	643

8,-10, L		
0	584	575
2	525	576
3	644	572
5	775	843
6	629	528
7	860	929

8, -9, L		
-9	791	762
-7	695	720
1	617	553
3	1224	1281
5	1737	1863
7	1414	1482
11	557	539
12	679	565

8, -8, L		
-10	872	893
-9	529	491
-8	934	872
-5	810	783
2	1056	1046
4	1757	1874
5	677	648
6	1808	1930
7	847	841
8	1345	1351
9	1055	1056
12	1100	997
14	1466	1366

8, -7, L		
-10	847	815
-9	680	643
-8	1112	1144
-6	1225	1304
-5	482	458
-4	1145	1210
-2	522	560
1	863	886
2	730	725
3	1344	1324
4	1062	1108
5	1670	1778
6	1445	1482
7	1453	1507
8	1481	1441
9	587	569
10	891	921
13	717	626
14	1024	879
16	1039	955

8, -6, L		
-12	746	682
-9	1441	1507
-7	1763	1729
-5	1959	1954
-3	1346	1337
1	576	532
2	500	551
3	1450	1413
4	639	750
5	1561	1572
6	797	852
7	1861	1783
9	1308	1342
13	726	657
15	1195	1071
17	775	669

8, -5, L		
-13	710	639
-10	702	603
-9	1065	1134
-8	689	732
-7	1359	1296
-6	1357	1379
-5	741	707
-4	1796	1829
-2	1377	1320
0	577	617
2	520	488
4	1393	1355
6	1207	1211
8	1511	1442
10	447	412
11	697	561
13	866	841
15	966	851
17	453	469

8, -4, L		
-14	963	870
-10	826	879
-9	725	720
-8	1109	1089
-7	799	764
-6	1021	962
-5	681	669
-3	1702	1659
-1	2044	1917
0	690	681
1	1487	1467
2	1012	959
3	506	496
4	1198	1189
6	831	805
7	508	557
10	993	964

H, -4, L		
11	534	433
12	1635	1456
13	873	828
14	1586	1464
15	902	917
16	818	713
17	629	697

H, -3, L		
-15	657	656
-12	895	839
-10	1476	1412
-8	1650	1613
-4	915	893
-2	1836	1697
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2	2044	2057
4	1147	1182
5	410	467
6	751	842
7	425	443
10	841	813
11	1475	1323
12	1515	1447
13	1428	1297
14	2326	2128
16	2055	1763
18	687	638
19	882	865

H, -2, L		
-13	1021	924
-11	2014	1991
-10	878	912
-9	2340	2307
-8	858	902
-7	1011	992
-3	1412	1373
-1	2102	2015
0	864	872
1	2297	2229
2	887	830
3	1944	1993
4	752	771
5	1127	1167
7	480	435
9	325	227
11	1626	1604
12	766	668
13	2437	2445
15	2331	2242
16	1164	1116
17	1189	1101
18	989	1038
20	692	678

H, -1, L		
-16	626	572
-14	585	474
-13	753	685
-12	1658	1618
-11	1572	1575
-10	2060	2126
-9	2624	2566
-8	1634	1671
-7	1724	1715
-6	507	478
-4	510	450
-3	590	565
-2	1389	1356
-1	1014	966
0	1346	1254
1	1311	1282
2	1658	1586
3	1618	1675
4	1581	1556
5	1076	1086
6	911	928
7	451	466
9	787	732
10	643	607
12	1748	1766
13	449	528
14	1700	1695
15	1055	1105
16	1021	1017
17	1297	1201
19	599	629

H, 0, L		
-16	1028	981
-13	680	748
-12	1838	1806
-11	747	793
-10	3115	3129
-9	915	916
-8	3229	3170
-6	1195	1266
-2	1288	1249
-1	603	613
0	1790	1775
1	763	730
2	1674	1701
3	1174	1114
4	1622	1562
5	950	919
6	1287	1284
7	500	469
8	685	764
9	400	521
11	867	884
12	395	439
13	679	709
14	953	1022
16	1041	1097

H, 1, L		
-16	453	414
-15	495	435
-13	763	722
-11	1934	1965
-9	2324	2318
-8	1081	1113
-7	1257	1240
-6	572	546
-2	605	653
-1	924	936
0	654	696
1	1192	1138
3	1597	1625
4	537	395
5	1399	1446
6	435	429
7	1183	1220
9	529	563
16	776	717
22	734	669

H, 2, L		
-16	648	572
-12	708	708
-11	1166	1129
-10	842	768
-9	1154	1182
-7	663	684
-5	477	506
-3	1123	1091
-2	628	623
-1	1302	1311
0	700	687
1	935	910
2	455	415
5	1012	1024
6	1054	1105
7	677	710
8	1131	1172
9	592	605
10	813	828
13	636	628
14	656	670
16	1352	1360
18	792	838
21	687	704
22	849	859

H, 3, L		
-15	633	583
-13	680	606
-12	839	866
-10	1366	1339
-5	670	628
-4	832	764
-3	1423	1492
-2	889	831
-1	1781	1838
0	334	259
1	2041	2067
2	685	671
3	1502	1543
4	1660	1631
5	454	469
6	1324	1338
7	1150	1201
8	964	1079
9	1487	1516
11	1010	1039
13	1189	1328
15	1473	1594
17	1495	1536
18	851	845
20	685	604
21	1221	1181

H, 4, L		
-14	834	865
-12	1117	1061
-10	989	1043
-8	740	697
-7	987	981
-6	639	616
-5	623	586
-4	1696	1738
-2	2001	1959
-1	396	443
0	2024	1986
1	1754	1639
2	1311	1247
3	1848	1796
5	1781	1859
6	808	891
7	578	640
8	1154	1154
10	1174	1181
11	718	689
12	1110	1172
13	613	588
14	1492	1626
15	830	868
16	1474	1557
17	912	1002
19	532	597
20	626	553
22	1298	1222

H, 5, L		
-15	562	583
-13	1071	1006
-11	1356	1327
-10	940	953
-9	995	973
-8	1510	1508
-6	1003	1015

8, 5, L			9 608 741			3 546 557			8, 11, L			1 1504 1412			8 868 908		
-5	1859	1751	10	511	431	7	1095	1131	-9	533	510	2	557	471	10	604	632
-3	1973	2005	13	1385	1456	8	684	718	-4	934	933	3	1025	920	9, -7, L		
-2	964	971	15	1828	1868	9	1705	1608	-3	1276	1200	8	803	809	-10	1156	1197
-1	1847	1862	17	1499	1533	10	603	634	-2	1105	1090	10	695	600	-9	874	878
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2	2043	1976	-12	1287	1255	8, 9, L			1	2346	2236	-1	1024	954	-5	1147	1173
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4	1966	2030	-9	735	712	-2	1702	1640	6	563	576	6	557	556	-2	753	788
6	1100	1113	-8	1261	1324	0	1643	1539	7	1061	1020	7	1064	887	0	748	687
10	1006	1051	-7	854	801	2	1022	1000	8	763	731	9	939	820	1	603	607
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13	661	687	-5	1157	1164	8	2115	2210	10	985	977	5	1192	1090	3	788	788
14	1487	1484	-4	610	520	10	2461	2410	11	1397	1388	7	1326	1204	4	817	876
15	1013	1098	-2	1130	1135	12	1777	1759	12	987	1075	9, -10, L			5	1163	1207
16	1534	1575	-1	526	484	14	714	562	13	983	843	-1	467	523	6	1026	1036
17	771	762	0	1108	1219	19	579	586	14	656	711	0	523	388	7	1318	1306
18	738	799	1	936	922	20	949	1000	8, 12, L			1	601	541	8	676	754
22	581	573	2	579	628	8, 10, L			-8	666	736	9, -9, L			9	1216	1247
8, 6, L			3	851	828	-5	655	680	-5	438	477	-2	638	607	13	616	577
-13	1056	1049	6	596	519	-3	1616	1555	-4	842	850	0	832	845	9, -6, L		
-12	818	830	8	860	897	-2	951	896	-2	1762	1694	2	758	781	-11	569	593
-11	1436	1455	9	548	559	-1	1580	1541	-1	446	206	4	840	942	-10	1305	1334
-10	640	608	10	1175	1141	0	1529	1432	0	2259	2164	6	705	803	-8	1490	1495
-9	2017	1985	14	1191	1139	1	1155	1111	2	1847	1763	9	563	572	-6	1316	1337
-7	1675	1626	15	632	296	2	1369	1327	3	661	495	9, -8, L			-4	968	935
-6	1225	1221	16	1324	1380	4	564	619	4	766	635	-7	622	758	-3	611	605
-4	1539	1544	21	1109	1060	7	1646	1655	8	1188	1140	-6	713	704	-1	502	548
-3	1355	1344	8, 8, L			8	1491	1324	10	1206	1125	-4	657	617	0	421	421
-2	1201	1193	-11	569	572	9	1956	1993	12	773	769	-3	483	486	2	580	602
-1	1676	1692	-10	694	664	10	1347	1295	13	627	587	-1	836	875	4	803	867
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1	1709	1727	-8	723	773	12	895	899	8, 13, L			3	999	984	8	1490	1546
3	1257	1249	-2	796	745	13	1330	1383	-3	1105	1088	4	542	504	10	841	851
4	535	522	-1	443	427	19	956	899	-2	602	471	5	1224	1332	14	965	907
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7	726	731	2	870	774				0	763	539	7	855	992			

9, -5, L			-2	447	398	16	1619	1559	-3	493	418	14	422	499	-2	1870	1816
-11	853	831	-1	2195	2223	9, -1, L			-2	455	405	9, 2, L			-1	1035	993
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-7	898	943	3	1909	1901	-11	1147	1190	1	2526	2373	-9	709	649	2	1654	1591
-6	653	708	5	712	723	-10	1403	1430	3	2070	1939	-8	1206	1265	4	331	335
-5	560	715	6	343	336	-9	1373	1371	4	652	583	-7	938	874	5	1581	1625
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5	493	559	11	1885	1979	-4	692	692	11	389	407	-2	1544	1541	9	765	856
7	1308	1344	12	888	873	-3	879	879	12	733	763	-1	563	615	10	1499	1569
9	874	911	13	2032	1943	-2	496	517	13	730	782	0	2404	2327	11	753	744
12	788	679	14	868	796	-1	1359	1320	14	923	890	2	1603	1548	12	1247	1318
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16	828	749	17	768	726	1	1262	1234	16	614	690	4	480	485	15	503	541
9, -4, L			9, -2, L			2	2692	2673	17	610	681	5	881	876	16	648	689
-9	548	605	-12	869	851	3	753	677	9, 1, L			6	1489	1552	17	846	857
-7	690	685	-10	1261	1252	4	1829	1728	-12	1045	967	7	1311	1329	19	762	690
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-1	921	897	-8	1296	1301	7	527	591	-9	679	738	9	1048	1097	-13	956	980
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15	1095	943	4	1165	1196	18	412	413	3	564	567	-11	452	376	4	1389	1389
9, -3, L			5	746	802	9, 0, L			4	1402	1378	-10	465	439	5	1326	1386
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-9	742	792	7	691	619	-12	520	508	6	950	1044	-7	778	754	7	2003	2057
-7	837	822	10	1301	1381	-11	1710	1767	7	1243	1284	-6	848	731	9	1747	1834
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-4	588	551	14	2229	2242	-7	2153	2136	9	1013	1046	-4	1292	1349	11	1326	1494
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9, 4, L		
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15	679	674
16	765	754
18	601	681
21	895	909
9, 5, L		
-13	920	880
-12	980	945
-11	788	813
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-9	592	576
-8	525	466
-6	775	782
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3	1521	1450
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5	860	882
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9	1099	1095
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12	530	476
13	1012	992
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9, 6, L		
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2	1533	1563
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10	578	485
12	702	699
14	745	802
16	821	769
9, 7, L		
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-7	706	790
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15	632	554
17	776	793
19	649	622
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9, 8, L		
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-6	596	517
-1	678	721
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4	480	424
7	904	873
8	986	1043
9	462	444
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9, 9, L		
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-1	874	879
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4	687	590
5	670	784
6	778	979
7	1594	1570
9	2136	2143
10	467	486
11	1870	1914
12	740	818
13	914	949
14	781	685
19	865	859
9, 10, L		
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-6	703	698
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-2	944	922
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1	1084	1040
2	635	658
3	1149	1098
4	441	543
6	1364	1337
8	2101	2113
9	1420	1444
10	1870	1913
11	1638	1564
12	1138	1081
13	1085	1110
9, 11, L		
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-5	763	709
-4	627	668
-3	735	707
-2	1158	1002
-1	647	543
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2	1639	1539
4	938	902
5	837	724
7	1125	1113
8	1507	1432
9	1010	955
10	1929	1818
11	718	724
12	1298	1269
9, 12, L		
-3	848	827
-1	1590	1473
1	1708	1647
3	1117	1035
6	508	453
7	945	838
9	1357	1258
11	1115	1141
13	724	651
9, 13, L		
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-2	776	791
0	1210	1196
2	1087	995
4	581	557
9	1028	982
11	670	579
9, 14, L		
0	532	340
8	1159	1112
10	770	707
10, -9, L		
0	555	539
1	1147	1219
3	844	862
10, -8, L		
-4	577	600
-2	1372	1400
0	1411	1418
2	1066	1104
4	642	751
5	443	611
7	667	676
10, -7, L		
-7	843	862
-6	954	984
-3	1069	1129
-1	1402	1403
0	811	774
1	967	1018
2	819	805
3	615	631
6	846	873
8	731	774
10, -6, L		
-7	1476	1497
-5	921	924
-4	569	458
-2	892	929
-1	963	878
0	752	703
1	787	781
3	716	691
5	491	499
7	654	665
9	588	559
10, -5, L		
-8	1166	1163
-6	803	808
-2	645	696
1	452	439
3	433	328
8	592	632
10	438	447
11	643	617
13	589	554
10, -4, L		
-9	784	675
-2	695	728
0	1091	1055
1	988	982
2	724	735
3	976	1024
8	566	575
9	957	969
10	926	997
11	1310	1438
12	486	523
13	1026	1024
14	487	444
10, -3, L		
-3	715	674
-2	1183	1154
-1	533	531
0	1903	1887
2	1807	1827
4	1021	1037
7	530	574
8	946	1081
10	2005	2083
12	1955	1974
14	1304	1350
16	691	692

10, -2, L			12	958	968	-1	1414	1434	19	702	667	3	829	716	-4	527	488
-9	495	415	13	1016	1106	0	784	821	20	654	636	5	635	551	-3	1331	1312
-6	723	775	14	1196	1234	1	1711	1564	10, 3, L			6	1867	1899	-2	1081	1009
-4	867	941	15	538	662	2	639	554	-11	625	660	8	2189	2347	-1	1599	1548
-3	980	917	16	963	1044	3	1271	1305	-6	1078	1027	9	825	768	0	1365	1351
-1	2168	2029	18	535	619	5	883	866	-5	849	861	10	2109	2234	1	1639	1556
0	1060	1090	10, 0, L			6	613	565	-4	529	478	11	988	989	2	821	806
1	2082	1955	-12	954	942	8	1142	1211	-3	1649	1660	12	1503	1593	3	968	1019
2	1745	1740	-10	893	901	10	995	1020	-1	2319	2219	13	850	879	7	896	991
3	1233	1218	-8	1217	1201	12	711	785	0	630	555	16	414	389	8	445	383
4	1741	1699	-6	1225	1297	16	696	682	1	1884	1757	18	864	930	9	1466	1502
7	497	468	-5	383	492	17	640	643	3	715	687	20	909	1024	11	1063	1043
9	1242	1299	-4	673	678	18	715	723	4	826	840	10, 5, L			13	614	590
10	718	814	-3	946	920	19	569	570	5	1255	1339	-12	1377	1277	10, 7, L		
11	1817	1883	-2	868	875	10, 2, L			6	1084	1144	-10	826	788	-10	1250	1197
12	854	913	-1	866	828	-9	697	673	7	1998	2091	-6	605	692	-8	569	566
13	1695	1750	0	2276	2203	-8	610	598	8	769	813	-5	905	904	-7	664	570
14	560	596	2	2480	2406	-7	1003	967	9	1955	2221	-4	1097	1037	-4	869	847
15	1222	1246	4	1693	1620	-6	925	903	10	910	999	-3	1565	1506	-2	1358	1273
17	536	503	6	577	574	-5	573	645	11	1862	1917	-2	1274	1226	0	1808	1692
10, -1, L			7	371	443	-4	772	808	13	1129	1251	-1	2049	1990	2	988	854
-12	765	776	10	768	867	-3	854	861	14	469	553	0	1466	1425	8	544	575
-11	573	613	12	701	751	-2	806	751	16	650	633	1	1708	1611	9	627	631
-9	664	694	14	591	730	-1	1614	1653	17	865	854	2	1260	1156	15	558	721
-7	1010	1020	15	723	756	0	387	365	19	1065	1069	3	641	596	17	900	901
-5	1371	1406	16	565	692	1	1527	1463	10, 4, L			4	936	964	19	918	848
-3	538	531	17	935	976	3	526	604	-12	865	804	5	888	932	10, 8, L		
-2	1413	1426	18	466	473	5	847	796	-11	824	825	7	1215	1253	-9	860	850
-1	1338	1330	19	703	816	6	938	1041	-10	436	264	8	1294	1313	-8	514	428
0	1595	1510	10, 1, L			7	1360	1450	-6	954	868	9	1281	1409	-7	901	847
1	2454	2330	-11	658	635	8	939	1069	-5	928	932	10	1674	1703	-6	798	709
2	806	700	-9	946	987	9	1461	1582	-4	1339	1327	11	1028	1129	-5	478	593
3	2397	2404	-8	449	624	10	1117	1232	-3	603	582	12	1433	1500	-2	484	459
5	1127	1094	-7	987	959	11	1090	1240	-2	2250	2104	19	532	366	-1	798	796
7	344	381	-6	546	597	12	1079	1098	-1	580	500	10, 6, L			0	713	738
9	721	688	-5	650	666	14	503	446	0	2482	2486	-11	1537	1498	6	1040	1089
10	859	902	-3	566	467	17	875	863	1	1003	932	-9	800	762	7	457	424
11	1207	1312	-2	487	560	18	646	717	2	1510	1521	-5	944	865	8	986	1004

10, 8, L		
9	764	742
11	604	606
14	776	768
16	897	962
18	723	764
10, 9, L		
-8	1169	1113
-6	1471	1399
-4	1168	1088
4	735	754
5	929	934
6	1420	1403
7	1014	1059
8	1820	1724
10	1549	1555
11	721	691
12	841	848
13	1087	1108
15	1081	1031
17	671	743
10, 10, L		
-7	1499	1414
-5	1330	1373
-4	766	596
-3	919	914
-2	615	589
0	511	515
2	445	307
3	589	526
5	1382	1370
7	1992	2017
9	1749	1774
10	997	1013
11	939	939
12	1137	1190
14	1059	1106

10, 11, L		
-6	1064	1030
-5	877	813
-4	837	752
-3	1057	942
-1	775	691
1	853	860
3	524	478
4	774	729
6	1036	1072
7	768	659
8	1203	1200
9	1235	1169
10	727	734
11	929	1025
13	892	817
10, 12, L		
-4	860	773
-2	798	711
0	960	968
2	645	672
8	758	755
10	846	944
12	668	764
10, 13, L		
1	670	662
11, -7, L		
-2	1290	1309
-1	718	691
0	1390	1430
1	916	924
2	1244	1214
3	839	819
4	506	567
5	634	649

11, -6, L		
-3	731	623
-2	895	906
-1	843	894
0	1177	1150
1	771	764
2	1074	1061
11, -5, L		
-3	714	646
-1	960	927
1	726	705
8	497	536
10	649	656
11, -4, L		
-8	844	859
-3	714	746
-1	1001	967
1	704	736
5	496	505
7	1025	1049
8	485	487
9	1028	1165
10	892	988
11	659	678
12	889	937
14	615	658
11, -3, L		
-7	635	651
-5	640	662
-4	687	735
-3	890	955
-2	458	518
-1	1041	1066
1	1116	1057
3	846	820
6	1025	1104
7	642	712
8	962	999

9	1502	1660
11	1852	1926
13	1115	1095
14	615	672
15	431	420
11, -2, L		
-6	725	725
-4	1094	1164
-2	1326	1305
0	1132	1128
1	825	813
2	1068	1068
3	854	949
5	959	1064
6	548	702
7	490	558
8	1316	1358
10	1713	1843
11	997	1082
12	1363	1410
13	1045	1110
14	617	623
15	669	698
11, -1, L		
-5	585	595
-3	1237	1215
-2	497	478
-1	1161	1110
0	1004	1012
1	834	811
2	1446	1438
3	384	313
4	1270	1362
7	596	484
9	1058	1101
10	921	1003
11	699	674
12	1319	1406

13	571	616
14	928	987
15	521	555
17	505	538
11, 0, L		
-4	737	814
-3	406	385
-2	880	816
-1	1128	1138
0	658	657
1	1514	1507
3	1375	1395
5	895	947
9	439	502
11	820	882
13	608	651
15	489	469
16	702	764
18	897	920
11, 1, L		
0	943	928
2	1199	1124
4	924	875
6	418	354
9	883	935
11	1105	1133
13	385	432
16	473	590
17	718	750
18	699	815
11, 2, L		
-5	661	762
-3	553	476
2	471	439
6	747	862
7	683	772
9	1090	1160
10	1230	1333

11	1413	1604
12	597	578
13	849	893
16	605	650
17	855	829
18	741	830
11, 3, L		
-6	1081	1095
-5	501	548
-4	1189	1186
-2	1274	1236
0	943	943
2	671	595
5	589	577
6	1223	1224
7	573	651
8	1685	1803
9	740	787
10	2044	2268
12	1630	1696
14	586	600
15	699	679
16	743	722
18	1426	1504
11, 4, L		
-10	832	814
-9	528	519
-7	1094	1054
-6	827	780
-5	1144	1111
-4	1026	940
-3	1338	1319
-2	1027	941
-1	1529	1480
0	1060	1012
1	1310	1169
2	842	801
5	956	922

11, 4, L		
7	1697	1770
8	589	552
9	2108	2157
10	743	680
11	1885	1958
12	775	884
13	987	954
14	629	665
17	1169	1193

11, 5, L		
-8	545	552
-6	616	677
-5	1044	1007
-4	590	650
-3	1087	1013
-2	931	837
-1	1430	1359
0	774	747
1	1517	1525
2	860	786
3	794	753
4	491	340
6	478	491
7	1112	1083
8	1240	1311
9	1620	1624
10	1298	1305
11	1476	1578
12	1042	1170
13	874	869
17	659	705
18	658	620

11, 6, L		
-9	658	558
-6	830	757
-4	897	735
-2	1133	1133
0	1223	1205
1	489	418
2	1338	1313
4	904	842
8	1431	1568
10	1654	1684
12	1179	1124
13	597	588
15	496	678
16	482	367
18	478	554

11, 7, L		
-6	749	668
-4	633	606
-2	470	412
-1	1095	981
1	1108	1159
3	900	894
5	527	528
6	469	477
9	868	921
11	913	901
16	1028	1069

11, 8, L		
-7	957	868
-6	1014	847
-5	842	822
-4	714	572
-3	528	566
0	625	584
2	996	890
4	1083	990
5	802	754
6	790	752
7	651	763
8	423	324
9	505	631
15	1155	1189
17	1231	1222

11, 9, L		
-5	1868	1756
-3	1104	982
1	673	678
3	1484	1414
5	1808	1784
6	729	759
7	1670	1643
8	635	705
9	1077	1045
14	1101	1076
16	1041	1067

11, 10, L		
-5	1113	955
-4	1462	1384
-3	1195	1054
-2	637	551
2	830	766
4	1497	1495
6	1981	1899
8	1800	1793
10	955	974
13	725	834
14	610	550
15	710	688

11, 11, L		
-2	965	887
3	606	629
5	1023	954
6	778	595
7	1160	1142
8	714	588
9	1102	1058
12	529	552

11, 12, L		
10	523	508
11	522	493

12, -5, L		
0	864	841
2	941	983
4	512	485
7	632	744
9	786	795

12, -4, L		
-3	679	718
-2	769	740
0	604	593
2	535	556
6	878	945
8	1254	1336
9	540	504
10	1081	1174
11	482	548

12, -3, L		
-4	1344	1364
-2	1223	1194
0	733	732
5	578	618
6	698	775
7	1200	1317
8	1517	1625
9	1077	1042
10	1530	1673
12	859	950

12, -2, L		
-5	1360	1418
-3	1251	1320
-2	554	489
-1	1039	1006
1	752	746
4	417	340
5	579	594
6	634	622
7	1428	1529
9	1860	1991
11	1370	1462
12	718	726
13	635	657
14	631	715

12, -1, L		
-6	701	694
-5	708	690
-4	947	1016
-3	674	677
-2	1046	1034
-1	825	786
0	738	720
1	481	437
5	402	419
6	777	777
8	1153	1153
10	1204	1271
11	799	876
12	481	468
13	845	910

12, 0, L		
-6	764	716
-4	867	849
-3	600	608
-2	1025	977
-1	753	715
0	920	887
1	646	644
2	641	639
4	459	458
7	516	513
10	511	581

12, 1, L		
-3	502	508
-1	707	745
1	865	805
2	524	574
3	559	591
10	524	547

12, 2, L		
-7	844	875
-6	423	489
-5	724	739
1	573	617
2	600	598
3	554	508
5	499	526
7	395	513
8	455	537
9	711	700
10	1009	1136
11	610	576
12	811	902
14	399	445

12, 3, L		
-8	653	634
-7	1120	1108
-6	442	446
-5	1340	1342
-3	1148	1109
-1	695	640
0	868	858
2	674	655
3	607	569
5	911	968
7	1123	1115
9	1464	1603
11	1556	1703
13	745	767
14	622	656

12, 3, L
16 585 718
17 1088 1127
12, 4, L
-6 1434 1433
-4 1211 1209
-3 751 781
-2 1004 950
-1 1099 1046
0 485 403
1 975 958
4 600 731
6 939 889
8 1392 1493
9 649 556
10 1559 1662
11 729 827
12 1041 1092
13 852 922
15 524 556
16 832 901
12, 5, L
-7 1186 1108
-6 624 713
-5 856 866
-4 790 757
-3 659 559
-2 1045 1003
0 963 959
7 630 632
8 974 1048
9 1008 1023
10 1199 1176
11 977 1041
12 1106 1173
13 541 612

12, 6, L
-5 945 862
-3 890 809
-1 635 646
1 575 536
7 530 556
9 1125 1191
11 1207 1239
13 725 792
12, 7, L
-6 531 484
-4 449 474
-3 690 623
-1 530 482
2 642 642
4 751 702
10 754 801
12 743 763
15 760 861
12, 8, L
-4 646 605
-2 510 421
2 640 621
3 1163 1122
4 684 720
5 1381 1372
7 935 871
14 725 663
12, 9, L
-2 829 709
2 1304 1258
4 2088 1981
6 1797 1814
8 1089 1115
12, 10, L
1 887 864
3 1609 1554
4 705 648

5 1961 1896
6 617 594
7 1419 1375
9 848 831
12, 11, L
2 672 695
3 1025 878
4 934 916
5 1366 1211
6 739 764
7 888 805
8 806 751
13, -3, L
5 1160 1190
6 668 605
7 1458 1559
8 746 807
13, -2, L
-2 1280 1235
-1 602 641
0 817 834
4 467 518
6 1374 1441
8 1820 1944
10 1436 1561
13, -1, L
-3 920 915
-2 1252 1230
-1 715 678
0 559 606
7 942 955
9 1248 1357
11 811 862
13, 0, L
-3 1363 1431
-1 976 1001
2 612 570
8 502 558

13, 1, L
-4 978 942
-2 868 833
0 488 432
1 806 767
3 951 957
5 524 560
13, 2, L
-4 1015 1029
0 801 768
1 707 606
2 1251 1206
3 693 722
4 1108 1116
5 480 458
6 748 817
9 502 506
11 396 475
13, 3, L
-4 1345 1360
-2 899 868
-1 687 722
1 1003 931
2 1083 1070
3 740 739
4 1332 1349
5 634 536
6 1111 1182
8 876 941
10 893 1008
13 477 589
13, 4, L
-3 1184 1203
-2 988 934
0 1027 932
1 868 833
2 503 486
3 1197 1226

5 1111 1122
7 809 909
8 629 569
9 706 802
10 527 421
11 517 606
12 692 700
14 558 554
13, 5, L
-4 1047 988
-3 923 913
-1 765 697
0 636 523
2 986 985
4 717 661
5 663 547
7 691 710
8 480 587
9 530 631
11 481 507
13, 6, L
-2 742 698
-1 428 383
10 655 637
13 564 610
13, 7, L
4 445 455
13, 8, L
1 491 504
2 517 483
3 819 759
4 1188 1111
6 1161 1157
8 489 577
13, 9, L
2 857 820
3 1668 1585
5 1868 1825

7 1276 1280
8 625 606
9 627 576
14, 1, L
2 773 737
4 980 1058
6 773 836
14, 2, L
1 843 792
2 630 617
3 1238 1229
4 847 816
5 1265 1265
6 777 823
7 689 722
8 601 605
14, 3, L
1 768 785
2 853 794
3 1439 1403
4 847 771
5 1535 1643
7 1149 1222
9 559 591
14, 4, L
2 1410 1327
4 1757 1738
6 1404 1474
8 763 811
14, 5, L
2 441 430
3 996 949
4 998 904
5 948 893
6 930 941
7 740 745
8 555 605

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14,  6,  L
5  820   715
7  665   614
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CALCULATED AND OBSERVED STRUCTURE FACTORS OF
[CpMo(Pr^{i}SC(CO_2Me)C(CO_2Me)=C(CF_3)C(CF_3)=C(CF_3)CCF_3)]

0, 0, L		
2	2165	1885
4	1853	1703
6	1099	1019
8	302	291
10	337	315
12	285	251
13	178	74
14	425	411
16	533	513
0, 1, L		
-15	190	171
-13	316	316
-11	218	216
-9	478	478
-7	459	430
-5	764	736
-3	671	604
-1	2546	2323
5	1533	1433
7	453	461
9	419	462
11	495	512
13	294	280
15	536	510
0, 2, L		
-14	476	440
-12	604	581
-10	88	91
-8	1214	1196
-6	521	445
-4	1846	1755
-2	2706	2573
0	1933	1732
2	3408	3383
5	86	69
6	1599	1541
8	1243	1131
12	354	362
14	410	409
16	381	367
0, 3, L		
-13	208	252
-11	413	413
-9	897	878
-7	276	272
-5	1709	1621
-3	292	295
-1	963	878
1	905	872
3	913	881
7	1146	1151
8	321	139
9	1437	1397
11	897	916
13	365	386
15	330	313
17	512	511
0, 4, L		
-12	261	269
-10	154	107
-8	370	377
-6	1038	1007
-4	1281	1288
-2	1094	1048
0	1875	1706
1	75	54
2	1452	1345
4	114	89
8	623	602
9	122	105
10	327	322
14	378	371
0, 5, L		
-13	154	164
-11	537	534
-9	805	765
-7	913	848
-5	1303	1253
-3	1900	1749
-1	1145	1066
1	567	496
3	1193	1138
5	472	483
7	267	270
9	1908	1914
11	560	571
13	580	567
15	618	585
17	599	613
0, 6, L		
-10	231	206
-6	194	182
-4	369	332
-1	88	74
0	543	509
2	226	233
4	188	168
8	620	633
10	279	288
12	512	504
16	400	401
0, 7, L		
-11	433	400
-9	717	680
-7	633	576
-5	1339	1243
-4	77	82
-3	620	612
-1	1093	1007
1	1551	1464
2	107	81
3	446	436
5	1207	1155
7	531	538
9	800	785
13	366	350
15	269	264
17	300	294
0, 8, L		
-10	208	191
-8	403	374
-6	156	158
-4	480	429
-2	779	746
0	898	855
2	386	429
3	150	137
4	1445	1427
6	497	469
7	79	84
8	1183	1160
12	365	370
14	172	175
16	363	388
0, 9, L		
-9	316	278
-7	852	800
-5	480	457
-3	729	693
-1	227	185
1	265	255
3	80	83
5	379	383
7	211	96
9	702	718
11	194	163
13	287	301
0, 10, L		
-8	437	435
-6	431	388
-4	251	218
-2	184	161
0	727	687
4	1055	1036
6	938	928
8	740	735
10	484	457
12	448	450
14	282	255
16	224	212
0, 11, L		
-5	324	310
-3	140	103
-1	153	111
1	155	152
3	586	512
5	133	82
7	557	559
11	125	116
15	250	247
0, 12, L		
-4	631	593
-2	583	539
0	814	738
2	793	718
4	1091	1005
6	293	263
8	288	265
10	603	598
12	308	302
0, 13, L		
-3	164	153
-1	517	493
1	552	503
3	628	585
9	405	421
11	233	228
13	206	202
15	373	416
0, 14, L		
-2	360	346
0	283	263
2	416	362
4	556	493
6	571	562
8	194	189
12	131	152
0, 15, L		
1	461	450
3	327	311
5	274	271
7	376	365
9	175	183
11	207	213
0, 16, L		
6	249	240
8	200	182
1,-15, L		
-8	268	262
-6	209	202
-4	177	175
-2	341	328
1,-14, L		
-11	372	366
-9	217	223
-8	229	224
-7	196	184
-3	146	149
-2	145	155
-1	110	108
1	120	115

1,-13, L		
-12	405	397
-10	520	527
-8	394	362
-7	266	250
-6	269	254
-4	706	688
-3	163	149
-2	527	483
-1	181	175
0	490	483
1	85	84
2	338	320
1,-12, L		
-13	136	152
-12	201	180
-10	258	245
-8	358	355
-7	243	245
-6	231	255
-5	454	443
-4	263	257
-3	227	209
0	285	282
2	150	139
3	128	126
4	154	170
5	151	117
1,-11, L		
-14	293	316
-13	238	248
-12	479	476
-10	342	340
-8	757	736
-6	329	319
-4	817	785
-2	676	657
-1	143	159
0	657	632
1	144	120
2	545	533
3	131	144
4	158	143
6	326	309
1,-10, L		
-16	122	134
-15	101	89
-13	199	208
-12	350	360
-11	248	259
-10	364	362
-9	678	638
-8	202	204
-7	436	450
-5	544	495
-3	598	579
-2	302	322
-1	364	371
0	155	159
1	212	183
3	497	483
4	170	121
5	152	143
7	426	400
8	121	119
1, -9, L		
-16	369	397
-15	121	114
-14	222	226
-13	134	139
-12	464	481
-10	185	129
-9	146	187
-8	245	220
-7	171	166
-6	700	680
-4	503	531
-3	179	198
-2	693	695
-1	131	150
0	125	140
1	652	668
2	370	371
4	95	69
5	133	103
6	179	177
8	214	211
9	106	100
1, -8, L		
-15	203	220
-14	192	188
-13	490	517
-12	355	364
-11	668	676
-10	237	236
-9	753	723
-8	297	288
-7	1007	938
-6	346	334
-5	1187	1150
-4	595	552
-3	632	626
-2	280	265
-1	841	848
0	213	200
1	751	763
2	357	356
4	236	214
5	770	765
6	378	373
7	528	506
8	200	204
9	705	666
1, -7, L		
-16	139	148
-15	103	107
-13	157	159
-8	169	164
-7	145	155
-6	649	634
-5	530	483
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-3	198	159
-2	527	486
-1	438	442
1	324	338
2	111	97
3	127	133
4	488	500
6	401	384
8	372	361
10	153	105
1, -6, L		
-17	319	332
-15	581	599
-14	176	175
-13	438	470
-12	225	198
-11	556	586
-10	230	228
-9	1180	1207
-8	411	409
-7	1105	1111
-5	1135	1099
-4	768	746
-3	1310	1317
-2	728	680
-1	159	69
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1	588	608
2	158	169
3	540	560
5	580	612
6	310	305
7	627	598
9	711	705
11	531	525
12	141	149
1, -5, L		
-16	244	237
-14	266	249
-13	111	152
-12	309	306
-10	434	454
-9	163	162
-7	245	338
-6	345	321
-5	494	464
-4	1037	995
-3	200	180
-1	195	197
0	1115	1133
1	771	731
3	530	525
4	1034	1073
5	509	530
6	826	833
8	572	562
10	373	359
11	87	88
12	459	436
1, -4, L		
-15	434	456
-14	259	247
-13	277	282
-12	214	180
-11	553	532
-10	452	476
-9	1083	1089
-8	197	193
-7	1075	1127
-6	655	662
-5	347	303
-4	596	602
-3	1066	1073
-2	103	104
-1	128	143
0	795	829
1	878	864
2	435	457
3	87	120
4	199	188
5	621	629
6	225	239
7	327	341
9	293	284
10	317	306
11	385	368
13	154	192
14	92	102
1, -3, L		
-16	443	435
-14	509	503
-12	413	414
-11	177	183
-10	434	427
-9	256	300
-8	1206	1156
-7	264	250
-6	188	201
-5	1062	1029
-4	1381	1395
-3	341	357
-2	1038	1066
-1	1761	1737
0	1755	1719
1	614	582

1, -3, L		
2	1226	1254
3	226	238
4	1908	1944
6	621	639
7	212	193
8	811	829
10	625	616
12	459	444
14	331	310

1, -2, L		
-16	197	192
-15	321	327
-14	296	324
-11	533	547
-10	133	98
-9	381	425
-8	896	885
-7	454	478
-6	168	127
-5	1467	1454
-4	1804	1869
-3	449	461
-1	621	617
1	877	867
2	185	183
3	614	642
4	78	115
5	240	212
6	325	339
7	235	213
8	580	567
9	225	235
10	258	274
11	145	147
12	343	330
13	223	216
15	259	233

1, -1, L		
-16	534	524
-15	151	163
-14	484	452
-13	165	134
-12	792	778
-11	98	73
-10	556	588
-9	240	248
-8	1230	1266
-7	320	243
-6	602	639
-5	258	263
-4	775	873
-3	92	43
-2	297	297
-1	252	243
0	2958	2914
1	252	222
2	1215	1259
3	177	200
4	122	117
5	118	140
6	1746	1798
7	268	283
8	587	616
9	162	175
10	512	507
11	121	158
12	351	347
13	158	134
14	254	255

1, 0, L		
-14	190	189
-13	137	136
-10	127	101
-8	89	115
-7	889	901
-6	193	302
-4	420	429
-3	223	220
-2	215	230
-1	1870	1839
1	439	425
2	475	477
3	690	735
4	724	677
5	150	159
7	884	865
8	364	355
9	804	787
10	553	590
11	288	299
13	661	625
14	236	238
15	549	502

1, 1, L		
-14	480	482
-13	231	237
-12	617	637
-10	265	273
-9	575	598
-8	793	850
-7	362	399
-6	927	1001
-3	664	670
-2	719	742
-1	525	541
0	687	703
2	1782	1712
3	195	205
4	424	469
5	286	279
7	344	376
8	1030	1025
9	117	83
14	129	109
15	174	176

1, 2, L		
-13	235	265
-12	198	138
-11	324	331
-9	554	589
-8	217	232
-7	512	526
-6	237	221
-5	1681	1746
-4	186	186
-3	104	51
-2	135	128
-1	1249	1252
0	337	316
1	2752	2778
2	310	324
3	345	327
4	174	163
5	576	639
6	257	287
7	627	618
8	208	153
9	1271	1255
10	248	231
11	692	683
12	94	105
13	834	775
15	531	500
16	190	198
17	596	581

1, 3, L		
-14	255	265
-13	101	103
-12	231	254
-11	351	353
-10	150	146
-9	237	266
-8	111	87
-7	548	595
-6	257	231
-5	284	262
-4	94	41
-3	123	143
-2	658	694
-1	135	130
0	964	955
2	559	543
4	453	450
5	1821	1799
6	1624	1588
7	163	147
8	485	464
9	957	903
10	332	326
12	532	540
15	286	264
16	291	273
17	183	176

1, 4, L		
-13	281	316
-11	447	451
-10	121	182
-9	591	597
-7	746	739
-6	169	136
-5	623	663
-4	101	116
-3	1758	1856
-2	283	318
-1	1320	1356
0	649	634
1	1696	1692
2	1621	1603
3	1044	1045
4	332	346
5	1386	1362
6	1116	1111
7	142	150
8	300	283
9	1233	1188
10	271	275
11	452	428
12	148	120
13	450	437
15	565	541
17	454	465

1, 5, L		
-13	139	145
-12	171	166
-10	325	332
-9	293	308
-8	197	196
-6	251	279
-5	290	301
-4	566	575
-1	179	248
0	791	830
1	712	732
2	108	119
4	984	971
5	563	579
6	322	283
7	621	607
8	1070	1120
9	154	104
10	1123	1097
11	452	491
12	513	501
13	186	163
14	299	290
15	260	237
16	419	412

1, 6, L		
-11	458	464
-10	81	105
-9	411	411
-7	564	535
-5	825	813
-4	515	506
-3	1052	1117
-2	376	365
0	653	652
1	1119	1187
2	102	93
4	235	221
5	1011	992
6	527	510
7	312	316
8	229	201
9	124	173
10	120	131
11	469	469
13	376	395
15	326	295
16	170	161
17	276	293

1, 7, L		
-11	129	129
-10	491	491
-8	620	639
-6	572	595
-5	306	335
-4	551	560
-2	390	424
-1	98	107
0	616	667
1	447	452
2	299	182
3	843	766
4	1340	1365
5	680	647
6	1146	1119
8	1196	1220
9	443	443
10	1148	1119
11	270	284
12	608	647
13	237	203
14	433	409
15	156	117
16	580	558

1, 8, L		
-9	113	97
-7	368	378
-5	423	440
-3	423	445
-2	245	260
0	413	450
2	343	352
3	500	473
5	781	739
6	525	494
7	658	607
9	183	213
13	121	106
14	193	238
16	149	164
17	124	125

1, 9, L		
-8	675	678
-7	243	254
-6	469	455
-5	366	379
-4	761	782
-3	294	295
-2	122	111
-1	264	282
0	761	774
1	219	211
2	833	792
3	203	178
4	649	634
5	561	568
6	1187	1186
7	241	219
8	986	985
9	348	346
10	747	785
11	217	232
12	707	687
13	401	417
14	498	490
15	196	201
16	202	230

1, 10, L		
-8	108	133
-7	150	153
-5	145	127
-4	213	211
-2	150	161
-1	468	483
0	613	640
2	214	243
3	685	680
4	156	172
5	433	422
6	136	157
7	643	596
8	148	130
9	151	117
11	150	92
13	405	373
14	158	169
15	224	216
16	161	156
17	366	374

1, 11, L		
-7	177	165
-6	434	419
-4	154	155
-2	520	528
0	253	227
1	155	178
2	411	383
3	296	327
4	730	663
6	565	541
8	495	498
9	231	233
10	636	600
11	433	475
12	253	253
13	358	354
14	184	172
17	150	171

1, 12, L		
-5	259	257
-3	170	177
-2	161	183
-1	477	459
0	159	163
1	626	620
2	133	134
3	678	657
5	784	759
7	326	324
9	719	716
11	285	272
12	104	114
13	476	446
14	224	215
15	280	282

1, 13, L		
-4	152	166
-3	105	107
-2	104	111
-1	143	130
0	157	152
1	187	187
4	299	289
5	242	246
6	413	404
7	117	102
8	246	252
9	382	379
10	115	125
11	306	313
13	222	243

1, 14, L		
-1	336	320
0	99	105
1	449	431
2	238	239
3	511	489
4	154	129
5	667	651
7	225	222
8	277	266
9	409	403
11	507	509
12	146	150
13	440	437

1, 15, L		
0	116	120
4	166	176
8	226	237
9	260	283
10	186	188
12	354	369

1, 16, L		
5	212	212
7	208	201
9	266	261

2,-14, L		
-10	332	355
-9	216	209
-8	497	493
-6	393	377
-5	115	112
-4	421	405
-2	256	260
-1	172	187

2,-13, L		
-8	241	214
-6	182	174
-3	143	156
-2	181	209
1	197	193
2	139	133

2,-12, L		
-13	189	165
-12	417	406
-11	215	202
-10	450	427
-8	477	496
-7	138	160
-6	469	457
-4	345	346
-2	391	405
0	197	181
2	272	280

2,-11, L		
-13	257	264
-12	128	114
-11	442	411
-10	255	246
-9	532	508

2,-11, L			-1	692	683	-9	691	671	6	767	770	-4	1235	1235	2, -2, L		
-8	456	447	0	409	398	-8	167	157	7	296	290	-3	493	481	-16	425	473
-7	296	282	1	1020	1013	-7	845	817	8	459	442	-2	2045	2130	-14	440	474
-5	638	630	2	335	331	-6	534	491	10	499	499	-1	223	242	-13	112	112
-4	262	253	3	602	601	-5	967	912	11	182	174	0	800	851	-12	542	573
-3	448	476	4	182	187	-4	134	132	12	421	449	1	673	681	-11	328	342
-1	463	448	5	625	604	-3	460	456	2, -5, L			2	887	945	-10	666	691
1	195	206	7	339	323	-1	243	244	-16	220	230	4	857	890	-9	127	83
3	346	336	9	367	380	0	573	576	-15	193	211	5	98	112	-8	1154	1168
4	160	158	2, -8, L			1	489	468	-12	169	189	6	726	726	-7	266	224
5	244	222	-15	184	191	2	336	345	-11	207	207	8	451	465	-6	365	375
2,-10, L			-13	218	209	3	858	843	-10	303	288	10	540	532	-5	626	647
-15	265	247	-11	177	142	5	597	585	-9	294	328	11	208	215	-4	806	843
-14	277	274	-10	150	46	7	532	539	-7	457	474	12	517	518	-3	822	844
-13	188	186	-9	189	161	9	360	362	-6	264	252	13	142	143	-2	570	548
-12	287	310	-8	199	157	10	88	99	-5	355	365	14	413	425	-1	1108	1058
-11	204	221	-6	133	123	11	326	313	-3	412	418	2, -3, L			0	1830	1821
-10	188	192	-5	384	383	2, -6, L			-2	764	748	-10	128	123	2	1701	1652
-9	164	147	-4	89	74	-16	287	294	-1	99	147	-8	307	296	4	973	964
-8	162	159	-2	909	919	-14	302	298	0	857	846	-7	458	425	5	304	295
-4	149	160	-1	191	200	-13	268	282	2	629	639	-6	94	93	6	925	958
-3	254	267	0	341	336	-12	485	466	3	278	301	-5	1004	1001	7	112	56
-1	228	246	1	414	407	-11	110	115	4	458	460	-3	1038	967	8	421	409
1	365	373	2	173	172	-10	593	590	5	149	159	-2	258	238	9	636	625
3	224	217	3	337	338	-9	312	308	8	105	138	-1	676	704	10	254	248
4	169	190	4	459	451	-8	832	782	9	154	140	0	461	464	12	422	405
7	226	226	5	108	111	-7	411	389	11	101	90	1	107	132	13	87	106
2, -9, L			7	150	153	-6	819	792	13	80	30	2	511	494	14	165	177
-15	348	353	8	323	313	-5	451	449	2, -4, L			3	459	444	2, -1, L		
-13	589	582	9	248	250	-4	1050	1043	-16	288	317	4	330	325	-13	193	201
-11	669	648	10	180	194	-3	444	440	-14	468	500	5	252	165	-12	417	436
-10	261	241	2, -7, L			-2	122	92	-12	296	287	7	535	530	-11	231	248
-9	631	571	-16	130	154	-1	111	114	-11	206	215	8	274	299	-10	218	247
-8	617	556	-15	420	448	0	995	1034	-10	604	640	9	215	192	-9	318	355
-7	702	668	-13	507	493	1	283	281	-8	1068	1062	11	238	212	-8	110	134
-5	658	644	-12	157	170	2	238	253	-7	107	65	12	236	226	-7	597	574
-3	1113	1106	-11	727	715	3	455	473	-6	1206	1175	13	466	478	-6	292	282
-2	346	378	-10	269	268	4	702	713	-5	151	119	14	101	98	-5	763	789

2, -1, L		
-4	1054	1040
-3	246	233
-2	1226	1281
-1	382	413
0	1064	965
1	1322	1251
2	255	241
3	951	957
4	449	499
5	1471	1519
6	804	794
7	788	790
8	295	325
9	914	950
10	261	248
11	448	433
13	562	547
14	192	172
15	456	452

2, 0, L		
-15	85	113
-14	274	289
-12	338	353
-10	561	584
-9	443	471
-8	581	615
-7	603	606
-6	1062	1070
-5	211	244
-4	145	140
-3	541	532
-2	1447	1449
-1	290	306
0	448	440
1	721	605
2	220	223
3	1065	1107
4	513	505
6	297	296
7	683	667
8	370	349
9	606	624
10	293	270
11	231	228
13	137	108
16	137	137

2, 1, L		
-15	197	198
-13	417	433
-12	126	25
-11	601	636
-10	431	426
-9	832	921
-7	1254	1305
-6	351	334
-5	1196	1265
-4	369	389
-3	154	163
-2	600	586
-1	707	717
0	891	894
1	342	382
2	993	955
3	574	526
4	877	872
6	289	282
7	1308	1356
8	205	213
9	1232	1264
10	238	245
11	869	870
12	437	434
13	611	631
14	155	46
15	429	423

2, 2, L		
-14	155	177
-9	302	328
-8	131	150
-7	566	565
-6	219	212
-5	577	573
-4	464	466
-2	494	484
-1	1015	1015
0	137	151
1	731	763
2	353	354
3	368	371
4	1538	1555
5	307	277
6	280	262
7	284	300
8	950	979
9	580	578
10	578	561
11	462	481
12	494	476
14	344	307
15	158	156
16	287	289

2, 3, L		
-14	131	137
-13	402	427
-12	162	166
-11	536	592
-9	456	501
-8	177	161
-7	1032	1107
-6	355	373
-5	870	884
-4	835	811
-3	1471	1517
-2	463	495
-1	1174	1202
0	360	381
1	1394	1442
2	1008	1004
3	471	473
4	1494	1497
5	130	103
6	898	935
7	758	787
8	327	270
9	671	646
10	102	110
11	418	420
12	172	184
13	357	355
14	402	421
15	249	241
17	172	187

2, 4, L		
-13	118	126
-11	129	126
-10	334	360
-8	234	256
-7	533	539
-6	214	199
-4	944	962
-3	188	172
-2	758	778
0	1489	1502
2	1565	1608
3	1048	1059
4	420	413
5	580	555
6	785	752
7	727	715
8	323	332
9	290	274
10	1055	1087
11	128	90
12	646	659
13	410	430
14	524	518
15	201	224
16	488	503

2, 5, L		
-11	524	556
-10	200	198
-9	308	326
-7	268	255
-6	350	350
-5	495	508
-3	129	51
-2	262	248
-1	499	534
0	688	698
1	213	231
2	583	599
3	965	1037
4	400	429
5	1064	1083
7	1066	971
9	570	546
10	372	343
12	172	140
13	132	117
18	153	163

2, 6, L		
-12	406	458
-11	139	171
-10	442	488
-9	208	211
-8	457	455
-6	405	426
-4	658	723
-2	866	892
-1	90	117
0	850	897
1	589	584
2	815	872
4	1986	2054
5	508	475
6	1098	1144
8	1270	1244
10	1046	1017
12	643	629
13	268	270
14	396	387
16	501	502
18	313	314

2, 7, L		
-11	121	94
-9	178	176
-7	90	89
-2	536	530
-1	317	315
0	701	717
2	918	915
3	153	155
4	750	723
5	144	138
7	203	203
8	159	130
9	323	292
11	221	218
12	270	238
13	157	145
14	140	116
17	155	125
18	273	273

2, 8, L		
-10	393	411
-9	116	107
-8	451	443

2, 8, L		
-6	453	449
-5	243	271
-4	797	835
-3	126	190
-2	750	770
-1	459	474
0	314	319
2	967	1001
4	204	225
5	530	540
6	1060	1098
7	237	224
8	815	846
9	395	378
10	869	861
11	220	187
12	608	601
13	139	185
14	529	528
15	330	343
16	379	371
17	96	88
18	290	274

2, 9, L		
-9	268	276
-7	307	306
-5	543	556
-4	97	105
-3	489	496
-1	878	866
0	460	462
1	438	429
2	542	520
4	150	131
5	497	534
7	746	748
8	435	400
9	796	794
10	166	189
11	598	566
12	221	225
13	665	638
14	129	133
15	459	431
16	190	207
17	403	391
18	135	153

2, 10, L		
-8	143	160
-7	270	268
-6	351	355
-5	168	196
-4	152	141
-3	96	96
-2	424	444
-1	406	417
0	377	379
1	351	344
2	538	541
3	183	207
4	957	952
5	130	132
6	267	266
7	320	309
8	164	169
9	129	137
10	228	240
11	225	231
12	128	105
13	243	249
15	219	213
17	203	202

2, 11, L		
-7	335	358
-6	86	97
-5	275	274
-3	630	673
-2	119	149
-1	561	581
0	455	468
1	930	975
2	294	272
3	626	625
4	277	316
5	1056	1063
7	587	590
8	90	77
9	602	579
10	558	533
11	623	610
12	234	209
13	639	611
15	529	542
17	371	390

2, 12, L		
-5	240	235
-4	110	115
-1	219	234
1	367	360
3	168	188
5	170	189
6	226	238
11	257	271
13	247	263
14	228	214
15	197	233
16	234	239
17	258	268

2, 13, L		
-3	242	251
-2	178	186
-1	335	326
1	174	188
3	437	460
5	480	495
6	258	248
7	592	614
8	225	240
9	312	339
10	434	444
11	496	523
12	219	221
13	458	457
15	232	237

2, 14, L		
-1	104	125
0	236	232
2	152	150
4	323	329
6	334	324
8	435	423
10	389	392
12	384	386
13	229	224
14	352	340
15	159	161

2, 15, L		
0	109	113
1	171	189
2	173	196
3	135	152
4	187	213
5	200	222
6	172	178
8	231	236
9	132	146
10	285	293

2, 16, L		
3	157	187
4	272	286
5	108	81
6	380	390
8	379	386
9	163	170
10	416	422
11	184	196
12	297	305

3,-14, L		
-6	156	183
-5	328	345

3,-13, L		
-9	210	215
-7	255	292
-6	264	289
-5	174	139
-4	303	319
-2	240	248
0	235	252

3,-12, L		
-11	350	358
-9	335	341
-7	408	415
-5	615	588
-4	112	101
-3	354	379
-1	295	295
0	174	180
1	618	616
2	122	127
3	334	326

3,-11, L		
-9	317	317
-7	219	212
-5	154	159
-4	165	175
-1	155	187
0	135	149
1	237	261
2	120	137
4	161	145
5	132	140

3,-10, L		
-13	460	448
-11	727	688
-9	596	583
-7	466	454
-5	366	367
-4	119	91
-3	621	615
-1	243	246
1	367	362
2	325	338
3	542	554
4	187	187
5	328	306
6	148	155
7	479	468

3, -9, L		
-14	295	282
-12	370	310
-10	413	356
-8	161	119
-6	165	162
-5	244	259
-4	284	282
-3	130	91
-2	326	359
0	655	685
1	86	66
2	496	501
3	214	222
4	667	652

3, -9, L			3 97 124			0 1313 1350			-10 397 411			4 720 717			-9 541 522		
6	428	423	4	878	869	1	268	250	-9	175	136	5	1001	1034	-8	143	170
7	88	120	6	632	651	2	1298	1332	-8	227	229	6	184	193	-7	1117	1142
8	244	259	8	157	171	3	164	152	-7	289	141	7	727	765	-5	1379	1440
3, -8, L			10	320	306	4	1253	1222	-6	976	970	8	186	195	-4	259	248
-15	287	271	3, -6, L			6	746	745	-5	162	130	9	817	837	-3	1729	1740
-13	437	417	-14	331	338	7	136	146	-4	695	703	11	519	539	-2	274	279
-12	172	170	-13	228	231	8	225	215	-3	884	897	13	587	582	-1	1164	1200
-11	534	504	-11	377	384	11	214	228	-2	1395	1351	15	556	587	1	1516	1536
-9	474	446	-10	232	223	12	193	171	-1	956	968	3, -1, L			3	1411	1403
-7	596	573	-9	158	162	3, -4, L			0	796	833	-14	187	226	4	384	375
-6	145	143	-6	169	174	-13	175	183	1	304	298	-12	166	183	5	1048	1078
-5	452	468	-5	185	177	-12	270	292	2	535	549	-9	494	513	6	485	492
-3	248	251	-4	272	270	-10	133	122	3	197	183	-8	129	133	7	901	927
-2	119	134	-3	442	420	-8	253	242	4	573	581	-7	251	80	8	531	543
-1	307	309	-2	135	97	-7	441	436	5	158	140	-6	324	340	9	422	472
0	342	345	-1	413	399	-5	580	556	6	351	338	-5	544	506	11	875	870
1	270	283	0	457	469	-4	118	122	7	219	220	-4	1191	1182	13	603	590
2	506	505	1	124	106	-3	633	567	10	177	177	-3	664	680	15	472	461
3	399	407	2	612	612	-2	802	820	11	182	170	-2	143	135	3, 1, L		
4	287	250	4	118	130	-1	696	709	12	159	163	-1	570	579	-13	122	104
5	465	461	5	206	192	0	797	791	3, -2, L			0	478	494	-12	209	201
7	180	169	6	154	165	1	390	409	-15	133	164	1	371	379	-11	124	108
8	279	285	7	164	172	2	118	146	-14	154	171	2	273	264	-10	503	514
9	238	229	9	120	122	3	485	510	-13	271	283	3	788	801	-9	307	303
3, -7, L			10	183	201	4	239	266	-12	266	257	4	605	625	-8	155	144
-14	490	488	11	94	94	5	548	555	-11	486	496	5	141	136	-7	510	560
-13	168	192	3, -5, L			6	113	135	-9	619	639	6	476	453	-6	290	326
-12	554	516	-14	531	540	7	399	407	-7	1080	1098	7	472	449	-5	863	863
-10	344	308	-12	598	593	8	322	318	-6	298	321	8	595	611	-4	579	560
-8	330	298	-10	319	302	9	392	412	-5	1333	1364	9	242	237	-3	587	636
-6	161	135	-9	265	224	10	195	181	-4	383	382	10	357	345	-2	249	233
-4	506	512	-8	348	345	11	349	335	-3	993	1051	13	187	204	-1	131	124
-3	234	257	-6	395	366	13	473	485	-2	343	346	14	244	268	0	490	508
-2	957	957	-4	923	880	3, -3, L			-1	823	780	3, 0, L			1	457	459
-1	482	459	-3	108	108	-14	232	242	0	215	222	-13	197	218	2	723	754
0	865	910	-2	1252	1323	-13	124	174	1	677	677	-11	471	471	3	705	671
2	1028	1052	-1	384	398	-12	298	289	2	581	589	-10	477	518	4	1762	1750

3, 1, L			14	210	121	-3	715	693	15	129	143	0	702	713	15	656	637
6	650	616	15	228	229	-2	94	112	16	254	273	1	227	219	17	492	475
7	439	403	17	97	84	-1	616	599	17	156	154	2	640	652	3, 9, L		
8	523	519	3, 3, L			0	897	915	18	229	245	3	676	711	-8	101	100
9	793	815	-13	123	122	1	440	430	3, 6, L			4	904	945	-7	222	224
10	585	581	-12	382	395	2	377	381	-10	144	165	5	764	802	-3	149	125
11	265	262	-11	120	37	3	289	276	-9	236	283	6	816	854	-1	172	170
12	371	388	-10	536	562	4	691	705	-7	88	70	8	570	569	0	193	209
14	223	219	-9	102	98	6	907	902	-6	172	170	10	503	494	1	669	679
15	193	178	-8	769	785	7	972	880	-5	108	88	11	272	267	2	326	334
16	250	264	-6	253	281	8	339	311	-3	342	306	13	130	132	3	389	408
3, 2, L			-5	722	731	9	78	56	-2	272	259	14	155	159	4	583	577
-13	304	331	-4	687	711	10	170	92	-1	453	461	15	309	309	5	145	133
-12	163	147	-3	189	184	12	543	557	0	87	40	16	275	297	6	514	513
-11	299	305	-2	812	837	15	194	171	1	580	614	17	196	211	7	427	419
-9	599	631	-1	293	297	17	165	172	2	441	460	3, 8, L			8	208	206
-8	170	165	0	1066	1143	3, 5, L			3	599	631	-10	142	142	9	154	171
-7	678	674	1	156	172	-12	510	584	4	1226	1229	-9	125	83	12	165	171
-6	651	654	2	1403	1523	-10	489	541	5	1229	1238	-8	267	300	13	263	249
-5	670	677	4	1112	1144	-9	155	158	6	716	805	-7	126	137	14	278	224
-4	705	695	5	205	211	-8	510	559	7	441	441	-5	219	227	15	178	183
-3	847	846	6	1892	1917	-6	723	749	9	874	756	-4	280	308	16	149	123
-2	160	167	7	383	406	-4	680	711	11	129	74	-3	745	748	17	325	311
-1	1802	1840	8	1265	1270	-3	171	199	12	203	192	-1	1109	1100	3, 10, L		
0	675	698	10	1082	1076	-2	912	934	13	372	404	0	186	207	-7	317	329
1	905	949	11	184	183	-1	738	750	15	203	193	1	1264	1293	-5	126	156
2	350	386	12	511	518	0	97	64	16	129	144	2	383	358	-3	680	701
3	603	644	13	592	579	1	361	355	17	225	233	3	1170	1229	-1	932	945
4	122	132	14	354	338	2	631	686	3, 7, L			4	446	421	0	172	179
5	191	189	16	225	240	3	119	118	-10	468	511	5	945	1014	1	951	992
6	643	640	3, 4, L			4	890	930	-8	268	274	7	731	709	2	187	184
7	713	723	-11	337	370	6	993	1004	-7	164	169	8	118	139	3	839	870
8	935	925	-10	136	162	7	296	285	-6	378	401	9	247	212	4	541	522
9	425	455	-9	147	153	8	1684	1611	-5	302	319	10	105	102	5	841	873
10	441	470	-7	560	580	9	208	184	-4	442	452	11	303	283	6	113	141
11	317	308	-6	231	249	10	1039	1068	-3	130	160	12	300	263	7	391	410
12	190	196	-5	765	705	12	558	595	-2	734	740	13	395	372	9	187	183
13	629	586	-4	422	410	14	555	594	-1	216	221	14	202	209	11	340	343

3, 10, L		
13	409	413
15	532	519
17	538	543
3, 11, L		
-6	184	172
-5	282	276
-3	135	58
-2	306	313
-1	366	345
0	243	242
1	473	468
3	417	415
4	163	167
5	113	126
6	165	160
8	523	547
9	168	174
10	561	579
12	361	400
13	125	134
14	437	425
15	183	196
16	325	296
17	155	132
3, 12, L		
-5	328	365
-3	455	479
-1	689	698
0	146	168
1	539	557
3	555	600
4	156	145
5	396	439
7	246	252
11	264	252
13	439	461
14	125	151

15	431	439
17	292	311
3, 13, L		
-4	427	451
-3	117	157
-2	280	285
-1	250	251
0	460	471
1	337	339
2	194	198
3	134	114
4	210	208
5	129	136
6	616	602
8	335	337
9	89	57
10	453	457
12	501	521
13	172	192
14	565	596
16	363	358
3, 14, L		
-2	116	128
-1	194	202
1	187	216
2	302	303
3	212	221
4	278	283
10	334	368
11	128	119
12	342	356
15	121	149
3, 15, L		
0	265	287
2	583	615
3	214	200
4	302	295
6	468	475

8	614	599
10	366	377
12	296	320
14	305	343
3, 16, L		
3	165	179
4	145	139
5	156	170
7	254	256
8	237	233
9	133	137
10	326	339
12	186	217
4,-13, L		
-5	486	505
-4	191	200
-3	466	498
4,-12, L		
-8	237	246
-7	244	275
-6	237	249
0	216	223
4,-11, L		
-11	508	511
-9	319	328
-8	206	227
-7	424	394
-6	240	261
-5	525	541
-4	237	243
-3	543	564
-2	234	235
-1	250	256
1	101	98
3	369	367
4	199	198

4,-10, L		
-12	476	451
-10	343	312
-8	280	279
-7	188	209
-6	324	331
-5	111	96
-4	333	347
-2	210	212
-1	230	234
0	230	221
1	284	292
2	656	652
3	145	127
4	441	428
6	561	564
4, -9, L		
-11	358	344
-10	173	151
-9	504	473
-8	334	317
-7	248	238
-6	364	363
-5	506	480
-4	429	437
-3	157	167
-2	236	246
0	257	266
3	144	129
6	99	66
7	123	154
4, -8, L		
-12	502	457
-10	656	567
-9	221	173
-8	453	403
-6	508	532
-5	194	233

-3	154	184
-2	469	465
0	532	538
2	528	538
4	602	606
6	666	646
8	424	420
4, -7, L		
-12	170	192
-10	185	177
-8	311	286
-6	301	292
-4	424	424
-3	177	162
-1	137	128
0	252	264
1	426	428
2	275	277
3	225	216
4	131	153
5	378	358
6	154	157
7	181	172
8	181	201
9	158	145
10	193	202
4, -6, L		
-14	556	569
-12	541	508
-10	750	726
-8	369	347
-7	316	266
-6	344	342
-5	333	315
-4	342	326
-2	887	882
-1	258	258
0	538	537

1	345	338
2	512	532
4	307	317
6	721	724
7	119	151
8	213	225
9	267	270
11	123	129
4, -5, L		
-13	146	142
-12	190	206
-11	369	361
-8	115	104
-7	142	147
-6	246	251
-5	203	190
-4	543	531
-3	616	635
-2	359	371
-1	1017	1014
0	144	20
1	975	936
2	181	163
3	434	420
5	791	747
7	151	147
11	462	440
4, -4, L		
-14	429	440
-13	103	129
-12	458	436
-11	176	176
-10	662	656
-9	608	611
-8	273	254
-7	396	355
-6	488	471
-5	622	616

4, -4, L			9	295	294	-3	795	809	13	95	117	-4	530	524	12	341	325
-4	314	311	10	197	209	-2	340	339	14	684	679	-3	349	319	14	261	236
-3	686	646	11	194	196	-1	1954	2010	16	246	263	-2	2097	2116	16	377	385
-2	662	631	13	474	414	0	667	645	4, 1, L			-1	354	372	4, 4, L		
-1	116	115	4, -2, L			1	391	404	-12	298	287	1	481	489	-12	342	365
1	471	441	-14	168	187	2	117	158	-11	120	119	2	349	394	-11	127	92
2	412	381	-13	145	167	3	390	430	-10	169	166	3	107	115	-10	654	656
3	270	264	-10	131	116	4	152	187	-9	256	264	4	264	274	-8	525	476
4	586	563	-9	519	533	5	262	278	-8	110	72	5	446	437	-7	283	289
5	113	107	-8	215	220	8	167	175	-7	184	206	6	2416	2411	-6	982	953
6	373	385	-7	526	506	9	261	276	-6	312	284	7	471	433	-5	426	432
7	246	253	-6	170	172	11	404	387	-5	679	705	8	501	501	-4	483	503
9	200	210	-5	195	194	12	239	241	-4	87	69	10	1005	988	-2	446	478
10	236	209	-4	157	143	15	490	486	-3	1496	1470	12	824	831	-1	491	483
11	355	374	-3	460	480	4, 0, L			-2	206	196	14	627	617	0	140	123
12	136	139	-2	136	116	-13	253	274	-1	1090	1074	15	158	130	2	132	110
13	130	138	-1	468	454	-12	326	314	0	693	687	16	440	438	3	880	936
4, -3, L			0	349	328	-11	322	341	1	738	769	17	100	83	4	1103	1151
-13	358	354	1	122	143	-10	446	414	2	1049	1060	4, 3, L			5	374	347
-11	552	571	2	233	217	-9	408	400	4	649	634	-12	169	168	6	917	917
-10	130	130	4	291	264	-8	879	866	5	388	358	-10	356	360	7	375	334
-9	322	335	5	322	323	-7	302	292	6	133	135	-8	185	189	8	1241	1255
-8	151	170	6	243	228	-6	734	732	7	420	423	-7	339	333	9	171	103
-7	480	502	7	485	473	-4	1094	1052	8	638	608	-5	835	847	10	1022	1065
-6	234	235	8	369	333	-3	282	253	9	617	614	-4	492	504	11	285	294
-5	327	380	9	330	339	-2	649	671	12	193	193	-3	329	329	12	660	668
-4	93	128	10	323	326	-1	426	430	13	231	212	-1	712	724	13	266	283
-3	1368	1406	12	299	291	0	649	664	14	453	442	0	826	869	14	533	505
-1	91	28	13	325	308	1	788	796	15	199	199	1	229	239	15	329	364
0	383	386	14	319	328	2	333	321	16	193	180	2	650	690	16	263	275
1	1052	1069	4, -1, L			3	174	151	4, 2, L			3	585	636	17	121	136
2	162	142	-13	108	164	5	462	464	-12	482	499	4	575	576	4, 5, L		
3	1115	1068	-12	191	219	6	434	463	-11	304	291	5	1070	997	-11	388	395
4	90	73	-11	571	541	8	656	657	-10	625	600	6	90	66	-8	218	230
5	430	449	-7	690	717	9	421	427	-9	102	142	7	743	746	-7	313	297
6	213	215	-6	254	241	10	1033	1029	-8	776	766	9	600	630	-6	116	150
7	922	912	-5	1281	1279	11	241	243	-6	822	808	10	330	316	-5	161	114
8	134	129	-4	473	447	12	415	394	-5	258	239	11	237	232	-4	397	392

4, 5, L		
-2	112	120
-1	248	255
0	291	298
1	626	667
3	440	442
4	618	613
5	1822	1806
6	297	285
7	695	693
8	505	457
9	1030	976
10	158	123
11	363	397
12	249	255
15	443	462
17	182	179
18	120	119

4, 6, L		
-10	422	442
-9	304	317
-8	308	300
-6	425	411
-5	347	339
-4	486	448
-3	420	416
-2	229	238
-1	370	357
1	232	222
2	155	196
3	282	290
4	423	387
5	270	281
6	492	494
7	577	546
8	128	55
10	412	413
11	694	678
12	273	292
13	340	350
17	208	218
18	128	141

4, 7, L		
-9	369	342
-8	243	251
-7	148	115
-6	172	171
-5	243	253
-4	274	252
-3	936	936
-2	241	243
-1	492	496
1	1239	1242
2	322	332
3	933	960
4	330	308
5	278	285
6	426	402
7	1224	1210
8	193	204
9	452	459
10	214	246
11	355	283
13	439	437
15	610	627
17	347	353

4, 8, L		
-9	162	196
-8	265	264
-7	333	310
-6	206	181
-5	274	256
-4	144	164
-3	197	216
-2	94	52
-1	117	104
0	478	471
1	274	277
3	307	292
4	173	172
5	289	283
6	527	463
7	663	625
9	658	648
10	354	351
11	327	323
12	358	346
13	600	550
14	552	509
15	236	227
16	325	322
18	351	381

4, 9, L		
-7	409	416
-4	124	164
-3	338	337
-1	779	757
1	554	568
2	163	172
3	965	957
4	186	25
5	1118	1127
6	547	536
7	718	697
8	426	447
9	168	179
10	129	133
11	253	246
13	190	202
14	168	166
15	536	510
16	197	160
17	236	242

4, 10, L		
-7	188	180
-5	374	378
-4	324	329
-2	592	589
1	221	226
2	360	369
3	391	376
4	390	400
5	258	256
6	596	599
7	154	143
8	214	213
9	406	406
10	310	322
11	343	356
12	271	297
13	212	210
14	688	681
16	456	413
18	524	522

4, 11, L		
-6	213	220
-5	207	196
-4	140	156
-2	210	203
-1	529	515
0	242	233
1	302	302
2	255	250
3	532	535
4	223	240
5	240	234
6	171	189
7	182	160
8	460	443
10	284	291
12	264	273
14	184	179
16	250	251

4, 12, L		
-4	395	399
-2	681	660
0	479	466
2	490	475
4	416	405
6	403	400
7	175	206
8	216	211
9	287	299
10	518	534
11	138	115
12	412	415
13	216	222
14	546	614
16	399	405

4, 13, L		
-2	167	150
-1	104	103
1	251	261
2	231	238
4	397	395
6	337	343
8	541	524
9	398	394
10	364	367
12	397	403
13	376	414

4, 14, L		
-2	542	555
0	511	487
2	566	538
3	340	341
4	250	234
5	172	152
6	276	280
8	394	399
10	427	426
11	180	176
12	278	288
14	451	478

4, 15, L		
0	263	273
1	265	256
4	213	211
5	263	277
6	295	281
7	476	503
8	237	226
9	407	434
10	324	328
11	252	260
12	222	237
13	286	297
14	128	155

4, 16, L		
4	179	193
5	104	116
6	121	126
8	169	171
10	330	331
11	237	265
12	315	331

5,-12, L		
-5	316	336
-3	188	200
-2	173	205

5,-11, L		
-8	266	289
-6	437	446
-5	104	119
-4	447	461
-3	231	221
-2	207	230

5,-11, L			3	254	240	6	166	151	5	322	302	0	253	240	-10	301	281
2	314	339	4	100	90	7	737	691	7	671	677	1	345	347	-9	583	559
5,-10, L			5	395	386	8	158	165	9	428	435	3	775	746	-8	115	115
-9	284	288	7	232	231	9	238	246	10	273	273	4	421	433	-7	307	343
-4	185	202	5, -7, L			5, -5, L			11	414	440	5	665	636	-6	419	303
-2	208	230	-12	259	268	-11	268	282	5, -3, L			6	1048	1030	-5	237	235
0	352	386	-10	548	508	-10	251	264	-11	183	195	7	507	491	-3	112	130
1	116	152	-9	427	394	-8	205	229	-9	482	498	8	441	418	-2	313	324
2	250	254	-8	409	386	-7	340	352	-7	259	262	10	341	331	-1	109	89
4	184	191	-7	638	616	-6	262	264	-6	766	747	11	317	319	0	244	245
5, -9, L			-6	318	308	-5	499	451	-5	346	358	12	204	206	2	474	489
-10	522	495	-5	512	532	-4	295	305	-4	516	536	5, -1, L			3	1056	1016
-9	136	150	-4	359	330	-3	546	548	-3	419	385	-12	252	258	4	87	24
-8	250	239	-3	488	485	-2	191	222	-2	565	538	-11	222	224	5	329	343
-7	209	198	0	119	130	-1	590	612	0	694	715	-10	239	220	6	667	638
-6	635	658	2	177	177	0	213	218	1	128	109	-9	331	316	7	263	235
-5	245	268	4	130	107	3	195	182	2	853	835	-8	276	246	8	533	509
-4	348	364	5	305	309	4	228	221	3	245	226	-7	497	485	10	281	287
-3	194	199	6	290	268	5	313	292	4	96	133	-6	612	573	11	130	91
-2	444	455	7	313	307	6	106	86	5	220	203	-5	472	487	12	290	287
0	254	264	8	391	388	8	132	94	6	444	436	-4	561	537	13	122	135
2	288	295	9	201	200	9	465	457	7	499	482	-2	1426	1424	14	241	235
4	365	351	5, -6, L			11	282	279	8	218	229	-1	220	216	5, 1, L		
5	171	153	-11	416	396	5, -4, L			10	536	542	0	383	404	-12	267	285
6	299	320	-9	294	280	-13	252	244	11	286	274	2	1505	1580	-11	254	253
5, -8, L			-8	393	360	-12	276	278	12	204	203	4	513	484	-10	708	702
-11	133	110	-7	494	484	-11	382	380	5, -2, L			5	213	188	-9	364	377
-8	137	127	-6	156	167	-10	196	173	-13	238	244	6	771	771	-8	315	300
-7	281	284	-5	571	560	-9	590	580	-12	244	224	7	146	35	-6	1150	1121
-6	314	322	-4	469	479	-7	563	553	-11	629	617	8	561	551	-4	252	248
-5	118	155	-3	655	632	-6	150	150	-10	400	427	9	98	54	-2	873	849
-4	383	394	-2	666	670	-5	616	636	-9	426	422	10	422	425	-1	460	454
-3	316	314	-1	666	656	-4	326	318	-8	313	325	12	425	425	0	788	815
-2	589	605	0	617	628	-3	704	686	-6	188	180	14	472	476	1	278	270
-1	238	221	1	421	419	-1	681	703	-5	654	646	5, 0, L			2	266	293
0	369	380	3	519	507	1	549	564	-3	270	300	-13	244	252	3	279	269
1	427	402	4	255	231	3	901	919	-2	193	197	-12	289	287	4	638	596
2	454	468	5	765	725	4	348	328	-1	938	979	-11	161	197	6	1216	1144

5, 1, L		
8	505	519
10	512	514
11	157	160
12	648	649
14	393	377
15	218	206
16	371	365
5, 2, L		
-12	309	310
-10	328	320
-8	118	104
-7	269	274
-6	315	310
-4	89	81
-3	883	878
-2	237	256
-1	218	214
0	314	319
1	129	117
2	429	467
3	320	338
4	804	870
5	625	607
6	335	351
7	378	395
8	435	418
9	437	500
10	155	196
11	488	508
13	463	458
15	420	419
5, 3, L		
-10	501	488
-8	561	590
-6	629	646
-4	394	435
-3	490	486
-2	985	995
-1	339	355
0	555	566
1	841	866
2	313	337
3	267	287
4	108	151
6	688	658
7	209	214
8	756	737
10	480	478
11	136	113
12	322	328
13	240	210
14	290	309
15	437	443
16	110	136
17	310	308
5, 4, L		
-11	372	383
-10	231	224
-9	215	188
-8	141	126
-7	543	551
-6	185	194
-5	390	407
-4	123	80
-3	692	690
-2	231	208
-1	735	727
0	165	153
1	833	901
3	142	168
4	297	320
5	776	809
6	509	503
7	620	631
9	290	293
11	839	827
12	133	135
13	357	347
14	271	299
15	626	635
17	256	255
5, 5, L		
-10	252	244
-9	287	262
-8	197	191
-7	279	266
-6	324	315
-5	294	274
-4	124	49
-3	578	554
-2	133	103
-1	565	557
0	319	338
2	455	449
3	457	463
5	283	293
6	648	612
7	287	289
8	219	211
11	389	371
12	594	615
13	287	263
14	496	492
15	370	365
17	323	336
5, 6, L		
-9	381	399
-7	516	530
-5	312	305
-4	229	160
-3	690	683
-2	366	345
-1	882	870
0	360	372
1	625	629
2	105	97
3	1616	1752
4	86	78
5	638	672
6	182	166
7	1285	1298
9	725	711
10	613	611
11	622	578
12	272	265
13	148	142
14	196	199
15	501	486
16	101	128
17	195	185
5, 7, L		
-7	302	288
-6	142	90
-5	281	276
-4	120	123
-3	548	547
-2	232	204
-1	1039	1004
0	516	484
1	299	299
2	415	437
4	195	194
5	335	313
6	822	815
7	225	239
10	235	230
13	445	457
14	414	413
15	534	534
16	392	403
17	235	237
18	230	245
5, 8, L		
-8	155	126
-7	308	307
-6	229	203
-5	597	634
-3	120	90
-2	428	401
-1	490	484
1	489	505
2	334	265
3	867	891
4	151	114
5	645	685
6	126	115
7	950	918
8	527	513
9	605	581
10	266	294
11	835	839
12	295	279
14	435	425
15	266	261
5, 9, L		
-6	429	425
-5	422	404
-4	357	348
-2	778	759
-1	91	58
0	145	152
1	401	387
2	735	743
4	446	482
5	177	169
6	558	601
8	319	326
9	133	129
10	678	665
11	264	272
12	267	318
13	105	122
14	681	657
15	275	270
16	300	264
17	250	248
18	304	318
5, 10, L		
-6	338	330
-4	405	391
-3	194	156
-1	288	286
0	369	344
1	321	324
2	139	115
3	282	286
4	190	201
6	833	829
7	593	602
8	697	695
9	401	407
10	627	632
12	177	200
16	258	258
5, 11, L		
-5	98	78
-4	337	331
-3	329	322
-2	780	725
0	666	617
1	224	204
2	558	514
4	320	313
5	638	622
6	728	727
7	408	422
8	496	494

5, 11, L		
9	240	254
10	513	516
12	475	498
13	386	403
14	350	381
16	362	389
5, 12, L		
-4	267	276
-3	312	291
-2	201	186
0	267	264
2	182	178
4	219	206
6	307	292
7	176	178
8	763	726
9	268	239
10	627	620
11	112	71
12	621	641
13	319	323
14	290	320
15	273	361
17	173	199
5, 13, L		
-2	376	381
-1	135	151
0	349	346
2	312	305
3	511	489
4	477	458
5	433	416
6	307	274
7	492	473
8	276	286
9	160	212
10	398	387

12	230	233
16	186	202
5, 14, L		
-1	171	189
0	200	205
1	264	247
3	199	197
4	112	128
6	237	239
7	458	447
8	282	270
9	331	343
10	326	336
11	496	498
12	146	149
13	297	306
15	417	472
5, 15, L		
1	203	193
2	216	221
3	353	336
4	128	144
5	351	360
7	131	151
5, 16, L		
6	144	148
7	260	263
8	261	250
9	463	473
11	373	410
6,-10, L		
-6	216	199
-5	249	251
-4	316	340
-3	196	207
-2	270	260
-1	208	197
0	251	237

1	182	215
2	191	197
6, -9, L		
-7	221	225
-6	202	200
-5	299	321
-3	368	367
0	207	218
1	297	320
2	132	142
3	262	295
6, -8, L		
-10	181	153
-9	117	117
-8	143	126
-5	221	240
-4	214	207
-3	179	198
-2	304	331
-1	297	309
0	207	203
1	484	501
2	247	230
3	277	277
6, -7, L		
-9	317	287
-8	214	211
-7	462	453
-6	316	307
-5	653	694
-3	338	362
-2	115	134
-1	524	555
1	386	386
3	460	461
5	226	206
6	224	213
7	375	391

6, -6, L		
-9	153	132
-5	390	417
-3	537	510
-1	602	628
0	268	266
1	152	196
2	144	147
3	310	328
4	250	236
6	386	360
7	151	144
8	130	127
9	144	137
6, -5, L		
-10	337	326
-9	487	461
-8	332	314
-7	452	450
-6	472	449
-5	450	456
-4	214	222
-3	471	491
-2	327	349
-1	808	825
0	275	275
1	620	626
2	176	166
3	492	494
5	242	225
6	339	323
7	287	291
8	244	242
9	484	474
10	404	408

6, -4, L		
-10	361	359
-9	255	266
-8	202	179
-6	458	448
-5	285	296
-4	182	154
-3	371	355
-2	495	483
-1	540	539
0	248	239
1	189	199
2	277	302
4	300	304
6	458	477
8	482	484
10	480	505
6, -3, L		
-11	120	131
-10	512	494
-9	288	279
-8	216	203
-6	258	259
-5	414	417
-2	294	321
-1	323	345
0	280	287
1	430	420
2	354	342
4	525	523
5	178	170
6	554	561
7	189	158
8	449	465
10	388	403
11	301	315
12	346	347

6, -2, L		
-12	203	238
-10	447	446
-9	223	223
-8	321	295
-6	442	430
-5	361	359
-4	737	747
-3	226	239
-2	730	743
-1	332	339
0	578	573
1	498	505
2	645	631
3	466	457
4	802	781
5	358	384
6	484	496
8	366	381
9	122	98
10	766	772
12	463	466
13	202	194
6, -1, L		
-12	322	312
-10	495	470
-9	289	299
-8	429	391
-6	263	223
-5	165	209
-3	470	438
-2	503	496
-1	144	139
0	377	392
1	619	613
2	274	297
4	560	545
5	837	801

6, -1, L		
6	782	738
7	192	183
8	782	784
10	228	230
11	494	484
12	147	164
13	104	112

6, 0, L		
-10	656	652
-8	306	283
-6	436	400
-4	578	548
-2	532	559
-1	493	483
0	594	593
1	346	347
2	764	747
3	297	311
4	427	423
5	376	361
6	902	871
7	674	639
8	839	844
9	212	192
10	312	321
12	485	504
14	171	182

6, 1, L		
-10	443	444
-8	136	85
-6	343	302
-5	349	345
-4	297	295
-3	200	199
-2	335	300
-1	506	493
0	563	529
1	749	728
2	718	723
3	941	958
4	839	814
5	539	519
6	796	764
7	875	873
8	385	337
9	231	200
10	104	118
11	246	251
13	320	304
15	330	328

6, 2, L		
-11	188	209
-10	354	341
-8	482	443
-7	263	257
-6	217	193
-4	368	359
-3	417	404
-2	255	242
-1	689	664
0	110	70
1	600	575
3	580	612
4	659	648
5	524	574
6	337	314
7	725	718
8	617	568
10	233	258
15	311	321
16	101	95

6, 3, L		
-10	285	253
-9	164	159
-8	198	162
-6	128	114
-5	315	324
-3	189	181
-2	390	369
-1	1138	1154
0	168	151
1	977	1013
2	140	127
3	683	702
4	316	324
5	800	878
7	1130	1104
8	627	622
10	261	243
11	333	332
12	242	250
13	233	240
14	288	291
15	274	281
16	106	127

6, 4, L		
-9	218	221
-7	145	137
-6	106	90
-5	186	217
-4	203	194
-2	428	397
-1	997	1024
0	184	167
1	652	673
2	216	196
3	805	844
4	291	306
5	641	691
6	209	208
7	779	744
9	196	227
10	585	555
11	203	170
13	134	161
14	393	401
15	251	237
16	220	252
17	229	255

6, 5, L		
-9	347	349
-7	409	396
-5	289	277
-3	497	507
-2	285	252
-1	1281	1311
0	499	485
1	411	432
2	646	648
3	1122	1215
4	348	384
5	758	783
6	305	302
7	420	410
8	167	165
9	242	237
10	362	338
12	240	222
13	141	141
14	139	112
15	311	329
16	382	398
17	158	179

6, 6, L		
-6	367	327
-5	98	47
-4	294	288
-3	442	435
-2	710	722
-1	860	851
0	255	254
1	507	515
2	454	466
3	540	570
4	145	140
5	461	469
6	384	401
7	642	619
8	640	641
9	269	225
10	495	449
11	174	170
12	355	342
13	180	173
14	408	418
15	227	239
16	467	469
17	265	270

6, 7, L		
-8	201	181
-7	202	190
-6	204	190
-5	769	796
-4	344	339
-3	242	226
-2	765	760
-1	470	475
0	438	428
1	935	955
2	410	386
3	377	369
5	615	612
6	471	506
7	451	445
8	429	426
9	119	96
10	355	355
11	417	440
12	242	227
14	547	543
16	421	430

6, 8, L		
-6	625	633
-5	193	179
-4	475	466
-3	131	94
-2	395	388
-1	339	315
0	356	351
1	494	523
2	470	450
3	628	654
4	551	546
5	329	324
6	492	511
7	219	206
8	616	626
10	876	865
11	203	222
12	172	188
14	401	394
16	407	397

6, 9, L		
-6	437	421
-5	112	11
-4	365	380
-3	301	309
-2	541	536
-1	133	126
0	435	436
2	352	356
3	194	184
4	268	270
5	376	355
6	415	431
7	120	120
8	477	500

6, 9, L		
10	338	336
12	332	341
14	391	366
16	524	529
6, 10, L		
-4	593	606
-2	489	477
-1	170	143
0	439	433
2	456	453
4	255	278
5	341	352
6	563	533
7	392	371
8	540	536
9	281	273
10	221	214
12	495	483
14	282	270
16	306	286
6, 11, L		
-4	398	394
-3	321	310
-2	267	262
0	275	261
3	390	385
4	142	159
5	696	680
7	623	629
8	518	501
9	320	304
10	391	401
11	420	408
12	440	434
13	328	311
14	330	348
15	360	369
16	258	290
6, 12, L		
-2	304	301
0	410	403
2	249	240
3	426	412
4	280	291
5	266	260
7	655	631
8	207	234
9	408	394
10	264	261
11	241	268
12	242	256
16	178	163
6, 13, L		
-2	156	168
-1	263	274
0	198	209
1	137	117
2	145	161
3	498	485
4	127	128
5	351	338
6	223	227
7	555	564
9	374	376
10	149	158
11	617	616
12	365	376
13	366	345
14	118	119
15	277	282
6, 14, L		
1	184	186
3	358	361
5	575	566
6	145	126
7	229	241
9	176	183
11	137	167
15	157	169
6, 15, L		
3	326	333
5	343	311
6	144	130
7	187	180
8	170	164
9	436	429
11	355	362
12	179	199
13	172	183
6, 16, L		
5	254	282
6	207	191
7	264	271
8	200	183
9	204	201
10	152	176
11	255	248
7, -9, L		
-5	294	334
-3	358	377
-1	286	302
1	136	155
7, -8, L		
-7	136	119
-6	210	195
-5	425	435
-3	370	384
-2	167	177
-1	352	340
0	117	97
1	472	501
2	121	145
3	353	362
7, -7, L		
-6	268	264
-5	225	253
-4	383	376
-2	199	214
1	224	228
3	187	154
5	206	193
7, -6, L		
-9	157	147
-7	241	228
-5	302	270
-4	162	155
-3	424	412
-1	427	442
0	231	239
1	538	549
2	317	320
3	426	435
4	297	309
6	311	314
8	142	139
7, -5, L		
-9	206	191
-8	313	301
-7	294	300
-6	397	364
-4	536	522
-2	279	260
0	213	221
2	304	307
5	312	316
6	223	220
7	108	159
8	266	248
7, -4, L		
-10	306	315
-8	470	463
-7	245	213
-6	292	301
-5	255	251
-4	281	293
-3	270	262
-2	362	346
-1	464	480
0	340	333
1	373	381
2	151	167
3	177	161
4	106	114
5	227	227
6	295	306
7	297	294
8	319	344
9	109	95
10	215	220
7, -3, L		
-10	246	238
-8	586	572
-6	575	577
-4	369	349
-2	518	517
2	299	326
4	404	415
6	111	56
7	330	332
8	297	260
9	169	131
10	473	499
11	349	346
7, -2, L		
-10	284	275
-9	131	105
-8	264	258
-6	304	330
-5	123	111
-4	575	578
-3	214	189
-2	657	689
-1	333	316
0	310	314
2	196	192
3	281	291
4	320	320
5	393	399
6	320	336
7	460	469
8	284	296
9	476	458
11	296	295
12	329	349
7, -1, L		
-10	441	448
-9	125	123
-8	389	396
-6	415	413
-5	535	525
-4	565	540
-3	343	337
-2	127	129
-1	216	199
0	304	304
3	114	106
4	336	320
6	309	299
7	280	275
8	225	200
10	258	261

7, -1, L		
11	234	223
12	352	347
13	178	174
7, 0, L		
-10	220	211
-9	213	212
-8	348	334
-7	326	329
-4	320	300
-1	344	334
0	107	125
1	293	291
2	197	182
3	715	738
4	165	137
5	808	739
7	534	502
8	367	367
9	409	391
10	335	346
11	467	476
13	233	233
7, 1, L		
-10	310	341
-9	299	300
-8	321	333
-7	409	389
-5	300	333
-4	179	177
-3	133	138
-2	280	279
-1	401	383
0	232	228
1	170	198
3	595	587
5	500	466
6	205	160
7	730	721
8	191	146
9	489	501
10	348	350
11	191	189
13	157	155
7, 2, L		
-9	378	374
-7	134	129
-5	370	325
-4	206	187
-1	682	671
0	206	200
1	1053	1026
2	249	249
3	664	680
4	602	581
5	818	826
6	333	357
7	786	738
8	116	91
9	446	435
11	241	235
12	297	307
13	222	225
15	177	168
7, 3, L		
-9	386	384
-7	201	197
-5	605	588
-3	157	165
-2	292	292
-1	386	387
0	437	441
1	731	717
2	504	534
4	261	291
5	437	452
6	303	307
7	699	664
9	321	349
10	219	208
11	496	511
13	282	278
14	273	272
15	301	284
7, 4, L		
-9	306	307
-8	153	157
-7	297	286
-6	392	399
-4	322	319
-3	345	326
-2	370	375
-1	391	377
0	443	425
1	608	643
3	528	587
5	821	904
6	553	583
7	686	671
9	209	194
10	180	186
11	202	200
12	427	414
14	169	175
16	267	292
7, 5, L		
-7	202	176
-6	162	148
-5	122	137
-4	421	394
-3	211	164
-2	396	394
-1	516	514
0	681	685
1	528	556
2	555	574
3	728	739
4	498	547
5	189	215
6	584	593
7	489	492
8	534	509
12	317	310
13	259	244
14	277	285
16	444	419
7, 6, L		
-8	193	169
-7	94	91
-6	187	163
-5	202	160
-4	352	338
-3	144	94
-2	565	575
-1	202	161
0	430	426
1	278	292
2	346	361
3	433	449
4	295	318
5	190	207
6	124	145
7	466	468
8	192	185
9	165	145
10	363	334
12	303	308
14	430	427
15	183	175
16	385	397
7, 7, L		
-6	365	365
-4	535	526
-3	249	260
-2	515	514
-1	158	143
0	559	563
1	172	165
2	739	736
4	522	551
5	189	188
6	285	283
8	159	157
9	125	113
10	268	268
12	239	238
14	402	402
15	267	254
16	400	406
7, 8, L		
-6	358	358
-5	240	204
-4	261	252
-3	131	38
-2	248	233
-1	142	98
0	384	380
2	133	164
4	133	149
7	378	376
8	445	446
9	174	154
10	521	491
11	473	469
12	518	502
13	297	285
15	271	277
16	313	309
17	273	282
7, 9, L		
-5	148	131
-4	511	543
-2	520	509
-1	169	167
0	490	472
1	260	274
2	524	513
3	349	325
4	342	357
5	213	196
6	146	153
7	383	391
9	574	551
11	477	461
12	229	214
13	163	180
14	405	408
15	396	390
16	234	227
17	195	204
7, 10, L		
-4	408	394
-3	263	241
-2	234	212
0	437	454
1	148	167
2	175	201
3	306	293
4	166	156
5	319	307
7	320	289
8	247	210
9	560	554
10	213	222
11	432	432
13	601	606

7, 10, L		
14	180	174
15	336	332
16	197	200
7, 11, L		
-3	183	153
-2	225	209
-1	418	428
0	398	398
1	106	93
6	237	259
7	299	299
8	317	327
9	228	218
11	239	246
13	423	414
15	463	452
16	222	223
7, 12, L		
-1	228	219
2	383	390
3	156	179
4	164	162
5	482	451
7	392	382
8	99	96
9	501	493
11	574	570
13	383	385
14	229	218
15	282	296
7, 13, L		
1	363	360
3	322	321
4	414	400
5	344	344
6	392	404
7	191	200
8	198	218
10	178	150
11	289	284
15	205	198
7, 14, L		
1	154	188
2	204	174
5	258	255
6	141	138
7	282	252
9	372	366
10	147	129
11	545	547
12	170	152
13	212	227
14	182	163
7, 15, L		
4	356	336
5	181	192
6	367	373
7	184	162
8	243	230
9	299	284
10	204	211
11	336	347
12	194	214
13	203	196
7, 16, L		
8	361	344
9	215	205
8, -7, L		
-4	130	159
-2	261	279
1	262	250
2	300	293
3	218	227
8, -6, L		
-6	240	228
-4	386	372
-2	393	381
0	408	405
2	283	283
4	285	269
8, -5, L		
-6	285	287
-3	172	172
-1	129	167
0	328	329
2	220	208
4	257	241
6	390	400
8, -4, L		
-8	235	247
-6	413	415
-4	489	489
-2	288	302
-1	358	376
0	165	150
1	297	305
2	294	264
3	294	291
4	197	185
5	437	436
7	193	190
8, -3, L		
-8	288	286
-7	268	292
-5	301	319
-4	221	234
-3	294	296
-1	156	176
1	134	148
2	258	218
3	305	293
4	160	132
5	333	326
6	191	191
7	302	271
8	379	381
9	256	242
8, -2, L		
-8	238	251
-6	450	447
-5	309	300
-4	490	503
-3	330	319
-2	341	343
-1	208	186
0	311	299
1	598	594
2	191	185
3	488	505
4	190	179
5	527	531
6	133	119
7	322	325
9	245	233
10	257	236
11	277	290
8, -1, L		
-7	526	514
-5	462	437
-4	197	213
-3	199	180
-2	236	214
-1	283	270
0	223	234
1	186	198
3	466	499
5	454	435
6	247	204
7	311	278
9	387	374
11	410	427
12	165	134
8, 0, L		
-7	211	191
-4	252	242
-3	638	642
-2	243	233
-1	483	464
1	346	342
2	159	171
3	504	509
4	184	192
5	298	293
7	481	498
9	187	171
11	295	297
13	310	313
8, 1, L		
-7	352	347
-5	428	400
-4	422	405
-3	393	360
-2	356	345
-1	262	268
0	217	203
1	266	259
2	393	402
3	233	210
4	128	113
5	604	594
6	374	342
7	512	482
8	218	167
9	331	320
10	330	323
11	339	344
12	251	248
13	279	288
8, 2, L		
-5	283	291
-4	176	183
-3	361	359
-2	298	306
-1	356	342
0	327	317
1	430	411
2	576	564
3	214	223
4	337	319
5	152	149
6	504	486
8	321	295
9	270	271
10	116	119
11	279	275
12	310	334
13	194	171
8, 3, L		
-8	245	240
-7	428	417
-6	458	447
-5	136	116
-4	321	293
-3	154	134
-2	420	394
-1	240	246
0	525	532
2	128	121
3	285	278
4	215	218
5	467	456
6	437	444
7	390	412
8	646	622
9	400	364

8, 3, L

10	418	399
11	272	265
12	510	511
14	409	383
15	102	17

8, 4, L

-7	119	115
-6	297	300
-5	164	149
-4	264	270
-3	214	188
-2	471	457
-1	331	318
0	589	607
1	298	287
2	467	488
3	281	283
4	732	769
5	316	326
6	261	279
8	541	527
10	358	358
12	204	190
13	216	201
14	384	392

8, 5, L

-6	410	396
-4	558	556
-2	440	433
-1	154	98
0	495	509
2	314	332
3	207	224
5	260	256
6	459	461
7	200	207
8	575	548
10	552	531
12	431	405
14	381	364
15	295	260

8, 6, L

-6	208	238
-4	365	376
-2	274	277
-1	159	151
0	491	493
1	196	188
2	621	647
3	234	246
4	395	412
6	489	522
7	241	220
8	344	356
10	371	354
12	278	273
13	180	189
14	214	224
16	273	275

8, 7, L

-6	417	405
-5	286	284
-4	364	352
-3	173	160
-2	312	309
-1	216	198
0	353	352
1	330	324
2	265	269
3	247	255
4	212	195
6	505	544
8	415	407
9	278	262
10	611	574
11	322	296
12	377	339
13	331	316
14	141	143
15	318	313

8, 8, L

-5	171	148
-4	173	140
-3	224	202
-2	187	159
-1	155	137
0	190	184
1	493	500
2	231	212
3	305	295
4	367	378
5	549	566
6	148	184
9	520	507
10	145	101
11	303	298
14	278	260
15	277	269
16	163	150

8, 9, L

-4	235	253
-3	442	466
-1	325	328
1	191	188
2	175	152
3	407	419
4	207	187
5	369	386
6	340	343
7	247	262
8	199	199
9	343	327
11	494	468
12	355	340
13	617	583
15	500	486

8, 10, L

-3	217	212
-1	361	352
0	176	162
1	470	442
2	308	285
3	581	562
4	174	86
5	572	574
7	512	494
9	122	108
10	187	208
11	385	376
12	237	244
13	172	178
15	173	157

8, 11, L

-2	186	179
-1	207	216
0	252	248
1	258	232
2	104	105
3	289	285
5	321	305
7	181	191
8	232	242
9	300	330
11	472	470
12	210	231
13	542	546
14	156	165
15	351	343

8, 12, L

1	453	448
3	473	459
4	133	136
5	341	335
6	172	172
7	456	439
9	314	300
12	327	345

8, 13, L

2	256	245
6	196	168
8	260	269
9	370	350
11	283	285
12	212	240
13	200	198
14	343	347

8, 14, L

3	184	184
4	329	327
5	290	283
6	309	303
8	406	388
10	245	245
12	260	266

8, 15, L

6	177	163
9	167	168
10	347	379

9, -5, L

-3	143	142
-1	266	292
0	249	273
1	254	253
2	310	324
3	341	361
4	287	294

9, -4, L

-1	255	260
1	183	203
2	240	237
3	229	249
4	187	162
5	332	347
6	240	215

9, -3, L

-4	201	219
-3	223	217
-1	222	230
1	519	542
3	550	546
5	433	446
6	202	186
7	433	443

9, -2, L

-5	291	296
-4	155	141
-3	375	393
-2	189	208
-1	242	271
0	282	287
1	442	458
2	285	314
3	342	359
5	303	327
7	309	294
9	211	210

9, -1, L

-5	118	100
-1	325	318
0	224	221
1	154	157
3	573	590
5	528	491
7	275	246

9, -1, L		
8	185	172
9	234	215
9, 0, L		
-6	194	162
-5	337	347
-4	305	302
-3	365	360
-2	470	472
-1	387	395
0	225	215
1	222	223
2	416	435
3	226	210
4	590	610
5	356	345
6	318	299
8	306	319
9	244	257
10	298	288
11	268	288
9, 1, L		
-6	304	309
-4	138	144
-3	255	234
-1	365	356
1	527	541
3	383	378
4	330	322
5	487	460
6	152	119
7	177	142
8	267	270
9	167	158
10	231	209
12	331	326

9, 2, L		
-6	336	351
-5	141	99
-4	516	527
-3	397	389
-2	539	519
-1	433	410
0	654	659
1	393	389
2	337	321
3	164	158
4	337	326
6	412	409
8	113	124
10	233	238
12	320	328
9, 3, L		
-6	265	265
-5	142	126
-4	254	252
-2	235	239
-1	155	113
0	504	512
1	292	296
3	535	538
4	230	212
6	209	231
8	271	253
9	207	221
10	273	271
11	314	319
12	222	220
13	216	205
9, 4, L		
-4	456	476
-2	418	413
0	360	356
2	639	639

3	251	268
4	121	93
5	171	180
6	299	297
8	178	177
9	228	214
10	181	158
11	184	185
12	314	333
13	265	281
14	274	278
9, 5, L		
-5	105	121
-4	336	349
-2	287	282
0	263	270
4	148	132
5	392	405
6	131	119
7	554	592
8	223	220
9	410	378
11	372	378
13	321	327
9, 6, L		
-4	320	322
-2	348	362
-1	154	183
0	167	159
1	186	191
2	168	143
3	215	216
6	251	287
7	160	144
8	241	205
9	547	532
10	140	150
11	325	311

12	337	330
13	237	237
14	358	348
9, 7, L		
-4	219	239
-3	247	270
-2	172	181
0	216	220
1	199	199
3	592	598
4	280	260
5	496	510
6	209	201
7	637	670
8	317	319
9	644	646
11	631	592
12	203	198
13	409	384
15	196	183
9, 8, L		
-3	327	335
-2	218	215
-1	241	235
0	230	239
3	291	282
4	158	67
5	252	261
8	245	246
9	383	357
11	237	204
13	380	364
15	310	321
9, 9, L		
-2	111	115
-1	290	286
1	299	291
3	525	524

4	214	203
5	786	834
7	392	391
9	488	490
10	284	291
11	458	456
12	292	285
13	295	268
15	188	166
9, 10, L		
-1	205	188
0	194	176
1	280	286
2	154	125
4	383	397
5	265	291
6	193	195
7	238	268
9	261	253
13	188	198
9, 11, L		
0	159	170
1	207	195
2	258	257
3	290	289
4	298	298
5	291	290
6	253	260
7	521	527
8	336	335
9	264	278
10	134	131
11	312	324
12	409	411
14	146	140

9, 12, L		
2	478	452
4	480	462
6	595	597
8	340	344
9	170	170
10	174	162
12	165	168
9, 13, L		
4	417	428
6	286	289
8	279	278
9	208	201
10	132	135
12	242	249
9, 14, L		
7	220	232
8	203	208
10	234	253
10, -3, L		
0	225	252
1	141	152
2	142	153
10, -2, L		
0	154	150
1	248	262
3	296	325
4	206	214
5	332	341
10, -1, L		
-2	368	369
0	406	414
1	158	155
2	338	362
3	146	148
4	231	241
5	371	374

10, 0, L
0 287 295
2 285 295
3 243 213
4 416 419
5 353 355
8 273 242
10, 1, L
-2 457 468
0 411 407
1 145 93
2 349 345
4 437 437
5 114 109
6 335 316
9 150 134
10, 2, L
-3 135 142
0 582 597
2 181 208
4 189 187
5 119 83
6 459 447
10 182 175
10, 3, L
-2 336 345
-1 140 109
0 392 403
2 276 269
4 266 269
6 175 163
8 149 153
9 237 227
11 226 228
10, 4, L
-3 177 185
-2 329 352
-1 307 320
0 290 280
1 160 158
2 420 428
5 223 237
7 275 259
9 268 262
10 154 177
11 190 188
10, 5, L
-3 237 228
-2 137 135
0 147 135
1 224 232
2 245 254
7 195 188
9 292 289
11 303 276
10, 6, L
-2 204 200
-1 163 127
0 288 285
1 293 302
3 246 230
5 318 328
7 185 196
8 380 407
9 331 340
11 391 394
12 171 190
13 362 362
10, 7, L
-1 232 236
3 284 287
5 202 215
8 245 248
9 479 508
10 305 303
13 206 202
10, 8, L
-1 182 196
3 183 149
4 350 357
5 276 267
7 155 125
8 302 302
9 244 193
10 232 231
11 338 323
12 128 124
13 379 347
10, 9, L
1 243 253
4 455 470
5 346 360
6 434 445
7 216 216
8 354 350
9 251 264
10 373 389
11 185 170
12 444 465
10, 10, L
2 142 120
4 397 390
6 281 290
8 281 293
9 222 224
11 256 232
10, 11, L
4 311 319
5 153 70
6 404 411
8 431 433
10 361 359
12 309 332
10, 12, L
6 324 357
8 135 135
11, 1, L
2 356 362
3 262 282
4 254 264
5 197 174
11, 2, L
1 243 278
3 211 242
6 343 330
11, 3, L
1 366 353
2 177 156
3 264 257
4 190 181
5 502 494
6 160 148
7 285 272
11, 4, L
1 364 389
4 194 206
11, 5, L
1 357 380
3 340 326
5 448 431
6 164 154
7 367 369
9 317 325
11, 6, L
1 163 178
2 159 154
4 278 273
8 185 187
9 221 223
11, 7, L
3 202 176
5 385 387
7 260 278
8 119 143
9 257 250
10 294 326
11, 8, L
4 396 384
6 315 315
8 167 163
11, 9, L
6 211 207
7 182 154
8 361 398

CALCULATED AND OBSERVED STRUCTURE FACTORS OF
[CpMo(F_3CCC(CF_3)C(CF_3)=C(CO_2Me)C(SPr^i)C(OMe)=O)]

0, 0, L
2 3426 2917
6 1169 1069
8 687 621
10 291 275
12 854 794
14 607 572
18 170 184
0, 1, L
2 1149 1016
3 179 172
4 1381 1230
5 684 654
6 1060 954
7 1202 1088
8 918 862
9 535 508
11 106 106
12 328 308
13 201 193
15 198 199
16 148 142
17 133 131
18 93 109
0, 2, L
0 1075 1031
1 1731 1708
2 98 86
3 65 44
4 367 331
5 1252 1146
6 213 205
7 242 241
8 230 204
9 529 500
10 294 277
11 474 466
13 436 405
14 132 158
15 247 244
16 94 118
17 173 185
0, 3, L
1 421 430
2 1211 1190
3 669 592
6 1005 969
7 788 753
8 755 702
9 407 396
11 453 447
12 221 218
13 274 286
14 213 232
15 147 146
16 265 297
0, 4, L
0 1427 1447
1 216 209
2 844 845
3 309 299
4 837 781
5 628 620
6 462 447
7 418 377
8 417 395
9 390 377
10 272 250
11 380 349
12 347 332
13 123 160
14 474 452
16 229 240
0, 5, L
1 583 558
3 810 824
4 118 121
5 913 885
6 776 714
7 781 725
8 543 513
9 799 782
12 205 183
13 109 133
14 139 140
15 120 133
17 269 285
0, 6, L
0 191 197
1 1354 1405
2 385 395
3 566 562
4 397 392
6 190 171
8 269 249
10 445 415
11 621 626
12 338 318
13 429 430
15 238 242
16 228 240
17 140 161
0, 7, L
2 124 138
3 335 334
4 711 734
5 410 405
6 449 458
7 492 482
8 771 757
9 162 139
10 542 567
11 134 125
16 275 301
0, 8, L
1 763 765
2 560 557
3 815 814
4 140 127
6 166 165
10 672 659
11 407 403
12 515 530
14 182 183
15 134 109
16 257 279
0, 9, L
1 309 303
2 271 277
3 530 537
4 303 313
5 902 901
6 504 513
7 209 205
8 267 267
9 506 522
10 263 258
11 242 245
12 209 211
0, 10, L
0 1030 1028
1 606 618
2 416 422
3 941 938
9 236 241
10 277 264
11 467 488
12 250 254
13 153 176
15 261 282
0, 11, L
1 199 183
3 176 180
4 791 804
6 407 394
8 373 366
9 134 131
10 329 340
0, 12, L
0 299 315
1 591 549
2 496 501
3 290 273
4 323 330
6 384 381
8 436 450
10 296 316
11 211 217
12 212 219
13 168 173
0, 13, L
3 508 497
4 189 181
5 415 406
6 305 306
7 210 209
8 166 151
9 399 419
10 115 133
11 196 219
0, 14, L
0 445 432
1 349 339
2 309 315
3 447 444
4 377 388
6 197 215
7 129 161
8 194 212
9 226 241
10 176 181
11 281 301
12 178 186
0, 15, L
2 256 265
4 417 419
6 649 669
8 440 490
9 120 131
10 212 241
0, 16, L
0 244 249
1 278 278
2 225 227
0, 17, L
1 162 160
3 219 240
5 287 276
7 331 343
0, 18, L
0 193 174
4 110 123
1, 0, L
-18 291 309
-16 339 337
-14 490 468
-12 216 232
-10 572 502
-8 1855 1772
-6 859 843
-4 2665 2397
2 677 651
4 3097 2578
6 1075 914
8 257 206

1, 0, L		
10	1114	1027
12	186	177
14	320	323
16	175	161

1, 1, L		
-17	151	162
-16	101	79
-15	256	233
-14	249	231
-13	371	358
-12	471	463
-11	307	293
-10	938	900
-9	324	301
-8	702	646
-7	681	626
-6	869	814
-4	303	276
-3	229	235
-2	2467	2468
-1	1302	1334
0	2366	2427
1	459	454
2	935	884
3	358	326
4	929	812
5	1318	1118
6	657	544
9	563	520
10	155	151
11	589	542
12	603	559
13	128	114
14	189	195
16	135	154
17	134	120

1, 2, L		
-17	359	358
-14	165	158
-13	325	331
-12	129	146
-11	183	168
-10	245	254
-9	874	815
-8	172	156
-7	451	463
-6	405	381
-5	106	69
-4	1144	1036
-3	89	69
-2	981	976
-1	311	328
0	220	228
1	245	255
2	1336	1269
3	1798	1671
4	814	753
5	1836	1668
6	501	445
7	1192	1098
8	218	187
9	783	716
10	337	325
11	695	671
13	114	124
14	159	183
15	193	199
17	204	222

1, 3, L		
-16	454	454
-15	269	263
-14	515	496
-13	108	134
-12	324	308
-11	308	300
-10	122	116
-9	510	484
-8	320	313
-7	131	135
-6	544	517
-5	540	490
-4	1226	1173
-3	1033	988
-2	2337	2319
-1	93	113
0	969	997
2	173	182
3	1624	1571
4	982	898
5	272	265
6	479	448
7	585	530
8	616	588
10	929	895
11	324	312
12	390	380
13	131	122
14	217	212
15	156	153
16	161	168
17	194	217

1, 4, L		
-18	283	284
-16	297	303
-12	221	216
-10	509	494
-9	152	157
-8	872	860
-7	842	793
-6	280	283
-5	793	763
-4	151	159
-3	1476	1425
-2	407	396
-1	1173	1200
0	960	1019
1	127	119
2	587	603
3	507	506
4	385	410
5	366	349
6	889	896
7	718	694
8	575	557
10	544	522
11	259	232
13	152	160
14	426	396
15	176	169
16	110	107

1, 5, L		
-17	271	270
-16	208	187
-15	284	256
-14	201	205
-13	574	563
-11	362	337
-10	318	304
-9	127	131
-7	305	278
-5	1366	1339
-4	663	646
-3	525	519
-2	757	750
-1	953	972
0	794	789
1	915	934
2	338	338
3	504	503
4	417	419
5	262	249
6	488	478
7	350	367
8	240	219
9	478	466
10	150	141
11	384	354
12	354	361
13	363	365
14	98	115
15	347	375

1, 6, L		
-15	163	177
-12	159	160
-11	326	300
-9	623	571
-8	198	170
-7	822	745
-5	1161	1131
-4	650	639
-3	306	295
-1	487	471
0	733	753
1	348	364
2	792	814
3	1612	1650
4	534	565
5	997	1037
6	305	309
7	819	845
8	408	415
9	464	472
12	377	376
15	210	236
16	180	173

1, 7, L		
-16	338	347
-14	365	381
-12	641	603
-11	290	255
-10	191	184
-8	173	144
-7	626	579
-6	228	240
-4	1113	1092
-3	370	363
-2	946	956
-1	1326	1326
0	1048	1051
1	899	925
2	582	567
3	647	643
4	529	528
5	416	422
6	298	317
7	598	594
8	184	191
9	203	209
10	614	630
11	344	370
12	394	402
13	318	334
14	265	290
16	139	158

1, 8, L		
-12	405	395
-11	345	328
-10	521	491
-9	222	206
-8	575	551
-7	714	722
-6	742	765
-5	543	558

1, 8, L		
-3	351	351
-1	221	205
0	209	182
1	302	299
2	575	619
3	678	705
4	640	645
6	923	929
7	406	421
8	709	719
9	188	208
10	240	254
12	230	242
14	148	163
16	217	244
1, 9, L		
-16	194	196
-15	236	225
-13	613	609
-11	306	292
-8	227	220
-7	465	437
-6	146	152
-5	319	321
-4	393	376
-3	1084	1121
-2	221	237
-1	1135	1165
0	265	259
1	1115	1129
3	169	184
4	166	142
9	693	720
10	277	304
11	326	367
13	164	171
15	265	306

1, 10, L		
-11	557	537
-10	262	255
-9	314	321
-8	312	308
-7	588	594
-6	362	367
-5	688	707
-4	251	248
-3	146	166
-2	205	198
-1	493	501
2	267	275
3	273	278
4	594	565
5	146	148
6	175	155
7	622	623
9	208	214
15	196	225
1, 11, L		
-14	252	246
-12	388	405
-10	232	224
-8	405	406
-5	135	159
-4	513	490
-2	553	545
-1	102	87
0	645	636
1	503	510
2	354	346
3	197	170
7	301	302
8	433	440
9	259	277
10	251	242
12	107	133

14	276	297
1, 12, L		
-12	208	241
-11	101	134
-10	388	426
-9	231	233
-8	364	392
-7	177	170
-6	570	563
-5	207	214
-4	394	399
0	192	198
2	563	553
3	468	441
4	375	361
5	282	255
6	218	225
8	409	403
9	248	252
1, 13, L		
-13	279	318
-11	240	252
-9	217	221
-8	261	275
-7	227	228
-5	385	385
-4	157	165
-3	477	478
-1	397	394
1	673	660
3	429	395
4	404	384
5	199	205
9	283	278
11	252	255

1, 14, L		
-11	255	277
-10	176	182
-9	322	326
-8	372	392
-7	429	422
-6	380	415
-5	385	401
-4	501	524
-3	241	243
-2	200	211
-1	279	268
0	164	152
3	126	137
4	607	556
6	658	627
7	340	334
8	220	228
9	180	181
1, 15, L		
-10	166	182
-7	175	191
-4	258	283
-2	518	523
0	530	516
2	490	479
3	143	167
4	185	183
6	136	152
7	163	146
8	198	192
10	254	274
1, 16, L		
-9	184	181
-8	219	253
-7	178	177
-6	318	328
-5	213	237

-4	187	208
-3	197	201
1	196	195
3	156	156
4	158	112
5	291	264
6	208	157
7	188	190
8	188	168
9	138	140
1, 17, L		
-5	250	262
-3	418	422
-1	430	436
1	186	189
3	167	140
4	159	140
6	154	142
1, 18, L		
4	267	252
2, 0, L		
-18	273	278
-16	327	317
-14	404	412
-12	846	826
-10	661	625
-8	413	360
-6	501	435
-4	1289	1299
-2	507	515
0	879	969
2	483	504
4	820	785
6	1256	1136
8	1263	1094
10	1319	1135
12	434	381
14	389	391

16	184	184
2, 1, L		
-18	267	285
-17	160	173
-13	202	201
-12	138	145
-11	332	289
-10	791	754
-9	825	817
-8	449	429
-7	411	393
-6	845	735
-5	211	195
-4	381	399
-3	623	660
-2	566	605
-1	754	780
0	857	888
1	1330	1361
2	128	59
3	1016	1021
4	861	873
5	530	503
6	112	93
7	799	732
8	1070	932
9	726	643
10	398	360
11	217	197
12	145	121
13	279	271
15	224	226
16	281	288
17	207	222
2, 2, L		
-17	407	413
-16	183	190
-15	446	452

2, 2, L			-5	200	219	4	277	269	2, 6, L			-5	653	613	2, 9, L		
-14	223	221	-3	285	295	5	636	590	-17	251	228	-4	531	512	-13	366	365
-13	552	544	-2	926	967	6	727	703	-15	410	396	-2	552	546	-12	283	282
-12	113	116	-1	167	159	7	631	616	-14	243	238	0	88	108	-11	469	469
-11	199	187	0	137	140	8	476	448	-13	481	483	1	89	115	-10	141	162
-10	375	386	1	409	430	9	220	227	-11	524	524	2	585	625	-9	605	596
-9	333	308	2	2310	2362	10	987	939	-10	191	192	3	781	805	-7	648	626
-8	162	149	3	715	735	12	416	408	-9	466	454	4	696	684	-5	270	267
-7	273	263	4	843	813	13	229	232	-7	481	468	5	188	167	-3	564	576
-6	352	355	5	306	319	14	365	350	-6	989	938	6	996	987	0	200	190
-5	799	797	6	832	812	16	231	245	-5	786	767	8	371	383	1	1147	1158
-3	1117	1160	7	90	75	2, 5, L			-4	84	97	10	381	382	2	112	76
-2	1493	1574	8	501	479	-13	370	346	-3	1426	1478	11	155	179	3	507	494
-1	884	920	9	261	249	-11	518	486	-2	617	646	12	125	127	4	227	208
0	757	782	10	264	247	-10	502	507	-1	1434	1465	14	197	206	5	724	697
1	234	224	12	271	270	-9	647	600	0	1049	1102	2, 8, L			6	554	554
2	530	522	14	361	365	-8	167	141	1	1007	1038	-16	297	289	7	698	687
3	293	281	16	81	100	-7	1422	1282	2	569	585	-15	179	178	9	236	255
4	573	554	17	292	329	-6	370	350	3	519	534	-14	327	334	10	143	147
5	597	547	2, 4, L			-5	807	798	4	427	389	-13	275	270	11	199	211
6	154	146	-18	262	256	-4	483	500	5	466	467	-12	241	239	13	279	296
8	398	366	-16	425	430	-3	271	275	6	265	285	-9	208	198	15	203	237
9	946	885	-15	240	235	-2	354	349	7	693	706	-5	356	338	2, 10, L		
10	328	312	-14	433	433	-1	615	605	8	112	103	-4	688	698	-15	251	271
11	599	545	-12	643	639	0	185	190	9	250	241	-2	1317	1384	-14	236	235
12	125	119	-10	334	320	1	1726	1827	10	121	105	-1	456	485	-13	390	400
13	256	249	-9	896	839	2	84	121	11	405	429	0	530	551	-12	224	229
15	318	338	-7	646	528	3	1094	1088	12	245	262	2	902	889	-11	240	245
2, 3, L			-6	251	249	4	679	684	13	435	438	3	352	360	-10	165	172
-18	148	147	-5	170	176	5	647	648	15	241	253	4	839	820	-7	480	475
-17	165	174	-4	986	1015	6	325	320	2, 7, L			6	212	206	-6	331	311
-12	349	326	-3	1138	1159	7	1045	1067	-14	196	175	7	418	411	-5	498	504
-11	455	459	-2	967	1053	8	534	540	-12	447	422	9	426	437	-4	444	432
-10	850	798	-1	190	209	9	145	143	-11	427	417	10	432	448	-3	662	672
-9	773	752	0	255	266	12	473	453	-10	530	494	12	311	328	-2	442	450
-8	462	480	1	476	475	13	185	160	-9	188	180	13	166	175	-1	1115	1095
-7	159	143	2	1336	1366	15	219	214	-8	686	626	14	116	120	1	672	664
-6	132	105	3	870	876	16	213	225	-6	683	676				2	211	210

2, 10, L		
3	302	278
6	321	319
7	613	594
8	352	352
9	345	348
10	221	221
11	231	235
12	205	209
13	308	336

2, 11, L		
-13	119	130
-12	272	276
-11	122	126
-10	488	490
-8	587	571
-7	319	301
-6	471	453
-5	260	273
-4	293	285
-3	303	316
-2	174	194
0	614	625
2	500	475
3	258	246
4	413	383
5	271	265
6	548	558
8	525	522
10	273	258

2, 12, L		
-14	182	178
-13	125	152
-7	175	175
-6	663	649
-5	284	278
-4	572	567
-2	495	498
0	547	537
1	176	184
3	208	194
6	197	201
8	328	333
9	276	282
11	152	144
12	268	276
13	164	157

2, 13, L		
-13	194	201
-9	377	390
-7	410	408
-5	173	165
-3	233	238
4	135	139
5	584	537
6	164	169
7	488	484

2, 14, L		
-12	218	245
-9	133	151
-7	159	183
-5	413	419
-4	280	272
-3	342	356
-2	327	328
-1	577	584
0	331	331
1	298	297
2	401	378
7	204	193
9	176	176
10	263	264
11	171	169

2, 15, L		
-10	267	293
-8	313	323
-6	433	456
-4	400	408
0	385	373
2	469	469
3	148	130
4	453	425
6	459	431
8	213	218

2, 16, L		
-6	203	214
-5	225	223
-4	163	147
-3	381	384
-2	277	269
-1	352	350
0	415	404
1	354	340
3	274	256

2, 17, L		
-7	285	298
-5	245	233
1	232	230
2	162	175
3	350	320
5	299	272

2, 18, L		
-5	195	224
-4	216	254
-3	226	244
-2	274	298
-1	185	190
0	188	159
1	145	168

3, 0, L		
-18	128	160
-14	348	346
-12	1078	1020
-10	646	615
-8	553	511
-6	1259	1322
-4	209	215
-2	428	453
0	601	690
2	907	978
4	184	212
6	1337	1289
8	599	532
10	133	121
12	263	255
14	429	417
16	372	392

3, 1, L		
-18	232	233
-17	251	254
-16	133	167
-15	404	421
-14	618	627
-13	336	334
-12	605	589
-10	112	125
-9	207	179
-6	1667	1691
-5	612	652
-4	1265	1350
-3	920	978
-2	556	597
0	1162	1218
1	578	601
2	659	691
3	282	296
4	456	472
6	637	660
7	240	242
8	953	906
9	602	580
10	377	357
11	325	304
12	229	211
13	501	485
14	279	280
15	95	99
16	100	110

3, 2, L		
-15	349	349
-13	582	569
-11	762	723
-10	249	246
-9	805	772
-8	398	387
-7	955	984
-5	308	328
-4	282	277
-2	1512	1555
-1	274	304
0	261	271
1	132	148
2	454	442
3	218	211
4	286	292
5	998	1005
6	198	194
7	620	632
10	151	148
12	184	184
13	367	366
15	378	381

3, 3, L		
-17	207	214
-16	285	285
-14	458	451
-13	580	563
-9	409	424
-8	204	215
-7	251	254
-6	697	732
-5	896	942
-4	577	619
-3	543	579
-2	530	550
-1	786	832
0	863	909
1	1144	1149
2	499	509
3	1046	1071
4	995	983
5	281	305
6	893	892
8	652	635
9	543	517
10	492	473
11	220	214
12	409	415
13	318	315
14	385	409

3, 4, L		
-17	178	199
-12	511	526
-10	687	640
-9	286	252
-8	1057	974
-7	304	309
-6	1306	1431
-5	664	672
-4	133	145

3, 4, L			10	182	168	-1	123	144	-8	201	180	10	191	207	8	200	177
-3	333	332	11	419	397	0	570	588	-7	559	563	12	233	252	10	133	141
-2	335	328	13	263	266	1	151	144	-5	469	471	13	154	171	12	144	141
-1	515	550	14	233	232	2	614	643	-3	1056	1090	3, 11, L			3, 13, L		
0	302	313	3, 6, L			3	219	205	-2	251	250	-14	264	276	-11	177	169
1	711	700	-14	257	251	4	339	332	-1	663	662	-12	265	273	-9	206	230
2	1407	1427	-13	325	314	5	173	178	0	203	216	-11	297	312	-7	415	433
3	424	413	-11	693	660	6	276	285	1	410	428	-10	140	130	-5	343	349
4	1268	1260	-10	315	295	8	227	244	2	263	267	-8	334	328	-3	683	674
6	843	846	-9	448	390	9	179	185	3	273	307	-7	269	252	-2	327	335
7	300	313	-8	467	469	10	564	576	5	648	620	-6	610	625	-1	601	578
8	263	251	-7	919	912	12	326	346	7	617	607	-5	122	123	1	432	422
9	173	172	-6	455	450	3, 8, L			8	170	172	-4	939	957	5	241	247
12	192	179	-5	980	1053	-15	116	135	9	449	438	-3	252	253	7	304	280
14	285	281	-3	183	211	-14	198	182	10	106	115	-2	738	728	9	370	348
16	305	334	-2	159	139	-12	389	386	11	504	508	-1	352	347	11	366	398
3, 5, L			-1	499	510	-10	546	516	13	179	181	0	207	203	3, 14, L		
-17	221	222	0	694	653	-9	416	395	3, 10, L			1	311	295	-12	193	225
-15	445	459	1	820	857	-8	481	450	-13	195	206	2	257	269	-10	213	225
-14	245	235	2	550	516	-6	745	783	-12	179	174	6	304	295	-9	246	246
-12	460	439	3	760	787	-4	597	600	-11	311	337	8	422	413	-8	254	270
-11	338	351	4	313	306	-3	197	209	-10	379	375	10	479	498	-6	463	464
-9	369	395	5	729	732	-1	603	647	-9	534	510	12	356	386	-2	242	259
-8	149	128	7	488	464	0	314	333	-8	158	155	3, 12, L			-1	337	304
-7	819	819	8	162	196	1	511	514	-4	156	139	-14	116	136	0	444	452
-5	290	318	11	228	217	2	550	571	-3	188	203	-12	133	142	1	193	162
-4	705	730	13	255	251	3	483	456	-2	300	304	-11	300	333	2	444	437
-3	472	479	15	240	254	4	787	742	-1	392	396	-10	366	372	3	421	393
-2	409	429	3, 7, L			5	697	661	0	265	291	-9	346	375	4	368	348
-1	234	248	-16	366	345	6	600	593	1	281	260	-8	298	292	5	601	533
0	1133	1161	-14	311	282	7	222	234	2	297	275	-2	367	372	6	378	359
1	533	509	-10	327	318	8	286	300	3	587	543	-1	187	203	7	195	174
2	378	370	-7	187	206	13	230	257	4	192	173	0	481	471	3, 15, L		
3	476	495	-6	201	218	3, 9, L			5	727	678	2	267	244	-6	277	280
4	383	359	-5	309	328	-15	324	339	6	274	272	3	215	180	-4	390	376
5	688	699	-4	775	823	-13	251	253	7	304	307	4	657	615	-3	170	163
7	391	380	-3	269	287	-11	326	330	8	450	457	5	449	414	-2	503	508
8	523	514	-2	1012	1094	-9	177	144	9	400	384	6	461	450	0	459	433

3,	15,	L	10	260	248	-5	961	1018	15	98	97	0	968	1012	-11	221	221
8	236	236	12	443	431	-3	919	975	4,	4,	L	1	626	681	-10	545	502
3,	16,	L	4,	1,	L	-2	411	416	-17	155	167	2	716	717	-8	399	433
-9	250	253	-15	203	215	-1	1211	1278	-16	307	312	3	998	971	-6	775	840
-7	314	341	-14	702	685	0	472	455	-14	305	292	4	620	614	-5	287	314
-5	314	325	-13	532	508	1	682	697	-9	280	270	6	328	336	-4	177	160
-4	162	177	-12	1063	1013	2	166	167	-8	690	732	8	105	95	-2	226	274
0	303	301	-11	477	414	4	587	620	-7	378	390	10	246	244	0	139	182
1	240	229	-10	597	530	6	323	323	-6	1189	1287	11	412	433	1	354	356
2	271	249	-9	545	578	7	422	425	-5	250	277	12	141	139	2	571	592
3	304	285	-8	665	686	8	105	122	-4	1095	1147	13	233	241	3	209	215
4	356	331	-7	695	731	9	397	405	-3	831	852	14	224	233	4	776	773
5	243	222	-6	113	137	11	369	371	-2	1262	1291	15	305	317	5	181	186
6	214	200	-5	291	300	12	157	172	-1	204	212	4,	6,	L	6	461	463
3,	17,	L	-4	199	206	13	324	324	0	868	879	-17	273	283	7	410	425
-7	162	179	-3	487	494	14	262	279	1	271	259	-15	334	325	8	165	156
-5	326	333	-2	608	613	4,	3,	L	2	375	345	-12	178	144	10	206	205
-3	388	387	-1	546	567	-15	210	228	3	94	83	-9	360	385	11	111	135
-1	343	347	0	1286	1336	-13	426	467	4	177	204	-8	259	249	12	248	267
1	153	169	1	726	757	-12	225	242	6	419	418	-7	764	806	14	186	200
3,	18,	L	2	291	311	-10	521	518	8	679	677	-5	630	684	4,	8,	L
0	228	218	3	296	310	-9	805	812	10	281	281	-3	1221	1313	-16	306	298
1	177	181	4	474	496	-8	874	901	11	202	214	-2	230	226	-14	281	268
2	319	306	5	1004	1038	-7	439	493	12	479	490	-1	330	350	-12	309	297
4,	0,	L	6	656	675	-5	439	452	14	183	169	0	237	242	-9	269	254
-18	132	135	7	372	374	-4	154	140	4,	5,	L	2	167	159	-8	301	325
-16	493	519	11	145	155	-3	426	434	-14	237	232	4	758	759	-7	211	234
-14	604	599	12	194	198	0	351	363	-13	141	164	5	423	431	-6	255	249
-10	207	191	13	365	369	1	86	101	-12	192	198	6	196	174	-5	248	266
-8	1057	1058	14	376	381	2	501	518	-11	823	775	7	652	639	-4	624	650
-6	1954	2007	15	160	190	3	828	830	-9	182	185	8	261	262	-3	458	451
-4	1484	1570	4,	2,	L	4	644	663	-8	427	476	9	616	630	-2	686	705
-2	1694	1833	-17	202	199	5	1012	1043	-7	413	423	10	358	347	0	207	216
0	1038	1057	-15	401	396	6	247	257	-5	411	461	11	438	466	1	667	651
2	436	440	-13	211	200	8	92	119	-4	214	233	4,	7,	L	2	425	407
4	231	258	-8	138	117	12	190	198	-3	572	586	-16	220	234	3	167	174
6	426	397	-7	509	552	13	226	223	-2	121	134	-13	100	75	4	437	407
8	756	744	-6	137	146	14	246	252	-1	377	382	-12	343	313	5	346	313

4, 8, L		
6	241	244
7	162	161
8	280	278
9	271	286
10	385	399
12	265	288
14	155	168

4, 9, L		
-15	197	203
-13	209	189
-11	644	633
-10	161	160
-9	374	372
-5	367	365
-3	263	280
-2	727	708
-1	376	369
0	329	346
1	316	312
3	902	865
5	272	271
7	185	187
9	178	175
11	356	385
13	138	151

4, 10, L		
-15	148	137
-13	359	381
-11	343	352
-9	362	374
-7	314	326
-6	232	225
-5	701	710
-4	594	633
-3	652	651
-2	306	314
-1	307	302
0	374	367
1	469	463
2	398	386
3	176	169
5	340	318
6	204	187
7	354	340
8	434	441
9	478	469
10	290	302
11	185	193

4, 11, L		
-14	198	189
-12	472	491
-10	627	606
-9	127	135
-8	247	253
-4	198	223
-2	430	422
-1	119	116
0	493	479
2	655	603
3	399	379
4	609	577
5	207	214
6	363	347
8	293	285
10	155	158
12	216	238

4, 12, L		
-13	199	197
-12	293	289
-9	371	375
-8	201	211
-5	228	225
-4	391	378
-3	297	285
-2	253	256
-1	204	179
1	174	177
3	222	228
4	252	228
5	187	204
6	160	146
8	320	318
9	265	255
10	350	357
11	235	224

4, 13, L		
-13	176	173
-11	358	372
-9	409	398
-8	213	226
-7	360	346
-6	110	122
-1	171	168
0	224	221
1	388	371
3	691	651
5	521	489
7	284	275
8	188	191

4, 14, L		
-6	393	413
-5	307	284
-4	309	301
-3	420	403
-2	444	428
-1	388	375
0	292	272
1	269	255
5	161	147
7	196	198
8	212	216
9	333	348

4, 15, L		
-10	250	253
-8	367	360
-2	204	200
0	462	431
2	525	486
4	465	432
6	200	210

4, 16, L		
-7	264	258
-6	184	196
-5	221	227
-4	258	277
-3	277	286
-1	321	310
0	172	153

4, 17, L		
-1	228	216
0	191	186
1	354	346
3	300	264

5, 0, L		
-14	400	408
-12	465	462
-10	650	673
-8	427	455
-6	282	272
-4	1187	1230
0	369	417
2	218	224
4	1029	1056
6	465	476
10	125	80
12	380	381
14	249	265

5, 1, L		
-18	229	241
-17	239	233
-16	418	420
-15	272	263
-12	193	187
-10	152	148
-9	318	320
-8	689	698
-7	482	499
-5	900	949
-4	1034	1107
-3	1158	1204
-2	827	833
-1	373	394
0	262	246
1	362	399
2	239	245
4	388	407
5	378	387
6	734	735
7	241	242
8	146	129
10	441	453
11	250	248
13	115	129
14	176	200

5, 2, L		
-15	313	303
-13	331	310
-11	335	325
-10	132	135
-9	574	598
-5	91	98
-4	766	819
-3	518	576
-2	697	725
-1	1371	1510
0	254	256
1	619	683
2	244	229
3	1092	1140
5	771	815
6	189	170
11	269	273
13	222	229

5, 3, L		
-17	252	255
-16	276	264
-14	172	169
-10	213	222
-9	610	619
-8	586	612
-7	214	199
-6	1131	1189
-5	301	322
-4	1063	1138
-3	532	556
-2	229	263
-1	211	197
3	322	318
5	507	541
6	556	566
7	238	248
8	486	487
9	108	103
10	161	141
11	181	167
12	379	403

5, 4, L		
-16	266	275
-14	359	329
-13	458	462
-12	227	244
-11	372	385
-10	581	608

5, 4, L		
-9	169	201
-8	412	457
-7	354	360
-5	118	134
-3	305	306
-2	745	789
-1	324	346
0	708	746
1	905	919
2	938	948
3	169	165
4	1232	1239
5	255	258
8	178	182
9	342	336
12	416	424
14	252	275

5, 5, L		
-17	190	216
-16	179	195
-15	415	426
-13	152	189
-11	256	267
-10	109	129
-9	329	355
-8	155	148
-7	756	793
-5	1148	1237
-4	768	849
-3	648	712
-2	507	555
-1	565	606
0	201	191
1	181	175
2	339	346
6	361	368
7	572	542
8	164	166
9	412	412
10	400	431
11	234	234
12	93	114
13	156	155

5, 6, L		
-13	428	451
-12	359	378
-11	757	786
-9	335	366
-8	231	268
-7	159	204
-5	209	241
-4	309	337
-3	419	427
-1	299	316
0	302	328
1	1172	1201
2	291	317
3	934	924
4	235	209
5	141	150
6	318	301
7	268	263
9	224	217
11	308	325
13	277	307

5, 7, L		
-16	165	170
-15	191	192
-14	370	359
-9	359	381
-8	292	312
-7	363	363
-6	869	899
-4	626	674
-3	312	350
-2	656	675
-1	228	223
0	787	801
1	205	184
2	124	138
4	133	139
5	425	413
6	343	336
7	217	213
8	522	532
9	249	259
10	258	272
11	321	356
12	256	288

5, 8, L		
-16	168	198
-14	247	224
-13	360	348
-12	401	385
-10	297	299
-9	152	150
-8	295	304
-7	370	394
-6	417	426
-4	206	216
-2	778	785
0	719	710
1	215	210
2	681	652
4	484	489
6	460	472
8	261	272
9	159	146
10	247	257
12	228	247

5, 9, L		
-15	210	197
-14	149	174
-13	260	254
-11	166	181
-7	519	554
-6	173	179
-5	1095	1128
-1	288	299
0	147	125
1	120	132
2	198	182
3	472	486
5	133	132
6	222	219
7	651	624
9	314	312
12	145	153

5, 10, L		
-14	227	210
-13	437	420
-12	324	333
-11	462	470
-9	525	501
-7	523	531
0	386	377
1	616	619
2	371	331
3	422	407
4	299	301
6	208	183
7	154	144
9	166	175
11	117	120

5, 11, L		
-14	240	227
-10	269	293
-8	283	308
-7	218	237
-6	483	455
-5	325	326
-4	581	564
-3	158	148
-2	330	328
0	165	174
1	183	194
2	275	274
4	333	334
6	409	384
7	271	265
8	409	412

5, 12, L		
-13	148	153
-12	314	313
-11	216	209
-9	193	200
-8	210	199
-2	218	210
-1	263	261
0	345	316
1	243	228
2	635	600
3	202	165
5	201	187
6	242	211

5, 13, L		
-7	399	412
-5	469	458
-4	196	191
-3	410	386
-1	432	421
3	265	246
5	282	259
7	442	399
9	356	350

5, 14, L		
-11	112	84
-10	386	421
-9	284	269
-8	202	213
-7	371	365
-3	158	150
-2	338	336
0	344	338
1	437	403
2	294	281
3	218	200
4	236	216
5	255	231
7	231	210

5, 15, L		
-8	233	230
-6	286	286
-4	274	271
-2	248	244
6	313	267

5, 16, L		
-1	257	255
0	192	167
1	235	212
2	188	157
3	361	324
4	149	115

5, 17, L		
-3	308	299

6, 0, L		
-16	195	188
-14	282	285
-12	605	586
-10	225	228
-8	380	389
-6	655	712
-4	843	922

6, 0, L			-4	179	187	12	242	251	2	936	960	0	633	646	5	432	407
0	132	133	-3	312	339	13	117	137	3	587	573	1	364	346	9	144	134
2	454	451	-2	227	248	6, 4, L			5	503	501	2	477	477	11	146	145
4	1495	1494	-1	483	511	-16	219	206	9	156	169	3	441	434	6, 10, L		
6	507	528	0	135	127	-15	172	193	10	405	423	4	718	705	-10	217	246
8	561	578	3	719	732	-14	316	311	11	159	156	5	159	172	-9	256	267
10	447	478	4	603	623	-13	191	199	13	239	275	6	447	443	-8	226	181
6, 1, L			5	387	394	-10	550	584	6, 6, L			12	286	309	-7	687	693
-15	225	213	6	153	136	-8	523	553	-15	203	225	6, 8, L			-6	222	224
-13	328	322	7	382	415	-7	319	339	-11	257	265	-15	122	154	-5	573	564
-12	321	335	9	409	432	-6	952	992	-9	407	431	-8	521	525	-4	591	628
-7	162	152	11	190	194	-5	268	298	-8	501	502	-7	408	400	-3	565	575
-6	204	196	12	106	125	-4	796	864	-7	607	638	-6	655	684	-2	440	423
-4	492	516	13	150	162	-3	434	439	-6	188	178	-4	349	345	1	459	451
-3	755	808	6, 3, L			-1	310	316	-5	123	156	-3	166	187	2	270	249
-1	1048	1079	-15	138	152	1	340	334	-2	481	502	-2	570	544	3	187	168
0	519	551	-14	355	338	2	281	307	-1	234	232	-1	179	183	4	389	386
1	658	686	-13	253	256	3	180	167	0	215	238	0	438	423	5	471	452
2	841	852	-12	473	470	4	579	553	2	167	169	1	323	312	6	307	297
3	429	438	-11	154	110	6	613	596	5	394	359	5	170	134	7	431	418
4	193	205	-10	482	502	7	237	231	6	283	295	6	288	274	8	195	194
5	300	297	-9	321	327	8	605	636	7	309	315	7	319	295	9	155	161
6	118	108	-8	352	346	9	147	170	8	108	102	8	198	196	6, 11, L		
7	185	195	-6	152	162	10	370	390	9	320	338	10	266	277	-12	241	252
9	291	293	-5	171	166	6, 5, L			11	306	342	11	113	126	-11	149	137
10	346	363	-4	182	173	-15	255	251	12	123	146	6, 9, L			-10	297	309
11	205	199	-3	524	514	-13	497	516	6, 7, L			-15	286	291	-9	236	247
13	166	158	-2	1133	1179	-12	354	364	-14	328	343	-13	378	388	-8	158	156
6, 2, L			-1	296	312	-11	580	598	-12	287	297	-11	261	271	-6	214	206
-17	289	279	0	663	670	-10	237	241	-11	317	343	-10	294	295	-5	160	166
-15	227	224	1	353	355	-9	557	580	-10	415	421	-9	476	475	-4	157	165
-13	292	300	2	632	641	-6	313	306	-9	231	244	-8	250	246	-3	195	209
-12	286	287	4	723	734	-5	269	288	-8	312	340	-6	207	225	-2	403	400
-11	282	296	5	258	257	-4	436	437	-7	328	327	-5	237	226	0	815	789
-9	670	663	6	299	310	-2	424	454	-5	207	219	-3	219	195	1	216	223
-8	210	209	7	342	354	-1	845	889	-4	180	187	-1	749	743	2	578	563
-7	532	557	10	223	235	0	420	410	-2	621	662	1	223	221	3	146	145
-5	900	965	11	273	291	1	1023	1008	-1	210	191	3	280	289	4	341	316

6, 11, L			6, 16, L			7 521 543			-4 231 236			-10 271 275			7, 7, L		
8	180	173	-5	241	236	8	173	176	-2	217	213	-9	528	552	-10	367	367
6, 12, L			-4	212	189	9	226	232	-1	219	231	-8	355	370	-8	378	397
-9	242	261	7, 0, L			11	116	156	0	246	269	-7	259	263	-7	300	336
-8	402	415	-16	158	146	7, 2, L			1	194	231	-6	591	626	-6	384	404
-7	365	364	-14	532	529	-17	194	183	2	511	508	-5	306	301	-5	338	330
-6	426	402	-12	450	462	-15	356	357	4	321	324	-3	334	329	-4	210	202
-5	280	291	-10	241	213	-13	625	629	6	526	553	-2	365	365	-1	125	118
-4	442	432	-8	806	776	-11	314	307	7	362	383	1	175	186	2	231	214
-3	147	137	-6	381	372	-9	399	375	8	559	576	2	359	375	4	589	547
-2	610	607	-4	826	824	-8	143	150	9	135	142	3	422	432	6	332	327
3	244	219	-2	443	474	-7	267	255	10	194	232	5	570	564	7	193	185
5	257	228	0	860	833	-6	341	350	11	103	118	6	278	284	8	307	319
6	436	398	2	631	622	-5	175	192	7, 4, L			7	216	199	9	145	157
7	214	189	4	653	646	-4	207	207	-15	123	86	8	280	280	10	320	350
8	121	116	6	391	388	-3	474	510	-14	541	513	9	320	328	7, 8, L		
6, 13, L			8	615	630	-2	126	146	-12	653	657	11	162	171	-15	162	186
-11	271	264	10	113	134	-1	906	898	-10	451	455	7, 6, L			-14	248	254
-9	376	401	7, 1, L			0	413	410	-8	197	200	-15	256	240	-12	235	234
-2	172	171	-17	131	142	1	670	675	-7	228	229	-13	186	164	-11	254	256
-1	452	443	-16	135	174	2	179	187	-6	195	202	-11	281	291	-7	354	363
1	502	459	-14	136	113	3	231	241	-4	458	479	-9	329	340	-4	208	208
2	118	106	-11	152	140	4	237	229	-3	443	434	-7	184	194	-3	536	529
3	336	299	-9	189	187	5	372	371	-2	562	571	-6	331	344	-2	393	399
5	212	180	-8	368	362	7	220	225	-1	299	294	-5	132	137	-1	203	203
6, 14, L			-7	373	408	8	132	161	0	989	969	-3	436	447	0	165	168
-9	174	160	-6	550	551	9	342	367	2	758	755	-2	392	402	2	397	381
-7	363	379	-5	359	358	11	189	203	3	530	540	-1	267	273	3	359	365
-6	178	178	-4	280	276	7, 3, L			4	318	312	0	235	251	4	173	170
-5	293	296	-3	580	563	-16	224	232	6	170	158	1	377	375	6	127	126
-3	331	312	-1	259	281	-15	167	187	7	289	291	3	529	539	8	141	140
-1	179	143	0	154	137	-14	201	212	8	244	235	4	165	155	10	262	272
4	188	175	1	531	549	-12	275	264	10	259	269	7	116	89	7, 9, L		
5	262	220	2	595	633	-10	540	542	12	223	243	9	311	305	-11	172	198
6, 15, L			3	220	226	-8	452	466	7, 5, L			11	182	201	-9	521	517
-2	239	216	4	254	253	-7	698	715	-14	170	146				-7	331	328
0	321	311	5	318	334	-6	489	495	-12	302	314				-5	502	506
2	301	291	6	296	315	-5	309	311	-11	269	286				-4	203	236

7, 9, L			-3	291	270	6	405	449	5	590	592	4	340	308	8	269	287
-3	381	366	-2	435	423	8	164	159	6	312	329	6	478	480	9	234	240
-1	181	187	-1	219	209	8, 1, L			7	427	429	7	144	143	8, 7, L		
3	368	356	0	375	354	-16	170	174	8	237	286	8	269	274	-14	256	257
5	473	439	1	249	234	-15	284	298	9	228	233	10	223	253	-12	319	316
7	203	199	2	398	380	-14	306	293	11	110	114	8, 5, L			-9	213	232
9	362	359	3	185	175	-13	241	245	8, 3, L			-15	237	251	-5	296	282
7, 10, L			4	149	133	-12	143	121	-16	314	333	-14	196	195	-4	382	376
-12	157	140	7, 13, L			-11	364	350	-15	213	216	-13	286	291	-3	455	448
-11	371	376	-9	378	387	-10	374	364	-14	305	306	-11	361	342	-2	412	398
-9	194	192	-8	166	170	-9	265	253	-13	311	303	-10	264	293	-1	383	371
-8	272	273	-7	424	420	-8	352	351	-12	319	328	-6	185	164	0	572	545
-4	518	516	-5	346	347	-7	211	187	-11	391	396	-5	477	461	2	352	359
-3	580	570	-3	233	230	-4	106	112	-10	415	421	-3	708	711	3	174	188
-2	511	534	3	248	231	-3	199	202	-9	287	295	-2	432	445	5	119	131
-1	531	488	5	440	424	-2	382	392	-6	226	204	-1	563	550	7	236	234
0	386	394	7, 14, L			-1	374	377	-2	406	386	0	409	375	8	245	248
1	568	557	-3	301	263	0	311	296	-1	313	322	1	557	557	8, 8, L		
2	485	456	-2	184	175	1	346	323	0	782	741	2	341	314	-12	228	229
3	601	582	-1	341	316	3	349	313	1	158	130	5	202	234	-11	222	232
4	289	295	0	274	287	4	298	279	2	654	630	6	164	150	-10	223	211
7, 11, L			1	238	241	7	247	258	3	267	260	7	321	317	-9	187	153
-10	329	348	2	202	187	8	197	198	4	197	186	9	352	362	-8	191	222
-8	453	464	3	324	287	9	122	157	5	110	104	8, 6, L			-7	132	123
-6	485	491	7, 15, L			11	239	267	10	152	185	-11	358	350	-6	303	288
-5	262	241	-6	338	338	8, 2, L			8, 4, L			-9	385	404	-5	203	204
-4	731	713	-4	214	191	-13	154	149	-12	338	335	-7	517	534	2	352	319
-3	224	242	8, 0, L			-11	314	326	-11	265	231	-5	516	506	3	208	210
-2	313	308	-16	236	214	-9	821	825	-10	490	506	-4	212	227	4	377	370
2	151	170	-14	275	235	-8	172	148	-8	659	654	-2	296	300	6	391	376
4	509	488	-12	291	269	-7	609	592	-6	379	370	0	208	237	7	212	197
5	119	121	-10	479	447	-5	253	255	-5	294	264	1	255	230	8	333	358
6	251	260	-8	718	721	-4	129	116	-4	506	525	2	456	469	8, 9, L		
8	185	178	-6	374	382	-3	422	434	-2	532	523	3	382	354	-13	309	318
7, 12, L			-4	687	680	-1	235	278	0	270	285	4	174	173	-11	301	321
-11	175	177	-2	359	334	1	361	363	1	242	249	5	289	293	-10	177	177
-10	285	285	0	682	669	3	196	179	2	341	313	6	208	200	-5	369	396
-4	186	204	4	301	293	4	174	177	3	345	341	7	310	308	-3	365	379

8, 9, L		
-2	256	228
0	235	230
1	642	608
3	218	196
8, 10, L		
-11	291	302
-10	214	238
-9	295	301
-8	272	262
-7	459	445
-6	389	381
-5	463	453
-4	253	220
0	202	196
1	194	204
2	227	216
3	458	450
4	197	218
5	276	274
6	133	137
7	287	256
8, 11, L		
-10	143	163
-4	407	417
-3	204	181
-2	208	224
0	426	401
1	193	182
2	352	348
8, 12, L		
-10	272	272
-8	245	251
-6	321	323
-5	203	192
3	225	202
4	238	223
5	239	239

8, 13, L		
-5	143	156
-3	348	337
-1	364	357
1	416	403
3	219	203
8, 14, L		
-5	249	220
9, 0, L		
-14	203	186
-12	278	272
-8	239	234
-4	466	474
-2	726	684
0	242	226
6	146	118
8	147	145
9, 1, L		
-13	199	211
-11	345	338
-10	521	524
-9	463	468
-8	490	486
-7	300	276
-6	272	277
-5	201	206
-4	387	377
-2	359	364
-1	172	135
0	217	201
2	275	252
3	246	223
4	503	477
5	440	415
6	174	178
7	242	239
8	165	178

9, 2, L		
-15	257	258
-13	233	225
-11	210	206
-9	329	307
-7	378	393
-5	279	268
-4	120	143
-3	485	471
-1	405	386
0	245	230
1	518	509
2	299	282
5	222	211
9	261	279
9, 3, L		
-14	207	190
-12	258	267
-10	336	335
-9	393	387
-8	414	409
-6	432	430
-5	154	174
-4	333	338
0	135	115
3	315	294
4	296	300
5	331	318
6	319	336
7	118	101
8	131	144
9	180	196
9, 4, L		
-14	201	213
-12	343	349
-10	341	367
-9	275	276
-5	189	185

-4	589	562
-2	723	701
-1	338	339
0	534	545
2	421	405
3	299	314
6	158	162
9, 5, L		
-11	485	476
-10	283	298
-9	412	404
-8	169	192
-7	540	524
-6	263	264
-5	367	339
-4	254	268
1	371	344
3	375	344
4	237	245
5	227	221
7	222	204
9, 6, L		
-14	212	168
-13	332	335
-11	242	249
-9	169	185
-5	426	421
-3	615	586
-2	262	257
-1	678	665
0	383	373
1	309	301
9, 7, L		
-12	318	316
-10	224	197
-9	167	140
-8	377	360
-6	452	440

0	223	231
2	334	333
3	262	250
4	333	320
6	417	391
9, 8, L		
-6	199	208
-5	201	224
-4	447	415
-2	504	482
0	522	515
2	285	273
3	137	190
6	159	150
9, 9, L		
-11	252	282
-9	235	251
-7	564	543
-5	194	191
1	264	266
2	121	82
3	259	249
5	347	333
9, 10, L		
-6	196	204
-5	361	345
-3	239	234
-1	302	293
1	236	237
9, 11, L		
-8	343	360
-6	271	288
2	266	248
9, 12, L		
-6	229	204
-5	191	188
-3	236	202
-2	171	185

-1	171	174
0	231	216
1	141	144
10, 0, L		
-12	374	363
-10	545	536
-8	329	350
-6	222	221
-4	356	342
-2	233	222
2	675	636
4	558	493
6	253	284
10, 1, L		
-14	227	219
-12	271	265
-10	234	228
-8	254	270
-7	305	288
-6	379	381
-5	424	405
-4	517	511
-3	313	288
-2	362	366
-1	335	327
0	390	367
1	203	170
7	162	158
10, 2, L		
-14	141	139
-13	279	275
-11	366	337
-9	288	273
-8	186	166
-7	388	382
-5	205	194
1	428	388
2	234	223

10, 2, L		
3	506	476
5	247	230
7	211	233
10, 3, L		
-13	207	178
-12	170	138
-10	165	166
-9	150	151
-6	308	284
-5	417	397
-4	448	410
-3	338	313
-2	411	393
-1	338	319
0	335	315
1	475	449
5	103	71
10, 4, L		
-12	378	378
-10	384	365
-9	421	423
-8	324	318
-6	357	334
0	238	205
2	473	447
4	272	250
6	221	208
10, 5, L		
-11	151	188
-7	343	330
-6	248	230
-4	387	370
-3	490	486
-1	511	499
4	138	151

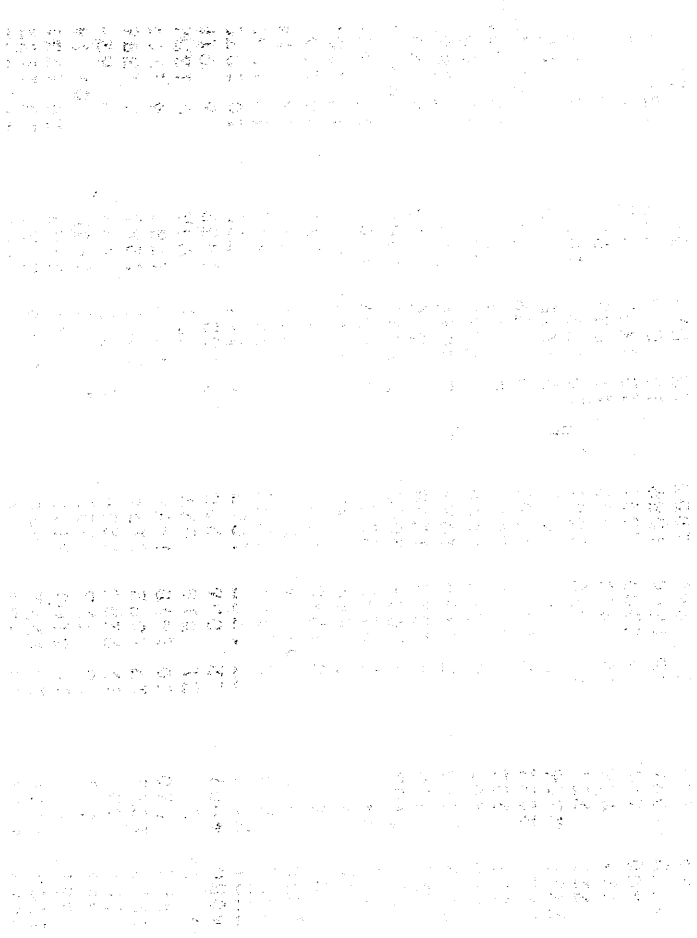
10, 6, L		
-11	358	341
-9	370	365
-8	302	298
-7	316	323
-5	199	178
-4	255	274
1	333	303
3	347	324
5	206	205
10, 7, L		
-6	272	238
-4	241	245
-3	208	219
-2	511	518
0	272	283
10, 8, L		
-10	268	267
-9	289	275
-8	362	369
2	205	189
3	144	128
4	302	285
10, 9, L		
-7	260	258
-5	271	270
-3	392	373
-1	349	308
10, 10, L		
-8	167	200
-1	241	217
1	250	223
10, 11, L		
-4	330	296
-2	394	388

11, 0, L		
-8	253	235
-6	484	490
-4	272	266
-2	495	474
0	471	439
11, 1, L		
-12	211	219
-11	142	147
-9	313	323
-8	381	363
-7	249	204
-1	258	230
0	294	296
1	342	314
2	341	322
3	178	169
4	216	207
11, 2, L		
-12	136	59
-7	359	336
-5	440	415
-4	201	189
-3	346	332
-1	324	316
11, 3, L		
-10	195	218
-8	187	169
-7	292	271
-6	201	91
-3	142	152
-1	159	173
0	317	280
1	418	399
2	258	236
4	219	184

11, 4, L		
-9	317	308
-7	181	215
-6	434	396
-4	391	379
-3	276	239
-2	407	398
0	251	237
11, 5, L		
-9	228	267
-3	183	201
-1	216	208
0	224	207
1	155	165
3	339	323
11, 6, L		
-9	193	165
-7	370	357
-5	440	442
-4	267	251
-3	383	386
-1	243	226
2	152	185
11, 7, L		
-2	253	233
11, 8, L		
-6	234	250
-5	183	172
-4	328	330
-3	249	229
-2	156	166
12, 0, L		
-8	345	320
-2	316	295
0	319	286

12, 1, L		
-8	260	249
-5	187	194
-4	216	196
-3	184	199
-2	298	284
12, 2, L		
-6	151	77
-1	400	387
12, 3, L		
-8	169	156
-6	315	304
-4	335	324
-3	280	256
-2	285	260
12, 4, L		
-3	194	179
12, 5, L		
-4	165	175

CALCULATED AND OBSERVED STRUCTURE FACTORS OF $[CpMoI(CO)(C_4Ph_4)].CH_2Cl_2$



0, 0, L		
4	3611	3678
6	4753	4714
8	2019	2111
10	1288	1191
12	631	676
16	663	601
22	759	639
24	1277	1213
26	963	960

0, 2, L		
0	4080	4081
1	2321	2186
2	2458	2633
3	1838	1762
4	504	448
5	805	798
8	3758	3624
9	1087	1106
10	775	728
11	2167	2095
12	494	405
13	818	783
15	2127	2033
17	2289	2306
19	727	751
21	916	904
22	480	609
23	1578	1596
25	642	903

0, 4, L		
1	459	360
2	1105	1068
3	4707	4572
4	1629	1676
5	2464	2490
6	1177	1278
7	3412	3365
8	1056	1083
9	3097	3135
11	1942	1993
12	932	870
14	1772	1690
15	3103	3118
16	773	720
17	2283	2289
19	1092	1124
20	1498	1496
21	516	579
22	836	708
23	1782	1862
25	1341	1235

0, 6, L		
0	1268	1183
1	648	645
2	2163	2182
3	1936	2010
4	1222	1228
5	1934	1963
6	1642	1598
7	3179	3076
8	1040	1158
9	966	997
12	1890	1661
13	820	867
14	2589	2631
15	1644	1589
16	949	1053
17	1545	1591
19	892	983
20	1254	1374
22	644	703
23	1125	1252
24	632	668
25	720	684
26	965	1040

0, 8, L		
0	3147	3297
1	1394	1422
2	1920	1881
3	3840	3939
5	3011	2963
6	1573	1455
8	1935	1999
9	1308	1266
10	1760	1787
11	955	946
13	1530	1459
14	764	738
15	742	643
16	703	793
24	748	782

0, 10, L		
0	1939	1902
1	1493	1564
2	690	713
3	2049	2140
5	2213	2146
6	816	860
8	929	891
9	1155	1183
10	1774	1871
11	955	974
12	1472	1455
13	845	789
15	527	561

0, 12, L		
0	769	770
1	966	977
3	1591	1586
4	1386	1390
6	1779	1814
9	1082	899
10	1931	1901
12	2195	2202
14	1548	1553
15	630	459
17	545	488
18	1132	1207
20	1731	1732

0, 14, L		
0	624	575
3	1396	1440
4	1117	1117
5	1356	1388
6	918	1036
10	1078	1090
12	1569	1531
13	714	707
14	1149	1187
18	1001	1065
20	1596	1614

0, 16, L		
3	1788	1786
5	1839	1859
11	1057	970
17	654	766

0, 18, L		
0	823	728
3	1376	1363
5	1473	1477
6	917	898
13	681	609

1, 0, L		
2	663	614
6	1169	1028
8	1836	1922
10	1369	1432
12	825	776
14	1898	1922
16	1023	996

1, 1, L		
1	1631	1598
2	5028	5029
3	387	337
4	3203	3286
5	566	436
6	4138	4213
7	2633	2568
10	1547	1542
12	1777	1760
13	899	898
15	1170	1089
19	803	1078
28	781	818

1, 2, L		
1	606	573
2	684	625
5	1649	1710
6	2675	2710
8	2819	2941
9	706	672
10	617	611
12	1169	1231
13	784	784
14	960	1085
16	591	589

1, 3, L		
1	1864	1725
2	916	1029
3	914	807
4	1283	1331
5	2099	2200
6	796	844
7	618	723
9	608	550
10	960	903
11	2907	2857
13	3315	3187
14	1119	1091
15	1513	1510
16	582	597
17	913	935
18	719	740
19	1698	1683
21	1504	1460
23	552	589
27	869	946

1, 4, L		
1	972	955
3	2728	2697
4	472	497
6	1347	1384
7	889	916
8	1802	1953
9	1054	1136
11	785	774
12	578	558
16	589	683

1, 5, L		
1	2657	2636
2	992	1073
5	1146	1079
8	1223	1143
9	1246	1280
10	1498	1444
11	1818	1909
12	1513	1424
13	2514	2523
14	669	688
15	1251	1208
16	1495	1443
17	779	904
18	988	970
19	1181	1193
21	1404	1263
23	777	725

1, 5, L		
24	943	942
27	747	663
1, 6, L		
2	2722	2674
3	1579	1596
4	512	579
7	747	730
8	566	617
9	1025	1011
11	812	820
12	564	681
13	555	544
21	724	746
1, 7, L		
1	2512	2601
2	1115	1113
4	2539	2488
7	441	475
9	1595	1624
10	1663	1684
11	897	897
12	1307	1373
13	675	706
16	705	798
17	597	553
18	728	666
19	628	666
22	912	849
24	702	624
1, 8, L		
1	1138	1087
2	1293	1284
11	1131	1184
13	840	824
16	564	584

1, 9, L		
1	2711	2843
2	850	881
3	1224	1221
4	1977	2057
5	810	875
6	1687	1729
7	2311	2313
9	1311	1372
12	769	846
13	627	732
15	626	658
23	581	500
25	738	805
1, 10, L		
1	570	569
2	1294	1252
4	983	1010
11	687	781
1, 11, L		
1	1595	1607
6	1469	1371
7	1188	1163
8	1291	1319
10	1066	1021
13	642	601
14	1094	1050
15	748	624
16	1289	1289
18	885	929
19	759	820
22	798	718
1, 12, L		
2	858	877
4	734	740
6	849	808
16	541	652

1, 13, L		
2	504	563
8	1626	1641
10	1183	1157
14	1066	1052
16	1398	1327
18	1679	1663
22	695	813
1, 14, L		
1	631	601
4	586	552
6	607	600
1, 15, L		
1	1899	1864
5	885	845
7	1066	1058
8	739	666
10	865	903
15	759	808
16	847	916
18	716	648
1, 17, L		
1	1388	1263
3	953	895
5	663	709
7	1286	1254
9	1106	1022
1, 19, L		
1	731	686
2, 0, L		
0	5345	5403
2	2393	2329
8	2142	2113
10	1983	2045
12	622	536
14	2725	2675
16	727	817
18	817	801

20	1003	955
24	555	508
26	956	944
2, 1, L		
0	1504	1387
2	1218	1179
3	861	818
4	973	973
5	1565	1497
6	1327	1315
7	2081	2080
8	1209	1222
9	582	506
10	2382	2430
11	869	907
12	2782	2834
14	1049	1017
18	712	784
20	1062	1114
22	929	952
24	416	324
2, 2, L		
0	2785	2608
2	393	438
3	3726	3659
4	1332	1414
5	735	774
6	509	400
7	949	975
8	2188	2174
9	2063	1908
10	1222	1235
11	1332	1299
15	1563	1516
16	761	755
17	1119	1135
23	936	1000

2, 3, L		
0	1996	1914
1	2167	2119
2	1764	1695
3	3306	3218
4	1337	1315
5	2197	2126
7	2156	2081
8	883	867
9	869	873
10	2362	2364
11	906	947
12	1231	1224
14	1159	1136
15	531	573
18	688	666
22	816	773
2, 4, L		
0	907	893
1	1219	1192
6	1120	1207
7	1670	1746
8	1140	1059
9	1633	1671
10	988	968
11	2048	2024
12	1104	1071
14	693	615
15	1838	1844
17	1645	1631
23	1252	1198
25	957	972
2, 5, L		
1	407	500
2	664	638
3	2925	2980
4	638	623
5	1356	1457

7	1657	1772
8	450	396
10	607	672
11	994	1003
13	933	894
15	1100	1051
17	672	749
2, 6, L		
0	3962	4133
2	1978	2076
3	979	979
4	1520	1482
6	3068	3006
7	1019	968
8	1825	1837
9	947	985
10	647	676
12	2301	2270
13	620	615
14	1385	1404
15	1167	1103
17	485	466
18	525	599
19	503	469
22	477	499
26	632	735
2, 7, L		
0	998	1012
1	830	810
2	410	407
3	1194	1237
4	517	444
5	1591	1647
7	1078	1121
9	1111	1182
12	1095	1019
13	557	690
14	1168	1113

2, 7, L
15 1589 1610
17 1183 1213
2, 8, L
0 947 992
1 525 581
2 1979 1964
3 1313 1335
4 515 569
5 1347 1349
6 1317 1384
7 1030 1057
8 1231 1198
9 1286 1185
11 1323 1329
13 701 653
14 575 517
2, 9, L
0 593 667
2 982 1104
5 674 712
7 1443 1499
8 799 845
9 1035 1035
10 754 728
12 733 802
14 499 585
15 1030 1043
17 950 855
18 479 429
19 628 519
20 864 851
22 521 521
2, 10, L
0 1839 1829
1 961 890
3 1804 1800
5 2008 1939
6 1080 1096
9 1158 1170
11 1071 1057
12 605 592
20 603 605
2, 11, L
0 2044 2104
2 1528 1550
4 392 442
6 1246 1267
8 909 913
9 791 856
10 1125 1057
12 702 645
18 503 419
22 727 651
2, 12, L
5 624 611
6 796 844
12 1434 1308
14 1014 1068
18 965 924
20 1239 1205
2, 13, L
0 1492 1492
2 1117 1079
4 684 632
8 1138 1138
2, 14, L
5 1277 1274
6 1016 1006
12 955 927
14 1031 970
16 504 399
18 654 629
20 920 975
2, 15, L
0 1030 1087
2 1027 1074
9 924 913
15 553 689
2, 16, L
0 471 514
3 1502 1438
5 1050 1061
9 765 803
2, 18, L
3 1025 954
5 821 939
6 747 675
3, 0, L
2 2276 2203
4 1210 1216
6 1020 1079
8 2974 2917
10 723 756
14 2060 1986
16 1627 1622
18 1205 1227
22 515 466
24 1349 1339
26 855 870
3, 1, L
1 1215 1149
2 1003 1047
4 657 592
6 853 799
9 1073 1072
10 2233 2188
12 1605 1527
13 1110 1315
15 759 871
16 1167 1265
18 1137 1111
22 803 771
24 1071 1035
3, 2, L
1 2467 2599
2 1998 2007
3 1053 1137
4 2455 2462
6 1627 1550
7 1971 1930
8 1086 1033
9 1437 1454
11 452 449
14 729 691
16 2115 2125
18 1456 1460
3, 3, L
1 2691 2738
5 2184 2183
6 539 541
7 2338 2250
8 1310 1282
9 1318 1236
10 894 853
11 1607 1586
13 2218 2186
15 670 649
18 423 400
19 480 616
21 888 938
25 813 777
27 780 797
3, 4, L
1 2859 2895
2 864 859
3 1138 1056
4 1373 1427
5 688 665
6 928 922
7 787 780
8 490 489
9 1312 1309
12 419 357
13 774 739
16 888 969
17 476 520
23 842 778
3, 5, L
1 750 818
2 2351 2347
4 2657 2735
6 467 349
7 1171 1170
8 1400 1442
9 1245 1162
10 1742 1639
12 915 905
13 1193 1205
14 722 734
16 1051 1024
19 783 649
21 526 490
22 650 621
24 573 553
3, 6, L
1 2368 2496
2 1711 1772
3 2127 2174
4 1415 1403
5 328 374
7 1216 1242
8 697 674
9 1983 1999
10 762 780
11 1352 1408
13 947 1002
16 715 621
17 594 666
21 954 936
23 918 930
3, 7, L
1 497 528
2 1448 1554
4 1816 1813
6 784 796
8 1381 1465
10 2139 2160
13 567 595
14 934 1011
15 706 500
16 1116 1191
24 763 783
3, 8, L
1 1139 1102
3 1003 954
6 1176 1238
7 720 682
8 1475 1511
9 724 627
11 1704 1695
13 1463 1425
14 683 684
16 719 778
17 447 618
21 1177 1125
3, 9, L
1 2069 2101
2 939 1026
4 873 928
5 740 811
7 2192 2205
11 988 1039
13 1237 1209
14 614 575
19 1090 1154

3, 10, L		
2	1055	1075
4	1021	1028
6	1170	1112
8	1458	1470
12	812	754
13	900	955
14	867	847
16	826	790
18	499	591
19	840	754

3, 11, L		
1	854	785
2	682	725
4	734	708
6	466	618
7	937	937
9	817	703
10	673	753
13	904	918
15	712	678
16	541	563
19	910	902
21	620	666

3, 12, L		
2	957	1024
4	1485	1577
6	1615	1602
7	428	475
12	849	885
14	767	734
16	759	715

3, 13, L		
4	1571	1592
6	729	713
10	1131	1076
16	827	868
18	740	711

3, 14, L		
4	1174	1142
6	1209	1189
11	925	821
12	548	535

3, 15, L		
1	823	729
5	1129	1120
7	905	902

3, 16, L		
3	537	466
11	1216	1157
13	726	705

3, 17, L		
7	983	1100
8	523	502
13	738	686

3, 18, L		
11	622	689

4, 0, L		
0	2306	2322
2	831	828
4	2994	2864
6	2288	2209
10	801	920
12	3010	2879
14	1723	1747
18	1079	992
20	1244	1244
22	1081	1098
26	522	536

4, 1, L		
0	1979	2028
1	476	438
2	1606	1622
3	638	647
5	1215	1261
7	582	638
8	692	605
9	644	473
10	884	916
12	1500	1548
14	1782	1733
18	996	967
20	1313	1265
22	1005	974

4, 2, L		
1	1041	1030
2	505	547
3	2115	2072
4	1025	1003
5	1049	1057
9	974	986
10	1118	1167
11	1158	1209
12	1220	1253
14	824	766
20	1122	1102
23	876	940

4, 3, L		
0	1449	1472
1	965	957
2	653	651
3	2594	2555
5	1785	1796
6	708	770
7	677	736
8	913	844
9	821	790
10	814	818
11	1037	1083
13	854	861
14	823	881
20	996	1027
22	793	767

4, 4, L		
1	2333	2223
2	1063	1037
3	2714	2708
4	785	763
5	2106	2191
8	760	756
9	788	702
10	1136	1138
11	1268	1284
13	1127	1013
14	617	701

4, 5, L		
0	1966	1941
1	708	729
2	1314	1392
3	2274	2311
4	871	745
5	1765	1734
6	1406	1370
7	908	898
8	405	464
12	798	717
13	658	543
15	889	861

4, 6, L		
0	1264	1252
1	636	583
2	990	1008
3	686	761
5	1669	1627
6	1578	1607
7	973	986
8	1174	1168
12	785	741
14	1179	1278
18	723	739
20	746	802

4, 7, L		
0	1148	1101
3	1400	1447
4	540	578
5	2020	2044
6	1078	1092
7	1162	1259
10	1042	1029
12	991	983
13	506	568
15	1262	1326
17	894	863
18	747	713
25	534	476

4, 8, L		
1	564	472
4	579	654
5	556	530
6	927	981
7	1102	1131
9	1707	1695
11	996	1002
12	632	559
14	859	887
15	1022	962
17	939	985
20	920	928
22	824	831

4, 9, L		
6	742	729
9	852	824
10	1453	1448
12	756	695
14	488	448
15	1036	993
17	1093	1193
18	729	689
20	681	659
23	607	579

4, 10, L		
0	1034	967
1	708	751
2	774	747
3	912	955
8	880	942
9	1147	1154
11	973	936
14	499	451
15	979	897
17	1205	1268
19	563	609

4, 11, L		
0	1571	1560
2	1090	1028
5	493	480
8	1072	1099
9	710	852
10	1124	1184
12	754	785

4, 12, L		
0	1974	2058
1	512	464
2	1567	1563
3	1142	1092
6	1159	1097
8	1512	1571
9	678	670

4, 13, L		
0	1258	1272
2	1066	1056
4	515	508
6	863	841
8	1015	959

4, 14, L			14 1934 1957			12 581 578			18 645 589			5, 11, L			24 435 535		
0	1166	1154	16	1822	1880	13	435	446	19	781	799	2	1531	1518	6, 1, L		
5	597	482	18	1092	1014	15	858	770	21	600	653	4	1640	1647	0	2244	2188
6	1018	1062	20	424	295	5, 5, L			23	585	645	5	887	843	1	365	357
8	932	949	24	937	992	1	2085	2143	24	871	858	6	1108	1056	2	1052	1032
9	633	632	26	792	822	3	935	924	5, 8, L			7	641	757	4	1328	1254
14	479	386	5, 2, L			4	1024	1056	1	707	708	11	754	719	6	1802	1687
15	632	540	2	406	314	6	748	669	5	539	601	13	577	692	8	1041	1105
4, 15, L			5	673	700	7	1961	2019	6	542	532	5, 12, L			11	649	594
2	744	690	6	669	740	9	1822	1827	8	451	481	2	1059	1012	12	808	699
9	570	681	7	1047	1082	11	1404	1454	10	824	735	4	1185	1148	14	537	495
11	471	444	8	719	753	12	1110	1122	11	689	664	6	589	675	15	488	518
15	617	695	9	1186	1114	16	536	512	13	834	775	7	815	802	24	468	481
4, 16, L			13	827	873	17	513	375	16	837	760	10	714	721	6, 2, L		
15	756	756	16	1052	1046	24	670	623	22	597	548	5, 13, L			0	967	1055
4, 17, L			18	727	501	25	467	462	5, 9, L			2	1304	1248	1	833	760
7	727	605	5, 3, L			5, 6, L			2	679	608	4	1923	1853	2	588	535
4, 19, L			1	2691	2807	1	847	936	3	591	684	6	1353	1327	3	1522	1496
0	741	724	2	775	683	2	944	1038	4	583	494	10	746	740	4	1075	1051
5, 0, L			3	1065	1068	3	1132	1060	5	1210	1195	5, 14, L			5	1903	1920
2	448	546	4	994	999	4	679	786	6	763	755	4	834	751	7	793	740
4	1214	1171	5	351	438	7	691	744	7	775	838	5, 15, L			9	1187	1213
8	1815	1792	6	1685	1625	10	802	819	11	1583	1580	2	806	831	10	1085	1057
10	1694	1592	7	2556	2545	13	489	417	13	1463	1450	4	1156	1095	11	813	784
12	612	600	8	1804	1685	14	446	396	14	510	529	6	598	557	12	1661	1591
14	1262	1327	9	1987	1913	16	992	1072	16	1393	1426	11	482	566	14	781	815
16	942	946	11	489	506	18	606	664	18	691	656	13	874	835	18	706	682
18	530	544	12	639	639	5, 7, L			19	1044	1150	6, 0, L			20	1107	1173
22	769	669	13	646	686	1	811	814	21	807	889	0	913	834	22	676	708
24	839	866	14	1048	1011	3	884	853	5, 10, L			2	639	702	6, 3, L		
5, 1, L			15	501	507	4	682	715	1	618	672	4	803	832	0	1121	987
1	797	760	16	796	772	8	594	650	2	748	659	6	564	584	1	1216	1199
4	535	545	5, 4, L			9	1101	1065	5	542	652	10	1738	1555	2	350	314
5	557	588	1	1310	1224	10	1114	1175	13	507	601	12	2481	2353	3	1894	1950
6	1667	1691	3	880	855	11	996	1085	19	559	624	14	1213	1233	5	791	810
8	1866	1870	5	561	668	12	664	674				18	1273	1248	6	634	552
9	785	673	7	1699	1574	13	1034	985				20	1273	1403	7	852	789
10	2039	2013	9	996	975	16	1361	1369				22	967	1087	9	1171	1118

6, 3, L		
10	682	652
11	1015	1070
15	920	817
17	934	977
6, 4, L		
0	807	866
1	1201	1237
2	1094	1130
3	2063	2093
4	575	539
5	1845	1957
6	404	433
7	1187	1202
8	678	631
10	673	692
11	1088	1027
12	473	401
13	856	983
23	430	166
6, 5, L		
1	607	527
6	573	594
8	728	753
9	476	508
11	507	419
12	708	755
14	956	903
17	1078	1093
18	548	617
20	588	715
6, 6, L		
0	1219	1159
1	857	877
2	934	871
3	1283	1285
4	749	715
5	1693	1707
6	1246	1177
7	809	749
8	759	769
11	445	436
12	762	765
13	685	625
14	826	818
15	873	915
17	830	839
6, 7, L		
0	1306	1369
2	614	617
3	687	569
4	505	484
6	598	631
8	870	938
20	1016	1127
6, 8, L		
0	689	766
2	708	603
3	576	611
5	565	616
7	924	1005
9	1057	1007
11	671	699
12	798	828
14	1028	961
15	1043	992
17	870	915
19	595	617
20	735	614
6, 9, L		
1	811	850
3	1558	1486
5	803	846
9	651	692
11	511	521
15	651	640
6, 10, L		
0	1217	1322
3	473	461
4	593	466
8	974	1011
9	883	890
10	1033	968
11	822	891
12	587	477
15	732	715
17	1066	1071
6, 11, L		
0	1076	976
3	922	883
4	693	701
5	971	945
6	849	807
7	451	303
9	939	806
6, 12, L		
0	1588	1500
2	1206	1205
6	980	902
8	1450	1432
10	573	606
6, 13, L		
4	482	506
6	861	882
12	740	739
14	756	727
6, 14, L		
0	1188	1199
2	971	956
8	1131	1140
10	656	637
15	595	641
7, 0, L		
2	1459	1507
4	2460	2529
6	1239	1202
10	907	941
14	508	519
22	653	607
7, 1, L		
1	857	877
4	551	554
6	537	565
7	798	782
8	509	697
9	693	744
10	1211	1250
14	1100	1115
16	1304	1273
18	1066	1123
22	584	641
7, 2, L		
2	1061	1057
4	1598	1553
5	1488	1567
6	762	755
7	786	775
11	571	528
12	578	512
13	920	943
15	881	873
19	900	876
7, 3, L		
1	2346	2375
4	786	746
5	884	817
6	652	662
7	1355	1361
9	876	823
7, 4, L		
4	488	494
5	718	842
7	707	852
9	428	493
11	665	679
13	1202	1226
15	522	490
16	649	601
19	1203	1197
21	931	904
7, 5, L		
1	1614	1637
2	1325	1242
4	1520	1481
7	975	1077
9	1230	1284
11	759	800
22	424	416
7, 6, L		
1	522	577
2	1570	1587
4	1000	949
9	816	857
10	928	900
11	895	909
12	586	615
15	601	667
16	858	911
18	1001	994
19	668	755
22	683	635
7, 7, L		
1	797	661
2	827	813
4	702	746
8	1008	981
9	686	720
10	700	742
16	876	802
19	761	723
21	513	505
7, 8, L		
1	1492	1480
4	864	929
6	577	530
7	682	654
9	779	806
11	611	641
14	520	491
7, 9, L		
6	832	837
8	739	724
13	1076	1149
14	763	679
16	726	739
19	845	921
7, 10, L		
1	1100	1062
5	830	875
6	772	822
7	1174	1187
7, 11, L		
2	877	941
4	1028	981
12	532	564
14	813	770
7, 12, L		
8	772	791
10	818	873
16	936	917
7, 13, L		
2	567	547
4	1050	1171
6	1067	1164

7, 14, L
1 654 586
8 865 815
7, 16, L
1 856 884
8, 0, L
12 541 654
14 604 535
20 848 857
8, 1, L
0 1708 1795
2 1441 1409
6 1067 1119
7 604 505
8 1364 1439
10 1172 1100
8, 2, L
3 585 614
20 517 511
8, 3, L
0 602 547
2 1072 1160
3 665 597
4 651 647
7 964 896
8 835 868
9 1247 1281
10 753 744
11 598 714
13 574 392
15 1464 1422
17 1196 1235
8, 4, L
0 945 907
3 1012 1025
5 854 804
6 418 380
13 691 752

8, 5, L
0 1164 1100
4 829 728
6 891 814
7 1429 1439
8 808 863
9 922 865
12 795 713
15 909 949
17 1200 1195
8, 6, L
0 584 730
3 610 533
6 482 412
14 551 604
8, 7, L
0 1480 1346
3 717 829
4 478 372
5 840 771
6 1149 1089
7 1248 1098
8 980 894
9 789 758
12 523 527
15 482 358
17 429 460
8, 8, L
4 597 597
8, 9, L
0 786 715
2 916 856
3 1214 1343
5 1291 1288
6 732 735
11 715 815
13 483 417

8, 11, L
0 933 923
5 775 747
12 1005 1058
14 797 771
8, 13, L
4 762 785
10 490 554
8, 15, L
3 789 748
9, 0, L
2 1633 1637
4 2066 2016
6 1415 1407
10 1565 1564
12 854 901
9, 1, L
2 920 742
9, 2, L
1 506 437
4 1226 1412
5 712 875
6 1426 1343
7 674 613
10 600 634
11 987 883
12 892 756
13 1214 1134
19 796 901
9, 4, L
5 718 648
7 1142 1111
8 481 467
10 628 705
11 1469 1448
13 1571 1541
14 582 588
17 585 651

9, 6, L
1 648 663
2 1274 1213
3 448 461
4 1294 1269
8 850 751
9 668 764
10 1076 1036
11 1002 912
13 788 804
16 823 744
9, 8, L
1 1206 1244
2 777 690
3 710 739
4 1280 1183
6 743 613
7 1020 1053
9 836 788
10 914 1011
9, 9, L
1 758 730
9, 10, L
1 734 706
4 515 521
6 752 738
7 1084 1265
9 676 646
9, 12, L
8 847 954
10 713 869
9, 14, L
1 827 683
10, 0, L
0 1375 1377
2 535 455
6 683 586
8 642 575

10, 1, L
0 1487 1449
2 1016 1028
6 1236 1215
8 1002 1051
9 470 550
10, 2, L
0 839 771
2 669 614
8 694 745
10, 3, L
2 777 785
9 999 1051
15 863 854
10, 4, L
0 744 690
10, 5, L
7 662 686
8 623 644
12 602 673
14 551 453
15 550 639
10, 7, L
0 726 735
2 749 823
3 817 751
6 808 868
8 769 829
11 449 456
10, 9, L
3 985 938
5 709 828
11 558 650
11, 0, L
2 896 801
4 1117 1104
8 854 741
10 751 766

11, 1, L
4 682 619
6 790 821
11, 2, L
2 542 513
4 825 814
11, 3, L
1 770 706
6 570 647
11, 4, L
7 636 702
11, 5, L
9 640 662
11, 6, L
4 666 815
12, 0, L
0 421 491
12, 3, L
1 616 535
3 863 988

CALCULATED AND OBSERVED STRUCTURE FACTORS OF $[WBr(CO)_2(SC_6F_5)(C_7H_8)]$

0, 0, L			7 561 556			9 502 453			3 1070 1050			0 147 149			13 420 428		
2	3423	3365	10	906	928	10	495	492	4	440	437	1	1989	1987		1, 3, L		
4	1773	1766	12	435	480	11	349	366	5	1064	1102	2	652	653	-12	286	246	
6	2302	2403	14	392	427	12	482	450	7	1048	1060	3	1738	1758	-10	267	279	
8	1592	1604	0, 4, L			13	330	311	9	908	912	4	390	401	-9	409	360	
10	576	574	0	1231	1242	0, 7, L			0, 12, L			5	1043	1039	-6	476	444	
12	846	829	1	383	382	2	870	843	1	933	927	7	853	853	-5	848	834	
14	537	537	2	1100	1155	3	681	703	3	747	773	8	657	581	-4	471	459	
0, 1, L			3	564	544	5	763	707	5	702	752	9	1016	1064	-2	572	560	
1	608	562	4	1733	1747	7	622	572	7	881	950	10	423	391	-1	837	878	
2	158	172	5	593	588	8	573	582	0, 14, L			11	617	613	1	831	792	
3	372	346	6	2299	2397	9	693	646	1	1063	1036	12	358	311	3	1272	1280	
4	1097	1041	7	633	683	10	400	413	3	673	728	13	623	606	5	499	507	
5	1046	999	8	1471	1495	11	478	391	5	537	729	1, 2, L			6	322	318	
6	883	861	9	760	798	0, 8, L			1, 0, L			-13	867	980	7	900	953	
8	1247	1283	10	988	997	0	1521	1543	-13	481	571	-12	284	349	8	542	556	
10	887	911	11	493	528	1	1984	1966	-11	838	912	-11	901	962	9	1380	1405	
11	274	269	12	847	846	2	1377	1444	-9	1538	1645	-10	255	287	10	646	624	
12	479	468	0, 5, L			3	1488	1526	-7	1988	2018	-9	1310	1333	11	1105	1105	
14	436	462	2	378	403	4	596	563	-5	2863	2638	-8	286	246	12	381	350	
0, 2, L			3	286	288	5	1281	1262	-3	3745	3175	-7	2205	2086	13	554	562	
0	2781	2901	4	557	483	6	845	795	-1	3100	2662	-6	509	466	1, 4, L			
2	2758	2610	5	703	659	7	1052	1034	1	2418	2995	-5	2400	2221	-13	772	808	
3	1257	1171	6	407	367	8	506	506	3	509	541	-3	2403	2250	-12	501	517	
4	1875	1874	7	439	408	9	418	430	5	281	285	-2	475	466	-11	862	875	
5	426	423	8	392	358	10	343	311	7	669	701	-1	2856	3011	-10	677	647	
6	1986	1969	10	532	508	0, 9, L			9	1144	1136	0	1594	1663	-9	807	819	
7	919	936	12	448	435	1	334	291	11	479	467	1	2515	2589	-8	812	768	
8	1509	1516	0, 6, L			2	527	515	1, 1, L			2	1110	1185	-7	1123	1109	
9	642	651	0	960	949	4	479	484	-13	394	434	3	1924	1957	-6	936	924	
10	934	951	1	2103	2106	6	628	653	-9	632	636	4	1842	1814	-5	1421	1408	
11	404	438	2	906	871	7	392	340	-8	307	326	5	1204	1252	-4	661	696	
12	647	689	3	1416	1415	8	544	616	-7	514	491	6	596	644	-3	441	457	
14	579	609	4	782	716	9	470	491	-5	542	527	7	1277	1299	-2	887	907	
0, 3, L			5	1360	1267	0, 10, L			-4	403	329	8	724	742	-1	687	650	
1	491	493	6	1315	1264	0	932	956	-3	1085	965	9	1022	1046	0	970	1044	
3	284	277	7	945	864	1	1094	1119	-2	625	592	10	339	408	1	2307	2502	
4	766	769	8	1159	1099	2	758	725	-1	1026	1071	11	436	478	2	1052	1116	

1, 4, L			-5	1113	1061	1, 8, L			-4	685	750	-8	1783	1730	-3	1131	1138
3	2059	2252	-4	2051	1947	-12	582	572	-2	874	887	-6	2413	2190	-2	872	930
4	1026	1025	-3	1309	1180	-11	416	427	-1	705	707	-4	3223	2776	-1	786	786
5	1657	1702	-2	1479	1492	-10	786	740	0	1406	1291	-2	731	650	0	1697	1703
6	1164	1141	-1	1593	1635	-9	564	580	1	781	765	0	3029	2930	1	1734	1738
7	1637	1685	0	2065	1968	-8	1116	1112	2	1412	1427	2	977	985	2	1512	1517
8	915	923	1	1779	1831	-7	978	935	4	894	852	4	534	498	3	995	1020
9	816	884	2	1005	1009	-6	1598	1591	6	1221	1211	6	891	884	4	515	520
10	574	543	3	1708	1641	-5	1308	1259	8	872	795	8	1189	1087	5	932	918
11	384	423	4	468	451	-4	1825	1660	10	509	519	2, 1, L			6	780	818
13	361	323	5	1333	1381	-3	855	895	1, 11, L			-10	271	298	8	890	873
1, 5, L			6	487	512	-2	1915	1854	5	412	290	-8	429	430	10	493	464
-5	432	387	7	1224	1220	-1	1192	1272	6	488	453	-6	1882	1691	2, 3, L		
-4	639	620	8	559	537	0	1151	1074	8	744	752	-5	878	816	-11	266	247
-2	698	617	9	758	699	1	937	997	1, 12, L			-4	2136	2000	-10	312	306
-1	754	697	12	441	443	2	1280	1263	-8	596	673	-3	1181	1151	-6	280	298
0	504	520	1, 7, L			4	980	951	-6	571	631	-2	2913	2903	-5	421	455
2	1477	1444	-10	420	373	6	667	687	-4	489	655	-1	214	129	-4	765	774
3	730	749	-9	438	386	7	530	513	-2	738	781	0	2085	2026	-3	611	645
4	1125	1158	-8	278	298	10	529	458	0	1401	1301	1	299	276	-2	531	579
5	542	590	-6	268	319	1, 9, L			2	1112	1143	2	1118	1171	-1	305	311
6	661	646	-4	647	560	-7	354	404	4	896	950	4	1637	1589	0	1268	1202
7	950	922	-2	919	862	-1	579	598	6	846	741	5	292	259	1	737	788
8	664	595	-1	615	619	0	458	441	8	850	809	6	1193	1136	2	2124	2124
9	1195	1135	0	1203	1186	1	978	1010	1, 13, L			7	370	426	3	845	860
10	502	480	1	456	518	2	742	752	-1	422	408	8	985	922	4	2389	2595
11	963	909	2	1080	1068	3	1046	1129	4	540	451	9	366	369	5	1558	1546
12	429	339	3	832	833	4	852	841	1, 14, L			10	1489	1404	6	1839	1868
13	664	584	4	1030	1014	5	458	421	-4	780	810	12	1218	1093	7	872	893
1, 6, L			5	956	870	6	732	695	0	904	846	14	753	640	8	1268	1325
-13	672	630	6	622	632	8	599	579	2	669	654	2, 2, L			9	624	601
-12	554	536	7	548	445	10	781	716	4	573	505	-14	649	722	10	1329	1333
-11	665	600	9	478	496	1, 10, L			1, 15, L			-12	1065	1146	11	501	468
-10	777	698	10	433	392	-10	712	739	2	516	554	-10	1045	1080	12	879	850
-9	782	746	11	679	669	-8	682	693	2, 0, L			-8	1141	1162	2, 4, L		
-8	1250	1152				-7	870	866	-14	862	931	-6	2250	2190	-13	387	417
-7	1432	1320				-6	1099	1076	-12	1313	1362	-5	721	691	-12	735	778
-6	1732	1669				-5	875	904	-10	1420	1421	-4	1810	1786	-11	488	507

2, 4, L		
-10	760	714
-9	468	431
-8	956	987
-7	482	488
-6	1918	1924
-5	1113	1071
-4	1831	1866
-3	619	625
-2	1147	1344
-1	967	1068
0	2740	2859
1	941	991
2	3080	3262
3	702	808
4	902	953
5	566	579
6	701	738
7	622	640
8	589	564

2, 5, L		
-5	621	578
-3	772	747
-2	339	329
-1	367	362
0	896	787
1	399	401
2	1616	1635
3	823	795
4	1945	1949
5	464	448
6	1537	1441
7	329	344
8	1366	1251
9	476	486
10	1168	1096
12	823	692

2, 6, L		
-13	523	477
-12	608	554
-11	837	803
-10	509	552
-9	1090	1020
-8	801	776
-7	1186	1144
-6	1145	1081
-5	1261	1202
-4	995	996
-3	754	746
-2	1410	1396
0	1345	1317
1	899	866
2	1594	1486
3	396	354
4	969	936
5	375	320
6	353	401
7	787	705
8	437	369
9	722	648
11	414	352

2, 7, L		
-7	671	680
-5	1249	1238
-4	900	930
-3	1184	1196
-1	1253	1269
0	544	575
1	994	915
2	1034	954
3	388	399
4	993	985
5	605	630
6	767	725
7	513	405
8	528	510
9	533	460
10	662	617
11	830	701
12	622	545

2, 8, L		
-12	521	545
-11	741	740
-10	657	693
-9	822	892
-8	748	781
-7	1087	1079
-6	996	1009
-5	887	918
-4	754	776
-3	774	770
-2	581	544
-1	889	924
1	792	765
2	279	258
3	755	760
6	468	449
7	401	441
8	542	499
9	406	433

2, 9, L		
-5	623	645
-4	940	941
-3	776	732
-2	774	711
-1	710	721
1	809	780
2	529	493
3	911	873
4	318	243
5	761	780
7	929	869
9	707	695
11	731	746

2, 10, L		
-9	656	651
-7	627	660
-6	315	388
-5	1146	1159
-4	411	304
-3	995	1122
-1	1117	1121
1	1329	1345
3	1198	1154
5	454	412
7	520	532

2, 11, L		
-1	474	476
1	769	837
3	1266	1259
5	1212	1206
7	1111	1028
9	919	876

2, 12, L		
-7	710	783
-5	844	943
-3	965	1020
-1	1098	1054
0	430	342
1	1110	1076
2	352	223
3	800	765

2, 13, L		
1	660	660
3	796	795
5	713	764
7	697	603

2, 14, L		
-5	572	748
-3	545	655
-1	519	525
3	502	492

2, 15, L		
-1	527	500
1	574	464

3, 0, L		
-13	748	836
-11	1008	1080
-9	704	690
-7	476	469
-5	1602	1441
-3	2433	2144
-1	1252	1049
1	1194	1172
3	1884	1856
5	1018	1044
7	652	619
9	1057	907

3, 1, L		
-11	787	801
-9	1041	1038
-7	936	888
-5	2001	1901
-4	504	466
-3	2111	2045
-2	2025	1956
0	745	742
1	440	443
2	1010	1060
3	2041	2049
4	1092	1142
5	1672	1752
7	1338	1305
9	1599	1577
10	287	275
11	1319	1269
13	970	894

3, 2, L		
-13	810	891
-11	988	1004
-10	272	233
-9	1037	1027
-8	296	301
-7	1246	1245
-6	703	704
-5	1410	1429
-4	1436	1426
-3	1270	1283
-2	331	354
-1	1643	1669
0	626	635
1	907	886
2	442	433
3	960	1021
5	605	565
6	820	782
7	226	153

3, 3, L		
-11	553	556
-9	421	437
-8	314	317
-7	386	382
-6	227	228
-5	1056	1082
-4	838	857
-3	1635	1755
-2	1143	1186
-1	2040	2069
0	1336	1318
1	2588	2609
2	1688	1700
3	1794	1924
4	932	969
5	1673	1779
6	709	776

3, 3, L		
7	1484	1554
8	325	274
9	888	957
11	912	959
13	691	675
3, 4, L		
-13	589	582
-12	366	400
-11	711	699
-10	517	522
-9	1048	1079
-8	707	703
-7	1275	1358
-6	683	676
-5	1516	1538
-4	605	629
-3	1415	1567
-2	706	756
-1	919	932
0	346	290
1	1116	1157
2	456	447
3	844	872
4	286	305
5	704	736
7	389	453
3, 5, L		
-12	408	331
-10	515	429
-9	601	560
-8	706	695
-6	1021	979
-5	782	711
-4	822	825
-3	1595	1665
-2	1017	1039
-1	2259	2266
0	1222	1029
1	2279	2337
2	1151	1120
3	2286	2327
4	1310	1250
5	1662	1600
6	1080	1025
7	868	864
8	908	788
9	885	801
10	864	742
11	819	709
12	625	616
3, 6, L		
-12	576	557
-11	844	781
-10	558	551
-9	615	615
-8	618	540
-7	1115	1037
-5	1512	1482
-3	794	860
-1	529	468
1	1202	1157
2	771	773
3	436	458
4	831	809
6	416	452
3, 7, L		
-10	775	764
-9	487	447
-8	822	846
-7	338	288
-6	875	860
-5	808	837
-4	1010	1025
-3	1287	1351
-2	530	568
-1	821	804
0	383	384
1	750	712
2	531	555
3	1209	1188
4	652	585
5	1105	1073
6	821	827
7	685	618
8	994	882
9	671	588
10	1095	934
11	788	770
12	865	742
3, 8, L		
-11	552	557
-10	540	573
-9	373	380
-8	360	427
-6	683	735
-4	542	578
-2	297	335
0	562	577
2	973	994
3	524	552
4	412	342
7	379	395
3, 9, L		
-8	618	674
-7	446	533
-6	457	452
-5	420	491
-4	930	990
-2	1049	1105
0	991	1030
2	1059	1000
4	1445	1387
5	633	665
6	1189	1123
7	512	513
8	949	862
9	555	488
10	854	737
3, 10, L		
-10	515	524
-8	620	694
-6	843	911
-4	927	1016
-2	947	955
0	649	582
2	530	554
3, 11, L		
-6	497	532
-4	741	841
-2	954	1026
0	1388	1370
2	1263	1201
4	1164	1103
6	1042	976
8	688	674
3, 12, L		
-6	773	819
-4	910	972
-2	683	728
0	588	581
3, 13, L		
-6	466	532
-4	631	753
-2	808	913
0	766	739
2	917	908
4	1011	955
6	755	739
3, 14, L		
2	465	377
4, 0, L		
-12	673	689
-10	517	460
-6	345	347
-4	1139	1038
-2	1020	909
0	827	798
2	988	998
4	740	717
8	860	818
10	761	787
12	669	599
4, 1, L		
-12	614	645
-10	998	1002
-8	938	942
-7	427	408
-6	1466	1445
-5	885	856
-4	1390	1325
-3	189	112
-2	1930	1786
-1	577	566
0	1663	1650
2	1901	1915
3	314	297
4	2464	2427
6	2150	2309
8	1220	1286
10	1073	1137
12	947	949
4, 2, L		
-12	632	673
-11	331	325
-10	780	777
-9	436	461
-8	288	264
-7	633	636
-6	697	722
-5	237	283
-4	1098	1130
-3	318	275
-2	202	232
-1	434	447
0	169	161
1	471	492
2	451	471
3	922	940
4	334	351
6	524	510
12	466	450
4, 3, L		
-12	409	457
-11	291	300
-10	1013	1035
-8	1193	1263
-7	556	568
-6	984	1024
-5	1259	1293
-4	1859	1952
-3	1718	1789
-2	2609	2632
-1	1186	1196
0	2031	1960
1	900	831
2	1473	1459
3	597	583
4	1660	1816
5	413	423
6	1494	1528
7	360	323
8	886	876
10	772	781
12	766	782

4, 4, L			4, 6, L			1 544 616			3 800 744			-4 1045 1070			2 343 400		
-12	710	731	-12	575	573	2	420	434	5, 0, L			-3	370	361	5, 5, L		
-11	479	498	-10	623	575	4	358	414	-11	353	300	-2	604	603	-11	769	725
-10	794	835	-8	430	383	8	422	304	-9	310	237	0	280	220	-10	612	572
-9	528	525	-6	646	639	4, 9, L			-7	542	515	1	776	781	-9	1331	1217
-8	876	902	-5	407	395	-9	569	576	-5	617	651	3	430	419	-8	663	624
-6	845	896	-4	498	504	-7	665	639	-3	1661	1508	5	797	817	-7	1193	1127
-5	492	544	-3	885	909	-5	845	844	-1	456	426	7	1057	1096	-6	591	574
-4	776	813	-1	270	275	-3	1099	1187	1	576	544	9	725	734	-5	1235	1222
0	862	865	1	811	757	-1	1209	1229	3	590	656	11	484	495	-4	675	676
2	257	284	3	991	950	1	1110	1159	5	713	744	5, 3, L			-3	1275	1247
4	568	638	4, 7, L			2	464	492	7	1710	1679	-12	318	281	-2	1302	1254
6	834	838	-11	555	562	3	899	900	9	645	676	-11	842	875	-1	1171	1180
4, 5, L			-10	585	571	4	1143	1196	11	506	629	-10	548	553	0	1209	1201
-12	313	291	-9	881	868	5	1022	992	5, 1, L			-9	1328	1352	1	849	744
-11	562	490	-8	670	637	6	743	732	-13	417	446	-8	544	563	2	1212	1108
-10	763	719	-7	585	531	7	1052	994	-11	731	713	-7	1200	1223	3	562	500
-9	527	473	-6	512	466	8	481	429	-10	261	276	-6	520	566	4	1106	1106
-8	1236	1107	-5	599	608	9	667	664	-9	1322	1236	-5	1043	1096	5	762	820
-7	572	588	-4	979	1046	4, 10, L			-8	257	199	-4	410	410	6	701	780
-6	1196	1131	-3	570	594	-9	568	587	-7	1245	1172	-3	2083	2220	7	720	731
-5	484	472	-2	799	779	-7	493	464	-6	592	604	-2	506	513	9	581	557
-4	1757	1816	-1	902	923	-5	591	560	-5	1643	1578	-1	1683	1737	10	431	426
-2	2281	2210	0	942	851	-3	356	396	-4	534	556	0	291	345	11	679	623
-1	853	838	1	1475	1494	1	278	336	-3	2274	2160	1	1109	1074	5, 6, L		
0	2197	2040	2	1117	1134	4, 11, L			-2	331	313	3	1127	1132	-4	401	386
1	1005	897	3	1315	1350	-7	691	802	-1	2333	2199	5	1318	1284	-2	529	534
2	1233	1139	4	1156	1087	-5	1066	1150	1	2233	2187	7	1038	1089	-1	629	689
3	978	990	5	1378	1282	-3	1360	1413	2	205	196	9	765	793	1	512	475
4	935	959	6	942	877	-1	1084	1170	3	2334	2491	11	632	659	4	313	353
5	1141	1127	7	1429	1313	1	888	908	5	2041	1930	12	371	329	6	703	697
6	638	642	8	723	665	3	1073	1022	7	1324	1324	5, 4, L			8	912	811
7	802	800	9	1106	968	5	886	909	9	734	715	-5	325	374	9	650	571
8	475	458	11	798	682	4, 13, L			11	470	458	-3	318	295	11	408	361
9	703	624	4, 8, L			-5	678	804	5, 2, L			-2	542	554	5, 7, L		
10	784	695	-5	434	416	-3	861	881	-11	462	454	-1	860	846	-9	630	614
11	669	551	-4	364	403	-1	833	826	-9	530	538	0	393	377	-8	645	638
12	662	607	-1	614	661	1	722	695	-6	506	512	1	1024	998	-7	613	604

5, 7, L		
-6	620	566
-5	449	479
-4	981	1003
-3	978	961
-2	1397	1275
-1	1094	1082
0	1611	1483
1	995	980
2	1546	1441
3	754	777
4	990	1067
5	710	700
6	900	867
7	482	488
8	691	640

5, 8, L		
2	374	378
4	616	623
5	644	704
6	568	597
7	727	673
8	611	573

5, 9, L		
-8	935	951
-6	816	877
-4	1068	1148
-2	1257	1152
-1	935	931
0	1137	1144
1	738	740
2	744	874
3	697	699
4	1012	1034
5	823	899
6	1061	965
8	725	725

5, 10, L		
0	538	460
2	430	427
5	468	433

5, 11, L		
-6	886	872
-4	871	921
-2	909	814
0	632	683
2	489	517
4	615	650
6	712	665

5, 13, L		
-4	616	653
-2	889	808
0	556	700
2	557	660

6, 0, L		
-10	365	342
-6	286	266
-4	524	470
-2	700	664
0	1957	1910
2	1731	1821
4	1233	1274
6	1363	1352
8	1408	1341
10	576	527

6, 1, L		
-12	505	520
-10	1007	932
-8	1580	1472
-6	1639	1557
-4	1306	1231
-3	506	492
-2	2266	2114
0	2061	2001
2	1009	1034
4	623	670
5	494	507
6	696	727
7	436	425

6, 2, L		
-7	480	545
-6	354	371
-5	495	507
-3	278	333
-2	852	880
0	1157	1161
1	302	306
2	1047	1044
3	277	309
4	949	1022
6	1053	1071
8	793	792
10	747	721
11	387	337

6, 3, L		
-12	630	656
-10	910	941
-9	452	473
-8	1106	1103
-7	401	431
-6	996	1029
-4	885	956
-2	1071	1086
-1	350	414
0	1018	968
1	420	410
2	924	1000
3	785	807
4	1033	1047
5	639	609
6	1163	1134
7	637	603
8	850	825
9	566	530

6, 4, L		
-8	357	396
-6	614	676
-5	217	255
-4	588	637
-1	260	259
0	403	406
2	700	695
4	395	365
6	627	587
7	462	448
8	1074	1013
9	423	380
10	855	844

6, 5, L		
-11	511	448
-10	603	616
-9	509	449
-8	957	872
-7	599	536
-6	541	576
-5	951	896
-4	866	850
-3	865	818
-2	822	844
-1	934	909
0	889	867
1	1411	1208
2	571	520
3	601	547
4	996	931
6	1113	1080
7	547	528
8	560	582

6, 6, L		
-6	545	560
-1	712	721
0	642	639
1	1077	1037
3	1036	940
5	713	678
6	538	617
8	770	779
10	617	568

6, 7, L		
-10	480	418
-9	809	784
-8	806	859
-7	894	901
-6	554	568
-5	1094	1127
-4	614	620
-3	1529	1452
-2	1173	1121
-1	1386	1391
0	1044	1015
1	977	943
2	487	485
3	712	673
4	586	541
5	476	450

6, 8, L		
-5	346	321
-1	593	665
0	749	718
1	1106	1078
2	1095	989
3	667	610
5	653	683
6	681	696
7	552	635
8	564	532
9	402	545

6, 9, L		
-9	682	672
-8	375	429
-7	853	830
-5	700	716
-4	681	657
-3	911	862
-2	723	743
-1	778	798
0	670	715
1	821	828
3	571	536
5	654	645

6, 10, L		
0	469	481
1	560	535
2	539	471
7	477	492

6, 11, L		
-5	501	554
-3	553	496
-1	374	442
1	579	617
3	618	752
5	571	687

6, 12, L		
3	379	366

7, 0, L		
-9	481	426
-7	760	682
-5	1129	1031
-3	1426	1359
-1	1427	1328
1	1618	1540
3	1383	1530
5	683	653
7	823	803

7, 0, L		
9	759	669
11	636	562
7, 1, L		
-11	712	667
-9	1319	1246
-7	1459	1360
-5	1164	1115
-3	1026	987
-2	229	206
-1	1039	988
0	369	327
1	474	452
2	657	695
3	305	333
4	310	319
7	386	370
7, 2, L		
-9	286	227
-7	631	619
-5	1170	1207
-3	829	862
-2	282	300
-1	1102	1113
1	1727	1787
3	1152	1223
5	830	842
6	271	314
7	1240	1217
8	602	622
9	985	935
10	450	425
7, 3, L		
-11	462	512
-9	665	670
-7	891	936
-5	566	568
-3	793	832

-2	524	531
-1	1166	1204
0	692	683
1	1055	1033
2	768	757
3	651	731
4	574	599
5	721	696
7	453	402
7, 4, L		
-7	365	415
-5	495	560
-3	287	289
-2	289	311
-1	250	261
0	400	409
1	996	979
2	695	704
3	1083	1066
4	362	393
5	927	921
6	571	563
7	1168	1106
8	547	528
9	1144	1065
10	409	399
7, 5, L		
-10	413	425
-9	576	503
-8	656	574
-7	557	532
-6	648	591
-5	612	592
-4	538	490
-3	862	807
-2	691	679
-1	1003	920
0	531	427

1	1086	966
3	759	678
5	806	668
6	305	236
7, 6, L		
-7	359	355
-6	580	515
-5	553	539
-4	1076	1026
-3	408	361
-2	850	787
-1	434	447
0	791	696
1	849	837
2	811	778
3	817	772
4	710	591
5	1021	872
7	880	785
9	821	781
7, 7, L		
-8	800	761
-7	682	639
-6	796	720
-5	380	424
-4	828	773
-3	589	558
-2	631	574
-1	684	661
7, 8, L		
-6	539	573
-5	477	436
-4	780	725
-3	635	581
-2	801	737
-1	647	697
0	765	759
1	694	666

2	827	788
4	762	700
7, 9, L		
-7	599	592
-6	531	588
-4	558	559
-2	449	468
0	494	469
4	352	438
7, 10, L		
-2	418	359
0	509	495
1	481	530
2	907	865
4	700	653
6	545	659
7, 11, L		
-2	477	533
0	771	839
7, 12, L		
0	425	541
8, 0, L		
-10	564	521
-8	963	882
-6	1136	1062
-4	1335	1301
-2	1084	1081
0	1017	980
2	852	876
4	756	842
6	479	467
8	1002	961
8, 1, L		
-10	517	523
-8	718	673
-6	660	626
-5	334	317
-3	358	346

-1	319	298
0	368	332
8, 2, L		
-10	495	486
-8	597	577
-6	823	806
-4	942	935
-2	925	897
-1	479	500
0	1080	1074
1	704	715
2	1238	1303
3	650	722
4	846	917
5	551	504
6	779	793
7	411	405
8	767	786
9	361	250
8, 3, L		
-10	383	326
-8	588	587
-6	837	876
-5	568	600
-4	377	373
-3	478	458
-2	508	505
-1	599	601
0	672	665
1	386	386
2	272	301
5	357	318
8, 4, L		
-6	681	718
-5	469	537
-4	840	896
-3	433	491
-2	847	882

-1	639	668
0	1134	1114
1	739	765
2	1488	1553
3	647	668
4	1274	1359
5	455	443
6	1016	975
7	638	599
8	855	834
8, 5, L		
-8	604	544
-7	374	329
-6	619	547
-4	748	790
-2	700	709
0	726	693
8, 6, L		
-7	618	587
-6	642	599
-5	908	826
-4	863	815
-3	818	781
-2	633	597
-1	461	471
0	739	700
1	391	400
2	936	922
3	539	517
4	1009	904
5	598	519
6	739	678
8	641	579
8, 7, L		
-8	535	440

8, 8, L		
-7	516	489
-6	559	588
-5	754	741
-4	691	562
-3	655	685
-2	445	474
0	392	420
1	671	622
2	614	587
3	559	537
5	554	552

8, 10, L		
-3	581	581
-1	635	702
1	793	867
3	1009	925

9, 0, L		
-9	685	650
-7	679	667
-5	890	840
-3	887	900
-1	493	462
1	820	813
3	1078	1241
5	946	950
7	855	792

9, 2, L		
-9	619	603
-7	628	672
-5	1046	1074
-4	524	549
-3	1038	1093
-2	577	576
-1	925	933
0	553	518
1	1117	1145
3	1059	1189
5	713	721
7	763	771

9, 3, L		
-7	375	376
-6	413	431
-5	301	284
5	487	494

9, 4, L		
-7	614	621
-6	432	337
-5	887	930
-4	501	487
-3	1123	1145
-2	599	616
-1	1116	1124
0	476	490
1	985	983
2	543	547
3	931	966
4	433	451
5	639	675

9, 5, L		
-7	549	531
3	574	572
5	634	559
7	407	337

9, 6, L		
-5	873	870
-4	522	510
-3	894	851
-1	572	520
0	288	211
1	814	794
2	339	386
3	751	709
4	780	733
5	587	459
6	588	555

9, 8, L		
-4	536	568
-2	511	513
2	658	710
3	427	392
4	817	709

10, 0, L		
-6	574	591
-4	886	836
-2	987	947
0	1034	1000
2	908	898
4	900	1037
6	670	704

10, 1, L		
1	302	298
4	422	457
6	532	614

10, 2, L		
-7	358	351
-6	568	548
-5	352	344
-4	889	886
-3	380	360
-2	936	908
0	685	658
2	784	859
4	802	861
6	451	432

10, 3, L		
-3	267	272
-2	554	565
-1	311	346
0	418	449
1	328	355
4	550	551
6	325	409

10, 4, L		
-6	756	801
-5	426	475
-4	791	891
-3	403	447
-2	749	770
-1	346	323
0	503	513
2	414	443
3	339	332
4	370	418

10, 5, L		
-2	506	503
0	398	387
4	504	455

10, 6, L		
-4	554	581
-2	502	498
-1	426	492
1	707	646
2	301	351
3	713	666

11, 0, L		
-3	990	959
-1	759	735
1	504	560

11, 1, L		
-3	363	392
-1	598	569
1	637	661
3	545	648

11, 2, L		
-3	744	776
-1	617	627
3	425	481

11, 3, L		
-3	458	473
-1	544	557
1	412	426

CALCULATED AND OBSERVED STRUCTURE FACTORS OF $[Ru(SC(NH_2)_2)_6][CF_3SO_3]_2$

0, 0, L

2	781	826
3	424	393
4	356	364
6	43	56
7	751	758
8	480	472
9	146	143
10	563	552
11	153	157
12	304	300
14	217	213
15	208	212
17	106	105

0, 1, L

1	17	20
2	27	8
3	788	788
4	725	729
5	151	145
6	419	427
8	142	146
9	233	236
10	139	137
11	128	133
12	42	29
13	153	158
15	44	38
17	38	42

0, 2, L

0	911	914
1	37	38
2	416	412
3	468	472
4	171	159
5	201	212
6	410	404
7	965	983
8	735	744
9	465	463
10	512	520
11	54	50
12	445	441
13	310	312
14	367	361
15	273	276
17	143	147

0, 3, L

1	95	98
3	988	995
4	169	164
5	341	349
7	210	214
8	82	83
9	255	266
10	127	129
11	160	163
12	112	114
13	222	225
14	69	71
16	114	110
17	60	58

0, 4, L

0	818	818
1	901	884
2	55	56
3	578	595
4	184	192
5	706	704
6	553	585
7	704	702
8	453	466
9	127	115
10	193	189
11	41	39
12	256	259
13	248	250
14	281	283
15	309	314
16	110	117
17	114	115

0, 5, L

1	475	460
2	217	211
3	740	728
4	198	197
5	37	41
6	156	170
7	267	282
8	218	228
9	381	387
10	171	168
11	59	49
12	49	52
13	158	159
16	88	84

0, 6, L

0	672	657
1	454	447
2	589	590
3	529	543
4	346	342
5	756	739
6	607	599
7	468	460
8	342	336
9	70	73
10	117	124
12	75	72
13	301	298
14	282	285
15	298	299
16	147	154

0, 7, L

1	100	102
2	258	252
3	139	142
4	422	421
5	130	127
6	217	233
7	208	197
8	180	183
9	238	238
10	138	137
11	63	74
12	113	112
13	44	52
14	44	52
15	60	54

0, 8, L

0	361	359
1	262	260
2	167	160
3	89	86
4	318	317
5	506	501
6	679	655
7	551	545
8	394	396
9	326	327
11	136	134
12	180	182
13	350	341
14	273	275
15	243	243

0, 9, L

1	136	135
2	85	83
3	312	309
5	145	151
6	238	246
7	139	143
8	258	257
10	56	53
12	155	149
14	76	71

0, 10, L

0	489	490
1	779	743
2	410	408
3	213	213
4	196	200
5	125	117
6	324	321
7	188	189
8	285	283
9	166	164
11	109	106
12	53	58
13	146	148

0, 11, L

1	76	70
2	272	274
3	208	201
4	151	148
5	97	94
7	43	57
8	127	129
12	81	81

0, 12, L

0	275	275
1	416	399
2	196	197
4	67	72
6	331	330
7	112	111
8	277	270
9	230	226
10	148	152
11	176	184

0, 14, L

0	152	144
1	290	281
2	151	150
4	108	111
5	48	43
6	175	178
7	166	163

0, 15, L

2	44	47
3	100	95
4	93	95

1, 1, L

-17	52	42
-16	86	84
-15	182	182
-14	474	468
-13	250	254
-12	533	524
-11	460	457
-10	377	369
-9	447	445
-8	120	122
-7	701	710
-6	673	673
-5	798	802
-4	945	978
-2	847	844
-1	738	729
0	728	708
1	899	923
2	559	539
3	879	927
4	309	299
5	273	271
6	764	769
7	475	450

1, 1, L		
8	928	933
9	323	317
10	185	173
11	144	150
12	118	126
13	186	186
14	178	183
15	332	332
16	158	167
17	130	139

1, 2, L		
-17	88	91
-14	188	182
-12	70	70
-11	398	407
-10	67	60
-9	522	535
-8	408	408
-7	128	133
-6	66	79
-5	121	125
-4	77	73
-3	873	868
-2	400	393
-1	305	285
0	468	449
1	60	48
2	383	396
3	153	140
4	670	688
5	444	438
6	184	219
7	419	417
8	172	173
9	229	233
10	101	95
11	319	317
12	49	50
13	75	67
15	44	48

1, 3, L		
-17	62	62
-16	130	131
-15	248	252
-14	566	568
-13	331	327
-12	537	543
-11	371	371
-10	116	114
-9	492	487
-8	399	392
-7	477	467
-6	487	511
-5	68	68
-4	200	214
-2	28	31
-1	260	276
0	982	999
1	858	847
2	576	571
3	428	430
4	112	112
5	461	475
6	471	477
7	735	743
8	874	883
9	472	467
10	242	242
11	428	429
12	169	166
13	312	308
14	220	217
15	270	271
16	155	160

1, 4, L		
-15	51	61
-14	166	165
-13	71	69
-12	107	111
-11	75	78
-10	247	263
-9	98	105
-8	112	108
-7	405	421
-6	306	301
-5	616	610
-4	270	276
-3	85	88
-2	260	273
-1	1248	1300
0	697	693
1	859	859
2	763	760
4	147	118
5	319	321
6	148	147
7	101	108
8	99	108
9	469	462
10	40	39
11	106	105
12	75	70
13	60	59
14	141	135
15	242	248
16	55	54

1, 5, L		
-17	116	124
-16	132	136
-15	103	107
-14	143	146
-13	105	102
-12	101	105
-9	286	294
-8	570	579
-7	834	819
-6	968	931
-5	819	790
-4	520	520
-3	40	50
-2	721	705
-1	714	716
0	740	726
1	885	891
2	554	557
3	528	504
4	443	437
5	99	92
6	566	571
7	134	133
8	323	323
9	162	152
12	41	43
13	247	238
14	328	326
15	263	258
16	200	203

1, 6, L		
-14	98	100
-11	250	259
-10	70	79
-9	228	215
-8	464	481
-7	116	114
-6	265	274
-4	153	168
-3	204	186
-2	685	669
-1	572	585
0	488	483
1	55	47
3	83	90
4	158	135
5	406	418
6	123	139
7	323	319
8	134	136
9	61	67
10	49	49
11	225	223
14	114	108

1, 7, L		
-16	145	146
-15	188	192
-14	245	253
-13	300	310
-12	127	123
-11	139	138
-10	203	209
-9	309	301
-8	447	453
-7	618	618
-6	538	548
-5	188	182
-4	98	111
-2	92	102
-1	229	218
0	625	608
1	786	755
2	723	706
3	204	208
4	463	457
5	130	122
6	390	400
7	302	288
8	466	458
9	274	269
10	236	219
11	197	204
12	326	323
13	256	267
14	269	266
15	178	184

1, 8, L		
-13	70	67
-12	73	73
-10	155	155
-9	150	149
-7	273	295
-6	293	283
-5	83	89
-4	325	324
-3	52	46
-2	71	62
0	174	172
1	302	296
2	112	110
3	155	156
4	242	247
6	360	352
9	79	80
10	191	191
12	108	108
14	62	60

1, 9, L		
-14	197	197
-13	289	283
-12	155	152
-10	218	210
-9	129	128
-8	338	337
-7	371	350
-6	529	522
-5	387	380
-4	104	110
-3	202	211

1, 9, L

-1	327	312
0	482	473
1	378	383
2	642	625
3	203	207
4	203	196
5	276	270
6	207	213
7	431	424
8	193	185
9	287	287
10	173	167
11	106	106
12	155	157
13	167	178

1, 10, L

-12	47	46
-11	50	66
-10	214	220
-9	148	145
-8	113	114
-7	98	106
-6	103	102
-4	256	270
-3	131	134
-2	59	56
0	218	215
1	136	134
2	63	68
4	332	330
5	65	61
6	160	156
7	197	198
8	52	55
10	175	173
11	56	54
12	81	90

1, 11, L

-12	130	129
-10	136	129
-9	71	61
-8	247	250
-7	316	322
-6	392	381
-5	449	447
-4	208	210
-3	362	370
-2	295	299
-1	416	412
0	423	402
1	308	310
2	299	301
3	102	106
4	109	113
5	151	151
6	116	121
7	336	331
8	90	92
9	273	265
10	62	65

1, 12, L

-11	75	73
-8	68	66
-7	99	97
-6	180	176
-5	144	130
-3	53	47
-2	151	148
-1	109	102
0	121	112
1	97	93
2	161	151
3	72	73
4	43	28

1, 13, L

-10	196	191
-9	46	48
-8	115	109
-7	91	78
-6	65	65
-5	172	164
-3	205	202
-1	200	200
0	287	267
1	90	95
2	248	242
4	84	76
5	144	144
6	192	197
7	385	385
8	235	236
9	260	277

1, 14, L

-8	76	73
-7	75	81
-5	82	77
-4	53	55
-1	59	57
0	81	88
1	139	138
2	83	83
3	63	53

1, 15, L

-4	130	123
-3	230	228
-2	180	175
-1	227	233
0	240	238
1	106	110
2	193	197

2, 0, L

-18	104	104
-15	231	236
-14	287	294
-13	597	590
-12	340	335
-11	458	457
-10	145	139
-8	598	605
-7	783	785
-6	1028	1064
-5	844	849
-4	728	687
-3	1044	1126
-2	232	234
-1	1242	1248
0	158	123
1	548	537
2	486	473
3	287	251
4	432	451
5	376	354
6	564	576
7	387	375
8	329	343
9	565	550
10	75	81
11	66	67
12	73	69
13	166	165
14	404	401
15	289	280
16	348	348

2, 1, L

-18	55	59
-15	65	53
-13	275	280
-12	269	264
-11	202	197
-10	272	273
-8	143	139
-7	321	321
-6	204	184
-5	327	342
-4	212	208
-3	238	242
-2	289	298
-1	381	363
0	522	499
1	575	557
2	613	592
3	873	882
4	149	140
5	303	302
6	340	335
7	68	61
8	195	196
9	278	265
10	296	297
12	56	49

2, 2, L

-18	165	167
-16	216	214
-15	383	377
-14	369	372
-13	536	530
-12	255	258
-11	482	477
-10	185	183
-9	90	92
-8	484	486
-6	763	763
-5	745	739
-4	936	936
-3	366	382
-2	722	714
-1	616	588
0	661	636
1	417	389
2	594	602
3	752	759
4	441	442
5	235	248
6	1072	1088
7	828	829
8	530	530
9	584	586
10	106	100
11	147	142
13	84	76
14	309	307
15	201	203
16	243	250

2, 3, L

-18	50	54
-17	74	84
-16	102	100
-14	106	112
-13	191	197
-12	166	162
-11	169	166
-10	128	133
-9	202	216
-8	136	131
-7	543	528
-5	236	224
-4	130	120
-3	847	824
-2	406	407
-1	28	9
0	251	238
1	490	503
2	507	507
3	349	359

2, 3, L		
4	242	260
5	138	139
6	40	37
7	201	210
8	183	181
11	170	164
12	51	53
13	177	179
15	72	68
2, 4, L		
-17	40	32
-16	71	79
-15	111	117
-14	241	258
-13	422	413
-12	296	298
-11	422	429
-10	122	132
-9	158	151
-8	575	575
-7	529	531
-6	976	959
-5	314	332
-4	398	371
-3	77	85
-2	262	256
-1	537	497
0	975	983
1	743	726
2	831	838
3	421	446
4	396	389
6	154	141
7	391	388
8	355	355
9	629	610
10	209	202
11	240	232
12	129	135
13	120	114
14	255	253
15	179	185
2, 5, L		
-14	120	122
-13	112	110
-12	207	212
-11	219	219
-10	291	292
-9	174	163
-8	141	147
-7	425	434
-6	49	43
-5	91	95
-4	146	142
-3	392	403
-2	78	84
-1	172	175
0	517	496
1	416	392
2	334	337
3	384	389
4	200	201
5	212	219
6	129	141
7	338	357
8	125	129
10	61	66
11	83	80
13	153	153
15	56	48
2, 6, L		
-14	181	182
-13	260	267
-12	302	313
-11	220	221
-10	380	377
-9	339	350
-8	498	495
-7	629	621
-6	604	593
-5	501	517
-4	180	176
-3	405	421
-2	85	89
-1	558	526
0	802	783
1	1018	978
2	939	892
3	182	178
4	82	82
5	222	218
6	259	262
7	333	330
8	328	331
9	386	392
10	252	258
11	271	272
12	237	244
13	153	149
14	201	205
15	135	145
2, 7, L		
-15	102	101
-14	103	98
-13	131	131
-12	136	140
-11	110	105
-10	239	238
-8	182	189
-7	154	164
-6	86	84
-5	259	260
-4	414	428
-3	115	120
-2	182	188
-1	103	103
0	171	170
1	436	435
2	56	42
3	174	184
4	102	96
6	212	208
7	232	228
9	176	167
10	146	156
12	74	78
14	115	115
2, 8, L		
-15	117	118
-14	222	217
-13	224	220
-12	294	293
-11	170	177
-10	231	239
-9	136	129
-8	247	246
-7	315	315
-6	328	330
-5	298	307
-4	180	189
-3	98	94
-2	74	65
-1	162	162
0	629	611
1	713	698
2	516	515
3	455	447
4	317	324
5	354	346
6	282	291
7	374	373
8	504	505
9	350	354
10	368	370
11	194	193
12	96	94
13	64	72
2, 9, L		
-14	139	148
-13	129	123
-12	190	189
-11	179	181
-10	42	35
-8	49	50
-7	157	153
-6	50	45
-5	194	199
-4	210	207
-3	70	74
-2	266	272
0	405	417
1	141	134
2	484	482
3	323	331
4	152	154
5	213	208
6	179	169
8	237	244
9	262	252
11	90	74
2, 10, L		
-14	161	165
-13	187	182
-12	220	217
-11	107	116
-10	200	195
-9	286	282
-8	160	161
-7	447	445
-6	444	441
-5	444	445
-4	367	352
-3	239	248
-2	493	490
-1	170	177
0	455	446
1	495	484
2	352	350
3	101	94
4	62	55
5	95	92
7	176	172
8	301	306
9	123	122
10	142	146
12	97	96
2, 11, L		
-10	62	60
-8	144	143
-7	100	100
-5	69	80
-3	96	98
-2	136	137
-1	184	176
0	110	108
1	163	159
2	38	46
3	79	83
4	89	92
6	139	141
8	81	73
10	74	77
2, 12, L		
-11	65	57
-9	93	85
-7	331	318
-6	192	190

2, 12, L			-15	284	290	-11	153	145	-4	245	235	4	407	394	10	347	336
-5	361	361	-14	185	183	-10	65	59	-3	388	385	5	319	322	11	181	181
-4	269	262	-13	215	213	-8	309	315	-2	350	367	6	172	164	12	118	115
-2	306	315	-12	604	607	-7	218	224	-1	283	264	7	102	87	13	87	83
0	169	172	-11	37	37	-6	258	267	0	923	917	8	52	43	14	159	160
1	175	173	-10	258	261	-5	123	130	1	870	854	9	234	236	3, 6, L		
2	135	139	-9	238	238	-4	381	379	2	1046	1047	10	186	192	-14	141	149
3	280	271	-8	823	824	-3	213	228	3	727	742	11	144	144	-12	241	239
4	80	81	-7	580	596	-2	168	183	4	658	662	12	232	226	-10	44	40
5	334	332	-6	1082	1113	-1	250	236	5	405	425	13	71	75	-9	241	239
6	224	224	-5	1027	1078	0	722	695	6	260	258	14	50	59	-8	295	299
7	299	306	-4	434	406	1	316	302	7	388	393	15	102	98	-7	145	149
8	298	296	-3	218	220	2	237	238	8	526	519	3, 5, L			-6	54	60
9	123	130	-2	176	157	3	220	216	9	454	435	-16	90	95	-5	144	153
2, 13, L			-1	606	595	4	30	18	10	410	403	-15	116	122	-3	491	502
-9	88	85	0	836	819	5	447	453	11	76	73	-14	232	228	-2	83	99
-5	74	70	1	583	558	6	110	110	12	133	129	-13	412	419	-1	535	522
-1	43	40	2	1048	1055	7	223	229	14	141	138	-12	542	545	0	316	324
4	56	55	3	734	735	8	313	314	15	205	201	-11	564	560	1	210	203
2, 14, L			4	412	407	9	44	40	3, 4, L			-10	331	354	3	123	120
-7	180	187	5	325	331	10	80	87	-18	105	104	-9	306	304	4	119	116
-6	174	173	6	66	59	12	42	36	-14	40	44	-8	297	294	5	370	362
-5	273	282	7	408	402	15	100	95	-13	106	115	-7	598	604	8	268	281
-4	189	182	8	321	317	3, 3, L			-11	301	301	-6	480	471	10	80	74
-2	161	157	9	265	259	-18	161	163	-10	266	277	-5	872	840	11	41	47
0	158	163	10	317	305	-17	196	196	-9	84	80	-4	824	806	13	94	87
1	217	212	11	154	153	-16	92	89	-8	280	273	-3	845	819	3, 7, L		
2	122	126	12	293	286	-15	283	284	-7	254	241	-2	268	274	-15	66	66
3	217	224	13	138	137	-14	156	160	-6	157	151	-1	232	253	-14	267	269
5	253	254	14	305	295	-13	432	416	-5	644	626	0	616	624	-13	380	382
6	204	211	15	298	305	-12	517	515	-4	553	540	1	224	221	-12	393	394
2, 15, L			3, 2, L			-11	168	169	-3	378	359	2	104	104	-11	364	372
-3	82	83	-17	43	46	-10	172	166	-2	772	743	3	300	284	-10	264	253
-2	83	86	-16	62	56	-9	105	105	-1	424	401	4	258	263	-8	140	149
3, 1, L			-15	73	71	-8	72	66	0	144	139	5	73	67	-7	170	174
-18	158	163	-14	206	202	-7	271	279	1	76	73	7	522	530	-6	160	149
-17	180	178	-13	95	104	-6	415	417	2	139	132	8	525	521	-5	353	354
-16	94	102	-12	286	284	-5	956	950	3	114	107	9	328	332	-4	438	433

3, 7, L			3, 9, L			7	283	263	3, 13, L			-7	403	408	0	172	171
-3	396	400	-14	204	200	9	82	78	-8	87	81	-6	670	697	1	164	157
-2	425	423	-13	280	291	10	102	102	-7	92	98	-5	857	858	2	96	102
-1	592	567	-12	249	261	3, 11, L			-6	348	346	-4	448	479	3	566	546
0	576	570	-11	356	352	-13	169	177	-5	71	72	-2	96	79	4	250	255
1	696	682	-10	157	158	-12	73	68	-4	188	186	-1	119	114	5	226	228
2	455	442	-9	36	30	-11	220	209	-1	217	207	0	63	65	6	138	138
3	434	436	-8	75	77	-10	113	126	0	69	70	1	619	625	7	228	240
5	285	290	-7	328	321	-9	271	268	1	450	452	2	741	744	8	57	48
6	206	207	-6	300	307	-8	313	305	2	351	352	3	894	899	11	77	71
7	462	470	-5	360	360	-7	332	344	3	352	352	4	244	218	4, 2, L		
8	462	470	-4	395	378	-6	602	587	4	324	329	5	45	39	-18	217	221
9	521	499	-3	207	215	-5	265	283	5	137	144	6	115	113	-17	222	219
10	316	326	-2	243	243	-4	456	447	6	215	222	7	92	97	-16	75	79
11	123	124	-1	361	358	-3	78	79	3, 14, L			8	411	408	-15	43	43
3, 8, L			0	387	406	-1	79	75	-5	89	85	9	598	578	-14	178	172
-15	85	83	1	468	460	1	357	358	-4	127	123	10	492	486	-13	62	64
-13	118	106	2	354	358	2	322	327	-3	106	101	11	526	507	-12	487	473
-12	131	126	3	293	294	3	200	203	-2	114	115	12	258	256	-11	474	480
-11	47	48	4	217	216	4	131	128	-1	96	91	13	268	256	-10	46	41
-10	56	58	6	221	230	6	226	214	0	81	78	14	93	89	-9	336	329
-9	272	270	7	230	232	8	194	187	3, 15, L			15	196	197	-8	110	116
-8	115	113	8	366	372	9	170	174	-4	214	210	4, 1, L			-7	507	507
-7	176	182	9	307	322	10	128	132	-3	112	104	-18	78	84	-6	497	505
-6	176	189	10	186	194	3, 12, L			-1	75	86	-17	106	103	-5	668	665
-4	118	122	11	106	100	-12	87	81	1	171	179	-16	137	136	-4	797	810
-3	344	351	3, 10, L			-11	43	40	4, 0, L			-15	107	108	-3	387	375
-2	251	256	-13	177	176	-10	67	73	-19	272	265	-14	141	134	-2	332	349
1	181	190	-9	116	113	-9	134	131	-18	140	147	-13	67	66	-1	575	573
2	77	72	-4	50	58	-7	69	67	-17	179	177	-12	37	39	0	793	785
3	329	334	-3	160	157	-6	95	89	-16	102	113	-11	60	63	1	1016	1010
4	236	231	-2	86	83	-5	204	210	-14	251	269	-10	252	247	2	747	739
5	42	39	-1	81	83	-4	116	122	-13	323	305	-8	56	61	3	990	998
7	198	197	0	173	187	-3	228	224	-12	623	630	-5	520	522	4	429	417
9	144	146	1	234	233	-2	79	75	-11	777	761	-4	250	238	5	328	317
10	144	139	3	166	163	-1	118	114	-10	434	410	-3	370	378	6	168	171
13	55	50	4	124	118	3	74	69	-9	824	827	-2	771	748	8	441	431
			5	119	118	8	74	81	-8	644	651	-1	88	84	9	351	347

4, 2, L		
10	271	260
11	276	271
12	76	76
13	87	85

4, 3, L		
-16	88	90
-12	352	358
-11	188	189
-10	94	92
-9	161	156
-8	125	112
-7	539	528
-6	602	573
-5	337	339
-4	303	314
-3	247	243
-2	671	645
-1	414	396
0	254	271
1	135	137
2	223	213
3	275	264
4	193	208
5	58	47
6	50	39
7	180	181
8	322	315
9	178	181
10	174	170
13	94	90
14	125	120

4, 4, L		
-18	132	144
-17	145	154
-16	114	115
-15	85	91
-14	339	335
-13	280	285
-12	549	545
-11	364	380
-10	153	141
-9	325	317
-8	174	180
-7	506	507
-6	476	488
-5	665	675
-4	828	830
-3	293	321
-2	392	401
-1	286	262
0	174	181
1	543	544
2	584	573
3	717	737
4	268	262
6	358	347
7	188	187
8	520	526
9	338	341
10	328	321
11	173	179
13	109	111
14	123	119

4, 5, L		
-16	104	104
-14	72	84
-13	100	106
-12	242	241
-10	130	123
-9	65	40
-7	353	338
-6	401	414
-4	63	69
-2	308	322
-1	97	83
0	88	96
1	165	162
3	200	194
4	373	359
5	165	162
6	72	71
7	200	209
8	165	170
9	50	56
11	75	71
12	57	57
13	64	64
14	111	114

4, 6, L		
-17	87	91
-16	132	134
-15	178	184
-14	328	329
-13	368	351
-12	484	494
-11	491	486
-10	277	268
-9	67	66
-8	130	134
-7	205	193
-6	675	676
-5	739	723
-4	827	801
-3	270	268
-2	226	227
0	392	385
1	204	190
2	221	221
3	262	243
4	256	261
5	191	183
6	422	414
7	292	293
8	425	433
9	334	318
10	331	334
11	180	183
13	71	68

4, 7, L		
-16	108	117
-14	95	89
-13	140	143
-12	50	65
-11	105	102
-10	40	36
-9	67	71
-8	45	42
-7	513	499
-6	57	70
-5	536	546
-4	161	164
-2	354	371
-1	207	212
0	256	261
1	103	102
2	89	90
4	78	79
5	110	108
6	348	346
7	170	169
8	82	74
9	109	118
11	107	108
12	74	72

4, 8, L		
-16	49	45
-15	90	91
-14	163	169
-13	266	275
-12	240	246
-11	158	153
-9	94	95
-8	81	75
-7	204	200
-6	372	386
-5	382	372
-4	727	717
-3	532	510
-2	505	503
-1	224	219
0	331	330
1	421	439
2	554	549
3	570	573
4	481	472
5	264	261
6	152	157
7	346	336
8	269	279
9	201	194
10	111	108

4, 9, L		
-15	162	174
-14	90	87
-13	46	46
-12	66	60
-11	153	148
-10	73	77
-9	63	66
-8	59	56
-7	153	149
-6	220	218
-5	81	82
-4	186	190
-3	215	219
-2	293	301
-1	530	534
1	63	68
2	130	126
3	268	280
4	113	106
5	266	278
6	67	68
7	139	138
8	77	69
9	134	133

4, 10, L		
-14	105	108
-13	301	305
-12	313	313
-11	329	328
-10	385	373
-9	140	144
-8	196	189
-7	209	209
-6	385	380
-5	493	508
-4	208	219
-3	270	265
-1	81	70
0	42	45
1	221	233
2	275	268
3	117	131
4	179	172
5	118	119
6	86	81
7	175	183
8	106	117
9	273	271
10	235	242

4, 11, L		
-13	62	54
-11	147	143
-9	58	37
-8	59	52
-7	248	245

4, 11, L		
-6	173	167
-5	143	149
-1	113	121
3	98	91
5	104	102
6	115	116
7	100	103
8	105	103
9	133	130
4, 12, L		
-12	123	122
-11	145	144
-10	258	253
-8	200	185
-7	101	101
-6	207	210
-5	294	292
-3	381	371
-1	164	164
0	267	262
1	286	299
2	460	463
3	171	175
4	284	281
5	106	111
7	135	136
8	90	94
4, 13, L		
-10	57	44
4, 14, L		
-8	143	148
-7	114	128
-6	191	193
-5	186	186
-3	164	164
-2	72	72
-1	149	151
0	211	207
1	218	222
2	354	365
3	138	142
4	162	163
5, 1, L		
-19	173	177
-18	235	239
-17	140	140
-16	103	97
-13	538	544
-12	531	527
-11	794	805
-10	626	623
-9	481	459
-8	152	157
-7	148	151
-6	481	491
-5	268	275
-4	297	310
-3	886	895
-2	287	290
-1	413	425
0	733	719
1	530	536
2	474	486
3	260	270
4	558	563
5	152	157
6	161	159
7	343	332
8	415	409
9	611	584
10	407	395
11	402	386
12	108	112
13	43	41
14	115	116
5, 2, L		
-18	113	108
-17	52	50
-14	124	114
-13	77	88
-11	85	95
-10	186	182
-9	50	52
-8	47	49
-7	388	390
-6	146	142
-5	304	302
-4	236	248
-3	404	402
-2	170	174
-1	201	206
0	510	525
1	90	79
2	453	464
3	144	145
4	88	92
5	166	159
6	68	59
8	72	60
10	101	105
11	66	65
12	76	72
5, 3, L		
-18	242	240
-17	97	97
-16	133	129
-13	255	250
-12	282	289
-11	438	429
-10	168	158
-9	220	214
-8	346	335
-7	166	155
-6	791	799
-5	717	709
-4	896	897
-3	1035	1036
-2	168	182
-1	647	643
0	443	456
1	618	606
2	783	775
3	670	658
4	498	499
6	116	107
7	230	236
8	112	108
9	327	319
10	198	197
11	244	242
12	50	49
5, 4, L		
-18	91	83
-16	130	125
-15	49	41
-14	198	205
-13	145	139
-12	77	73
-11	43	50
-10	352	358
-9	334	328
-8	459	457
-7	418	429
-6	265	249
-5	121	120
-4	65	67
-3	147	151
-1	56	54
0	84	93
1	192	194
2	124	134
3	118	117
4	112	122
5	228	222
6	446	458
7	121	119
8	110	114
9	96	90
10	111	101
11	65	73
12	120	115
5, 5, L		
-18	263	267
-17	195	200
-16	245	261
-15	163	167
-14	226	228
-13	367	366
-12	428	432
-11	534	530
-10	362	372
-9	229	213
-8	246	251
-7	322	321
-6	606	605
-5	606	591
-4	525	533
-3	159	166
-2	137	133
-1	201	189
0	225	239
1	228	235
2	468	459
3	579	583
4	639	645
5	392	393
6	249	249
7	185	185
8	200	198
9	363	362
10	259	260
11	272	274
12	176	181
13	127	138
5, 6, L		
-17	69	76
-15	106	108
-14	92	96
-11	248	244
-10	110	100
-9	174	170
-8	85	89
-7	241	247
-6	208	222
-5	173	178
-4	490	503
-3	38	34
-2	96	94
-1	87	78
0	145	148
2	497	479
4	95	81
5	198	205
7	109	116
8	40	43
9	68	63
10	86	84
5, 7, L		
-17	146	162
-16	172	177
-15	139	141
-14	106	107
-13	129	122
-12	162	167
-11	224	224
-9	85	68
-8	258	255

5, 7, L

-7	329	311
-6	586	580
-5	799	789
-4	819	795
-3	307	316
-2	180	172
-1	164	157
1	335	335
2	635	622
3	698	692
4	510	504
5	292	293
6	218	211
8	64	61
9	123	121
10	148	148
11	104	111
12	75	81

5, 8, L

-15	134	131
-13	120	108
-11	102	98
-10	73	79
-9	87	84
-8	77	71
-7	47	35
-5	331	337
-4	151	142
-3	288	279
-2	57	39
-1	35	30
0	63	71
1	232	234
2	94	112
3	169	177
4	53	56
5	114	115
6	106	107
7	124	120
8	54	54

5, 9, L

-15	102	101
-14	164	169
-13	131	139
-12	260	241
-11	221	228
-10	201	201
-9	141	143
-8	146	145
-7	246	241
-6	295	294
-5	427	437
-4	491	480
-3	374	365
-2	233	227
-1	130	133
0	79	83
1	298	300
2	441	435
3	367	362
4	203	202
5	270	267
6	94	106
7	71	76
8	158	164
9	160	165
10	181	175

5, 10, L

-13	149	145
-12	62	57
-9	68	72
-6	111	112
-5	202	209
-4	57	62
-3	218	220
-2	84	81
0	216	212
1	244	252
3	127	114
4	70	72
5	90	91
7	121	121

5, 11, L

-13	141	142
-12	348	332
-11	306	307
-10	361	349
-9	204	199
-7	238	236
-5	278	270
-4	160	160
-3	41	40
-2	253	253
0	204	203
1	166	172
2	193	204
3	253	249
4	100	109
5	229	223
7	128	118
8	234	240

5, 12, L

-9	131	119
-8	98	100
-7	206	201
-6	143	145
-3	72	83
0	50	50
2	77	77
4	92	85
5	142	146
6	93	92

5, 13, L

-10	162	163
-9	121	119
-7	141	143
-5	238	237
-4	292	288
-3	295	293
-2	403	410
-1	148	159
0	343	332
1	245	251
2	240	235
3	182	191
5	85	93

5, 14, L

-7	83	90
-4	56	44
1	79	71

6, 0, L

-19	90	96
-18	236	239
-17	325	329
-16	178	176
-15	388	394
-14	409	397
-13	335	321
-12	795	784
-11	393	384
-10	391	384
-9	111	108
-7	73	77
-6	61	52
-5	760	765
-4	884	876
-3	731	734
-2	234	245
-1	233	227
0	161	175
1	404	413
2	446	462
3	614	637
4	576	529
5	600	610
6	384	345
7	582	586
8	451	454
9	331	338
10	399	373
11	167	175
12	151	150

6, 1, L

-19	54	56
-18	55	49
-16	45	41
-15	44	54
-14	90	86
-13	149	148
-12	135	131
-11	90	92
-10	103	99
-9	92	95
-8	211	209
-7	101	101
-6	257	267
-5	387	395
-3	136	135
-2	212	218
-1	270	301
0	298	296
1	406	423
2	173	170
3	296	302
4	82	88
5	37	33
8	80	77
12	93	90
13	52	55

6, 2, L

-19	87	89
-18	158	161
-17	214	213
-15	110	112
-14	60	60
-13	164	161
-12	549	544
-11	405	402
-10	587	579
-9	186	177
-8	259	259
-7	191	196
-6	346	349
-5	976	993
-4	723	734
-3	842	858
-2	853	856
-1	229	233
0	569	569
1	30	23
2	559	547
3	506	492
4	283	286
5	434	434
7	116	109
8	107	108
9	210	200
10	284	270
11	124	119
12	157	149

6, 3, L

-18	44	49
-16	102	96
-15	92	90
-12	228	231
-11	281	275

6, 3, L		
-10	221	217
-9	291	301
-8	81	81
-6	286	297
-5	185	194
-4	95	96
-3	306	306
-2	50	53
-1	525	517
0	125	126
2	203	215
4	571	567
5	211	212
7	75	75
8	90	84
9	119	116
10	220	215
11	79	82

6, 4, L		
-18	225	227
-17	282	277
-16	111	123
-15	198	192
-13	171	165
-12	352	357
-11	474	455
-10	522	518
-9	400	395
-8	349	335
-7	109	106
-6	151	142
-5	633	651
-4	566	563
-3	534	550
-2	253	264
-1	107	112
0	358	345
1	250	250
2	564	572
3	614	603
4	315	338
5	376	365
6	86	98
7	192	182
8	132	138
9	218	214
10	308	306
11	236	235
12	201	208

6, 5, L		
-16	98	96
-15	99	96
-14	96	92
-13	71	68
-12	172	170
-11	81	80
-10	117	111
-9	312	312
-8	98	97
-7	145	156
-6	310	323
-5	267	267
-4	108	113
-3	100	104
-2	151	163
-1	152	138
3	162	160
4	442	443
5	60	69
8	134	135
9	62	60
10	144	138

6, 6, L		
-17	298	301
-16	172	172
-15	113	117
-13	195	202
-12	327	317
-11	428	428
-10	421	416
-9	400	389
-8	292	288
-7	237	238
-6	175	178
-5	232	247
-4	104	101
-3	327	342
-2	126	111
-1	349	346
0	59	54
1	342	340
2	573	561
3	623	606
4	508	478
5	281	276
6	93	83
7	74	78
8	157	156
9	292	294
10	325	323
11	220	229

6, 7, L		
-17	116	113
-13	174	169
-11	155	149
-10	101	94
-8	407	400
-7	158	159
-6	66	64
-5	57	53
-4	198	210
-3	282	281
-2	287	272
0	170	161
1	83	84
3	301	297
4	56	52
5	254	262
6	118	126
7	102	103
9	110	116
11	77	82

6, 8, L		
-16	106	108
-12	95	95
-11	316	314
-10	457	450
-9	432	431
-8	297	290
-7	270	261
-6	365	352
-5	545	540
-4	457	442
-3	491	472
-2	289	289
-1	257	246
0	312	307
1	482	500
2	495	491
3	327	326
4	226	237
5	63	56
7	121	113
9	109	109
10	165	167

6, 9, L		
-14	141	140
-12	111	113
-11	75	73
-9	158	160
-8	57	47
-7	178	179
-6	112	110
-5	173	175
-4	162	169
-1	359	346
0	279	284
1	280	267
2	88	98
4	85	95
7	57	63
9	63	74

6, 10, L		
-14	190	184
-13	211	205
-12	219	218
-11	310	302
-10	147	149
-9	142	128
-7	88	87
-6	254	252
-4	356	348
-3	159	165
-2	142	140
-1	59	43
1	183	177
2	175	185
3	359	347
4	352	368
5	193	193
6	185	189
7	121	128
8	211	215

6, 11, L		
-13	92	83
-11	165	163
-10	70	66
-9	75	69
-8	112	110
-7	77	82
-6	71	72
-5	86	87
-1	113	113
1	72	69
3	132	130
4	137	141
5	175	172
6	44	51

6, 12, L		
-11	236	233
-10	154	151
-9	143	134
-7	65	58
-6	273	279
-5	147	153
-4	463	452
-3	307	315
-2	269	271
-1	160	169
1	228	235
2	91	95
3	178	177
4	189	193
5	102	108

6, 13, L		
-2	60	62

6, 14, L		
-6	168	173
-5	164	162
-4	302	307
-3	231	232

6, 14, L		
-2	170	176
-1	108	116
7, 1, L		
-19	184	182
-18	205	207
-17	378	366
-16	335	329
-15	163	169
-14	292	294
-13	54	50
-12	289	301
-11	437	440
-10	145	139
-9	588	580
-8	71	68
-7	305	305
-6	203	197
-5	375	399
-4	881	884
-3	525	530
-2	393	428
-1	184	167
1	205	209
2	121	113
3	964	956
4	486	494
5	515	494
6	469	467
7	123	119
8	125	121
10	219	211
11	191	192
12	88	88
7, 2, L		
-17	124	119
-14	35	29
-13	144	151
-12	64	57
-10	328	327
-9	184	183
-8	327	318
-7	297	318
-6	38	61
-5	138	136
-4	314	311
-3	527	546
-2	322	315
-1	516	524
0	134	126
1	61	65
2	28	45
3	153	130
4	59	37
5	113	98
6	136	124
10	72	68
11	59	59
12	119	114
7, 3, L		
-18	120	119
-17	267	265
-16	215	213
-15	77	83
-14	144	137
-12	355	355
-11	504	495
-10	437	435
-9	565	556
-8	258	240
-7	518	525
-6	566	577
-5	630	619
-4	947	960
-3	569	592
-2	557	550
-1	218	234
0	101	96
1	65	57
2	89	74
3	494	483
4	322	323
5	188	193
6	206	194
8	137	135
9	113	112
10	265	259
11	254	245
7, 4, L		
-17	91	96
-16	105	107
-15	109	104
-14	114	113
-13	310	317
-12	106	102
-11	243	237
-9	178	176
-8	130	131
-7	308	305
-6	252	245
-5	73	71
-2	195	200
-1	166	173
0	531	552
1	172	168
2	252	256
3	289	304
5	80	69
6	305	309
7	93	98
8	141	137
9	130	127
7, 5, L		
-18	197	203
-17	257	262
-16	199	197
-14	130	128
-13	129	129
-12	381	385
-11	357	358
-10	510	496
-9	439	440
-8	132	132
-7	220	223
-6	171	181
-4	169	162
-3	324	319
-2	529	524
-1	341	333
0	408	406
1	466	438
2	639	633
3	528	532
4	394	382
5	283	281
6	248	245
7	88	95
8	211	214
9	256	246
10	282	282
11	230	236
7, 6, L		
-17	96	102
-15	80	81
-14	69	70
-13	66	65
-12	89	83
-10	252	243
-8	80	86
-7	319	318
-6	251	250
-5	166	172
-4	278	281
-3	272	274
-2	227	239
-1	489	488
0	73	74
1	167	169
4	69	76
5	95	106
6	90	89
7	47	41
10	77	80
7, 7, L		
-17	148	153
-16	116	112
-13	90	90
-12	333	323
-11	400	402
-10	543	538
-9	405	398
-8	291	292
-7	187	192
-6	228	222
-5	296	306
-4	425	427
-3	503	492
-2	516	511
-1	283	279
0	263	269
1	229	220
2	265	263
3	130	129
4	209	219
5	130	129
7	43	40
8	154	160
9	210	207
10	199	204
7, 8, L		
-16	95	91
-12	109	105
-10	85	78
-9	211	206
-8	86	103
-6	192	213
-5	205	205
-4	130	129
-3	115	118
-2	128	132
0	148	148
1	178	175
2	69	76
4	95	93
7	108	106
7, 9, L		
-15	99	90
-13	134	130
-12	168	174
-11	309	313
-10	433	427
-9	260	267
-8	221	225
-6	138	138
-5	260	261
-4	259	255
-3	414	402
-2	346	343
-1	264	270
0	117	112
1	148	151
2	245	237
3	122	118
4	265	261
5	196	207
6	83	85

7, 9, L		
7	90	92
8	100	103
7, 10, L		
-12	83	76
-10	63	70
-9	202	200
-8	126	125
-7	70	69
-5	115	119
-4	111	94
-3	193	192
-2	178	171
-1	96	97
1	88	102
4	85	86
7, 11, L		
-13	146	143
-12	96	105
-11	184	187
-10	202	204
-8	148	145
-6	60	49
-5	165	173
-4	137	136
-3	374	372
-2	123	126
-1	141	134
0	64	66
1	137	140
2	308	311
3	219	229
4	358	351
5	261	265
6	147	144

7, 12, L		
-10	68	70
-6	50	68
-2	85	82
-1	138	148
0	80	81
1	114	109
2	89	95
7, 13, L		
-9	106	96
-8	186	188
-7	179	187
-6	266	268
-5	322	329
-4	288	290
-3	333	333
-2	105	106
-1	94	91
2	54	66
8, 0, L		
-19	154	165
-18	367	372
-17	341	331
-16	450	432
-15	301	282
-14	82	74
-13	81	80
-12	216	209
-11	268	275
-10	130	124
-9	408	423
-8	552	544
-7	242	228
-6	583	571
-5	257	256
-4	444	453
-3	428	427
-2	203	227

-1	554	570
0	214	213
1	546	551
2	588	591
3	530	507
4	730	726
5	384	371
6	388	385
9	117	119
10	97	102
11	263	265
8, 1, L		
-16	50	46
-15	63	61
-14	105	104
-13	131	124
-12	181	180
-11	292	280
-9	83	78
-8	224	223
-7	121	129
-6	304	311
-5	361	388
-4	241	247
-3	228	227
-2	113	125
-1	80	87
0	75	80
2	221	219
3	50	48
4	72	65
5	60	55
7	61	61
8	125	125
9	107	103
10	133	135
11	103	98

8, 2, L		
-18	254	254
-17	217	210
-16	310	306
-15	164	171
-13	142	141
-12	221	226
-11	572	562
-10	470	470
-9	786	792
-8	835	846
-7	142	137
-6	430	441
-5	185	185
-4	302	299
-3	409	413
-2	222	231
-1	487	484
0	95	97
1	105	107
2	415	406
3	362	373
4	442	436
5	77	77
6	184	182
9	185	177
10	171	168
8, 3, L		
-18	47	45
-17	72	58
-16	89	95
-15	193	188
-14	57	53
-13	122	122
-12	104	105
-11	167	173
-9	291	285
-7	133	128

-6	85	81
-5	105	104
-4	83	83
-3	41	39
-2	62	67
-1	79	74
0	161	174
1	384	393
2	97	95
3	93	101
4	152	150
5	250	251
6	99	97
7	79	76
8, 4, L		
-18	188	194
-17	196	202
-16	282	288
-15	166	164
-14	118	121
-13	158	159
-12	222	221
-11	426	425
-10	368	375
-9	371	374
-8	160	170
-6	213	220
-5	316	320
-4	480	479
-3	642	644
-2	470	491
-1	440	435
0	119	124
1	103	115
2	195	182
3	210	224
4	464	435
5	350	362

6	298	283
7	145	152
8	94	99
9	182	184
10	130	132
8, 5, L		
-15	188	179
-13	106	105
-11	186	184
-10	122	121
-9	198	203
-8	40	45
-7	125	130
-5	256	257
-4	131	133
-3	91	106
-2	116	135
-1	73	58
0	97	96
1	208	218
2	253	251
3	125	126
4	77	65
5	197	203
6	77	67
7	59	53
8	69	63
10	54	43
8, 6, L		
-17	173	176
-16	211	216
-15	149	153
-14	190	199
-13	208	204
-12	180	176
-11	270	266
-10	292	302
-9	194	196

8, 6, L

-7	101	105
-5	248	243
-4	571	582
-3	764	739
-2	623	627
-1	377	385
0	186	185
1	101	101
2	103	111
3	220	214
4	308	308
5	374	365
6	266	271
7	249	254
8	157	166
9	145	144

8, 7, L

-16	130	128
-14	141	143
-11	129	127
-10	69	74
-8	172	176
-7	136	139
-6	99	97
-5	225	236
-4	59	57
-3	261	253
-2	51	63
-1	98	89
0	50	46
1	68	72
2	221	214
3	58	57
6	142	134
8	96	100

8, 8, L

-16	106	114
-15	109	105
-14	132	141
-13	194	204
-12	351	347
-11	417	419
-10	526	507
-9	347	359
-8	211	206
-7	254	242
-6	104	108
-5	218	213
-4	319	314
-3	432	437
-2	394	387
-1	220	221
0	94	101
1	65	74
2	42	36
3	89	96
4	143	139
5	219	220
6	110	114
7	138	135
8	114	119

8, 9, L

-15	90	99
-13	120	122
-12	76	73
-11	139	141
-10	165	174
-7	154	149
-6	232	230
-5	178	171
-4	227	227
-3	42	57
-2	122	117
-1	51	54
0	99	98
3	52	51
6	41	41
7	83	85

8, 10, L

-14	111	111
-11	60	54
-10	211	215
-9	136	137
-7	186	180
-5	159	161
-4	275	266
-3	349	334
-2	356	343
-1	123	124
0	244	242
1	166	171
2	202	203
3	271	276
4	263	261
5	273	282
6	146	143

8, 11, L

-10	94	86
-8	101	103
-4	50	54
-3	85	85
-2	94	91
-1	91	109
0	120	117

8, 12, L

-10	284	270
-9	256	257
-8	217	212
-7	250	250
-6	90	91
-5	157	153
-4	129	139
-3	96	98
-2	155	160
-1	62	66
0	190	186
1	107	106
2	143	149

9, 1, L

-18	154	154
-17	268	262
-16	152	157
-15	209	205
-14	57	46
-12	262	271
-11	225	222
-10	643	647
-9	436	446
-8	536	548
-7	69	67
-6	68	72
-5	269	270
-4	66	66
-3	556	553
-2	532	539
-1	593	606
0	584	590
1	79	82
2	435	443
3	267	277
4	210	209
5	274	273
6	141	138
7	114	115
9	160	161

9, 2, L

-17	44	43
-13	102	94
-12	93	96
-11	163	162
-10	116	119
-9	230	233
-8	58	59
-7	345	358
-6	225	218
-5	170	174
-2	70	65
-1	170	179
0	46	53
1	131	119
3	58	43
4	98	92
6	164	159
7	129	129
8	81	83
9	81	84

9, 3, L

-18	147	158
-17	313	309
-16	254	258
-15	343	338
-14	203	198
-13	233	234
-12	282	269
-11	266	264
-10	544	539
-9	529	533
-8	515	512
-7	241	243
-6	95	97
-5	251	251
-4	174	168
-3	486	479
-2	362	373
-1	165	168
0	81	81
1	165	163
2	132	135
3	151	150
4	176	181
5	361	354
6	249	251
7	247	239
8	138	134
9	165	169

9, 4, L

-18	73	79
-17	234	227
-16	126	124
-13	113	111
-11	317	315
-10	60	68
-9	127	134
-8	170	173
-7	310	308
-5	91	92
-4	375	387
-3	374	374
-2	180	183
-1	323	324
1	124	114
2	253	243
3	388	390
4	177	164
5	256	247

9, 5, L

-17	241	239
-16	228	224
-15	239	243
-11	115	119
-10	267	254
-9	274	272
-8	250	241
-7	231	239
-6	122	132

9, 5, L

-5	294	299
-4	365	375
-3	512	513
-2	518	498
-1	485	477
0	423	414
1	191	189
2	211	214
3	344	350
4	379	374
5	370	369
6	205	204
7	125	131

9, 6, L

-13	67	67
-12	40	36
-11	79	80
-10	144	150
-9	208	210
-8	115	114
-7	255	271
-6	63	65
-5	93	90
-4	166	160
-3	105	98
-2	213	217
-1	111	114
0	123	116
2	106	116
3	38	41
4	146	148
6	117	112
7	81	83

9, 7, L

-16	262	266
-15	271	274
-14	244	253
-13	195	191
-12	106	104
-11	175	178
-10	255	252
-9	324	310
-8	216	223
-7	306	309
-6	233	235
-5	260	263
-4	354	347
-3	386	382
-2	322	320
1	40	36
3	154	156
4	288	288
5	331	341
6	242	249
7	160	164

9, 8, L

-14	80	71
-12	117	115
-8	155	160
-7	41	36
-6	86	88
-5	44	48
-2	170	173
1	51	44
2	82	83
4	69	71
6	59	65

9, 9, L

-14	162	168
-13	77	85
-12	106	98
-11	196	205
-10	199	197
-9	294	280
-8	182	190
-7	175	175
-6	159	153
-5	86	90
-4	321	312
-3	260	258
-2	265	271
-1	177	160
0	63	72
1	120	123
3	195	200
4	262	260
5	209	214

9, 10, L

-12	111	114
-9	53	47
-8	138	139
-7	80	73
-6	143	141
-5	98	89
-2	170	169
2	81	76

9, 11, L

-11	166	175
-10	161	168
-9	203	205
-8	130	131
-7	97	93
-6	121	115
-4	220	224
-3	217	218
-2	304	300
-1	293	294
0	188	193
1	244	243
2	116	118

9, 12, L

-5	77	74
-4	124	126
-2	107	106
-1	62	59

10, 0, L

-18	45	38
-17	193	185
-16	179	178
-15	96	93
-14	138	136
-13	61	64
-12	277	272
-11	105	112
-10	177	166
-9	587	593
-8	91	95
-7	299	284
-6	178	192
-5	347	346
-4	363	370
-3	646	657
-2	1008	999
-1	638	645
0	358	358
1	115	111
2	88	89
3	88	98
5	278	272
6	224	225
7	131	130
8	164	172

10, 1, L

-15	70	68
-14	77	71
-12	57	62
-11	201	195
-10	221	216
-9	248	260
-8	173	164
-7	186	202
-6	175	182
-5	89	86
-3	168	175
-2	125	123
-1	38	31
1	81	78
2	125	129
3	111	106
4	72	71
5	69	71
6	73	54
7	75	79

10, 2, L

-17	238	224
-16	271	281
-15	288	288
-14	339	325
-13	167	170
-12	323	325
-11	289	288
-10	413	415
-9	662	655
-8	208	203
-7	127	125
-6	84	95
-4	105	99
-3	240	235
-2	460	462
-1	259	262
0	297	299
1	203	209
3	151	153
4	125	128
5	311	310
6	308	304
7	232	225
8	213	214

10, 3, L

-18	82	80
-16	52	47
-15	136	126
-12	60	59
-11	94	89
-10	48	46
-9	152	152
-8	111	117
-7	116	119
-6	124	135
-5	377	381
-4	102	102
-2	151	155
-1	137	134
0	104	99
1	262	271
2	116	117
5	66	63
7	62	67
8	71	73

10, 4, L

-17	234	227
-16	263	263
-15	208	212
-14	216	210
-13	46	42
-12	118	121
-11	97	93
-10	238	242
-9	440	441
-8	354	360
-7	335	339
-6	267	263
-5	162	159
-4	246	245

10, 4, L			-2	311	294	5	211	214	11, 1, L			1	112	111	-6	89	91
-3	251	247	-1	259	259	10, 9, L			-17	118	120	2	123	125	-5	81	87
-2	448	457	0	190	188	-12	86	80	-16	276	277	3	164	163	-4	92	97
-1	310	315	1	165	167	-11	72	73	-15	268	270	4	102	104	-3	250	250
0	219	218	2	175	174	-10	197	194	-14	339	329	5	61	61	-2	98	99
1	157	155	3	242	254	-9	135	143	-13	255	253	11, 3, L			-1	225	224
2	113	117	4	266	263	-8	147	144	-12	43	30	-17	197	196	0	246	247
3	275	268	5	197	209	-7	134	129	-11	110	108	-16	359	348	1	76	82
4	248	251	6	161	165	-5	56	53	-10	89	87	-15	329	328	2	72	65
5	278	283	10, 7, L			-4	74	73	-9	354	345	-14	300	295	11, 5, L		
6	235	236	-12	44	34	-3	73	69	-8	392	403	-13	212	206	-16	97	103
7	82	87	-11	97	94	-1	109	103	-7	281	287	-12	55	62	-15	93	93
10, 5, L			-9	171	173	1	83	77	-6	475	475	-11	140	139	-14	73	77
-15	83	85	-8	140	142	10, 10, L			-5	210	216	-10	115	110	-13	80	78
-12	66	71	-7	117	124	-11	95	92	-4	354	345	-9	262	272	-12	52	53
-11	83	89	-6	231	235	-10	154	163	-3	383	382	-8	253	250	-11	229	232
-9	126	122	-4	73	80	-9	149	154	-2	368	373	-7	81	80	-10	336	339
-7	76	79	-3	58	56	-8	247	255	-1	363	360	-6	167	169	-9	505	501
-5	239	245	-2	77	80	-7	177	178	0	119	116	-4	90	92	-8	555	553
-3	64	67	0	187	188	-6	161	163	1	86	89	-3	156	157	-7	388	384
-1	178	173	2	97	95	-5	196	195	2	58	53	-2	241	239	-6	262	259
0	52	47	3	84	85	-4	233	230	3	65	63	-1	389	397	-5	64	63
1	218	214	10, 8, L			-3	356	344	4	205	204	0	202	200	-4	127	127
5	40	49	-15	260	261	-2	286	282	5	218	227	1	148	148	-3	309	311
10, 6, L			-14	204	207	-1	335	330	6	286	295	2	129	130	-2	327	327
-16	251	251	-13	116	120	0	174	183	7	152	155	3	146	147	-1	457	449
-15	190	200	-11	202	197	1	99	101	11, 2, L			4	257	259	0	303	306
-14	131	129	-10	276	284	2	113	109	-14	69	71	5	296	288	1	248	242
-13	65	61	-9	283	284	10, 11, L			-13	159	155	6	337	340	2	129	134
-12	59	54	-8	372	376	-8	90	82	-12	165	156	11, 4, L			3	61	58
-10	186	179	-7	220	228	-7	54	56	-11	173	179	-17	65	65	4	78	74
-9	341	341	-6	79	80	-6	136	126	-10	211	207	-16	115	117	11, 6, L		
-8	441	444	-1	148	148	-5	84	88	-7	57	76	-14	65	62	-16	42	35
-7	446	435	0	130	123	-4	99	104	-6	72	59	-12	108	108	-15	65	62
-6	347	368	1	112	122	-3	48	43	-5	181	194	-11	65	69	-13	152	157
-5	225	224	2	169	159	0	128	127	-4	63	67	-9	173	177	-12	90	91
-4	367	358	3	200	205				-3	39	51	-8	73	80	-11	110	111
-3	229	236	4	269	270				-1	76	75	-7	132	128	-10	206	212

11,	6,	L
-5	44	44
-4	116	114
-3	68	69
-2	65	61
1	125	134
3	130	130
11,	7,	L
-15	211	208
-14	124	124
-13	101	96
-12	94	91
-11	153	157
-10	249	246
-9	322	316
-8	320	320
-7	168	160
-3	94	97
-2	183	182
-1	343	340
0	272	278
1	196	194
2	155	156
3	117	124
4	120	125
11,	8,	L
-14	55	44
-12	79	73
-11	95	86
-9	72	73
-8	65	59
-7	63	65
-6	56	58
-5	72	72
-3	58	60
-2	88	91
2	96	100

11,	9,	L
-12	63	77
-11	92	89
-10	180	183
-9	204	207
-8	237	239
-7	240	247
-6	95	96
-5	66	70
-3	121	124
-2	208	205
-1	218	224
0	259	253
1	153	160
11,	10,	L
-8	56	62
-6	76	72
-5	122	112
11,	11,	L
-7	252	248
-6	145	143
-5	163	170
-4	156	159
12,	0,	L
-17	155	149
-16	155	164
-15	297	301
-14	261	264
-13	200	194
-12	72	75
-10	279	284
-9	400	393
-8	577	562
-7	533	531
-6	455	453
-5	348	346
-4	165	170
-3	260	254

-2	104	108
-1	88	84
0	169	178
2	87	85
3	99	103
4	112	116
5	152	156
12,	1,	L
-15	113	112
-14	143	141
-13	141	139
-12	119	117
-11	60	50
-9	53	58
-8	57	43
-6	52	51
-5	82	79
-4	58	66
-3	43	42
-2	110	111
-1	145	154
0	150	149
1	115	115
2	73	74
4	58	54
5	62	58
12,	2,	L
-17	224	220
-16	216	215
-15	304	300
-14	227	225
-13	161	166
-11	72	70
-10	121	117
-9	148	142
-8	252	260
-7	288	293
-6	272	276

-5	140	136
-4	54	59
-3	156	158
-2	202	206
-1	262	262
0	350	353
1	217	221
2	220	221
3	180	182
4	217	216
5	257	255
12,	3,	L
-15	89	84
-14	55	66
-11	83	86
-10	124	119
-9	108	113
-8	157	161
-6	50	55
-5	199	206
-4	205	205
-3	156	157
-2	97	91
1	51	53
2	62	62
4	38	22
12,	4,	L
-16	115	126
-15	249	255
-14	217	209
-13	219	219
-12	145	145
-11	70	72
-10	200	196
-9	257	263
-8	369	354
-7	288	285
-6	169	171

-5	151	149
-4	63	61
-3	225	229
-2	274	273
-1	317	311
0	308	302
1	129	135
2	133	130
4	49	62
12,	5,	L
-15	72	61
-14	67	66
-12	46	56
-11	56	55
-10	66	65
-9	74	72
-8	124	119
-7	82	85
-6	50	43
-5	117	112
-4	113	110
-3	84	81
-2	108	102
1	59	62
2	76	74
12,	6,	L
-15	207	205
-14	185	185
-13	197	197
-12	184	185
-11	172	172
-10	242	245
-9	287	288
-8	317	316
-7	237	248
-6	153	146
-5	161	159
-4	93	93

-3	160	170
-2	262	252
-1	293	300
0	259	258
1	117	113
12,	7,	L
-14	85	81
-12	98	93
-10	92	95
-9	97	88
-6	94	97
-5	93	96
-4	97	100
-3	110	114
-1	121	120
12,	8,	L
-12	116	117
-11	73	82
-10	64	68
-9	105	112
-8	134	129
-7	83	89
-3	127	129
-2	279	276
-1	317	314
0	256	255
12,	9,	L
-10	49	50
-9	68	79
-7	93	97
-2	152	140
-1	83	85
12,	10,	L
-6	191	187
13,	1,	L
-16	107	110
-15	177	182
-14	241	245

13, 1, L		
-13	113	111
-12	138	142
-11	145	140
-10	170	176
-9	414	404
-8	372	361
-7	415	416
-6	251	253
-5	92	90
-3	70	63
-2	134	137
-1	215	219
0	284	283
1	266	273
2	146	150
3	130	128
13, 2, L		
-16	92	94
-15	98	96
-14	60	54
-12	43	48
-11	54	51
-10	80	79
-5	35	36
-3	92	95
-2	129	132
-1	70	69
0	82	76
2	56	56
3	65	67
13, 3, L		
-15	148	150
-14	222	216
-13	91	90
-12	77	79
-9	161	158
-8	197	192
-7	289	291
-6	201	201
-5	133	132
-4	139	136
-3	131	130
-2	276	274
-1	291	285
0	317	315
1	274	271
2	186	183
13, 4, L		
-13	68	73
-12	91	90
-8	106	109
-7	182	188
-6	248	250
-5	114	118
-4	147	143
-3	58	49
0	65	59
13, 5, L		
-14	333	329
-13	290	286
-12	265	266
-11	130	131
-10	146	149
-9	207	210
-8	205	202
-7	273	270
-6	275	277
-5	225	224
-4	147	152
-3	88	84
-2	164	165
-1	112	118
0	94	95
13, 6, L		
-10	60	64
-5	103	105
-3	105	99
-2	91	95
0	56	52
13, 7, L		
-12	125	129
-8	81	85
-7	158	155
-6	170	173
-5	172	169
-4	179	184
-3	197	192
-2	213	214
-1	200	203
13, 8, L		
-6	44	43
-4	55	54
14, 0, L		
-14	274	276
-13	337	327
-12	281	283
-11	319	313
-10	209	203
-9	198	193
-8	230	217
-7	129	132
-6	194	192
-1	207	203
0	196	193
14, 1, L		
-12	37	43
-11	71	70
-9	52	49
-8	71	70
-7	96	96
-6	85	81
-5	89	90
-4	121	115
-3	51	57
0	68	65
14, 2, L		
-14	178	174
-13	198	197
-12	113	109
-11	94	94
-9	116	118
-8	204	201
-7	181	181
-6	298	287
-5	176	167
-4	170	173
-3	184	185
-2	209	205
-1	315	320
0	253	255
14, 3, L		
-14	95	96
-11	38	25
-10	101	95
-9	107	105
-8	168	170
-7	131	132
-6	91	91
-4	101	95
-3	64	63
-2	81	82
14, 4, L		
-13	205	203
-12	106	109
-11	102	103
-10	76	73
-9	161	159
-8	204	202
-7	237	234
-6	276	278
-5	162	157
-4	107	110
-3	93	84
-2	70	69
-1	138	143
14, 5, L		
-10	74	71
-9	55	53
-8	106	108
-7	69	66
-6	47	46
-4	77	77
14, 6, L		
-11	65	67
-9	119	120
-8	173	183
-7	287	273
-6	262	263
-5	144	145
14, 7, L		
-7	94	89
15, 1, L		
-12	267	263
-11	106	106
-10	69	68
-8	74	75
-7	94	93
-6	165	161
-5	224	221
-4	99	98
-3	162	161
15, 2, L		
-8	88	84
-6	69	69
-5	47	40
-3	39	24
15, 3, L		
-11	102	97
-10	136	129
-9	116	116
-8	193	185
-7	243	237
-6	293	291
-5	278	274
-4	132	137
15, 4, L		
-10	160	157
-9	139	132
-6	76	75
-5	49	42

CALCULATED AND OBSERVED STRUCTURE FACTORS OF $C_4Cl_4O_2S$ at 295K

0, 0, L		
2	1390	1400
4	1242	1274
6	978	1068
8	202	210
10	221	221
12	145	151
16	38	46

0, 2, L		
0	136	117
1	920	933
2	1341	1323
3	718	711
4	87	97
5	863	847
6	398	411
7	1060	1067
8	443	470
9	477	472
10	204	215
11	354	361
12	207	211
13	150	135
15	111	103

0, 4, L		
0	153	144
1	1278	1280
2	600	598
3	531	509
4	568	546
5	286	278
7	545	528
8	404	393
9	137	140
10	134	143
12	49	42
14	62	67
15	81	87

0, 6, L		
0	579	549
1	144	139
2	50	36
3	853	873
4	182	193
5	417	449
6	162	143
7	124	130
8	151	141
9	164	172
10	75	75
11	50	42
12	143	139
13	71	81
14	52	50

0, 8, L		
0	234	202
1	76	95
3	297	326
5	214	211
6	218	219
7	128	139
9	46	27
10	67	67

0, 10, L		
0	260	227
1	91	80
2	151	152
3	56	42
4	96	79
5	84	94
6	130	141
7	42	49

1, 1, L		
-16	68	66
-13	147	138
-12	96	97
-11	85	101
-10	585	589
-9	88	99
-8	525	540
-7	458	450
-5	639	637
-4	690	677
-3	918	901
-2	183	194
-1	1019	980
0	728	613
1	636	586
2	81	54
3	213	215
4	261	256
5	147	148
6	450	428
7	38	42
8	247	235
9	431	436
11	250	244
12	214	221
13	139	133

1, 3, L		
-14	57	41
-13	96	101
-12	57	50
-11	254	246
-10	154	152
-9	364	385
-8	377	419
-7	142	136
-6	259	256
-5	140	159
-4	916	935
-3	64	61
-2	388	387
-1	1468	1394
0	1593	1350
1	453	432
2	240	256
3	151	133
4	635	611
5	426	392
6	266	224
7	521	516
8	215	199
9	243	237
10	201	204
11	193	200
12	61	50
13	113	98
14	135	134

1, 5, L		
-14	74	78
-13	91	97
-12	36	17
-10	130	149
-9	296	308
-8	426	438
-7	423	442
-6	58	65
-5	86	106
-4	45	59
-3	55	73
-2	215	218
-1	189	189
0	214	189
1	417	426
2	42	16
3	98	103
4	321	304
5	721	720
6	536	537
7	212	189
8	314	310
10	117	132
11	128	121
12	81	82
13	91	87
14	134	117

1, 7, L		
-13	76	65
-12	64	69
-11	72	73
-10	115	128
-9	56	41
-8	99	101
-7	245	258
-4	117	122
-3	205	239
-2	45	44
-1	186	206
0	295	282
1	34	51
3	184	186
4	171	169
5	185	156
6	204	212
7	110	116
8	89	79
9	111	99
11	119	120
12	139	129

1, 9, L		
-9	54	47
-8	80	93
-7	220	235
-6	44	51
-5	69	69
-4	138	133
-3	183	185
-1	292	305
0	132	107
1	113	133
2	205	234
3	164	165
4	179	206
5	226	224
7	63	53

1, 11, L		
0	92	95
2	160	170

2, 0, L		
-14	244	232
-12	75	61
-10	598	619
-8	947	938
-4	2518	2567
-2	732	728
0	254	260
2	1249	1340
4	765	770
6	1534	1585
10	528	543
12	212	227
14	118	108
16	59	59

2, 2, L		
-16	67	77
-15	65	67
-14	106	109
-13	108	102
-12	40	34
-10	262	272
-8	189	187
-7	199	183
-5	379	387
-4	93	85
-3	2135	2085
-2	1693	1660
-1	1551	1421

2, 2, L		
0	63	74
1	1517	1466
2	528	539
3	925	941
4	1275	1330
5	1018	1025
6	326	318
7	207	219
8	184	176
10	183	181
11	256	249
16	62	60

2, 4, L		
-15	85	74
-14	92	87
-13	68	70
-11	197	188
-10	168	165
-9	62	59
-8	195	206
-7	335	362
-6	48	46
-5	621	683
-4	287	291
-3	586	603
-2	430	440
-1	364	328
0	275	265
1	1243	1102
2	183	175
3	232	232
4	949	922
5	201	178
6	143	130
7	607	606
8	270	254
9	65	70

10	115	132
11	133	143
12	60	51
13	139	123

2, 6, L		
-13	97	100
-11	163	173
-10	79	48
-9	67	87
-8	63	68
-7	301	324
-6	46	66
-5	242	260
-4	45	44
-2	290	265
-1	534	518
0	358	341
1	487	488
2	74	78
3	356	351
4	310	295
5	414	418
6	50	53
7	178	179
8	57	32
10	117	113
12	87	59
13	77	74

2, 8, L		
-9	65	52
-8	171	188
-7	185	210
-6	106	103
-5	183	197
-4	166	172
-1	275	262
0	167	155
1	293	245

2	205	199
3	265	265
4	82	94
7	84	80
8	188	184
9	72	86
10	93	93
11	55	44

2, 10, L		
-5	42	30
-4	139	138
-3	65	43
-2	237	244
-1	76	71
0	90	94
1	152	161
2	112	121
4	195	197
5	76	67

3, 1, L		
-15	120	112
-14	171	169
-13	171	158
-12	74	86
-11	150	156
-10	169	175
-9	187	191
-8	106	108
-7	752	758
-6	439	418
-5	78	79
-4	1242	1222
-3	496	459
-2	939	907
-1	126	135
0	536	506
1	1394	1373
2	630	599

3	104	98
4	436	404
5	478	480
6	31	43
7	448	440
8	198	182
9	364	351
10	170	186
11	106	104
12	255	255
13	63	53

3, 3, L		
-16	60	57
-14	78	89
-13	81	78
-12	240	263
-11	189	171
-10	134	146
-9	286	307
-8	364	372
-7	148	152
-6	193	206
-5	644	683
-4	433	413
-3	136	136
-2	93	76
-1	885	829
0	57	71
1	318	289
2	335	299
3	362	351
4	34	51
5	358	370
6	584	586
7	299	296
8	207	198
9	60	67
10	381	383

11	194	190
12	85	84
13	92	84
15	76	67

3, 5, L		
-14	51	59
-13	113	107
-12	225	222
-11	124	131
-10	47	71
-9	102	91
-8	50	68
-6	334	362
-5	83	54
-4	105	112
-3	1151	1194
-2	176	158
-1	92	93
0	41	58
1	562	537
2	485	463
3	35	31
4	643	627
6	198	167
7	74	70
8	224	222
9	145	140
10	309	295
11	93	91
12	93	87
13	43	37

3, 7, L		
-11	103	109
-10	225	214
-9	148	164
-8	93	89
-7	42	64
-6	69	61

-5	240	260
-4	137	161
-3	52	25
-2	181	178
0	68	71
1	125	92
2	157	155
3	260	271
4	272	264
5	63	67
6	77	71
7	149	163
8	101	100
9	169	159
10	57	53
12	54	46

3, 9, L		
-9	59	64
-8	61	57
-5	196	197
-3	184	194
-2	234	260
-1	124	120
0	237	239
1	173	177
2	122	111
3	247	251
4	68	67
6	118	107
7	116	116
9	95	94

3, 11, L		
0	162	164

4, 0, L		
-16	40	37
-12	249	226
-10	519	545
-8	392	418

4, 0, L		
-6	105	132
-4	1784	1814
-2	1202	1228
0	1443	1414
2	3463	3750
4	848	885
6	312	361
8	651	703
10	402	408
14	104	101
16	60	52
4, 2, L		
-16	80	75
-13	170	165
-11	153	131
-10	309	296
-9	601	615
-8	60	66
-7	759	793
-6	767	830
-5	847	848
-4	599	598
-3	1840	1760
-2	482	442
-1	847	802
0	1603	1504
1	1519	1488
2	166	151
3	1205	1173
4	645	652
6	254	252
7	439	417
8	204	210
9	360	351
10	131	128
11	215	198
12	200	204
14	81	87
15	60	60
4, 4, L		
-15	59	49
-14	132	132
-13	143	148
-12	75	85
-11	122	130
-10	167	164
-9	45	65
-8	362	386
-7	145	132
-6	799	821
-5	271	247
-4	328	301
-3	682	670
-2	710	664
-1	604	573
0	718	653
1	613	594
2	522	472
3	1288	1280
4	158	143
5	411	398
6	46	31
8	157	154
9	514	482
10	211	192
12	100	99
13	37	25
15	42	32
4, 6, L		
-13	63	66
-12	96	100
-11	63	66
-10	174	175
-9	100	107
-8	48	50
-7	118	117
-6	158	147
-5	170	170
-4	277	270
-3	525	565
-2	130	125
-1	843	815
0	197	189
1	148	139
2	444	421
3	410	387
4	74	63
5	629	608
6	268	278
7	46	61
9	64	74
10	93	78
11	83	86
12	63	58
4, 8, L		
-11	52	65
-10	91	94
-9	140	146
-7	86	72
-6	123	151
-5	200	207
-4	143	136
-3	227	219
-2	76	75
-1	296	307
1	121	141
2	251	234
4	146	145
5	109	128
6	115	115
7	62	64
8	95	84
9	79	74
10	71	55
4, 10, L		
-6	89	102
-4	148	160
-3	133	139
-1	74	65
0	186	170
1	61	50
2	182	161
3	51	31
5	42	22
6	103	87
5, 1, L		
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-14	110	98
-13	149	159
-11	189	188
-10	68	66
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-8	895	922
-7	116	128
-6	366	373
-5	937	929
-4	60	65
-3	139	108
-2	856	841
-1	547	514
0	302	317
1	383	371
2	1426	1422
3	189	230
4	161	139
5	52	48
6	192	194
7	33	12
8	365	360
9	260	268
11	292	304
12	159	155
13	59	52
14	120	125
5, 3, L		
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-14	43	36
-13	71	83
-12	86	94
-11	130	139
-10	41	26
-9	240	241
-8	64	52
-7	628	655
-6	556	603
-5	688	683
-4	522	517
-3	36	49
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-1	234	238
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3	287	276
4	98	110
5	491	458
6	276	292
7	241	221
8	185	188
9	145	148
10	129	104
11	160	140
13	124	124
14	35	37
5, 5, L		
-13	104	99
-12	50	52
-11	96	107
-10	156	168
-7	423	447
-6	200	200
-5	387	396
-4	112	104
-3	308	327
-2	228	240
-1	451	460
1	205	190
2	433	428
3	393	397
4	68	69
6	413	408
7	497	504
8	391	388
9	106	100
10	86	84
12	48	70
14	46	51
5, 7, L		
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-11	85	72
-10	155	169
-8	188	212
-7	177	153
-6	266	266
-5	172	175
-4	138	139
-3	169	146
-1	336	349
1	267	274
2	142	149
3	109	130
4	58	62
5	280	273
6	81	76
7	111	90
8	83	78
10	48	40

5, 7, L			-11	133	129	0	710	682	-5	184	203	5	193	178	7, 5, L		
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5, 9, L			-9	76	54	2	66	69	-2	152	139	7	398	406	-12	82	90
-7	102	102	-8	509	519	3	743	719	1	173	155	8	135	144	-11	190	186
-6	136	160	-7	70	71	4	362	341	3	92	58	9	413	397	-10	224	215
-5	209	220	-5	161	144	5	291	283	4	225	217	10	38	61	-9	190	203
-4	65	82	-4	251	279	6	391	382	5	90	83	11	57	40	-8	146	120
-2	182	174	-3	88	86	8	183	184	10	103	98	12	63	74	-7	160	136
-1	184	168	-2	335	343	9	229	244	6, 10, L			13	87	86	-6	61	72
1	263	263	-1	1044	1028	11	61	49	-5	43	44	14	59	59	-5	77	77
2	134	122	0	1165	1165	12	121	134	-3	42	36	7, 3, L			-4	293	308
3	57	41	1	53	44	13	58	67	-2	159	145	-15	87	91	-3	131	102
4	205	210	2	81	70	15	60	44	-1	74	53	-14	49	50	-2	92	90
5	180	174	3	315	352	6, 6, L			0	165	160	-13	72	78	-1	871	850
6	95	100	4	513	506	-12	94	80	3	105	112	-12	131	141	0	217	216
7	78	73	5	713	691	-11	185	184	4	97	104	-11	239	238	2	217	220
6, 0, L			6	716	697	-9	216	220	5	65	64	-10	265	306	3	176	193
-16	92	98	7	727	758	-8	67	31	7, 1, L			-9	137	114	4	545	538
-12	342	322	8	330	335	-7	323	360	-16	96	86	-8	165	169	5	217	215
-10	73	61	9	127	132	-5	368	388	-15	112	112	-7	98	104	6	363	342
-8	549	565	10	125	131	-4	181	195	-13	72	65	-6	667	663	7	120	126
-6	1729	1734	11	143	141	-3	234	254	-12	244	256	-5	499	512	8	53	27
-4	397	412	13	146	134	-2	153	157	-11	170	147	-4	70	94	10	115	115
-2	2685	2689	6, 4, L			-1	90	60	-10	97	104	-3	620	634	11	92	91
0	451	419	-14	56	39	0	227	197	-9	83	92	-2	1126	1095	12	134	126
2	560	578	-13	77	64	1	782	730	-8	285	301	-1	300	311	7, 7, L		
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6	336	348	-11	228	216	3	368	370	-6	316	326	1	930	903	-10	54	50
8	279	270	-10	202	202	4	82	73	-5	611	617	2	281	250	-9	192	201
10	270	271	-9	109	74	5	80	91	-4	599	592	3	191	176	-8	181	170
12	85	108	-8	77	86	6	305	287	-3	251	237	4	82	65	-7	85	96
14	57	54	-7	125	116	7	283	284	-2	746	721	5	125	131	-5	220	239
16	50	36	-6	158	174	8	43	41	-1	573	599	6	269	279	-4	99	110
6, 2, L			-5	785	814	10	42	16	0	283	297	7	228	225	-3	308	320
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-14	177	179	-3	494	538	-9	60	48	2	878	868	10	88	85	-1	72	52
-13	277	278	-2	159	152	-8	89	88	3	631	633	12	138	146	0	246	238
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7, 7, L		
2	149	149
3	212	180
4	237	237
5	117	121
6	182	171
9	65	73
11	71	66
7, 9, L		
-6	84	77
-5	38	22
-3	196	187
-1	111	108
0	264	269
2	215	217
3	185	192
4	76	61
7	41	49
8, 0, L		
-14	43	49
-12	119	111
-10	430	407
-8	704	756
-6	716	738
-4	400	368
-2	151	166
0	609	622
2	278	247
4	1927	2101
8	356	386
10	64	70
12	265	256
8, 2, L		
-15	106	95
-14	97	82
-12	178	177
-11	103	106
-10	54	16

-9	362	354
-8	325	309
-7	843	848
-6	437	459
-5	678	689
-4	916	956
-3	1039	993
-2	536	558
-1	1001	996
0	599	556
1	31	11
2	919	901
3	609	640
4	135	137
5	191	177
6	142	123
8	91	98
9	118	125
11	118	125
14	105	104
8, 4, L		
-14	80	78
-13	67	47
-12	135	148
-11	123	118
-10	131	131
-9	371	393
-8	107	72
-7	74	80
-6	425	454
-5	109	107
-4	721	760
-3	165	198
-2	171	212
-1	597	574
0	557	501
1	480	480
2	749	709

3	190	190
4	178	152
5	782	787
6	111	109
7	105	103
8	132	108
9	126	129
11	224	212
12	51	45
8, 6, L		
-13	68	71
-11	156	172
-10	103	111
-9	105	107
-8	205	209
-7	157	166
-6	216	226
-5	39	37
-4	210	194
-3	208	187
-2	287	254
-1	674	679
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1	549	531
2	200	195
3	155	153
4	162	147
5	146	144
6	96	81
7	173	174
8	135	141
8, 8, L		
-10	164	174
-9	99	110
-7	180	180
-6	38	37
-4	139	164
-3	198	195

-2	117	98
-1	169	149
0	148	132
1	84	100
2	115	117
5	37	34
6	152	138
8, 10, L		
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-3	59	67
-2	75	85
-1	99	98
0	60	64
1	62	64
2	127	131
3	85	75
9, 1, L		
-13	114	118
-12	70	61
-11	165	188
-9	260	272
-8	103	106
-7	303	313
-6	831	844
-5	220	215
-4	568	590
-3	304	265
-2	628	637
-1	246	267
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1	498	485
2	42	66
3	199	200
4	711	713
5	603	611
6	33	6
7	229	202
8	144	143

9	175	203
10	141	139
11	221	219
13	91	97
14	75	68
9, 3, L		
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-13	95	71
-11	97	109
-10	204	210
-8	54	45
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-6	163	172
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-2	83	87
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2	113	113
3	549	574
4	707	703
7	137	103
8	290	312
9	145	141
10	88	75
13	106	87
9, 5, L		
-13	88	95
-12	67	55
-11	86	57
-10	67	73
-9	175	194
-8	227	239
-7	78	54
-6	70	44
-5	572	588
-4	86	89

-3	452	443
-2	357	342
-1	288	290
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1	345	343
2	258	231
4	302	295
5	172	164
6	108	105
7	105	106
8	200	199
9	129	144
10	171	170
11	80	70
9, 7, L		
-11	121	116
-10	109	94
-8	133	154
-7	96	100
-6	138	158
-5	207	185
-4	241	227
-3	138	140
-2	115	111
-1	192	168
0	87	83
1	319	318
2	268	264
3	128	121
4	128	142
5	91	107
6	82	90
7	82	84
8	70	62
10	64	61

9,	9,	L
-7	55	49
-4	126	138
-3	135	128
-2	108	122
-1	113	109
0	208	191
1	150	138
4	70	69
5	113	108
6	95	94
7	95	94

10,	0,	L
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-12	146	149
-10	412	387
-8	44	38
-6	292	289
-4	1076	1057
-2	595	601
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2	102	103
4	879	913
6	603	647
8	348	361
10	53	58
12	92	98

10,	2,	L
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-13	180	155
-12	259	255
-11	403	396
-10	57	71
-9	184	190
-8	200	200
-7	91	96
-6	632	640
-5	627	654
-4	253	273
-3	572	557
-2	266	262
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2	496	500
4	51	66
5	92	80
6	205	210
7	47	58
8	174	168
9	284	291
10	185	185
15	67	63

10,	4,	L
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-13	81	91
-12	167	139
-11	59	47
-10	237	229
-9	339	325
-8	300	300
-6	54	67
-5	242	226
-4	62	62
-3	880	895
-2	212	199
-1	272	297
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1	631	589
2	119	118
3	485	477
4	85	83
5	155	163
7	222	212
8	214	224
9	59	42
10	102	98
13	60	48

10,	6,	L
-12	73	71
-11	102	103
-10	190	179
-9	148	138
-8	49	60
-7	147	153
-5	310	341
-4	159	159
-3	369	374
-2	135	137
-1	192	199
0	150	172
1	283	260
2	172	159
3	361	349
4	91	101
5	65	67
8	112	97
9	154	163

10,	8,	L
-8	92	113
-6	52	46
-4	79	92
-3	102	113
-2	105	110
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2	102	86
4	88	83
6	61	58

10,	10,	L
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11,	1,	L
-15	91	98
-14	145	141
-13	86	96
-12	68	74
-10	251	263
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-4	49	39
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-1	138	112
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2	389	408
3	377	383
4	365	369
5	478	475
6	272	288
7	96	112
8	128	107
9	171	180
10	126	118
11	124	104

11,	3,	L
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-12	74	87
-10	145	148
-9	286	289
-8	178	219
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1	153	144
2	105	122
3	458	439
4	165	180
5	95	105
6	259	247
8	94	86
9	124	105

11,	5,	L
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-12	88	101
-11	190	186
-10	57	64
-9	255	253
-8	111	104
-7	84	84
-6	181	149
-3	76	68
-2	237	238
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1	624	622
2	71	67
5	88	115
6	241	233
8	87	74
9	82	74
12	94	92

11,	7,	L
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-8	147	131
-7	215	214
-6	151	131
-5	73	84
-3	257	256
-2	247	237
-1	269	262
0	55	51
2	97	101
3	86	82
4	160	159
6	104	103
8	138	125

11,	9,	L
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-3	92	81
-2	64	81
-1	156	143
1	61	61
2	165	166
3	104	108
4	91	94
5	102	103
6	49	38

12,	0,	L
-14	181	162
-12	129	115
-10	167	145
-8	568	541
-6	1091	1126
-4	791	791
-2	222	210
0	236	209
4	408	399
6	480	487
8	105	114
10	69	73
14	104	102

12,	2,	L
-13	133	125
-12	52	35
-10	299	297
-9	81	74
-8	37	12
-7	223	225

12, 2, L	-7 135 134	-1 126 117	-3 373 359	-8 114 109	-5 129 160
-6 239 226	-6 200 200	0 308 306	-1 161 162	-6 133 128	-4 68 56
-5 486 501	-5 190 206	1 334 332	0 172 154	-4 259 258	-3 94 85
-4 482 506	-4 212 224	4 220 231	1 205 215	-2 598 594	-2 165 171
-2 578 591	-3 94 84	5 260 280	2 216 210	0 543 561	-1 565 576
-1 384 396	-2 109 90	6 352 369	3 285 275	2 690 709	0 113 104
0 366 373	-1 280 268	7 379 365	4 108 90	4 210 262	3 285 286
1 693 724	0 137 119	11 77 92	5 65 75	6 558 570	5 142 131
2 404 384	1 330 346	13 104 102	6 86 74	8 150 182	7 67 53
4 258 256	2 211 198	13, 3, L	7 78 73	10 98 100	9 100 95
5 483 523	3 95 101	-12 102 105	8 100 100	14, 2, L	14, 6, L
6 214 218	4 60 55	-10 56 54	10 132 130	-13 90 87	-10 101 104
9 80 85	5 60 59	-8 357 371	11 49 69	-12 77 52	-9 79 79
12, 4, L	6 116 109	-6 72 79	13, 7, L	-11 196 180	-8 233 223
-13 207 181	8 54 34	-5 55 54	-10 60 56	-10 255 249	-7 67 63
-10 98 122	10 52 50	-4 400 403	-9 115 110	-9 494 480	-6 55 69
-9 66 49	11 49 48	-3 368 391	-8 57 36	-8 161 174	-5 60 71
-7 536 563	12, 8, L	-1 463 460	-7 43 67	-7 61 67	-3 274 294
-6 182 146	-8 129 142	2 98 90	-6 77 98	-6 222 213	-2 179 166
-4 345 348	-7 98 108	3 51 39	-5 112 113	-5 214 227	-1 86 95
-3 37 58	-5 159 154	4 271 273	-4 48 45	-4 459 458	0 68 68
-2 588 592	-4 54 50	5 286 293	-3 152 134	-3 556 565	3 102 105
-1 219 241	-2 123 138	6 248 235	-2 237 225	-2 327 334	5 102 111
1 192 209	-1 184 179	7 77 70	0 142 132	-1 303 300	9 91 94
2 156 151	0 54 63	8 55 62	1 117 107	0 134 133	14, 8, L
3 121 133	1 60 50	9 67 46	2 135 140	1 319 329	-6 120 128
4 120 121	2 108 103	10 80 88	4 154 147	3 179 174	-5 64 67
6 156 147	8 75 76	12 44 33	13, 9, L	5 56 52	-3 63 69
7 205 225	13, 1, L	13, 5, L	-5 97 78	11 96 105	0 115 115
8 59 47	-13 55 51	-12 97 91	-2 94 91	12 85 81	4 77 72
11 101 101	-11 122 130	-11 74 89	0 88 89	14, 4, L	6 68 61
12 42 41	-9 124 154	-10 102 92	1 131 130	-12 83 91	15, 1, L
13 83 77	-8 44 25	-9 42 8	2 91 90	-11 164 168	-13 113 121
12, 6, L	-6 49 58	-8 77 78	3 64 53	-10 192 164	-12 168 169
-11 68 68	-5 229 233	-7 131 150	14, 0, L	-9 55 40	-10 138 145
-10 54 59	-4 324 322	-6 192 202	-14 88 77	-8 159 148	-9 100 83
-9 232 256	-3 65 66	-5 66 60	-12 282 254	-7 258 246	-8 92 95
-8 82 92	-2 346 366	-4 36 12	-10 239 256	-6 233 231	-6 151 147

15, 1, L
-5 152 152
-3 357 355
-1 115 119
0 300 320
2 61 54
3 403 409
4 215 209
5 240 232
6 123 136
7 106 96
8 43 51
10 66 52
11 37 43
15, 3, L
-12 80 84
-11 169 177
-9 155 164
-4 129 126
-2 238 235
-1 163 172
0 165 171
1 281 293
2 482 492
3 44 57
5 139 120
6 138 148
8 86 71
11 78 61
15, 5, L
-11 122 137
-10 77 91
-9 212 209
-7 235 223
-4 142 118
-2 101 91
-1 45 34
2 59 59
3 193 193
4 64 64
6 63 63
8 133 124
15, 7, L
-8 58 46
-7 141 129
-6 171 145
-5 155 146
-2 103 113
-1 171 162
0 240 238
1 63 40
2 53 54
3 69 78
4 69 68
6 67 67
8 56 61
15, 9, L
-1 87 84
1 63 47
16, 0, L
-12 112 92
-10 231 211
-8 127 111
-6 350 316
-4 777 817
-2 558 556
0 352 348
2 348 331
4 69 83
6 71 70
8 104 128
16, 2, L
-11 63 58
-9 35 41
-8 276 272
-7 282 281
-6 51 81
-5 169 159
-4 120 119
-3 294 295
-2 269 288
-1 88 79
0 162 171
1 253 291
2 129 110
3 282 288
4 154 146
5 90 85
7 68 87
8 124 139
16, 4, L
-11 207 188
-8 58 73
-5 421 426
-3 104 83
-2 178 185
-1 53 40
0 105 112
1 152 156
3 117 94
11 45 49
16, 6, L
-7 202 217
-5 125 128
-4 157 144
-3 74 74
-2 121 129
-1 138 140
1 93 96
2 122 123
3 122 122
4 104 95
7 62 71
16, 8, L
-5 83 94
-4 108 97
-3 91 89
1 67 80
2 74 70
17, 1, L
-11 158 146
-9 83 94
-8 141 142
-5 78 63
-4 138 143
-3 83 88
-2 119 128
-1 35 31
0 252 271
1 59 59
2 102 111
3 136 132
4 98 89
5 61 85
7 95 104
8 161 165
9 129 119
17, 3, L
-10 53 56
-8 80 75
-7 33 11
-6 260 266
-4 91 94
-2 309 304
0 146 130
1 280 282
2 90 81
4 152 145
5 49 54
6 84 80
7 162 163
8 76 69
17, 5, L
-9 56 52
-8 79 71
-7 65 80
-5 118 127
-3 48 46
-2 63 57
-1 179 183
0 45 50
1 106 116
3 104 113
4 122 121
5 94 76
6 84 69
10 80 81
17, 7, L
-7 73 73
-5 105 102
-3 85 83
-2 53 46
0 88 86
1 69 65
2 68 62
4 73 73
6 85 76
18, 0, L
-12 151 136
-10 249 222
-8 287 299
-4 86 82
-2 239 221
0 154 150
2 271 284
4 106 122
6 75 106
8 207 209
18, 2, L
-11 52 43
-10 61 47
-9 124 106
-8 159 146
-7 317 314
-6 135 150
-4 143 131
-3 106 110
-2 192 185
-1 406 409
0 270 268
1 182 187
3 188 203
4 58 68
5 42 31
6 59 45
7 60 48
18, 4, L
-9 181 178
-8 166 147
-7 71 63
-6 112 110
-5 65 69
-4 102 99
-3 149 158
-2 34 60
0 91 101
1 178 179
2 59 29
3 53 55
5 80 87
9 75 66
18, 6, L
-8 80 80
-6 183 171
-4 49 52
-3 38 37

18, 6, L		
-1	87	104
0	188	165
1	51	35
5	74	79
19, 1, L		
-11	81	86
-10	128	128
-9	84	61
-8	139	143
-7	56	58
-4	77	75
-3	118	113
-2	107	95
-1	246	248
0	79	63
1	122	116
2	108	127
4	74	71
5	160	145
6	62	59
7	79	65
19, 3, L		
-10	119	123
-9	132	141
-8	63	69
-7	84	82
-6	74	56
-4	83	69
-3	103	91
-2	57	66
-1	96	96
2	141	147
3	130	134
4	135	136
7	48	35
8	61	55

19, 5, L		
-7	132	135
-5	138	125
-4	65	55
-3	49	47
0	103	103
3	38	42
6	44	49
8	74	68
19, 7, L		
-4	121	111
0	67	75
2	116	113
4	56	52
20, 0, L		
-8	166	161
-4	181	170
-2	400	436
0	239	246
2	110	95
4	122	112
20, 2, L		
-8	81	84
-6	163	154
-5	230	216
-4	92	102
-1	78	101
0	60	72
1	103	101
4	50	26
5	67	68
6	39	35
20, 4, L		
-3	197	197
-1	121	119
0	70	71
1	70	60
3	64	45

5	100	88
7	66	57
20, 6, L		
-5	141	153
-4	71	51
1	65	64
2	78	75
4	60	72
21, 1, L		
-9	145	142
-8	74	64
-6	113	109
-3	95	80
-2	122	129
1	90	83
9	57	53
21, 3, L		
-5	99	80
-4	126	135
-2	104	106
0	183	179
1	54	50
3	139	146
4	70	66
21, 5, L		
-6	64	58
-5	73	77
-2	76	68
5	47	53
6	68	65
22, 0, L		
-8	120	102
-6	165	168
0	203	195
2	54	46
4	45	55

22, 2, L		
-7	72	62
-5	152	155
-4	72	82
-1	55	64
0	49	34
1	107	101
2	115	118
3	102	111
5	54	60
6	46	47
22, 4, L		
-6	73	56
-5	60	55
-1	87	93
2	62	73
23, 1, L		
-7	94	79
-6	109	110
-1	101	100
0	49	33
1	73	81
2	74	60
23, 3, L		
-6	41	45
-5	85	82
-4	89	74
-2	75	67
-1	49	53
1	84	77
4	57	56
5	58	60
24, 0, L		
-6	69	75
0	106	133
2	46	46
6	50	34

24, 2, L		
-3	119	114
-2	61	64
25, 1, L		
-4	63	58
0	61	62

CALCULATED AND OBSERVED STRUCTURE FACTORS OF $C_4Cl_4O_2S$ at 150K

0, 0, L		
2	1326	1354
4	1319	1342
6	1249	1307
8	246	263
10	525	539
12	384	402

0, 2, L		
0	135	102
1	1084	1077
2	1442	1430
3	667	664
4	172	196
5	1077	1059
6	476	494
7	1402	1406
8	735	780
9	803	833
10	328	346
11	609	634
12	366	382
13	351	339
14	85	81
15	238	241
16	92	89
17	123	115
18	130	136

0, 4, L		
0	207	201
1	1510	1537
2	762	769
3	436	429
4	810	827
5	227	222
6	155	171
7	779	786
8	719	731
9	63	53
10	297	317
11	93	106
12	136	128
13	55	50
14	177	185
15	284	288
16	213	214
17	82	77

0, 6, L		
0	927	979
1	79	84
2	79	75
3	1231	1296
4	281	276
5	554	577
6	280	286
7	190	206
8	180	170
9	300	322
10	309	312
11	189	188
12	346	330
13	133	141
15	115	114
16	119	105

0, 8, L		
0	283	279
1	129	136
2	240	247
3	479	496
4	73	83
5	382	381
6	375	364
7	271	266
8	141	133
9	106	91
10	100	98
11	172	175
0, 10, L		
0	192	171
1	267	251
2	248	255
3	59	54
4	226	206
5	269	293
6	267	282
7	138	151

1, 1, L		
-18	206	218
-16	235	241
-15	63	75
-14	113	107
-13	320	330
-12	110	113
-11	110	116
-10	975	1020
-9	38	33
-8	702	735
-7	461	465
-6	47	28
-5	780	805
-4	699	730
-3	1023	1010
-2	239	248
-1	987	977
0	635	597
1	552	506
2	72	35
3	203	208
4	308	304
5	274	259
6	492	493
8	361	352
9	732	744
10	59	28
11	457	471
12	457	472
14	243	240
15	476	472
16	174	173
17	169	166

1, 3, L		
-17	356	368
-16	54	54
-15	140	147
-14	228	223
-13	253	259
-12	84	75
-11	671	679
-10	263	271
-9	512	532
-8	598	627
-7	207	209
-6	381	388
-5	201	207
-4	1086	1069
-3	130	132
-2	384	376
-1	1538	1514
0	1622	1560
1	403	378
2	330	350
3	132	94
4	798	767
5	538	493
6	277	229
7	931	934
8	221	214
9	434	442
10	230	226
11	364	371
12	39	36
13	331	330
14	310	321
15	110	110
17	162	171
18	89	94

1, 5, L		
-17	162	169
-15	189	187
-14	182	198
-13	109	122
-11	35	24
-10	150	172
-9	638	689
-8	732	777
-7	780	815
-6	147	160
-5	232	255
-2	291	304
-1	188	201
0	158	149
1	702	713
3	59	47
4	403	398
5	1125	1148
6	693	679
7	394	394
8	497	479
9	92	91
10	265	274
11	334	316
12	242	260
13	302	299
14	462	450
15	203	202
16	80	86
17	122	116

1, 7, L		
-12	152	158
-11	105	110
-10	360	384
-9	89	65
-8	296	298
-7	495	514
-6	125	114
-4	119	109
-3	425	442
-2	93	91
-1	392	399
0	590	594
1	56	70
2	87	90
3	289	284
4	477	485
5	236	208
6	455	497
7	208	211
8	209	192
9	195	178
11	205	203
12	513	475

1, 9, L		
-9	94	92
-8	323	340
-7	621	616
-5	81	78
-4	194	173
-3	524	527
-2	33	6
-1	671	681
0	49	18
1	216	235
2	336	356
3	353	350
4	429	455
5	415	427
6	43	73
7	155	159
9	49	46

1, 11, L		
-1	160	162
0	174	185
1	73	87
2, 0, L		
-18	87	84
-16	91	111
-14	465	497
-12	135	121
-10	946	1078
-8	1181	1234
-4	2534	2770
-2	791	788
0	237	229
2	1299	1330
4	872	876
6	2025	2084
8	106	113
10	793	806
12	496	529
14	273	266
16	151	145
18	78	79
2, 2, L		
-18	152	165
-17	149	142
-16	234	237
-15	232	225
-14	208	224
-13	250	240
-12	30	30
-11	82	87
-10	410	429
-9	117	102
-8	255	275
-7	270	264
-6	118	131
-5	297	316
-4	85	59
-3	2214	2284
-2	1712	1789
-1	1397	1382
0	24	28
1	1570	1541
2	526	523
3	1025	983
4	1618	1543
5	1285	1291
6	373	370
7	216	225
8	105	106
9	31	6
10	296	319
11	417	431
12	85	89
13	137	132
14	60	52
15	58	66
16	167	177
17	87	85
18	74	82
2, 4, L		
-16	81	51
-15	242	229
-14	271	269
-13	90	79
-12	184	159
-11	339	328
-10	244	244
-9	144	143
-8	173	195
-7	393	404
-6	92	88
-5	928	985
-4	344	336
-3	753	791
-2	553	592
-1	269	255
0	506	535
1	1176	1124
2	371	380
3	441	443
4	1303	1273
5	343	345
6	169	147
7	974	964
8	438	433
9	63	45
10	150	162
11	271	275
12	99	93
13	325	310
14	94	81
15	95	102
16	89	91
17	193	182
2, 6, L		
-13	245	265
-12	120	119
-11	377	390
-10	174	150
-9	129	149
-7	617	653
-6	54	71
-5	245	257
-4	314	336
-3	45	35
-2	302	297
-1	637	653
0	497	496
1	370	388
2	139	133
3	481	466
4	363	353
5	660	667
6	355	373
7	138	129
8	86	69
9	194	198
10	222	210
11	87	101
12	231	185
13	237	228
2, 8, L		
-11	87	92
-9	96	86
-8	344	362
-7	415	437
-6	366	381
-5	376	393
-4	254	255
-2	191	188
-1	374	368
0	308	308
1	353	345
2	370	370
3	436	436
6	57	61
7	206	213
8	541	568
9	206	224
10	170	176
11	102	88
2, 10, L		
-5	148	150
-4	128	111
-3	123	102
-2	438	433
-1	112	121
0	113	121
1	415	440
2	161	175
4	412	409
5	214	201
6	63	89
3, 1, L		
-18	131	133
-17	116	131
-15	288	288
-14	463	480
-13	457	449
-12	205	208
-11	210	234
-10	285	309
-9	312	336
-8	173	181
-7	970	1016
-6	487	476
-5	36	21
-4	1260	1273
-3	456	445
-2	989	961
-1	195	203
0	540	532
1	1424	1354
2	643	586
3	44	39
4	538	507
5	706	718
7	684	693
8	253	249
9	420	423
10	333	348
11	405	421
12	602	601
13	123	124
14	72	71
16	81	78
17	64	69
18	171	171
3, 3, L		
-18	119	129
-17	118	131
-16	147	154
-15	220	215
-14	210	202
-13	197	197
-12	514	523
-11	443	427
-10	310	325
-9	439	460
-8	372	392
-7	130	129
-6	201	215
-5	871	909
-4	443	420
-3	149	133
-2	97	77
-1	960	935
0	123	148
1	237	212
2	403	370
3	534	507
4	74	55
5	613	600
6	796	754
7	441	424
8	352	337
9	110	115
10	723	733
11	455	450
12	182	177
13	415	410
14	118	124
15	260	261
16	159	164

3, 5, L		
-17	89	70
-16	71	63
-15	144	136
-14	65	77
-13	354	365
-12	534	541
-11	299	315
-10	208	245
-9	188	180
-8	120	136
-7	49	57
-6	460	491
-5	143	128
-4	45	40
-3	1748	1733
-2	159	153
-1	195	185
0	144	155
1	835	839
2	524	520
3	37	47
4	931	935
5	75	27
6	257	241
7	222	220
8	483	472
9	410	379
10	699	667
11	321	323
12	153	146
13	56	53
14	61	55
16	213	220
17	166	163

3, 7, L		
-12	76	67
-11	236	243
-10	634	620
-9	228	238
-8	152	143
-7	115	129
-6	167	146
-5	477	488
-4	351	376
-2	498	493
-1	48	50
1	145	123
2	340	350
3	465	469
4	529	522
5	180	196
7	236	244
8	330	319
9	368	367
10	219	212
12	198	194
3, 9, L		
-9	91	107
-8	182	165
-7	100	85
-6	63	50
-5	465	483
-4	36	70
-3	297	303
-2	490	516
-1	300	288
0	328	345
1	255	282
2	138	111
3	579	600
4	134	132
5	224	232

6	173	152
7	206	197
9	286	283
4, 0, L		
-18	276	286
-16	67	64
-14	163	202
-12	508	533
-10	789	883
-8	671	770
-6	119	137
-4	1972	1996
-2	1307	1249
0	1514	1355
2	3680	3702
4	1056	1022
6	429	465
8	1020	1103
10	786	830
12	110	85
14	401	392
16	176	183
18	74	79
4, 2, L		
-18	49	51
-17	300	299
-16	205	197
-14	92	95
-13	308	317
-12	56	16
-11	291	271
-10	431	440
-9	801	841
-8	53	62
-7	1132	1146
-6	1107	1140
-5	895	907
-4	667	700

-3	2016	1970
-2	423	386
-1	787	757
0	1715	1679
1	1743	1720
2	179	145
3	1537	1435
4	880	852
5	47	10
6	352	364
7	636	591
8	291	286
9	674	684
10	385	388
11	418	417
12	419	436
14	177	187
15	170	168
16	125	126
17	142	145
18	131	130
4, 4, L		
-17	65	59
-16	64	87
-15	134	115
-14	320	321
-13	377	368
-12	97	105
-11	289	283
-10	339	321
-9	162	176
-8	572	604
-7	46	30
-6	1249	1248
-5	331	348
-4	192	172
-3	664	670
-2	907	915

-1	492	498
0	855	860
1	746	776
2	592	556
3	1693	1656
4	209	189
5	371	362
6	236	218
8	187	174
9	895	867
10	567	554
11	101	96
12	304	298
14	165	163
15	98	87
16	68	82
17	129	134
4, 6, L		
-16	178	169
-15	71	72
-14	100	79
-13	263	273
-12	68	79
-11	67	65
-10	331	324
-9	130	136
-8	116	105
-7	167	190
-6	146	145
-5	293	294
-4	382	404
-3	597	636
-2	180	197
-1	1091	1151
0	237	247
1	150	152
2	861	871
3	470	472

4	137	125
5	1059	1063
6	463	456
7	83	87
9	88	93
10	181	165
11	260	264
12	303	291
13	188	173
4, 8, L		
-11	141	166
-10	251	266
-9	386	394
-7	190	186
-6	148	164
-5	347	347
-4	172	158
-3	327	326
-2	171	184
-1	436	449
0	120	119
1	245	249
2	384	389
3	43	40
4	513	526
5	246	251
6	148	147
7	151	144
8	142	115
9	208	199
10	266	254
11	35	13
4, 10, L		
-6	176	188
-5	91	104
-4	263	283
-3	386	404
-2	129	106

4, 10, L		
-1	127	125
0	288	289
1	159	148
2	130	105
3	158	147
6	270	253

5, 1, L		
-17	234	234
-16	142	140
-15	144	153
-14	284	291
-13	348	370
-11	354	371
-10	46	53
-9	214	220
-8	1223	1271
-7	39	6
-6	389	392
-5	1029	986
-4	80	82
-3	191	149
-2	937	878
-1	583	555
0	283	281
1	558	522
2	1664	1496
3	304	345
4	99	53
5	105	86
6	224	208
7	127	139
8	601	608
9	469	488
10	196	185
11	625	636
12	370	374
13	141	131
14	356	365
16	178	167
17	317	304
18	65	69

5, 3, L		
-16	147	169
-15	437	401
-14	64	53
-13	105	119
-12	65	53
-11	252	258
-10	49	29
-9	554	553
-8	93	83
-7	779	815
-6	802	815
-5	873	897
-4	742	748
-2	892	886
-1	209	224
0	353	342
1	941	896
2	1171	1121
3	371	348
4	176	155
5	689	658
6	533	515
7	366	336
8	377	373
9	459	450
10	85	75
11	405	397
12	162	162
13	329	326
15	287	282
16	131	138
18	80	69

5, 5, L		
-17	95	91
-16	260	251
-15	207	218
-13	278	267
-12	103	110
-11	47	52
-10	261	278
-9	53	36
-8	33	38
-7	795	831
-6	273	286
-5	640	656
-4	148	145
-3	526	540
-2	214	213
-1	562	576
0	52	47
1	375	356
2	605	626
3	781	795
5	86	63
6	681	659
7	1025	981
8	585	560
9	323	302
10	218	203
12	156	167
13	97	92
14	196	196
15	144	143
16	241	227
17	149	137

5, 7, L		
-12	133	116
-11	205	188
-10	367	375
-9	109	113
-8	509	531
-7	280	255
-6	620	624
-5	362	361
-4	278	267
-3	228	207
-2	72	26
-1	548	560
0	64	69
1	554	566
2	424	420
3	204	218
4	60	54
5	438	439
7	162	144
8	244	243
9	97	95
10	159	135
11	171	154
12	67	71

5, 9, L		
-9	57	36
-7	207	207
-6	450	476
-5	520	521
-2	274	252
-1	444	441
1	674	688
2	75	50
3	114	94
4	373	391
5	432	412
6	295	303
7	124	122
8	36	21

6, 0, L		
-18	61	67
-16	262	303
-14	58	84
-12	495	506
-10	138	126
-8	747	839
-6	2091	2097
-4	383	413
-2	3129	2869
0	511	475
2	586	592
4	719	768
6	598	638
8	610	607
10	293	309
12	76	79
14	252	260
16	187	173
18	63	69

6, 2, L		
-17	189	191
-16	102	119
-15	339	319
-14	437	430
-13	619	621
-12	84	83
-11	310	303
-10	236	254
-9	142	116
-8	753	769
-7	159	151
-6	53	57
-5	194	182
-4	464	476
-3	95	86
-2	408	425
-1	1277	1240
0	1356	1355
1	226	187
2	137	112
3	519	543
4	559	536
5	997	964
6	1086	1086
7	1259	1262
8	481	482
9	95	93
10	102	104
11	332	338
12	106	111
13	339	348
14	101	90
15	118	110
18	69	73

6, 4, L		
-17	236	249
-16	169	175
-15	118	113
-14	142	97
-13	164	136
-12	264	265
-11	308	293
-10	507	488
-9	126	102
-7	80	85
-6	391	382
-5	951	985
-4	162	137
-3	764	808
-2	128	121
-1	1201	1181
0	899	938
1	652	650
2	240	270
3	836	818

6, 4, L			9 83 70			-14 75 90			-10 517 521			-6 96 102			6 465 433		
4	564	535	10	64	45	-13	153	155	-9	251	233	-5	181	184	7	103	108
5	524	513	11	105	107	-12	524	555	-8	294	314	-4	353	375	8	91	99
6	755	738	12	122	115	-11	377	382	-7	131	130	-3	185	167	9	123	130
7	159	136	6, 8, L			-10	168	165	-6	755	780	-2	194	207	10	214	208
8	404	389	-9	123	113	-9	66	69	-5	591	601	-1	1388	1371	11	223	215
9	594	585	-8	60	48	-8	469	515	-4	83	95	0	313	328	7, 9, L		
10	185	184	-6	169	178	-7	304	314	-3	798	794	2	299	308	-7	40	19
11	160	159	-5	339	358	-6	428	441	-2	1416	1320	3	380	384	-6	195	176
12	322	332	-4	146	151	-5	773	765	-1	378	385	4	782	767	-5	162	157
13	132	136	-3	309	320	-4	688	664	0	325	295	5	456	455	-3	440	458
14	102	91	-2	147	146	-3	212	209	1	1267	1241	6	639	607	-2	154	180
15	173	161	-1	63	65	-2	744	724	2	352	315	7	255	241	-1	184	194
17	171	170	0	108	110	-1	731	741	3	233	211	8	129	116	0	564	586
6, 6, L			1	271	257	0	307	324	4	123	81	9	47	47	1	46	36
-16	178	158	3	128	113	1	255	250	5	337	336	10	345	334	2	350	363
-15	242	256	4	434	436	2	1117	1014	6	266	269	11	347	328	3	351	372
-14	114	109	5	173	175	3	782	747	7	441	435	12	465	433	4	143	124
-13	52	48	6	274	252	4	123	121	8	384	351	13	192	190	5	90	96
-12	146	130	9	73	74	5	145	119	9	46	23	16	178	171	6	114	112
-11	376	392	10	402	404	6	97	109	10	130	139	7, 7, L			8	81	75
-10	32	29	6, 10, L			7	824	843	12	371	369	-12	119	137	8, 0, L		
-9	449	451	-5	146	148	8	319	340	13	213	208	-11	148	125	-18	133	123
-8	107	84	-4	58	53	9	773	777	14	59	35	-10	159	157	-16	500	507
-7	547	590	-3	148	148	10	108	113	15	211	206	-9	447	450	-14	104	118
-6	151	167	-2	146	126	12	252	254	16	75	87	-8	474	436	-12	275	314
-5	620	649	-1	172	149	13	382	393	17	57	58	-7	96	96	-10	722	737
-4	266	279	0	293	281	14	291	283	7, 5, L			-5	401	412	-8	909	998
-3	245	260	1	53	42	15	107	102	-16	131	129	-4	159	177	-6	1076	1154
-1	78	63	2	111	103	17	38	20	-15	38	39	-3	606	620	-4	443	412
0	195	188	3	361	381	18	111	109	-14	53	32	-2	451	460	-2	145	158
1	1074	1089	4	182	193	7, 3, L			-13	336	328	-1	49	32	0	781	783
2	427	420	5	157	170	-16	147	142	-12	133	148	0	615	618	2	196	149
3	334	338	7, 1, L			-15	206	207	-11	488	499	1	127	120	4	2705	2667
5	162	169	-18	179	179	-14	63	67	-10	411	421	2	181	176	8	515	547
6	468	463	-17	103	128	-13	274	270	-9	391	410	3	282	270	10	239	255
7	536	518	-16	276	272	-12	257	243	-8	160	140	4	532	532	12	697	720
8	311	306	-15	261	277	-11	420	424	-7	289	280	5	214	225	14	93	69

8, 0, L

16	147	148
18	220	211

8, 2, L

-18	143	145
-17	126	114
-16	68	73
-15	251	234
-14	152	142
-12	395	394
-11	129	141
-10	62	62
-9	642	633
-8	419	420
-7	1024	1044
-6	558	563
-5	972	996
-4	1279	1278
-3	1206	1135
-2	654	676
-1	1201	1183
0	617	578
1	30	17
2	1238	1168
3	981	1018
4	156	142
5	366	339
6	382	369
7	191	205
8	175	181
9	259	276
10	44	34
11	465	469
12	141	144
13	178	163
14	317	317
15	51	40
17	174	173

8, 4, L

-17	194	178
-16	275	268
-15	283	276
-14	83	87
-13	130	110
-12	250	255
-11	310	282
-10	203	192
-9	711	704
-8	129	89
-7	257	261
-6	595	631
-5	31	25
-4	1115	1149
-3	257	251
-2	489	527
-1	621	625
0	817	797
1	460	474
2	1077	1070
3	393	397
4	222	199
5	1279	1256
6	243	242
7	82	80
8	301	285
9	194	189
11	562	531
12	222	217
13	254	236
14	140	133
17	67	56

8, 6, L

-16	98	69
-15	112	120
-14	210	200
-13	235	238
-11	429	454
-10	46	56
-9	323	326
-8	384	369
-7	229	239
-6	180	187
-5	115	96
-4	235	227
-3	307	296
-2	423	419
-1	890	919
0	353	360
1	778	792
2	241	247
3	275	263
4	505	509
5	107	107
6	132	120
7	541	525
8	337	322
9	95	99
10	39	42
11	90	98
12	185	174

8, 8, L

-10	427	442
-9	230	250
-8	39	44
-7	404	415
-5	94	91
-4	153	173
-3	331	322
-2	144	123
-1	251	244
0	310	316
1	169	177
2	107	111
3	74	65
5	82	70
6	502	503
7	51	61
8	80	72

8, 10, L

-4	63	80
-3	171	181
-2	142	158
-1	295	301
0	110	131
1	186	190
2	265	267
3	262	250
4	119	140

9, 1, L

-18	145	143
-17	185	181
-15	122	130
-14	101	108
-13	193	204
-12	171	189
-11	313	344
-10	73	69
-9	469	486
-8	94	105
-7	340	339
-6	1078	1093
-5	176	147
-4	700	710
-3	201	148
-2	858	852
-1	301	338
0	147	144
1	679	643
2	65	84
3	447	446
4	954	899
5	1007	1037
6	69	68
7	216	207
8	295	300
9	498	526
10	352	341
11	472	491
13	284	284
14	279	272
15	90	77
16	304	316
17	82	82

9, 3, L

-17	131	109
-16	177	186
-14	202	208
-13	262	225
-12	71	73
-11	174	187
-10	195	181
-9	27	2
-8	123	90
-7	349	335
-6	229	242
-5	701	719
-4	198	195
-3	705	703
-2	169	166
-1	37	33
0	186	168
1	495	481
2	81	77
3	912	900
4	1104	1078
5	121	135
7	341	308
8	693	680
9	340	310
10	223	208
11	224	213
13	354	328
14	93	104
16	87	85
17	198	193

9, 5, L

-16	162	153
-15	74	66
-14	355	338
-13	242	255
-12	83	63
-11	153	136
-10	182	178
-9	213	229
-8	360	379
-7	142	124
-6	100	85
-5	1063	1089
-4	118	121
-3	771	769
-2	530	542
-1	459	453
0	205	198
1	478	498
2	387	387
3	108	98
4	452	449
5	551	526
6	286	290
7	83	93
8	444	434
9	404	397
10	351	339
11	324	302
12	74	77
13	69	57
14	200	213

9, 7, L		
-11	270	255
-10	204	183
-8	289	289
-7	303	307
-6	396	402
-5	312	294
-4	557	556
-3	333	344
-2	204	190
-1	288	261
0	214	218
1	526	530
2	557	574
3	372	361
4	505	493
5	144	146
6	196	190
7	166	165
8	137	132
9	90	76
10	238	231

9, 9, L		
-7	129	127
-5	41	48
-4	400	419
-3	378	375
-2	135	162
-1	238	239
0	361	353
1	393	387
3	237	241
5	277	262
6	289	292
7	273	265

10, 0, L		
-16	96	91
-14	454	484
-12	344	403
-10	552	534
-6	443	479
-4	1358	1299
-2	648	631
0	1806	1783
2	89	79
4	1302	1295
6	935	975
8	873	912
10	127	113
12	156	159
14	46	54
16	83	90

10, 2, L		
-17	134	135
-16	108	104
-15	220	209
-13	436	408
-12	563	545
-11	689	670
-10	132	140
-9	429	428
-8	450	474
-7	176	183
-6	960	969
-5	953	964
-4	301	279
-3	800	798
-2	455	447
-1	869	840
0	389	385
1	779	748
2	758	764
3	43	10
4	60	52
5	144	140
6	287	272
7	79	69
8	481	470
9	683	676
10	412	407
13	115	112
15	316	315
16	166	155
17	78	68

10, 4, L		
-16	66	73
-15	266	291
-14	270	250
-13	351	331
-12	396	325
-11	59	39
-10	431	425
-9	498	472
-8	669	654
-7	116	134
-6	50	42
-5	250	246
-4	172	148
-3	1123	1157
-2	356	333
-1	474	496
0	346	331
1	887	885
2	222	242
3	598	591
4	354	376
5	255	244
7	453	460
8	628	634
9	307	282
10	277	267
11	156	161
12	147	146
13	185	178
14	69	87

10, 6, L		
-15	69	79
-14	137	105
-13	170	173
-12	192	189
-11	261	264
-10	286	272
-9	232	237
-8	90	96
-7	301	310
-6	60	84
-5	499	537
-4	358	365
-3	643	664
-2	177	185
-1	244	252
0	25	15
1	448	446
2	199	185
3	641	639
4	206	213
5	76	78
7	122	122
8	249	226
9	457	447
10	162	157
11	171	163

10, 8, L		
-9	67	60
-8	182	195
-6	67	78
-4	154	164
-3	212	224
-2	147	150
-1	79	92
0	136	133
1	98	90
2	381	383
3	92	91
4	158	161
6	150	146
8	230	210

10, 10, L		
-2	206	199
-1	116	116
0	156	133

11, 1, L		
-16	108	111
-15	221	247
-14	349	348
-13	168	194
-11	84	85
-10	488	511
-9	183	178
-8	155	150
-6	154	173
-5	471	492
-4	60	71
-3	342	324
-2	942	917
-1	268	256
0	631	601
1	667	690
2	635	662
3	540	549
4	719	716
5	700	680
6	481	461
7	336	342
8	157	154
9	506	502
10	370	368
11	398	378
14	72	78
15	272	278
16	116	109
17	78	68

11, 3, L		
-17	111	96
-16	57	57
-13	367	358
-12	145	146
-11	122	117
-10	254	249
-9	468	477
-8	380	388
-7	206	182
-6	548	555
-5	237	231
-4	491	488
-3	617	621
-2	277	257
-1	418	431
0	1043	1029
1	169	162
2	51	75
3	815	802
4	411	401
5	185	196
6	460	477
7	90	89
9	416	405
10	67	53
11	62	76
12	88	87
13	168	176
14	216	220

11, 5, L			-1	598	594	8	128	130	12, 4, L			-6	379	361	-5	276	271
-16	89	92	0	75	69	10	118	130	-15	99	76	-5	392	409	-4	456	453
-15	100	72	1	130	119	12	123	137	-14	268	269	-4	228	227	-3	215	225
-13	110	114	2	336	336	14	484	484	-13	507	450	-3	229	212	-2	512	517
-12	225	239	3	92	82	16	53	35	-12	112	97	-2	67	51	-1	83	55
-11	358	345	4	338	334	12, 2, L			-11	116	87	-1	525	512	0	534	524
-10	110	120	5	29	13	-17	73	68	-10	159	168	0	257	248	1	582	616
-9	609	618	6	304	290	-16	236	231	-9	195	176	1	534	541	3	147	144
-8	185	187	7	42	59	-15	280	270	-7	997	982	2	355	360	4	425	440
-7	170	177	8	481	450	-14	48	36	-6	295	260	3	207	216	5	692	704
-6	229	207	10	97	111	-13	294	277	-5	107	111	4	60	56	6	752	751
-5	25	16	11, 9, L			-11	55	36	-4	489	511	5	82	76	7	871	859
-3	122	116	-6	66	33	-10	629	622	-2	1045	1061	6	442	438	8	104	79
-2	270	277	-5	98	84	-9	201	180	-1	342	341	8	77	67	10	75	66
-1	146	156	-4	216	203	-8	54	37	0	250	265	9	123	125	11	318	331
0	375	402	-3	294	287	-7	392	388	1	216	217	10	133	122	12	243	235
1	1258	1281	-2	106	111	-6	305	307	2	285	264	11	105	95	13	361	367
3	56	47	-1	434	441	-5	534	532	3	189	191	12, 8, L			14	79	75
4	41	18	0	165	183	-4	686	694	4	397	389	-8	314	331	15	107	106
5	257	258	1	198	184	-3	211	225	5	127	126	-7	228	247	16	235	220
6	451	445	2	441	444	-2	877	884	6	358	352	-6	84	71	13, 3, L		
7	181	173	3	210	207	-1	462	457	7	534	541	-5	380	383	-16	89	90
8	240	221	4	231	238	0	560	550	8	98	98	-3	52	63	-15	127	98
9	181	181	5	239	245	1	1144	1147	9	155	153	-2	196	211	-14	197	225
10	72	76	6	196	178	2	521	493	10	88	81	-1	404	392	-12	227	237
11	117	105	12, 0, L			3	78	63	11	227	217	0	218	231	-11	60	30
12	342	333	-16	150	155	4	492	496	12	191	183	1	131	120	-10	149	149
13	77	83	-14	409	415	5	1044	1079	13	275	258	2	239	230	-9	58	74
14	134	125	-12	189	185	6	343	337	14	62	65	8	394	386	-8	525	506
11, 7, L			-10	344	369	7	198	201	15	290	277	13, 1, L			-7	72	79
-9	318	288	-8	932	947	8	138	134	12, 6, L			-16	231	232	-6	156	172
-8	364	359	-6	1614	1613	9	224	229	-14	126	93	-15	90	92	-5	204	186
-7	481	479	-4	1226	1252	10	56	46	-13	264	268	-11	197	199	-4	666	659
-6	397	363	-2	223	205	11	106	106	-12	246	235	-10	53	7	-3	551	541
-5	127	131	0	327	296	12	190	178	-11	221	221	-9	253	267	-2	160	148
-4	111	120	2	39	27	13	148	152	-10	84	104	-8	102	112	-1	838	847
-3	466	477	4	411	380	16	163	160	-9	599	627	-7	62	59	0	53	60
-2	448	461	6	958	968				-7	316	326	-6	59	33	1	138	135

13, 3, L
2 159 168
3 115 111
4 351 362
5 654 664
6 490 466
7 196 209
8 169 177
9 208 178
10 301 294
12 172 158
13 82 82
14 76 76
15 168 145
16 105 107
13, 5, L
-15 198 197
-14 301 283
-13 122 113
-12 270 262
-11 201 217
-10 165 147
-9 106 76
-8 166 163
-7 153 160
-6 341 353
-5 112 93
-4 51 46
-3 798 806
-2 32 8
-1 344 330
0 265 251
1 401 397
2 390 390
3 569 559
4 194 185
5 288 291
6 192 191
7 402 400
8 412 418
10 412 407
11 246 256
12 69 68
13 161 161
14 231 235
13, 7, L
-9 270 258
-8 56 23
-7 97 114
-6 228 217
-5 342 340
-4 207 206
-3 262 241
-2 651 640
-1 99 99
0 328 311
1 156 134
2 355 357
3 111 118
4 456 456
5 183 177
6 268 273
7 63 73
8 153 157
13, 9, L
-4 127 137
-2 325 337
0 136 153
1 317 317
2 279 271
3 179 166
14, 0, L
-14 204 215
-12 589 609
-10 517 582
-8 41 13
-6 144 143
-4 372 347
-2 987 1007
0 815 827
2 1291 1319
4 372 387
6 1018 1024
8 390 412
10 422 421
14 85 86
16 91 81
14, 2, L
-16 88 65
-15 48 46
-14 193 199
-13 200 190
-12 127 88
-11 468 436
-10 567 533
-9 879 855
-8 319 332
-7 199 193
-6 457 474
-5 424 428
-4 788 784
-3 928 935
-2 482 461
-1 504 485
0 252 236
1 708 701
2 102 99
3 194 183
4 165 175
5 242 242
6 79 69
7 32 37
9 168 172
10 114 118
11 424 425
12 291 282
14 60 51
15 118 111
16 130 122
14, 4, L
-15 122 109
-13 237 234
-12 247 229
-11 524 493
-10 410 339
-8 203 205
-7 406 381
-6 623 597
-5 278 295
-4 272 256
-2 371 364
-1 897 910
0 221 193
1 97 101
2 94 104
3 555 557
4 159 180
5 206 202
6 176 191
7 178 177
9 291 287
10 139 157
11 302 284
12 167 164
13 107 94
15 136 130
14, 6, L
-13 136 159
-12 81 53
-10 274 278
-9 202 208
-8 385 366
-7 100 107
-6 82 83
-5 193 196
-3 570 597
-2 390 407
-1 160 169
2 100 96
3 192 189
4 65 69
5 342 336
7 190 167
8 78 82
9 258 257
10 93 80
14, 8, L
-6 269 280
-5 178 185
-4 88 100
-3 177 175
-2 72 67
-1 51 68
0 246 245
2 137 130
3 68 72
4 298 289
5 82 82
6 215 207
15, 1, L
-13 272 287
-12 375 364
-11 64 94
-10 203 203
-9 182 182
-8 188 196
-7 26 17
-6 285 290
-5 349 360
-4 88 102
-3 581 583
-2 78 91
-1 87 102
0 568 569
1 82 81
2 113 109
3 856 889
4 464 473
5 358 356
6 406 405
7 190 167
8 113 103
9 171 173
10 232 217
11 207 199
12 229 215
13 165 140
15 119 131
15, 3, L
-13 76 53
-12 143 143
-11 356 352
-10 67 82
-9 77 85
-7 278 281
-6 53 52
-5 123 113
-4 249 239
-3 41 51
-2 355 349
-1 258 259
0 289 281
1 640 655
2 957 957
3 142 144
4 145 134
5 485 489
6 409 414
7 145 158

15, 3, L		
8	231	221
9	205	211
11	342	321
13	150	156
14	131	125
15	107	114
15, 5, L		
-14	86	76
-13	87	55
-12	164	174
-11	302	294
-10	179	201
-9	446	435
-8	70	74
-7	571	568
-6	50	49
-5	147	121
-4	230	210
-2	232	235
-1	76	78
0	64	66
1	98	99
2	146	159
3	652	653
4	221	220
6	171	176
7	49	28
8	367	365
9	179	175
10	83	95
11	187	184
12	199	217
14	152	160
15, 7, L		
-8	84	60
-7	311	278
-6	440	424

-5	396	379
-4	72	47
-3	40	34
-2	302	313
-1	337	332
0	594	591
1	205	207
2	65	70
3	173	163
4	280	263
6	255	247
7	68	67
8	224	217
16, 0, L		
-14	178	201
-12	251	243
-10	421	440
-8	295	310
-6	659	664
-4	1312	1338
-2	1095	1105
0	576	570
2	736	733
8	477	493
14	128	115
16, 2, L		
-15	56	55
-14	259	247
-13	372	362
-11	68	65
-10	133	139
-9	213	208
-8	620	613
-7	631	605
-6	117	127
-5	412	403
-4	202	204
-3	396	406

-2	523	513
0	357	358
1	429	439
2	277	284
3	605	620
4	298	297
5	124	129
6	38	33
7	316	326
8	339	338
11	99	99
12	158	143
13	102	105
14	193	182
15	147	153
16, 4, L		
-14	75	50
-12	299	317
-11	528	466
-10	98	79
-8	80	93
-7	102	89
-5	846	835
-3	147	131
-2	261	257
-1	115	102
0	368	367
1	300	307
2	289	306
3	289	283
4	52	58
5	61	54
6	228	234
8	55	42
9	126	140
10	40	36
11	209	216
12	116	101

13	173	175
14	59	52
16, 6, L		
-13	61	63
-12	109	90
-11	157	188
-10	194	211
-9	160	156
-7	554	575
-6	138	126
-5	359	355
-4	357	337
-3	197	202
-2	137	140
-1	369	355
0	170	176
1	217	194
2	290	284
3	332	330
4	259	262
5	39	30
6	90	98
7	184	173
8	284	290
16, 8, L		
-5	254	277
-4	322	305
-3	292	288
-1	95	91
1	262	251
2	234	238
3	127	117
4	99	93
17, 1, L		
-14	288	286
-11	271	254
-10	50	38
-9	117	123

-8	250	240
-7	53	45
-6	52	50
-5	71	51
-4	161	161
-3	117	114
-2	223	216
-1	159	166
0	558	572
1	208	221
2	367	383
3	328	341
4	124	121
5	268	278
6	68	71
7	348	350
8	502	499
9	503	500
10	121	110
12	54	47
13	276	294
15	169	159
17, 3, L		
-15	218	250
-14	81	89
-13	174	147
-12	253	262
-11	66	55
-10	97	107
-8	240	225
-7	41	23
-6	407	394
-4	206	218
-3	145	144
-2	647	637
-1	48	39
0	136	135
1	659	680

2	265	266
3	86	88
4	329	341
5	187	189
6	69	64
7	636	648
8	232	217
9	129	139
10	138	141
12	167	175
17, 5, L		
-13	190	210
-12	225	238
-11	64	49
-10	86	93
-9	145	151
-8	134	120
-7	137	160
-6	94	80
-5	246	254
-3	87	76
-2	146	144
-1	611	610
0	174	170
1	300	296
3	249	251
4	359	376
5	261	268
6	210	201
7	101	105
8	33	31
9	214	210
10	398	416
12	192	194
17, 7, L		
-6	44	7
-5	240	243
-4	48	31

17, 7, L
-3 251 247
0 328 319
2 214 205
4 244 253
6 357 362
18, 0, L
-12 391 425
-10 579 600
-8 688 770
-6 111 134
-4 158 165
-2 415 394
0 428 453
2 521 521
4 415 429
6 44 57
8 576 586
10 149 173
12 304 311
18, 2, L
-12 232 227
-11 62 49
-10 110 77
-9 313 280
-8 382 352
-7 628 610
-6 345 358
-5 177 175
-4 322 318
-3 239 243
-2 447 449
-1 960 970
0 540 541
1 456 469
2 32 24
3 489 510
4 113 119

6 53 52
7 193 186
8 139 122
10 78 71
12 37 19
13 89 97
14 115 115
18, 4, L
-14 65 63
-13 140 127
-12 133 134
-11 64 61
-10 128 116
-9 574 534
-8 442 368
-7 139 122
-6 199 202
-5 142 128
-4 385 364
-3 353 358
-1 158 147
0 203 197
1 436 443
2 145 125
3 125 126
5 223 237
6 134 131
7 60 45
9 298 292
10 82 76
11 141 144
12 106 122
13 252 248
18, 6, L
-11 146 183
-10 88 65
-9 78 81
-8 202 219

-7 200 195
-6 353 332
-5 156 142
-4 33 30
-3 32 22
-2 59 50
-1 250 265
0 508 500
1 96 84
2 87 72
3 71 74
4 180 179
5 203 211
6 129 132
19, 1, L
-14 85 87
-12 118 117
-11 196 217
-10 268 261
-9 172 143
-8 232 227
-7 134 133
-4 177 180
-3 296 298
-2 144 131
-1 571 600
0 84 80
1 123 129
2 275 297
3 248 256
4 269 277
5 492 493
6 314 316
7 135 123
8 69 78
10 55 38
11 186 191
12 81 68

19, 3, L
-14 63 63
-12 84 85
-11 190 165
-10 288 292
-9 317 312
-8 185 195
-7 102 93
-6 153 152
-4 88 64
-3 336 329
-2 137 137
-1 167 167
0 30 6
2 292 298
3 458 471
4 374 378
5 61 57
6 113 119
7 268 264
8 225 231
9 156 168
10 155 149
11 66 71
12 105 113
13 197 183
19, 5, L
-10 205 193
-9 296 298
-8 68 82
-7 317 312
-6 98 88
-5 418 412
-4 129 123
-3 75 74
-1 137 144
0 325 322
2 173 179

3 205 205
4 144 149
5 383 394
6 281 291
8 257 260
10 138 135
19, 7, L
-3 97 86
-2 55 40
0 265 272
1 144 146
2 402 400
3 32 33
20, 0, L
-14 79 84
-12 196 216
-10 64 91
-8 334 344
-6 139 143
-4 587 593
-2 966 1003
0 617 619
2 258 257
4 373 362
6 166 173
8 50 47
12 90 88
20, 2, L
-12 180 170
-11 411 407
-10 98 110
-8 221 217
-7 179 172
-6 443 430
-5 592 566
-4 251 253
-3 145 144
-2 76 82

-1 122 134
0 218 231
1 146 137
3 94 85
4 180 178
5 319 331
6 140 136
8 130 127
9 94 109
10 229 233
11 109 124
13 109 104
20, 4, L
-12 81 55
-11 58 69
-10 207 225
-9 265 264
-8 184 158
-7 105 116
-5 50 42
-4 188 180
-3 565 550
-1 322 320
0 129 128
1 156 149
2 174 184
3 165 164
5 384 376
7 113 116
10 87 84
11 60 49
20, 6, L
-10 147 119
-9 115 135
-8 167 163
-7 33 39
-6 56 41
-5 495 501

20, 6, L		
-4	286	265
-3	88	86
-2	166	147
-1	88	80
1	232	224
2	292	291
3	147	139
4	206	206
5	95	92
6	216	227
21, 1, L		
-12	328	323
-11	104	102
-9	304	281
-8	143	133
-6	233	225
-5	88	85
-4	72	72
-3	173	165
-2	210	210
-1	116	115
0	71	77
1	319	331
2	163	169
3	43	48
4	183	198
5	35	27
6	51	41
7	184	196
9	231	249
10	366	382
11	185	184
21, 3, L		
-11	174	159
-10	92	104
-9	111	95
-6	117	101

-5	290	259
-4	318	311
-3	60	35
-2	307	319
-1	82	86
0	500	509
1	159	153
3	553	564
4	259	259
6	205	210
7	225	226
9	328	334
11	95	97
12	107	105
21, 5, L		
-11	234	242
-10	155	150
-9	68	63
-8	148	133
-7	81	85
-6	155	137
-5	193	201
-4	114	109
-3	113	123
-2	215	213
-1	64	59
0	98	103
1	225	234
2	112	112
3	91	94
4	133	143
5	165	175
6	274	297
7	185	193
8	65	50
9	104	113
10	59	60

22, 0, L		
-10	401	366
-8	397	406
-6	483	539
-4	188	187
0	567	559
2	374	400
4	151	157
6	104	121
8	87	109
10	245	257
12	100	76
22, 2, L		
-12	92	110
-11	76	73
-10	166	166
-7	287	254
-6	163	148
-5	436	432
-4	270	283
-3	51	45
-2	143	140
-1	124	137
0	183	185
1	394	404
2	388	391
3	323	340
4	69	70
5	175	183
6	145	144
8	81	72
9	227	231
10	173	159
22, 4, L		
-11	80	69
-10	89	91
-9	104	110
-8	36	21

-7	444	446
-6	197	159
-5	193	178
-4	81	85
-3	118	113
-2	162	161
-1	293	298
1	241	240
2	228	236
3	203	209
4	99	90
5	120	123
6	71	82
7	53	69
22, 6, L		
-9	180	205
-8	106	89
-7	125	133
-6	109	113
-4	291	306
-3	184	189
-1	73	22
0	106	112
1	159	176
2	367	387
3	202	210
5	116	129
6	109	117
23, 1, L		
-12	82	78
-10	128	124
-8	256	240
-7	214	187
-6	282	282
-5	70	67
-4	77	80
-3	83	81
-2	111	119

-1	338	344
1	242	255
2	160	153
3	32	20
4	30	38
5	154	152
6	189	192
7	284	299
8	77	89
11	124	127
23, 3, L		
-10	108	102
-9	251	219
-8	244	244
-7	136	144
-6	164	172
-5	177	166
-4	255	250
-3	116	109
-2	134	129
-1	251	254
0	147	139
1	284	275
2	85	83
3	70	67
4	137	139
5	323	333
6	155	158
8	157	161
9	71	66
10	132	131
23, 5, L		
-8	200	186
-7	304	303
-6	120	109
-5	250	266
-4	144	148
-3	226	236

-2	106	106
-1	49	44
1	79	79
2	206	232
3	46	46
4	170	179
5	89	89
7	101	108
8	173	182
24, 0, L		
-10	217	226
-8	192	186
-6	200	208
-2	259	261
0	381	408
2	167	164
4	181	166
6	245	247
8	214	217
10	163	169
24, 2, L		
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-8	109	124
-7	99	87
-6	227	226
-5	156	154
-4	228	220
-3	420	426
-2	240	251
-1	219	231
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4	80	77
5	127	128
6	143	134
7	53	59

24, 4, L
-9 72 75
-8 203 212
-6 112 105
-5 146 153
-3 46 39
-2 94 91
-1 240 254
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1 235 246
2 88 94
3 85 88
5 82 74
7 293 297
8 51 32
24, 6, L
-6 51 53
-5 105 121
-4 93 89
-3 243 274
-2 282 293
0 60 53
3 115 132
4 197 214
25, 1, L
-10 244 240
-9 85 75
-7 235 221
-6 148 135
-5 114 104
-4 184 176
-3 150 151
-2 104 99
-1 46 34
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2 101 101
3 221 224
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5 60 42
6 112 135
7 96 104
8 81 70
9 180 195
25, 3, L
-9 216 200
-7 140 126
-6 70 55
-3 254 239
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2 230 235
3 178 177
5 248 253
6 222 228
8 116 119
25, 5, L
-6 223 221
-4 65 65
-3 241 258
-2 95 104
-1 90 106
0 209 216
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2 59 59
3 106 123
4 115 125
5 73 84
26, 0, L
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-6 177 154
-4 376 390
0 187 195
2 373 372
4 171 185
8 104 86
26, 2, L
-8 81 81
-6 32 44
-5 174 165
-3 75 88
-2 117 130
0 51 44
2 92 84
3 160 167
4 192 196
5 265 282
6 92 102
7 103 112
26, 4, L
-5 273 286
-4 125 118
-3 161 169
-2 84 93
-1 136 137
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1 140 147
2 55 63
3 183 190
4 66 82
5 87 96
27, 1, L
-7 90 67
-6 183 177
-5 249 228
-4 168 162
-3 85 79
-2 107 112
-1 163 159
1 197 196
2 41 26
3 93 98
4 187 181
27, 3, L
-6 162 163
-5 102 111
-4 207 211
-3 202 189
-2 195 192
-1 84 81
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3 164 155
4 110 107
5 120 115
28, 0, L
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-2 160 151
0 145 152
2 129 149
28, 2, L
-4 149 154
-3 106 113
-2 93 89
-1 177 181
0 133 140
1 125 136
2 64 68
3 66 59
4 65 57
29, 1, L
-2 81 77
-1 61 59
0 109 102