X-RAY STUDIES OF SOME ORGANIC CRYSTAL STRUCTURES

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by

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Preface

The work described in this thesis was carried out in the chemical laboratories of Sussex University (1969-70) and Glasgow University (1970-72).

I wish to express my gratitude to my supervisor, Professor G. A. Sim, for his advice and encouragement during the three years of my research. I would also like to thank Dr. P. D. Cradwick for much helpful guidance, especially in connection with computing problems.

In conclusion, I am indebted to the medicinal section of Beecham Research Laboratories for financial support.

Summary

This thesis describes the crystal and molecular structures of a number of organic molecules. Both the heavy atom method and direct methods were used in the elucidation of these structures.

Three derivatives of 2-(6'-methoxy-2'-naphthyl)-1-methyl-5-oxocyclopentane-1-acetate have been examined and the structures determined. The alcohol derivative possesses oestrogenic activity and X-ray analysis has shown that this molecule contains both intramolecular and intermolecular hydrogen bonds between two hydroxyl groups. The intramolecular oxygen-oxygen distance can be regarded as completing a six-membered ring of the chair type. Configurations of the lactone and ether derivatives, suggested by I.R. and N.M.R. spectra, were shown by X-ray analysis to be incorrect. These molecules were in fact found to contain cyclohexane rings and not the expected cyclopentane rings. This is direct evidence of a Wittig reaction involving a novel rearrangement.

The structure of 9-methylanthracene was previously obtained from two-dimensional X-ray data by H. K. L. Verma, this structure has been completely redetermined using diffractometer data. Although the unit cell dimensions in this study and in the previous study were almost identical the packing of the molecules in the crystal is different. Either the four molecules of the unit cell are capable of packing in two different ways or the structure obtained from the limited two-dimensional data was incorrect. Preliminary crystal data of 9-methyltetracene have also been obtained.

An X-ray study of 6β-Trimethylammonio-penicillanic acid hemihydroiodide was undertaken to determine if a short, symmetrical hydrogen bond was present. It was found that the carboxyl groups of the two penicillin moieties in the Zwitter ion are linked by a short crystallographically symmetrical hydrogen bond with the oxygen-oxygen separation 2.46 Å.

The stereochemistries of three sesquiterpene-lactones, supplied by Werner Herz of Florida University, have been determined via non-centrosymmetric direct method procedures. Dihydromikanolide contains a highly strained carbocyclic ten-membered ring which adopts an unsymmetrical conformation. The two epoxide groups on this ring are in the anti-position and the stereochemistry at C(13) has been determined. The atoms C(15) and H(5) in miscandenin are syn to each other and the remaining stereochemistry of the molecule has been obtained. The configuration of the third sesquiterpene, berlandin, was uncertain and the stereochemistry of the molecule was completely unknown prior to X-ray analysis. These have been fully determined; the acyl side chains were found at C(8) and C(9).

The appendix contains the crystal and molecular structures of 17,20β,21-trihydroxypregn-4-en-3-one 17,21-p-bromophenylborate and N-2-(2,4-dimethyl-1-pyrrolidinyl)-ethyl-p-iodobenzene-sulphonamide. The data obtained for the former were limited, and although the stereochemistry of the molecule was determined high standard deviations were associated with the final results. The crystal structure of the iodobenzene-sulphonamide derivative may be disordered as very high temperature factors were associated with many of the atoms in this molecule.

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CHAPTER 1

SOME ASPECTS OF CRYSTAL STRUCTURE ANALYSIS

1.1 Introduction

The mathematical theory of crystal structure was known in the first half of the nineteenth century but the practical study of structure analysis only became possible after the discovery of X-rays by Röntgen in 1895. In 1912 von Laue suggested that X-rays might be diffracted by crystals, and in the same year Friedrich and Knipping obtained the first diffraction pattern. Thus it was shown that the wavelength of X-rays was of the same order of magnitude as the distances between atoms in a crystal lattice.

The Braggs developed the technique of structure analysis and showed that the concept of diffraction by a three-dimensional grating could be replaced by the concept of reflection of X-rays from crystal planes.

Initially the structures of simple inorganic salts were elucidated but progress with organic structures was slower owing to the scale of calculation involved. As crystallographic techniques improved and computers became available crystal structures of greater complexity were solved. At the present time the structuresof a number of proteins are known and as direct method procedures improve fairly complex molecules containing no heavy atom are being studied.

1.2 Measurement of structure amplitudes

The observed structure amplitude $|Fo_{(hkl)}|$ of the reflection (hkl) is related to the intensity $(I_{(hkl)})$ by the equation:

$$|Fo_{(hkl)}| = \sqrt{\frac{I_{(hkl)}}{L.p}} \qquad (1)$$

where

p = polarisation factor
L = Lorentz factor

The polarisation factor allows for the partial polarisation of the reflected beam and is given by

$$p = \frac{1 + \cos^2 2\theta}{2} \quad (hkl) \qquad (2)$$

The Lorentz factor allows for the varying angular velocities when reciprocal lattice points pass through the surface of the sphere of reflection and is dependent on the experimental technique used. For the equi-inclination Weissenberg geometry the correction is

$$L = \frac{\sin\theta}{\sin 2\theta \sqrt{\sin^2\theta - \sin^2\mu}} \qquad (3)$$

where μ is the equi-inclination angle (the angle between the incident beam and the plane normal to the rotation axis of the crystal). For diffractometers with normal beam geometry and for zero layer Weissenberg photographs the Lorentz factor is reduced to:

$$L = \frac{1}{\sin 2\theta} \qquad (4)$$

The initial structure amplitudes ($|F_{rel}|$) can be placed on an absolute scale by comparison with the calculated values ($|F_{calc}|$) during structure factor calculations.

Part of the incident X-ray beam will be absorbed by the crystal; the relationship between the intensities of the incident and emergent beam is given by

$$I = I_o . e^{-\mu t} \qquad (5)$$

where

I_o = the intensity of the incident beam
μ = the linear absorption coefficient
t = the path length of the X-ray beam in the crystal

Approximate correction for the effect is possible if the crystal dimensions are known.

The X-ray beam passing through a crystal may also be attenuated by primary and secondary extinction. Primary extinction is a consequence of multiple reflections between sets of crystal planes but the effect on the structure amplitudes, in general, is small and can normally be neglected. Secondary extinction arises for reflections of such intensity that an appreciable amount of the incident beam is reflected by the first planes encountered in the crystal leaving a less intense beam to reflect from deeper planes.

1.3 The structure factor

The structure factor, $F_{(hkl)}$, is a complex quantity defined as:

$$F_{(hkl)} = \sum_{j=1}^{n} f_j \exp\left\{2\pi i(hx_j + ky_j + lz_j)\right\} \qquad (6)$$

where

n = the total number of atoms in the unit cell
f_j = the atomic scattering factor of the j^{th} atom whose fractional co-ordinates are x_j, y_j, z_j)

$F_{(hkl)}$ may be represented by the structure amplitude $|F_{(hkl}|$ and a phase constant, α.

$$F_{(hkl)} = |F_{(hkl)}|. \exp i\alpha_{(hkl)} \qquad (7)$$

As the structure factor can be regarded as a complex number it may be expressed as:

$$F_{(hkl)} = A_{(hkl)} + iB_{(hkl)} \qquad (8)$$

and from equation (6) it follows that

$$A_{(hkl)} = \sum_{j=1}^{n} f_j \cos 2\pi(hx_j + ky_j + lz_j) \tag{9}$$

and

$$B_{(hkl)} = \sum_{j=1}^{n} f_j \sin 2\pi(hx_j + ky_j + lz_j) \tag{10}$$

Then

$$|F_{(hkl)}|^2 = A^2_{(hkl)} + B^2_{(hkl)} \tag{11}$$

and the phase constant is given by:

$$\alpha_{(hkl)} = \tan^{-1} \frac{B_{(hkl)}}{A_{(hkl)}} \tag{12}$$

For crystals where a centre of symmetry is present the sine terms of $B_{(hkl)}$ must sum to 0 and hence the phase angle must be 0 or π depending on the expression for $A_{(hkl)}$ being positive or negative.

1.4 The electron density distribution

The three-dimensional periodic electron density in a crystal may be represented by a three-dimensional Fourier series of the form:

$$\rho(x,y,z) = \frac{1}{V} \sum_{-\infty}^{\infty}{}_h \sum_{-\infty}^{\infty}{}_k \sum_{-\infty}^{\infty}{}_l F_{(hkl)} \exp\left\{-2\pi i(hx+ky+lz)\right\} \tag{13}$$

when Friedel's law holds i.e.

$$F_{(hkl)} = A_{(hkl)} + iB_{(hkl)} \tag{14}$$

and

$$F_{(\bar{h}\,\bar{k}\,\bar{l})} = A_{(hkl)} - iB_{(hkl)} \tag{15}$$

then a combination of the terms for (hkl) and $(\bar{h}\,\bar{k}\,\bar{l})$ gives the expression:

$$\rho(x,y,z) = \frac{1}{V} \sum_{-\infty}^{\infty}{}_h \sum_{-\infty}^{\infty}{}_k \sum_{o}^{\infty}{}_l \left[\left(A_{(hkl)}+iB_{(hkl)}\right)\exp\left\{-2\pi i(hx+ky+lz)\right\}\right.$$

$$\left. +\left(A_{(hkl)}-iB_{(hkl)}\right)\exp\left\{-2\pi i(-hz-ky-lz)\right\}\right] \tag{16}$$

i.e.

$$\rho(x,y,z) = \frac{2}{V} \sum_{-\infty}^{\infty}{}_h \sum_{-\infty}^{\infty}{}_k \sum_{o}^{\infty}{}_l \left\{ A_{(hkl)} \cos 2\pi(hx+ky+lz) + B_{(hkl)} \sin 2\pi(hx+ky+lz) \right\} \quad (17)$$

Thus the summation may be carried out over only half the reflections within the limiting sphere.

1.5 The phase problem

The structure amplitudes required for the Fourier series may be obtained experimentally from the diffracted beams but the relative phase angles cannot be measured directly. The methods most widely applicable to surmounting the phase problem are the heavy atom method and the so-called direct methods.

1.5.1. The Patterson function

The function defined by A. L. Patterson (1934; 1935) represents the vectors between atoms in a crystal structure. The coefficients of this Fourier series are $|F_{(hkl)}|^2$ which can be obtained directly from the measured intensities, independent of any phase calculation. The expression is defined as:

$$P_{(u,v,w)} = V \int_0^1 \int_0^1 \int_0^1 \rho_{(x,y,z)} \cdot \rho_{(x+u,y+v,z+w)} \, dx\,dy\,dz \quad (18)$$

where u, v and w are fractional co-ordinates.

If the electron density expressions are substituted into this equation and Friedel's law is obeyed then

$$P_{(u,v,w)} = \frac{1}{V} \sum_{-\infty}^{\infty}{}_h \sum_{-\infty}^{\infty}{}_k \sum_{-\infty}^{\infty}{}_l |F_{(hkl)}|^2 \exp\left\{2\pi i(hu+kv+lw)\right\} \quad (19)$$

which may be expressed as

$$P_{(u,v,w)} = \frac{2}{V} \sum_{-\infty}^{\infty}{}_h \sum_{-\infty}^{\infty}{}_k \sum_{o}^{\infty}{}_l |F_{(hkl)}|^2 \cos 2\pi(hu+kv+lw) \quad (20)$$

a centrosymmetric function.

For a unit cell containing N atoms a Patterson map will show N^2-N non-origin peaks. When the vector defined by (u,v,w) corresponds to two peaks in the electron density distribution the value $P_{(u,v,w)}$ will depend on the scattering power of the atoms involved. If a heavy atom is present this gives rise to high vector peaks which stand out against the background of overlapping smaller peaks, present due to lighter atoms in the structure. Hence the co-ordinates of the heavy atom may be determined.

1.5.2. The heavy atom method

If the position of the heavy atom can be found from the Patterson function a phase angle which will approximate to the phase angle of the complete structure may then be calculated for each structure amplitude. The electron density distribution may then be approximated by Fourier calculation using observed structure amplitudes and calculated phases. At this stage it is possible to derive the approximate positions of the light atoms present. Including the light atoms in the structure factor calculation improves the phase angles and refinement of atomic parameters is possible by least squares calculation.

The main disadvantage of this method is that the heavy atom contributes a major part to the structure amplitude and the accuracy of the remaining light atom positions is correspondingly diminished. Furthermore absorption errors become more significant the greater the scattering power of the heavy atom present.

1.5.3. Direct methods

The term 'direct methods' usually implies that class of methods where an attempt is made to derive the phases of the structure factors without postulating any atomic positions.

In 1948 Harper and Kasper first introduced this idea by examining inequality relationships between structure factors and Sayre in 1952 introduced the concept of probable relationships between phases of reflections. For a centrosymmetric structure the relationship between the reflection (H) and the phase S(H) is given by:

$$S(H + H') \approx S(H).\ S(H') \qquad (21)$$

This is known as the Sayre sign relationship which is normally significant only when $F_{(H)}$, $F_{(H')}$ and $F_{(H+H')}$ are all large.

Karle and Hauptman (1952; 1953; 1954) formulated a statistical treatment by introducing the normalised structure factor, $|E_H|$, given by

$$|E_H|^2 = \frac{|F_H|^2}{\varepsilon \sum_{j=1}^{n} f_j^{\,2}(H)} \qquad (22)$$

where ε is an integer which is normally unity but may assume other values for special sets of reflections in certain space groups.

The distribution of the $|E|$ values should be independent of the size and content of the unit cell but it is usually dependent on the presence or absence of a centre of symmetry.

Sayre's relationship (21) indicates that any two reflections with indices K and H-K when added together give a third reflection of index H, the phase of H being equal to the sum of the two phases φ_K and φ_{H-K}. It is possible that a number of pairs of reflections will combine in this way to give the phase of H. This is known as the Sigma two relationship and for large $|E|$ values in the centrosymmetric case:

$$S(E_H) \approx S(\sum E_K \cdot E_{H-K}) \qquad (23)$$

In the non-centrosymmetric case general phases are present and the $|E|$ values cannot all be assigned phases of 0 or π. However for large $|E|$ values the general phase relationship may be applied.

$$\varphi_H \approx \langle \varphi_K + \varphi_{H-K} \rangle \qquad (24)$$

By regarding each phase indication as a vector of length $|E_K \cdot E_{H-K}|$ and direction $(\varphi_K + \varphi_{H-K})$ they may be summed vectorially. This operation leads to the tangent formula:

$$\tan\varphi_H = \frac{\sum_K |E_K \cdot E_{H-K}| \sin(\varphi_K + \varphi_{H-K})}{\sum_K |E_K \cdot E_{H-K}| \cos(\varphi_K + \varphi_{H-K})} \qquad (25)$$

In practice for both centrosymmetric and non-centrosymmetric space groups three reflections with large $|E|$ values, which are associated with a large number of sigma two relationships, are normally chosen to define an origin.

For the centrosymmetric space group the origin fixing reflections may have phases which may be all 0 or π. If necessary a further small number of reflections may be assigned phases of 0 or π and together with the origin fixing reflections these will form the initial starting set for future phase determination.

For the non-centrosymmetric space group a reflection, other than the origin fixing reflections, is chosen to define the enantiomorph and a small number of reflections are given initial phase values before tangent formula iteration proceeds.

The application of direct methods enjoys most success for centrosymmetric space groups where the phases to be determined are 0 or π.

For non-centrosymmetric space groups where general phases are involved the failure of single phase relationships in the early stages of phase determination is more common. Occasionally only partial structure information is obtained but if the calculated structure factors, based on the partial structure, agree reasonably well with the observed amplitudes then the phases associated with other large $|E|$ values may be included in further tangent formula calculation. This recycling process may be repeated until all the atoms are located.

1.6. Least-squares refinement

The object of structure refinement is to minimise a function of the difference between the observed and calculated structure factors. The quantity normally minimised is

$$M = \sum_{hkl} w \left(|F_{(obs)}| - |F_{(calc)}|\right)^2 = \sum_{hkl} w \Delta^2 \qquad (26)$$

where the summation is over all the structure factors and w has a value representing the accuracy of the observation for each phase.

If $(p_1 \ldots\ldots p_n)$ are the initial n parameters obtained from an electron density calculation then for M to be a minimum

$$\frac{\partial M}{\partial p_j} = 0 \qquad (\text{where } j = 1 \ldots\ldots n) \qquad (27)$$

i.e.

$$\sum_{hkl} w\Delta \frac{\partial |F_{(calc)}|}{\partial p_j} = 0 \qquad (28)$$

The parameters are varied until these n conditions are satisfied (the trial set of p_j parameters being close to the correct values).

Expanding Δ as a first order Taylor series yields:

$$\Delta(\underset{\sim}{p} + \underset{\sim}{e}) = \Delta(\underset{\sim}{p}) - \sum_{j=1}^{n} e_j \frac{\partial |F_{(calc)}|}{\partial p_j} \qquad (29)$$

where $\underset{\sim}{p}$ and $\underset{\sim}{e}$ are the complete set of parameters and changes and e_j is is the small change in the parameter p_j. Combining the two above equations gives:

$$\sum_{i=1}^{n} \left\{ \sum_{hkl} w. \frac{\partial |F_{(calc)}|}{\partial p_i} . \frac{\partial |F_{(calc)}|}{\partial p_j} \right\} e_i = \sum_{hkl} w\Delta \frac{\partial |F_{(calc)}|}{\partial p_j} \quad (30)$$

These n equations are solved to obtain the shifts e_i. In matrix notation the normal equations become:

$$\sum_{i=1}^{n} a_{ij}. e_i = b_j \quad (31)$$

Here e_i is given by

$$e_i = \sum_{i=1}^{n} (a^{-1})_{ij}.b_j \quad (32)$$

where

$(a^{-1})_{ij}$ is the inverse matrix of a_{ij}.

Several cycles of structure refinement are necessary before convergence is obtained due to the limitation of the expansion of Δ as a first order Taylor series. The course of the refinement may be followed by considering the discrepency index:

$$R = \frac{\sum(|F_{(obs)}| - |F_{(calc)}|)}{\sum |F_{(obs)}|} \quad (33)$$

The accuracy of the final parameters may be obtained from their standard deviation (σ), where the variance $\sigma^2_{(pi)}$ of the parameter pi is given by

$$\sigma^2_{(pi)} = (a^{-1})_{ii}. \frac{\sum_{w\Delta^2}}{(m-n)} \quad (34)$$

where

m = the number of observations

n = the number of parameters

$(a^{-1})_{ii}$ = the diagonal element of the inverse matrix of the normal equations.

CHAPTER 2

TRACE DETERMINATION OF

A(S-MATRIX)-MATRIX

A-MATRIX-DIAGONALIZATION

METHODS

CHAPTER 2

THREE DERIVATIVES OF 2-(6'-METHOXY-2'-NAPHTHYL) - 1-METHYL-5-OXOCYCLOPENTANE-1-ACETATE

2.1 Introduction

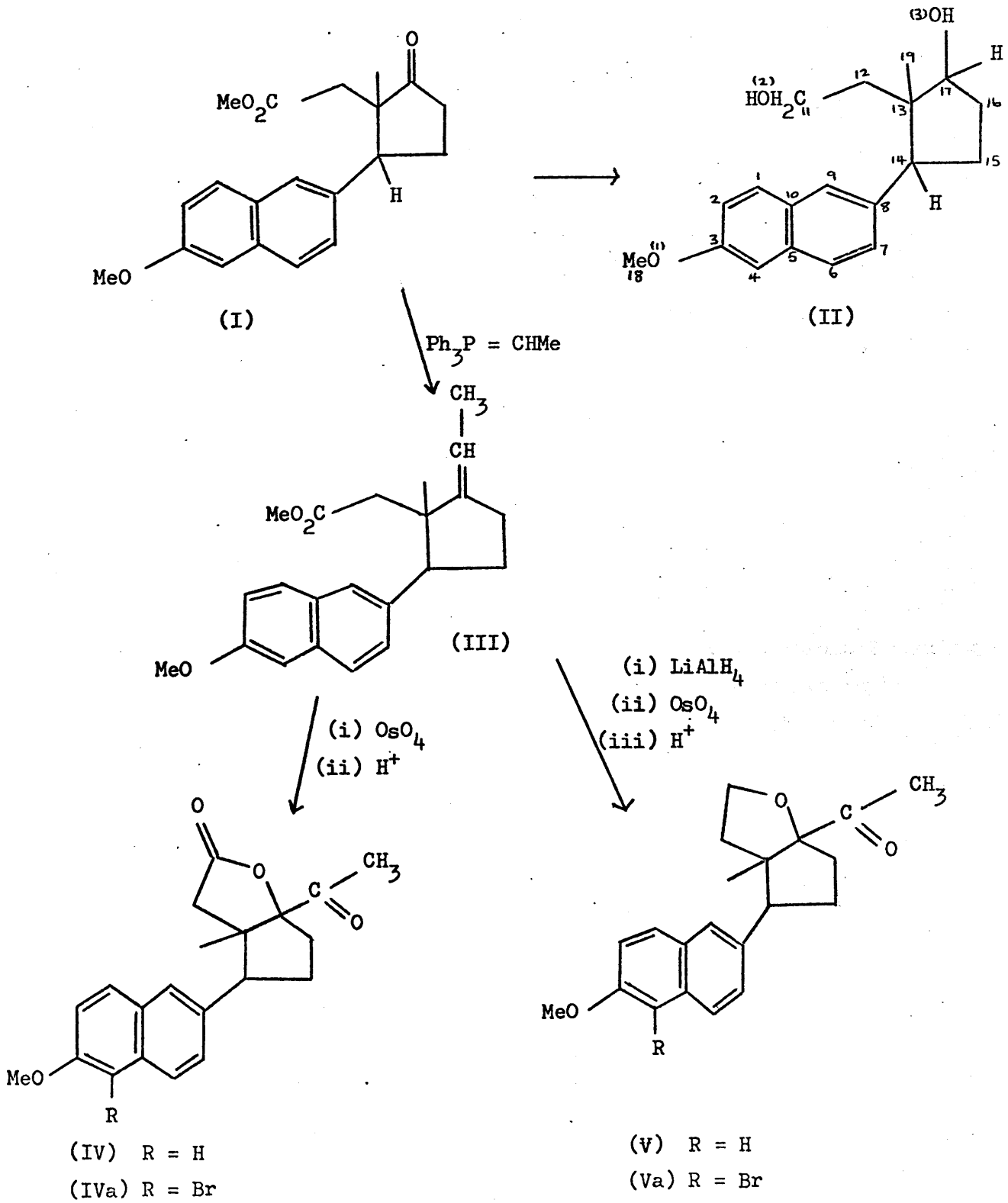
The importance of the biological functions of naturally occurring steroids,[1-3] e.g. cortisone, has been known for some time. During recent studies in the synthesis of secosteroids some disubstituted (methoxynaphthyl) cyclopentane derivatives[4] were prepared. The relative stereochemistries of these compounds were uncertain and the 2-(6'-methoxy-2'-naphthyl)-1-methyl-5-hydroxy-cyclopentane-1-ethanol (II) exhibited significant enough oestrogenic activity to warrant its conformational analysis by X-ray studies. /The names of the compounds in this chapter are those taken from the experimental section of the original paper, although for convenience, a steroidal numbering scheme has been used to present the crystallographic data./

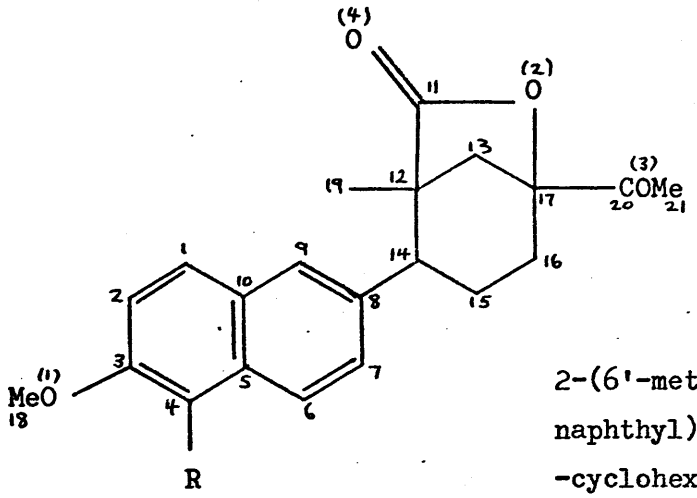
Further work in this field led to the reaction of 2-(6'-methoxy-2'-naphthyl)-1-methyl-5-oxocyclopentane-1-acetate (I) with five-fold excess of ethylidene triphenyl phosphorane. The product obtained was thought to be the ethylidene cyclopentane (III). Subsequent reaction of (III) with osmium tetroxide and triethylamine oxide peroxide, in tertiary butanol, gave a crystalline solid proposed as the 2-(6'-methoxy-2'-naphthyl)-1-methyl-4-carboxymethyl-cyclopentane-1,5-lactone (IV). Reduction of (III) with lithium aluminium hydride, followed by oxidation with osmium tetroxide, triethylamine oxide peroxide and acid cyclization was thought to give the 2-(6'-methoxy-2'-naphthyl)-1-methyl-4-carboxymethyl-cyclopentane-1,5-ether (V).

Compound (IV) was assigned a β-orientated side chain from I.R. and N.M.R. spectra whilst the side chain configuration of (V) was uncertain. Crystals of compounds thought to be (II), (IVa) and (Va) were supplied by Dr. A. W. Lake of Beecham Medical Research Centre, Harlow, Essex, for

X-ray analysis. The analysis showed that the compounds were not the expected cyclopentane derivatives but the cyclohexane derivatives (VIa) and (VIIa), whereas the configuration of (II) was verified.

Proposed reaction paths

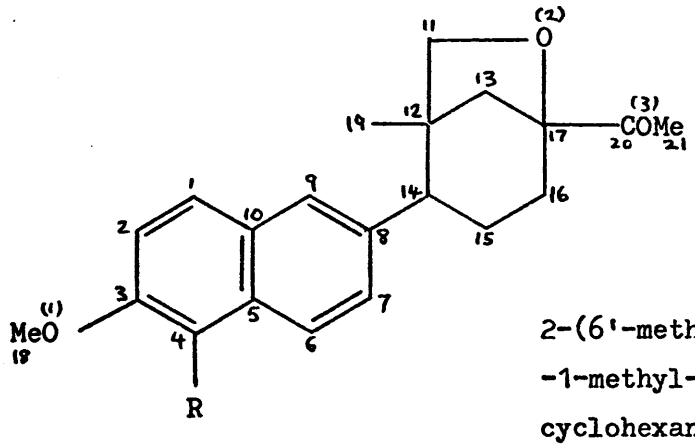




2-(6'-methoxy - 5'-bromo-2'-naphthyl)-1-methyl-5-carboxymethyl -cyclohexane-1,6,5-lactone.

(VI) R = H

(VIa) R = Br



2-(6'-methoxy-5'-bromo-2'-naphthyl) -1-methyl-5-carboxymethyl- cyclohexane-1,6,5-ether.

(VII) R = H

(VIIa) R = Br

2. 2.1 Experimental

Crystal data

2-(6'-methoxy-2'-naphthyl)-1-methyl-5-hydroxy-cyclopentane-1-ethanol.

Molecular formula	$C_{19}H_{24}O_3$
Molecular weight	300.4 a.m.u
Crystal system	monoclinic
Space group	$P2_1/c$ (C_{2h}^5)
Cell dimensions	$\underline{a}$ = 17.010(10)Å
	$\underline{b}$ = 7.264(5) Å
	$\underline{c}$ = 13.368(7) Å
	$\underline{\beta}$ = 93.52(4)°
Cell volume (u)	1656.5 $Å^3$
Density (observed)	1.19 $g.cm^{-3}$
Density (calculated)	1.20 $g.cm^{-3}$
Molecules per unit cell (Z)	4
Number of electrons per unit cell ($F_{(000)}$)	648
Linear absorption coefficient, μ(MoKα)	0.87 cm^{-1}

The crystal used in the analysis was a thick colourless plate which extinguished under polarising light. Weissenberg and precession photographs of the crystal were taken with CuKα radiation and MoKα radiation respectively, and the space group was determined as $P2_1/c$. The systematically absent reflections are h0l when l = 2n+1, and 0k0 when k = 2n+1; the preliminary cell dimensions were then obtained. The observed density was in close agreement with the calculated density giving the number of molecules in the unit cell as 4.

The crystal was transferred to a Hilger and Watts' Y290 four-circle PDP-8 computer controlled diffractometer and an initial orientation matrix was defined using the angular settings of two strong, low order reflections. The crystal was then positioned in an arbitary orientation with respect to the ϕ axis to reduce the possibility of multiple reflections.[5] This was achieved by offsetting the crystal by about -8° on the χ axis which also ensured χ values of less than 90° during data collection.

The initial matrix was redetermined and, with the preliminary photographic cell dimensions, was used to locate several other reflections with high θ values (15°-20°). The angular settings of two of these reflections were accurately determined by 2θ,χ and ϕ scans and used to define a better orientation matrix. The optimum angular settings of twelve reflections with θ values of 15-20° were then determined and the 2θ, χ and ϕ values of these reflections were adjusted together with the preliminary cell dimensions by least squares.[6] The orientation matrix determined was used to locate all the reflections in the automatic data collection.

The intensity data were collected by the θ-2θ scan procedure, each reflection being scanned by 60 steps of 0.01°. Each step was counted for 1 second, and at the start and end of each scan a stationary crystal-stationary counter background count was taken for 15 seconds. MoKα radiation with a Zr-filter was used and the stabilised X-ray generator was operated at 46 kV and 16 mA. The intensities of two strong standard reflections were measured after every 40 reflections to ensure that all the reflections could be placed on a common scale. The reflections of the

octants hkl and $hk\bar{l}$ were collected out to $\theta \leqslant 27^{o}$.

The integrated intensity (I) of each reflection was obtained from the scan count (P) and the background counts (B1, B2) by I = P-2(B1 + B2). The values of I were corrected for Lorentz and polarisation effects but absorption effects were neglected. A total of 3563 independent structure amplitudes was obtained, of which 2011 had $I > 3\sigma(I)$.

2 2.2 Structure analysis

Normalised structure factors (E's) were calculated for all the structure amplitudes based on an overall temperature factor of 4.5 $\mathring{A}^2$. This gave 251 E values above 1.80 which were used to calculate phases from Sigma two relationships after a suitable origin[7] had been defined (Table 1). The program used was a modified version of the 'Phase' program[8] adapted for the KDF9 computer. An initial E map showed 16 atoms including the naphthalene ring, but the remaining atoms were not clearly defined owing to the presence of a number of spurious peaks on the map. A structure-factor calculation with the sixteen atoms as carbons gave R = 0.557. A Fourier map computed at this stage revealed 5 more atoms and 2 cycles of least-squares calculation lowered R to 0.290. The missing atom was located from a difference Fourier synthesis. The three oxygens and nineteen carbons were refined isotropically to R = 0.220. Reflections for which $I \leqslant 3\sigma$ (where $\sigma = \sqrt{P + 4(B1 + B2)}^{\frac{1}{2}}$) were now regarded as 'unobserved' and removed from further calculations. The remaining 2011 reflections were used to refine the atoms isotropically to 0.168. The atoms were then allowed to refine with anisotropic temperature factors and R fell to 0.148. A Fourier difference map using data with $\sin\theta/\lambda < 0.5$ showed all the hydrogen positions but the hydroxyl and methyl hydrogens were less well defined at this stage. The R value

Table 1

(a) Origin determining reflections

Reflection	Parity	Phase	E
15 1 4	U U G	0	4.06
10 1 8	G U G	0	3.70
6 2 -3	G G U	0	3.43

(b) E statistics

Average values of	$\|E\|$	$\|E^2\|$	$\|E^2-1\|$
Found	0.733	0.959	0.954
Theoretical for centric	0.798	1.000	0.968
Theoretical for acentric	0.886	1.000	0.736

Percentage of values for:	$E > 1.0$,	$E > 2.0$,	$E > 3.0$
Found	27.56	4.53	0.40
Theoretical for centric	31.73	4.55	0.27
Theoretical for acentric	36.79	1.83	0.01

fell to 0.123 when the located hydrogens were included in the least squares as fixed atom contributors. The isotropic temperature factors of the hydrogens were set equal to those of the carbon atoms to which they were attached. Five reflections with large $F_{(obs)}$ values appeared to be affected by extinction, and when these reflections were removed from the calculations a further cycle of least-squares adjustment lowered R to 0.079. The hydrogens, except H(02) which was associated with a very small peak, were then allowed to refine isotropically. The final R value was 0.077; as $1/\Sigma\Delta w^2$ was approximately constant over various ranges of $F_{(obs)}$ and $\sin\theta$ the initial unit weighting scheme (w=1) was used throughout. The atomic scattering factors of Hanson et al[9] were employed.

The computing was carried out on the KDF9 computer at Glasgow University and the Univac 1108 computer at the National Engineering Laboratory, East Kilbride.

2.3.1 Experimental

Crystal data

2-(6'-methoxy-5'-bromo-2'-naphthyl)-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-lactone.

Molecular formula	$C_{21}H_{21}O_4Br$
Molecular weight	417.3 a.m.u.
Crystal system	triclinic
Space group	$P_{\bar{1}}$ (C_i^1)
Cell dimensions	$\underline{a}$ = 12.056(5) Å
	$\underline{b}$ = 13.026(5) Å
	$\underline{c}$ = 7.595(3) Å
	$\underline{\alpha}$ = 90.38(3)°
	$\underline{\beta}$ = 106.07(3)°
	$\underline{\gamma}$ = 124.42(3)°
Cell volume (u)	925.3 Å^3

Density (observed)	1.51 $g.cm^{-3}$
Density (calculated)	1.50 $g.cm^{-3}$
Molecules per unit cell (Z)	2
Number of electrons per unit cell ($F_{(000)}$)	428
Linear absorption coefficient, $\mu(CuK\alpha)$	35.43 cm^{-1}
Linear absorption coefficient, $\mu(MoK\alpha)$	23.86 cm^{-1}

Oscillation and Weissenberg photographs showed that the crystal system of this compound was triclinic and the initial cell dimensions were determined from precession photographs. Diffractometer data were collected using $CuK\alpha$ radiation and a fairly large, colourless crystal (cross-section ~ 0.5 sq.mm.) was employed. The position of the bromine atom was found from a Patterson synthesis and the remaining atoms (except hydrogens) were located by a subsequent Fourier calculation. However, as refinement converged at R = 0.145 it was decided to recollect the data using a smaller crystal (cross-section 0.30 x 0.14 mm and 0.50 mm long) with $MoK\alpha$ radiation. This would effectively lessen the absorption of radiation by the crystal.

The small crystal was transferred to the Hilger and Watts Y290 four-circle PDP-8 computer controlled diffractometer and an orientation matrix calculated as previously described. Each reflection was scanned by 72 steps of 0.01°. Each step of the scan was counted for 1 second and at the start and end of each scan a stationary crystal-stationary counter background count was taken for 18 seconds. The reflections of the octants hkl, $hk\bar{l}$, $h\bar{k}l$ and $h\bar{k}\bar{l}$ were collected out to $\theta \leq 28^{\circ}$. Only those reflections with $I \leq 3\sigma(I)$ were regarded as significantly above background. The 2928 independent reflections were corrected for Lorentz and polarisation effects but absorption corrections were neglected.

2.3.2 Structure Analysis

The atomic co-ordinates of the bromine, oxygen and carbons atoms were taken as previously defined by the CuKα radiation data. Allowing the atoms to refine isotropically gave a R value of 0.155. The bromine atom was then allowed an anisotropic temperature factor and one cycle of least-squares calculations lowered R to 0.086. With all atoms being refined anisotropically an R value of 0.065 was obtained and a difference Fourier synthesis showed all the hydrogen positions. The hydrogen atoms were allowed to refine isotropically and the calculations converged to a final R value of 0.055. The anomalous dispersion corrections for bromine with MoKα radiation were obtained from "International Tables".(10)

The computing was carried out on the ICL 1905E computer at Sussex University, the KDF9 computer at Glasgow University and the Univac 1108 computer at the National Engineering Laboratory, East Kilbride.

2.4.1 Experimental

Crystal data

2-(6'-methoxy-5'-bromo-2'-naphthyl)-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-ether.

Molecular formula	$C_{21}H_{23}O_3Br$
Molecular weight	403.3 a.m.u.
Crystal system	triclinic
Space group	$P_{\bar{1}}$ (C_i^1)

Cell dimensions	$\underline{a}$ = 12.076(6) Å
	$\underline{b}$ = 13.090(5) Å
	$\underline{c}$ = 7.490(3) Å
	$\underline{\alpha}$ = 92.65(5)°
	$\underline{\beta}$ = 104.90(5)°
	$\underline{\gamma}$ = 124.55(5)°
Cell volume (u)	914.5 Å^3
Density (observed)	1.45 g.cm^{-3}
Density (calculated)	1.46 g.cm^{-3}
Molecules per unit cell (Z)	2
Number of electrons per unit cell ($F_{(000)}$)	416
Linear absorption coefficient, μ(MoKα)	24.01 cm^{-1}

Oscillation and Weissenberg photographs showed that the crystal system was triclinic and the initial cell dimensions were determined from precession photographs.

The crystal was transferred to a Hilger and Watts Y290 four circle PDP-8 computer-controlled diffractometer and an orientation matrix was calculated. The reflections were scanned by 72 steps of 0.01°. Each step of the scan was counted for 1 second and at the start and end of each scan a stationary crystal-stationary counter background count was taken for 18 seconds. The reflections of the octants hkl, $hk\bar{l}$, $h\bar{k}l$, and $h\bar{k}\bar{l}$ were collected out to $\theta \leq 28^\circ$. Only those reflections for which $I \geq 2.5\sigma(I)$ were accepted as significantly above background. After correcting for Lorentz and polarisation effects, but not absorption, a total of 2006 independent structure amplitudes was obtained.

2 4.2. Structure Analysis

The co-ordinates of the bromine atom were found from a Patterson synthesis and a structure factor calculation based on these co-ordinates gave R = 0.510. A Fourier synthesis at this stage showed all the remaining atoms and 3 cycles of least-squares calculations lowered the R-factor to 0.128. All atoms were then allowed to refine anisotropically and the final R value obtained was 0.091. The hydrogen positions on a difference Fourier were not clearly defined and therefore these atoms were not included in the structure factor calculations. Unit weights were applied to all least-squares calculations.

The computing was carried out on the ICL 1905E computer at Sussex University.

2.5. Discussion

The molecular structures illustrated in Figures 1, 2 and 3 show that the configuration of the alcohol is verified and that the lactone and the ether contain heterocyclic bicyclo (3,2,1) octane systems. Figures 4, 5 and 6 show the molecular packing of the 3 molecules; the dotted lines in Figure 4 indicate hydrogen bonding. The tables of results (MoKα collected data) for the three compounds are listed. The final co-ordinates, with their standard deviations and thermal parameters for the alcohol, lactone and ether are listed in tables 3 and 4, 5 and 6, and 7 and 8 respectively. Similarly the bond lengths and valency angles are listed in tables 9 and 10, 11 and 12 and 13 and 14. The hydrogen atoms are numbered according to the carbon atoms to which they are attached. Table 11 for the lactone also lists the bond lengths

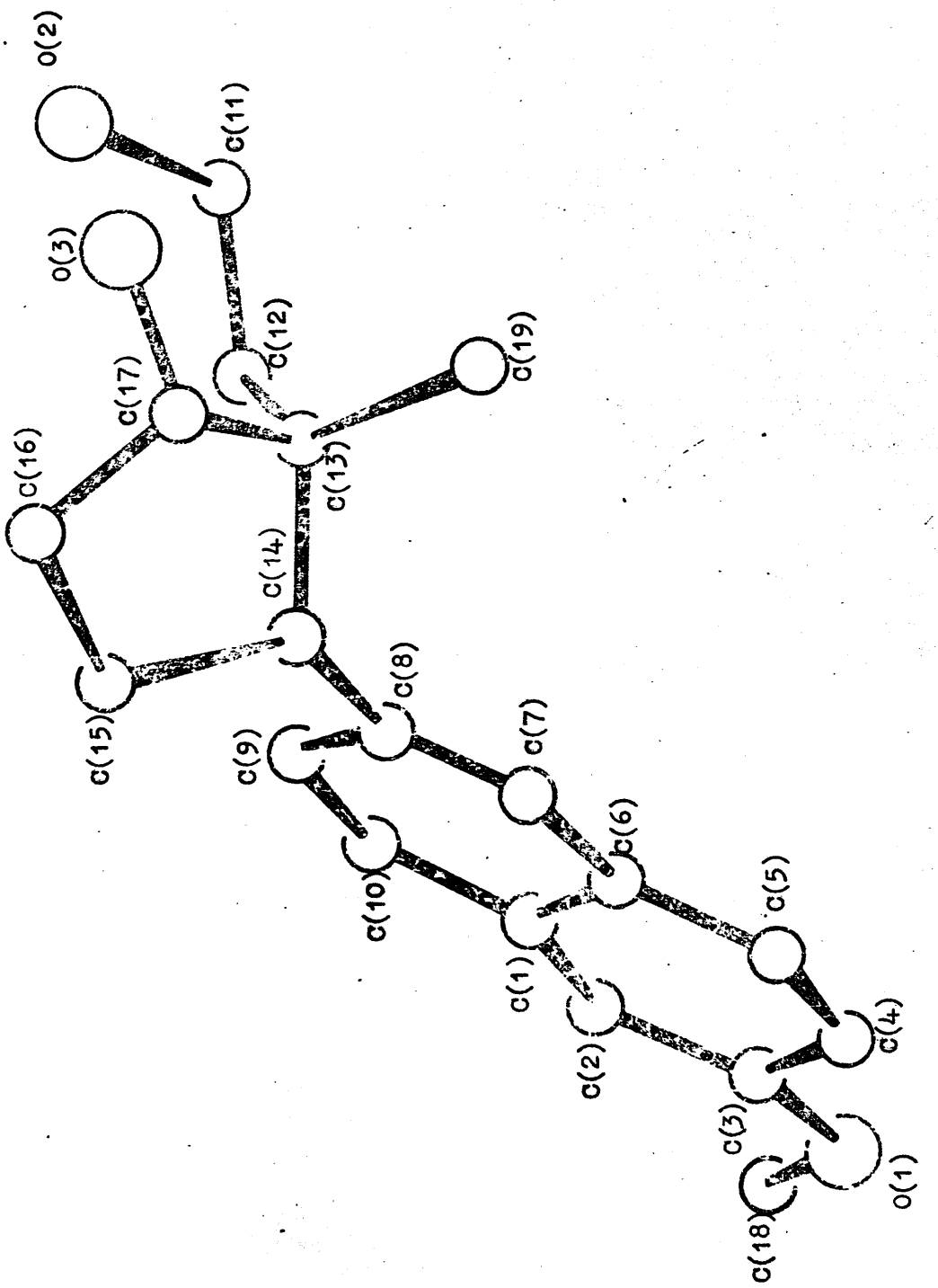


Fig. 1 A general view of the alcohol molecule.

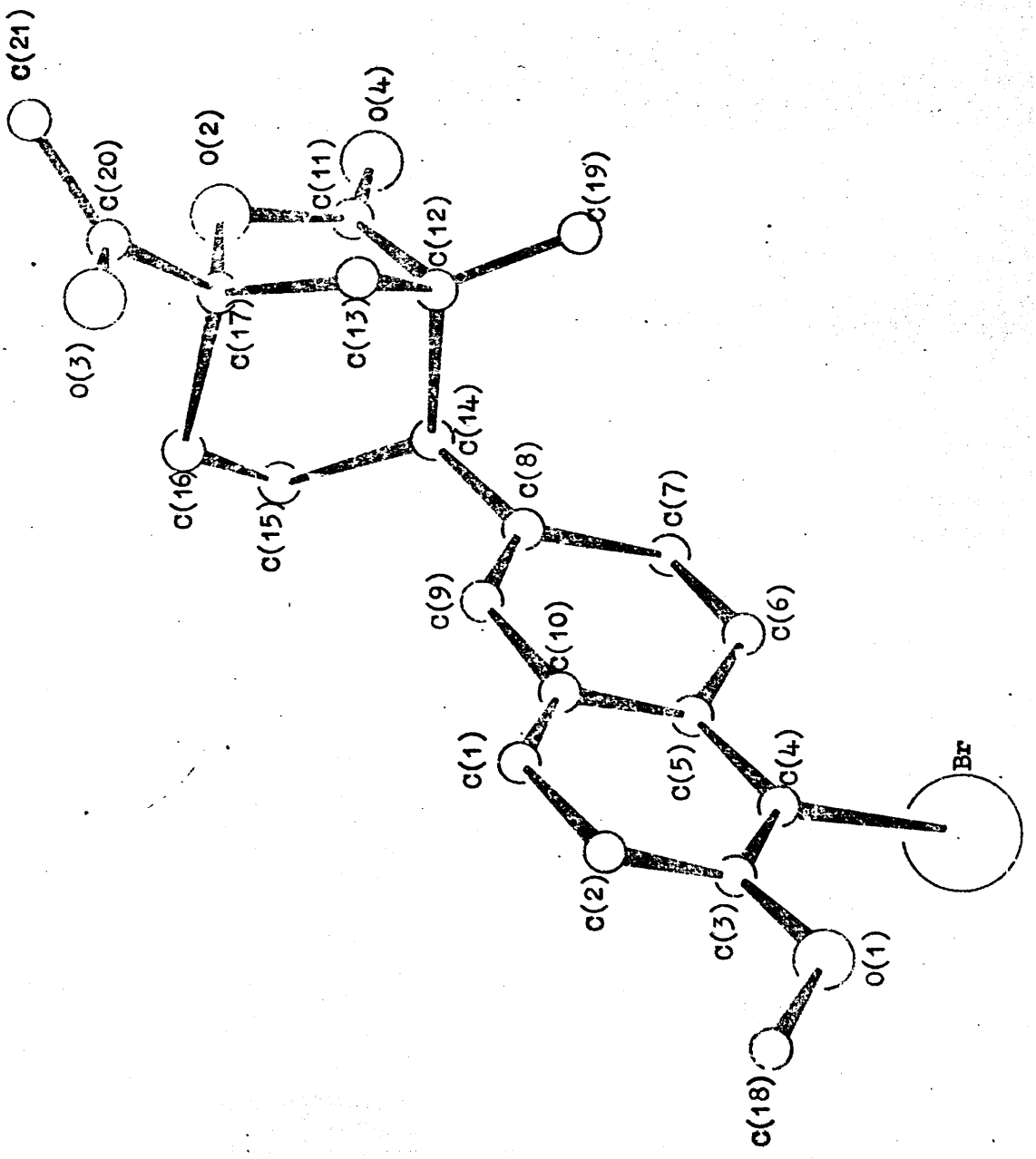


Fig. 2 A general view of the lactone molecule.

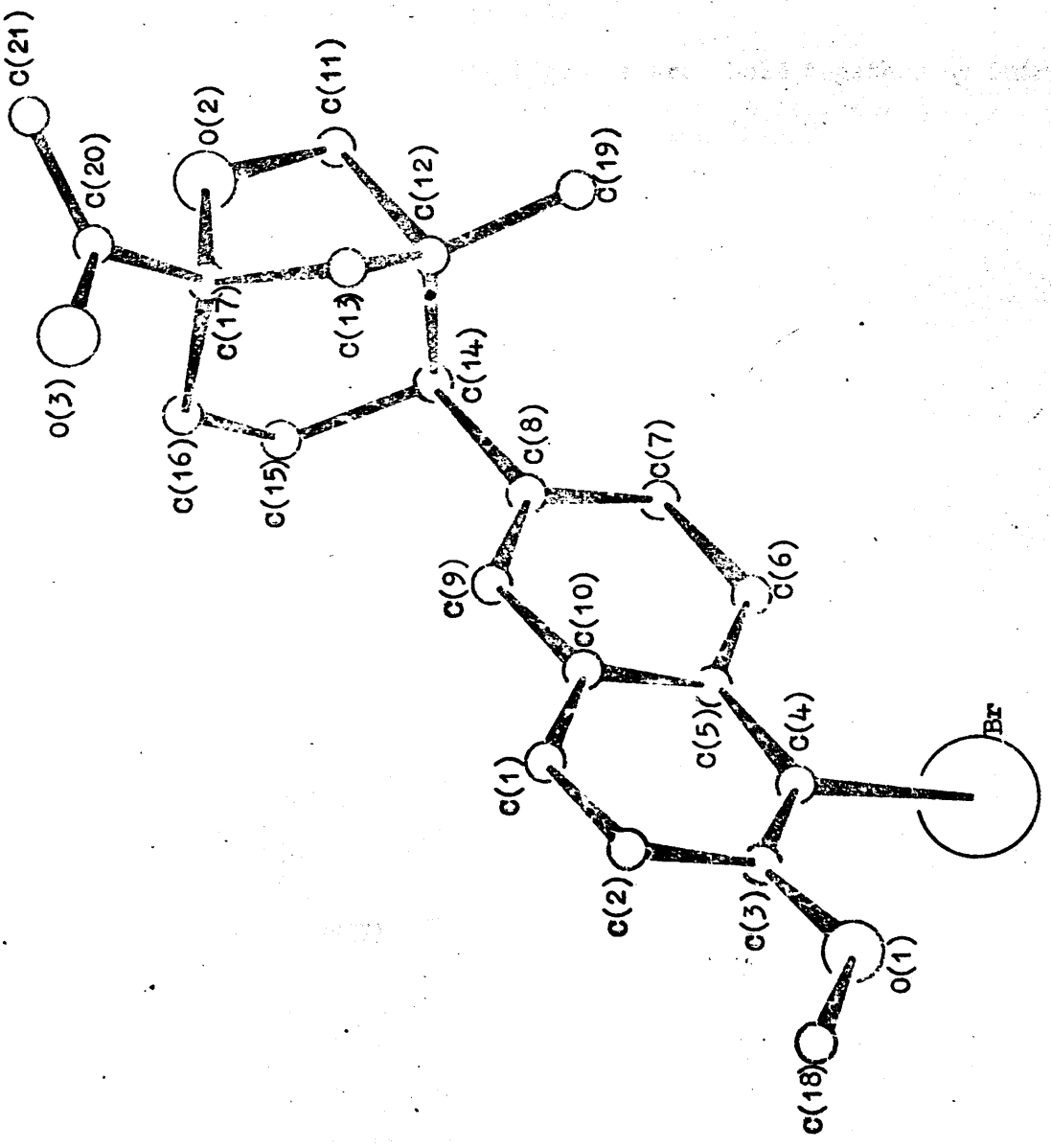


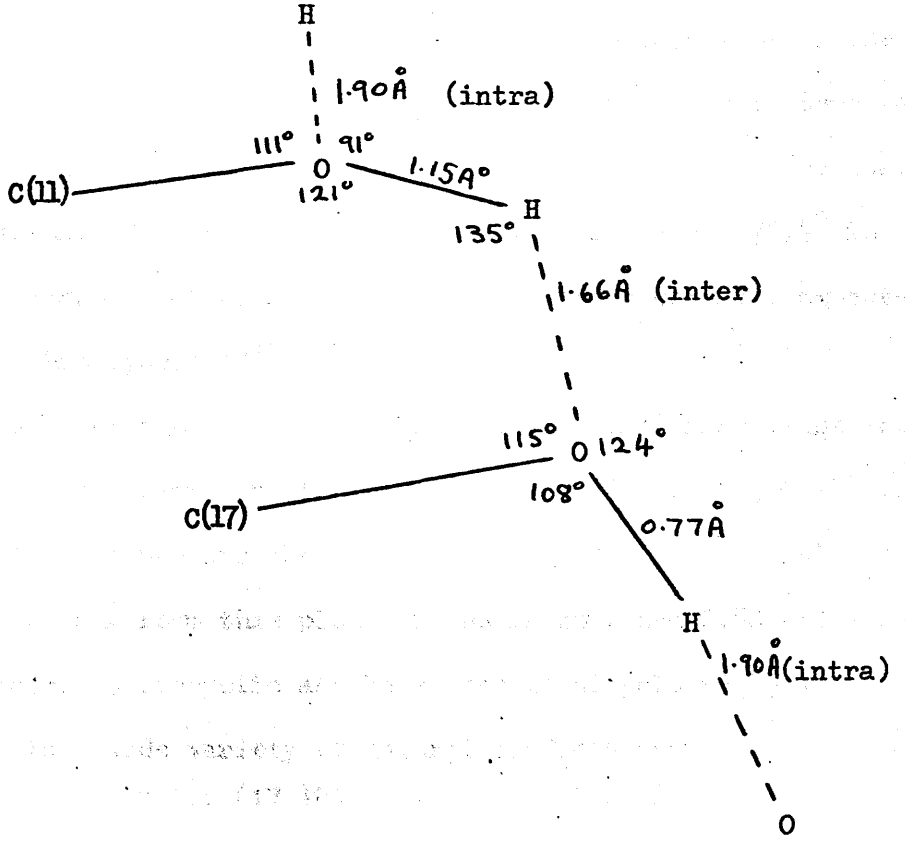
Fig.3 A general view of the ether molecule.

obtained using CuKα radiation and shows that these distances are associated with large standard deviations. The torsion angles and mean plane calculations are listed in table 15 and 16, 17 and 18, and 19 and 20 for the three compounds. Tables 21, 22 and 23 list the intermolecular contacts of less than 4 Å.

In the alcohol both hydroxyl groups are held together by intramolecular and intermolecular hydrogen bonding (Fig.7).

Fig. 7.

The hydrogen bonding of the alcohol



The intramolecular O(2)....O(3) distance is 2.597(5) Å and the intermolecular separation is 2.667(7) Å. The intramolecular O(2)....O(3) distance can be regarded as completing a six-membered ring of the chair type. Intramolecular and intermolecular hydrogen bonding is also found in salicylic acid[11,12] here the intramolecular O....O distance is 2.590 Å and the intermolecular distance is 2.627 Å. In salicylic acid the intramolecular hydrogen bonding forms a planar six-membered ring with the hydrogen as the sixth atom, a similar situation has recently been studied by neutron diffraction in the acid salt potassium tri-hydrogen di-malonate.[13] The O....O contact in potassium hydrogen chloromaleate forms[14] one side of a planar six-membered ring where the O - H•••O angle is 175.4°. For the alcohol this angle is 135° but here the preferential conformation of the atoms O(2), C(11), C(12), C(13), C(17) and O(3) is of the chair type and as such the position of the hydrogen is influenced by the stereochemistry of the system. The intramolecular O - H•••O angle of 175.4° in potassium hydrogen chloromaleate is of the order normally expected for angles of this type.[15,16]

The lactone and the ether both contain cyclohexane rings which adopt distorted chair conformations. Atoms C(12), C(14), C(16) and C(17) are closely coplanar and the atoms C(13) and C(15) are displaced by 0.88 and -0.48 Å from this plane in the lactone and 0.88 and -0.51 Å in the ether. Carbocyclic and heterocyclic bicyclo (3,2,1) octanes are found in a wide variety of natural products and a number of the available X-ray results[17,18] show that the displacement of the unique

bridging atom from the plane defined by atoms equivalent to C(12), C(14), C(16) and C(17) invariably exceeds the value of 0.73 Å appropriate to an ideal cyclohexane ring. For example the displacement of the bridging atom in Acety(bromoacetyl) dihydroenmein[19] is 0.90 Å and in verrucarin A p-iodobenzene sulphonate[20,21] 0.79 Å. The distortion of the cyclohexane ring is also apparent in the torsion angles of the ring; the average value of the angles C(13) - C(12) - C(14) - C(15) and C(13) - C(17) - C(16) - C(15) is 58°, that of the angles C(14) - C(12) - C(13) - C(17) and C(16) - C(17) - C(13) - C(12) is 73°, and that of the angles C(12) - C(14) - C(15) - C(16) and C(14) - C(15) - C(16) - C(17) is only 38°. The bridging valency angle C(12) - C(13) - C(17) is notably smaller than tetrahedral, 99.6 ± 0.7° in the lactone and 98.9 ± 1.4° in the ether. In bicyclo[2,2,1] heptanes the bridging angle is approximately 95°, e.g. 96° in norbornane,[22] 93° in 1,4-dichloronorbonane[22] and 95° in (+)-10-bromo-2-chloro-2-nitrosocamphane.[23] For the bicyclo [3,3,1]nonanes it is around the tetrahedral value, e.g. 112° in 2-chlorobicyclo[3,3,1]nonan-9-one[24] and 111° in 1-p-bromobenzenesulphonyl-oxymethyl-5-methyl bicyclo[3,3,1]nonan-9-ol.[25] The lactone ring approximates closely to an envelope configuration which is evident in the torsion angles of the ring and the C(13) atom is displaced from the plane containing O(2), C(11), C(12) and C(17) by -0.65 Å. Similarly the ether ring approximates to the envelope conformation with C(13) displaced by 0.74 Å. The lactone ring valency angles range from 99.6° to 109.8° with an average value of 104.3°, in the ether ring the similar angles range from 98.9° to 107.3° with an average of 103.1°, in both cases the values indicate the substantial deviation from planarity.

The cyclopentane ring in the alcohol also exhibits an envelope conformation with the out-of-plane atom C(13) displaced by 0.69 Å from the mean plane through atoms C(14), C(15), C(16) and C(17). The cyclopentane valency angles range from 97.2° to 107.0° with a mean of 104.1°, values again consistent with the substantial deviation from planarity of the ring.

The $C(sp^3)$ - $C(sp^3)$ bonds in the alcohol, lactone and ether have the same mean value of 1.54 Å. In the alcohol the $C(sp^3)$ - $C(sp^3)$ bonds range from 1.509 Å to 1.593 Å; the lengths of the bonds appear to be related to the number of hydrogen substituents on the bonds, which suggests steric effects. The bonds C(13) - C(14) and C(13) - C(17) have only one hydrogen atom and are 1.593 Å and 1.556 Å, C(13) - C(12) has only two hydrogen atoms and is 1.553 Å, while those bonds with three or four hydrogens range from 1.509 Å - 1.539 Å. Similar trends have been noticed in other molecules[26] e.g. in methyl melaleucate iodo-acetate[27] $C(sp^3)$ - $C(sp^3)$ bond lengths range up to 1.66 Å. In the lactone and ether the pattern is not so clear as the standard deviations are larger than those for the alcohol.

The bonds in the naphthalene residues have lengths very similar to naphthalene[28] itself and to perylene.[29] A comparison of average lengths of equivalent bonds in these molecules is given in table 2. The angle C(4) - C(5) - C(6) in both the lactone (125.1°) and ether (125.5°) is significantly larger than the angle C(1) - C(10) - C(9) in these molecules (121.8° and 122.2°) but the effect does not occur in the alcohol. Also, the angle Br-C(4)-C(3) exceeds the angle Br-C(4)-C(5) in both the lactone and ether and it is clear that there is a pronounced repulsion between the bromine substituent on C(4) and the hydrogen on C(6) leading to an in-plane displacement of the peri-bonds. The

Fig. 4

The crystal structure of the alcohol viewed on the ac plane.

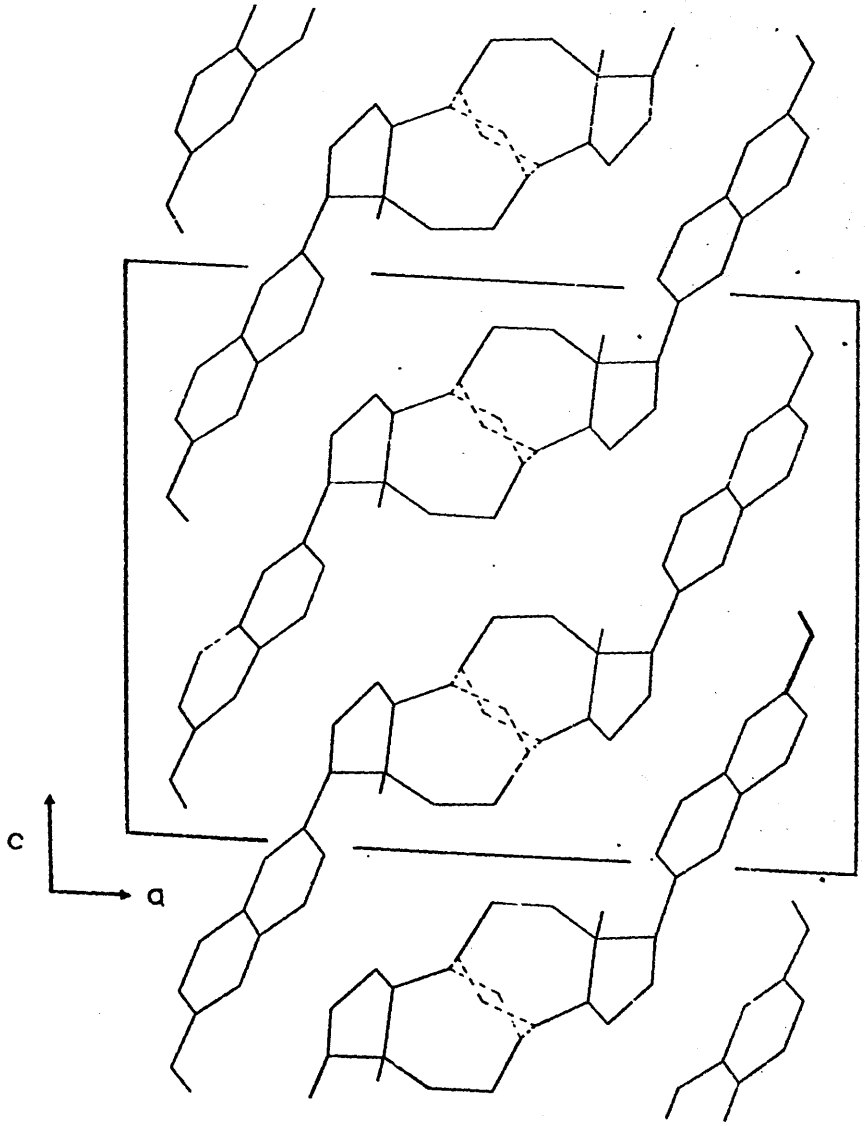


Fig. 5

The crystal structure of the lactone viewed on the ab plane.

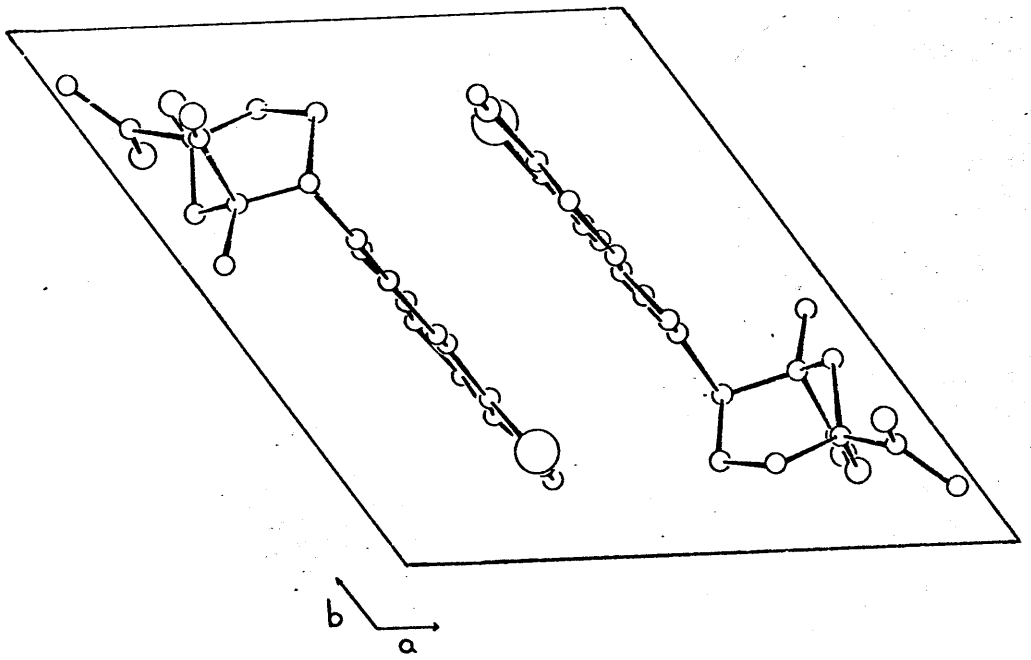
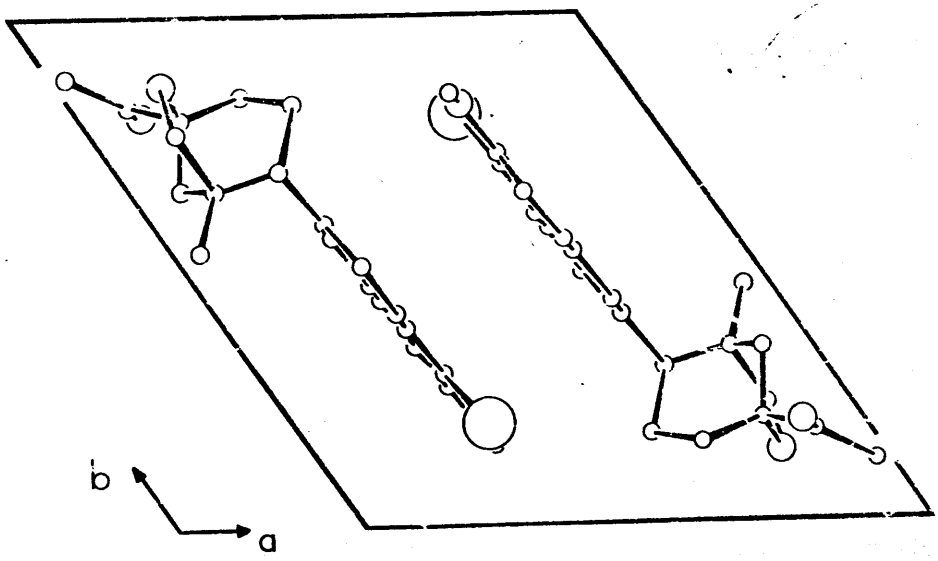


Fig. 6

The crystal structure of the ether viewed on the ab plane.



Br---H(6) separation in the lactone is 2.72 Å and this is less than the sum of the appropriate van der Waals radii (3.0 Å). An X-ray study of 3-bromo-1,8-dimethylnaphthalene[30] has revealed a still greater distortion of valency angles, caused by repulsive interaction between methyl substituents separated by 2.92 Å. The interplanar separation of the naphthalene rings is 3.74 Å in the alcohol, 3.66 Å in the lactone and 3.72 Å in the ether.

Revised Reaction Paths

A novel rearrangement during the Wittig reaction of (a) seems to have taken place as shown below. The product is the cyclohexane derivative (b) and not the expected ethylidenecyclopentane. The analogous reaction between androst-17-ones and the ethylidene Wittig reagent, on the other hand, is known to yield the expected pregn-17(20)-enes.[31,32] The mechanism of the rearrangement is by no means clear; several possibilities have been considered[33] but none has much in the way of precedent.

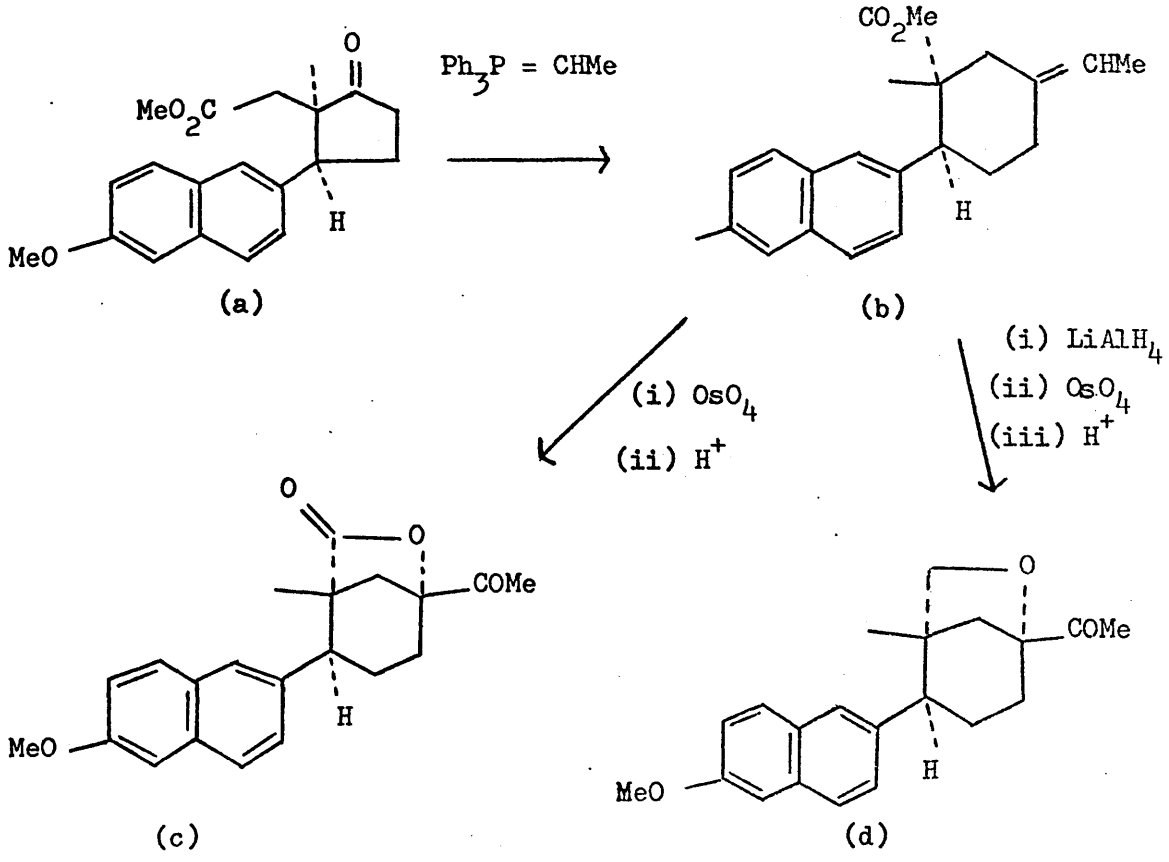
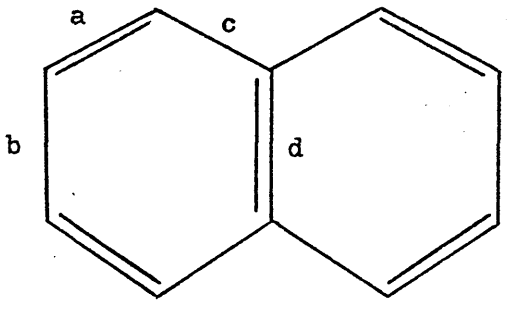


Table 2

A comparison of average lengths (Å) of equivalent bonds in naphthalene,[28] perylene,[29] the alcohol, lactone and ether. The theoretical valence-bond values for naphthalene are also listed.



Bond	Naphthalene	Perylene	Alcohol	Lactone	Ether	V.B.
a	1.364	1.368	1.370	1.368	1.369	1.375
b	1.410	1.410	1.410	1.422	1.427	1.421
c	1.421	1.421	1.417	1.417	1.410	1.421
d	1.418	1.426	1.422	1.431	1.428	1.421

TABLE 3

2-(6'-methoxy-2'-naphthyl)-1-methyl-5-hydroxy-cyclopentane-1-ethanol

Fractional Atomic co-ordinates and positional standard deviations.

Atom	x	y	z
O(1)	0.05934(19)	0.52858(58)	0.59867(27)
O(2)	0.54451(19)	0.29800(50)	1.18061(28)
O(3)	0.44145(21)	0.16143(49)	1.29473(26)
C(1)	0.09714(28)	0.25513(80)	0.81949(44)
C(2)	0.06782(29)	0.31572(87)	0.72754(43)
C(3)	0.09330(26)	0.48535(80)	0.69102(38)
C(4)	0.14886(26)	0.58717(71)	0.74391(36)
C(5)	0.18065(24)	0.52427(68)	0.83865(36)
C(6)	0.24019(27)	0.62088(68)	0.89418(36)
C(7)	0.26976(27)	0.55693(66)	0.98613(37)
C(8)	0.24320(25)	0.38963(68)	1.02636(35)
C(9)	0.18703(26)	0.29281(70)	0.97229(37)
C(10)	0.15559(25)	0.35311(70)	0.87727(37)
C(11)	0.50163(29)	0.25876(73)	1.08721(40)
C(12)	0.41661(25)	0.32934(68)	1.08362(34)
C(13)	0.35460(24)	0.21575(59)	1.13723(31)
C(14)	0.27335(26)	0.32369(67)	1.12876(33)
C(15)	0.28160(31)	0.47165(76)	1.21087(39)
C(16)	0.34271(35)	0.40108(79)	1.28983(37)
C(17)	0.36520(28)	0.21277(67)	1.25365(33)
C(18)	0.08122(37)	0.69780(107)	0.55609(47)
C(19)	0.34694(29)	0.02348(67)	1.09496(37)
H(02)	0.515(?)	0.285(?)	1.255(?)
H(03)	0.4425(21)	0.0559(53)	1.3011(27)
H(1)	0.0861(29)	0.1294(75)	0.8465(37)
H(2)	0.0374(28)	0.2546(72)	0.6759(36)

TABLE 3

Fractional Atomic co-ordinates and positional standard deviations (cont.)

Atom	x	y	z
H(4)	0.1679(23)	0.7098(58)	0.7223(30)
H(6)	0.2557(25)	0.7520(63)	0.8651(32)
H(7)	0.3069(23)	0.6222(57)	1.0256(30)
H(9)	0.1674(20)	0.1795(52)	0.9979(26)
H(11A)	0.5069(25)	0.1057(63)	1.0787(31)
H(11B)	0.5267(25)	0.2919(69)	1.0162(34)
H(12A)	0.3986(20)	0.3292(52)	0.9991(26)
H(12B)	0.4154(23)	0.4761(59)	1.1107(30)
H(14)	0.2319(23)	0.2305(58)	1.1453(30)
H(15A)	0.2959(26)	0.5942(62)	1.1877(32)
H(15B)	0.2326(26)	0.5051(67)	1.2460(34)
H(16A)	0.3903(28)	0.4899(72)	1.2935(36)
H(16B)	0.3225(22)	0.4022(57)	1.3646(29)
H(17)	0.3286(23)	0.1072(57)	1.2822(29)
H(18A)	0.1396(33)	0.6816(85)	0.5396(41)
H(18B)	0.3286(32)	0.1074(81)	1.2822(41)
H(18C)	0.0711(28)	0.8182(72)	0.5930(36)
H(19A)	0.3415(23)	0.0352(58)	1.0145(30)
H(19B)	0.3930(25)	-0.0677(63)	1.1021(32)
H(19C)	0.3048(28)	-0.0453(68)	1.1255(35)

TABLE 4

2-(6'methoxy-2'-naphthyl)-1-methyl
-5-hydroxy-cyclopentane-1-ethanol

Anisotropic temperature factors for the oxygen and carbon atoms ($\times 10^4$)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
O(1)	34(1)	344(19)	74(4)	-6(9)	-10(4)	38(16)
O(2)	33(1)	219(13)	104(5)	6(8)	-14(4)	-19(15)
O(3)	48(1)	230(13)	73(3)	-19(9)	-28(4)	53(14)
C(1)	31(2)	266(26)	94(6)	-59(10)	2(5)	37(23)
C(2)	33(2)	312(27)	84(5)	-47(10)	-20(5)	18(24)
C(3)	26(2)	281(26)	67(5)	19(9)	4(4)	19(21)
C(4)	28(2)	223(21)	64(4)	11(8)	9(4)	15(20)
C(5)	26(2)	202(20)	65(4)	9(8)	12(4)	3(19)
C(6)	35(2)	179(20)	64(4)	-17(8)	2(5)	18(18)
C(7)	35(2)	172(20)	69(4)	-18(8)	-1(5)	11(19)
C(8)	28(2)	195(20)	61(4)	4(7)	5(4)	10(18)
C(9)	30(2)	200(21)	70(4)	-29(9)	14(5)	30(20)
C(10)	25(2)	211(21)	73(4)	-22(8)	12(4)	16(20)
C(11)	37(2)	218(22)	80(5)	23(9)	19(5)	-30(21)
C(12)	31(2)	196(20)	58(4)	-5(8)	11(4)	36(18)
C(13)	32(2)	134(17)	48(3)	-15(7)	5(3)	1(16)
C(14)	34(2)	189(19)	53(4)	-19(8)	12(4)	3(18)
C(15)	50(3)	223(22)	67(4)	38(10)	32(5)	-26(21)
C(16)	63(4)	239(25)	53(4)	9(11)	5(6)	-17(21)
C(17)	39(2)	180(20)	49(3)	-7(9)	2(4)	29(17)
C(18)	56(3)	419(37)	85(6)	-30(20)	-25(6)	67(30)
C(19)	46(2)	167(20)	62(4)	-7(9)	0(4)	-15(18)

Anisotropic temperature factors used in this chapter are of the form:

$$T = \exp\left[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)\right]$$

TABLE 4 (cont.)

Isotropic thermal parameters for the hydrogen atoms.

H(02)	1.42 (fixed)	H(14)	2.44
H(03)	1.42	H(15A)	3.15
H(1)	5.52	H(15B)	3.82
H(2)	4.53	H(16A)	4.39
H(4)	2.27	H(16B)	2.12
H(6)	3.24	H(17)	2.10
H(7)	2.14	H(18A)	7.07
H(9)	1.09	H(18B)	5.86
H(11A)	2.97	H(18C)	4.62
H(11B)	3.68	H(19A)	2.29
H(12A)	0.78	H(19B)	3.08
H(12B)	2.04	H(19C)	4.18

The average standard deviation of the isotropic temperature factors is 1.0 $Å^2$.

TABLE 5

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-lactone
Fractional Atomic co-ordinates and positional standard deviations.

Atom	x	y	z
Br	0.38572(9)	0.22351(7)	0.17183(9)
O(1)	0.27032(62)	0.14398(48)	-0.23652(61)
O(2)	0.22271(50)	0.88701(41)	0.20325(58)
O(3)	-0.00377(79)	0.72883(74)	-0.26950(83)
O(4)	0.31859(66)	0.90003(55)	0.50664(66)
C(1)	0.23478(81)	0.40631(68)	-0.26607(82)
C(2)	0.22726(80)	0.30209(69)	-0.32261(84)
C(3)	0.27573(72)	0.24838(61)	-0.18965(82)
C(4)	0.32761(68)	0.30172(57)	-0.00218(78)
C(5)	0.33481(64)	0.40742(57)	0.06235(77)
C(6)	0.38183(73)	0.46283(63)	0.25470(78)
C(7)	0.38719(76)	0.56535(65)	0.30481(80)
C(8)	0.34697(64)	0.62532(57)	0.17084(78)
C(9)	0.29691(66)	0.57077(57)	-0.01526(76)
C(10)	0.28885(65)	0.46297(57)	-0.07391(76)
C(11)	0.26135(77)	0.83960(65)	0.34902(87)
C(12)	0.22503(68)	0.71231(58)	0.27546(79)
C(13)	0.10683(64)	0.67020(56)	0.08911(84)
C(14)	0.36311(63)	0.74338(55)	0.24174(77)
C(15)	0.41284(70)	0.84633(59)	0.12150(93)
C(16)	0.29181(71)	0.83598(60)	-0.03719(90)
C(17)	0.16600(67)	0.79665(56)	0.02919(80)
C(18)	0.22697(106)	0.09340(86)	-0.42921(103)
C(19)	0.17912(92)	0.62279(75)	0.41295(102)
C(20)	0.05236(78)	0.79869(69)	-0.12003(101)

TABLE 5

Fractional Atomic co-ordinates and positional standard deviations (cont.)

Atom	x	y	z
C(21)	0.01478(96)	0.88305(88)	-0.0711(129)
H(1)	0.1746(77)	0.4293(68)	-0.3595(98)
H(2)	0.1639(56)	0.2503(49)	-0.4509(70)
H(6)	0.4216(64)	0.4283(55)	0.3476(79)
H(7)	0.4315(70)	0.6036(62)	0.4383(88)
H(9)	0.2608(49)	0.6069(43)	-0.1025(61)
H(13A)	0.0200(61)	0.6408(53)	0.1052(77)
H(13B)	0.0887(60)	0.6078(52)	-0.0035(76)
H(14)	0.4378(51)	0.7765(44)	0.3653(64)
H(15A)	0.4762(66)	0.8423(58)	0.0779(83)
H(15B)	0.4864(57)	0.9380(50)	0.2001(72)
H(16A)	0.3325(65)	0.9287(57)	-0.0775(82)
H(16B)	0.2530(57)	0.7737(50)	-0.1398(71)
H(18A)	0.2295(64)	0.0264(56)	-0.4369(80)
H(18B)	0.1190(85)	0.0427(75)	-0.4861(109)
H(18C)	0.3117(90)	0.1873(79)	-0.4844(111)
H(19A)	0.1402(58)	0.5291(52)	0.3644(73)
H(19B)	0.0988(85)	0.6186(75)	0.4329(106)
H(19C)	0.2732(86)	0.6624(74)	0.5119(107)
H(21A)	-0.0987(88)	0.8294(77)	-0.1704(114)
H(21B)	0.1085(75)	0.9815(66)	-0.0292(92)
H(21C)	-0.0052(101)	0.8647(87)	0.0150(128)

TABLE 6

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-lactone

Anisotropic thermal parameters for the bromine, oxygen and carbon atoms ($\times 10^4$).

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Br	152(2)	99(1)	144(2)	196(2)	116(2)	881(1)
O(1)	220(11)	111(6)	146(9)	252(14)	131(14)	40(11)
O(2)	125(8)	77(4)	161(9)	149(10)	87(12)	26(9)
O(3)	259(19)	252(12)	210(13)	418(21)	-86(10)	-47(7)
O(4)	222(11)	149(8)	150(11)	278(14)	85(12)	-13(4)
C(1)	154(10)	110(7)	111(10)	200(17)	96(14)	70(10)
C(2)	153(10)	111(7)	120(10)	200(17)	101(15)	55(9)
C(3)	121(9)	84(7)	141(11)	153(14)	114(15)	50(9)
C(4)	105(9)	74(6)	125(10)	135(14)	79(13)	61(9)
C(5)	83(8)	73(6)	125(10)	111(12)	73(13)	50(8)
C(6)	123(9)	95(7)	102(9)	167(14)	32(13)	35(9)
C(7)	132(10)	98(7)	105(10)	172(15)	41(12)	20(8)
C(8)	81(9)	70(6)	129(11)	106(11)	47(13)	35(9)
C(9)	96(9)	77(7)	120(10)	131(14)	83(13)	61(9)
C(10)	90(9)	76(7)	117(10)	121(12)	76(13)	48(9)
C(11)	133(11)	93(8)	151(11)	173(15)	98(14)	29(7)
C(12)	102(9)	76(7)	130(11)	126(12)	111(14)	66(10)
C(13)	72(8)	59(5)	168(11)	76(11)	85(13)	43(7)
C(14)	78(8)	64(6)	126(10)	96(11)	45(12)	10(6)
C(15)	86(9)	62(6)	199(13)	81(11)	123(16)	51(7)
C(16)	100(9)	68(6)	182(12)	99(11)	131(16)	82(8)
C(17)	93(9)	66(6)	132(11)	108(11)	57(13)	22(7)
C(18)	247(18)	151(10)	170(14)	310(20)	78(16)	-36(10)
C(19)	197(13)	118(8)	213(15)	232(17)	262(21)	189(14)

TABLE 6

Anisotropic thermal parameters for the bromine, oxygen and carbon atoms ($\times 10^4$) (cont.)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
C(20)	114(11)	91(7)	199(15)	138(15)	64(18)	68(11)
C(21)	144(14)	139(10)	334(19)	231(20)	66(19)	68(13)

The form of the anisotropic temperature factors is:

$$T = \exp\left[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)\right]$$

TABLE 6 (cont.)

Isotropic thermal parameters for the hydrogen atoms

H(1)	3.92	H(16B)	0.82
H(2)	0.58	H(18A)	1.57
H(6)	1.68	H(18B)	4.89
H(7)	2.61	H(18C)	5.25
H(9)	0.40	H(19A)	0.88
H(13A)	1.21	H(19B)	4.60
H(13B)	1.22	H(19C)	4.91
H(14)	0.29	H(21A)	5.26
H(15A)	1.96	H(21B)	3.06
H(15B)	0.90	H(21C)	6.24
H(16A)	1.89		

The average standard deviation of the isotropic temperature factors is 0.9$\mathring{A}^2$

TABLE 7

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-ether

Fractional Atomic co-ordinates and positional standard deviations

Atom	x	y	z
Br	0.3807(2)	0.2188(1)	0.1517(2)
O(1)	0.2554(13)	0.1354(9)	-0.2635(11)
O(2)	0.2370(10)	0.8946(7)	0.2261(10)
O(3)	0.0480(18)	0.7690(14)	-0.2718(14)
C(1)	0.2321(15)	0.4008(12)	-0.2738(14)
C(2)	0.2209(17)	0.2962(13)	-0.3375(15)
C(3)	0.2657(15)	0.2405(11)	-0.2110(14)
C(4)	0.3185(15)	0.2966(11)	-0.0159(14)
C(5)	0.3310(13)	0.4022(11)	0.0548(14)
C(6)	0.3799(15)	0.4599(12)	0.2534(15)
C(7)	0.3855(15)	0.5604(12)	0.3116(15)
C(8)	0.3454(13)	0.6230(10)	0.1840(14)
C(9)	0.2972(13)	0.5673(11)	-0.0092(14)
C(10)	0.2867(14)	0.4594(11)	-0.0746(14)
C(11)	0.2496(17)	0.8320(12)	0.3787(15)
C(12)	0.2220(15)	0.7096(10)	0.2854(14)
C(13)	0.1120(13)	0.6761(10)	0.0890(15)
C(14)	0.3589(13)	0.7376(10)	0.2645(15)
C(15)	0.4294(16)	0.8481(11)	0.1570(18)
C(16)	0.3098(13)	0.8421(11)	-0.0086(16)
C(17)	0.1899(14)	0.8077(10)	0.0447(15)
C(18)	0.2095(24)	0.0800(16)	-0.4619(19)
C(19)	0.1571(17)	0.6044(13)	0.4007(18)
C(20)	0.0734(15)	0.8124(12)	-0.1086(18)
C(21)	0.0151(19)	0.8738(16)	-0.0470(22)

TABLE 8

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-ether

Anisotropic thermal parameters for the bromine, oxygen and carbon atoms ($\times 10^4$)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Br	187(3)	101(2)	143(3)	209(3)	107(4)	101(3)
O(1)	265(23)	125(12)	133(18)	273(29)	129(32)	56(23)
O(2)	168(17)	70(8)	132(17)	147(20)	89(25)	26(19)
O(3)	392(37)	278(24)	173(25)	526(53)	57(46)	78(39)
C(1)	125(21)	101(14)	92(21)	146(29)	77(32)	56(27)
C(2)	175(26)	115(16)	112(23)	207(35)	94(37)	57(30)
C(3)	162(24)	73(12)	121(23)	134(29)	142(36)	42(27)
C(4)	149(23)	71(12)	102(21)	123(28)	37(34)	50(26)
C(5)	84(17)	72(11)	117(22)	86(24)	61(30)	46(25)
C(6)	126(21)	101(14)	98(22)	144(30)	7(33)	30(28)
C(7)	125(22)	90(14)	126(24)	138(31)	10(35)	15(29)
C(8)	78(18)	62(11)	153(24)	95(24)	38(31)	34(26)
C(9)	90(18)	81(12)	121(22)	106(25)	104(31)	70(26)
C(10)	115(19)	76(12)	109(22)	115(26)	60(31)	60(26)
C(11)	203(28)	116(16)	152(25)	256(37)	157(41)	77(32)
C(12)	137(22)	64(11)	113(22)	112(27)	69(34)	50(25)
C(13)	74(17)	51(10)	170(25)	53(22)	92(32)	68(25)
C(14)	74(17)	61(11)	135(23)	70(23)	28(31)	9(25)
C(15)	134(23)	55(12)	223(32)	83(28)	42(42)	52(31)
C(16)	72(18)	83(13)	200(28)	97(26)	135(35)	113(31)
C(17)	107(19)	68(11)	137(23)	119(25)	76(32)	54(26)
C(18)	380(49)	148(21)	183(32)	361(56)	263(63)	41(41)
C(19)	175(27)	102(15)	211(31)	183(36)	228(46)	151(36)
C(20)	119(21)	95(14)	210(31)	156(31)	78(40)	105(34)
C(21)	155(28)	150(21)	287(40)	245(43)	13(51)	36(46)

TABLE 9

2-(6'-methoxy-2'-naphthyl)-1-methyl
-5-hydroxy-cyclopentane-1-ethanol

Intramolecular bonded distances and estimated standard deviations (Å).

O(1)	-	C(3)	1.368(6)	C(13)	-	C(17)	1.556(6)
O(1)	-	C(18)	1.415(8)	C(13)	-	C(19)	1.509(6)
O(2)	-	C(11)	1.437(6)	C(14)	-	C(15)	1.537(7)
O(3)	-	C(17)	1.432(6)	C(15)	-	C(16)	1.527(8)
C(1)	-	C(2)	1.371(8)	C(16)	-	C(17)	1.509(7)
C(1)	-	C(10)	1.417(7)	O(2)	-	H(02)	1.15(?)
C(2)	-	C(3)	1.404(8)	O(3)	-	H(02)	1.66(?)
C(3)	-	C(4)	1.366(7)	O(3)	-	H(03)	0.77(4)
C(4)	-	C(5)	1.423(7)	C(1)	-	H(1)	1.01(5)
C(5)	-	C(6)	1.409(7)	C(2)	-	H(2)	0.95(5)
C(5)	-	C(10)	1.422(7)	C(4)	-	H(4)	1.00(4)
C(6)	-	C(7)	1.381(7)	C(6)	-	H(6)	1.07(5)
C(7)	-	C(8)	1.415(7)	C(7)	-	H(7)	0.93(4)
C(8)	-	C(9)	1.361(7)	C(11)	-	H(11A)	1.12(5)
C(8)	-	C(14)	1.511(6)	C(11)	-	H(11B)	1.09(5)
C(9)	-	C(10)	1.418(7)	C(12)	-	H(12A)	1.15(4)
C(11)	-	C(12)	1.539(7)	C(12)	-	H(12B)	1.13(4)
C(12)	-	C(13)	1.553(6)	C(14)	-	H(14)	1.01(4)
C(13)	-	C(14)	1.593(6)	C(15)	-	H(15A)	0.98(5)
C(15)	-	H(15B)	1.01(5)	C(18)	-	H(18C)	1.01(5)
C(16)	-	H(16A)	1.04(5)	C(19)	-	H(19A)	1.08(4)
C(16)	-	H(16B)	1.08(4)	C(19)	-	H(19B)	1.03(5)
C(18)	-	H(18A)	1.04(6)	C(19)	-	H(19C)	0.99(5)
C(18)	-	H(18B)	1.17(6)				

The intramolecular O(2)...O(3) distance is 2.597(5)Å.

TABLE 10

2-(6'-methoxy-2'-naphthyl)-1-methyl
-5-hydroxy-cyclopentane-1-ethanol

Valency Angles (degrees) and estimated standard deviations.

C(18)	-	O(1)	-	C(3)		117.0(4)
C(2)	-	C(3)	-	O(1)		113.1(4)
C(13)	-	C(17)	-	O(3)		115.8(3)
C(5)	-	C(10)	-	C(1)		117.3(4)
C(6)	-	C(5)	-	C(4)		122.2(3)
C(10)	-	C(5)	-	C(6)		117.9(3)
C(9)	-	C(8)	-	C(7)		118.3(3)
C(13)	-	C(14)	-	C(8)		117.9(3)
C(17)	-	C(13)	-	C(12)		115.4(3)
C(19)	-	C(13)	-	C(14)		111.9(3)
C(16)	-	C(17)	-	C(13)		107.0(4)
C(17)	-	C(16)	-	C(15)		105.1(4)
C(4)	-	C(3)	-	O(1)		125.9(3)
C(12)	-	C(11)	-	O(2)		113.0(3)
C(16)	-	C(17)	-	O(3)		110.9(3)
C(10)	-	C(1)	-	C(2)		122.3(4)
C(3)	-	C(2)	-	C(1)		119.3(4)
C(9)	-	C(10)	-	C(1)		123.3(4)
C(4)	-	C(3)	-	C(2)		121.0(4)
C(5)	-	C(4)	-	C(3)		120.2(4)
C(10)	-	C(5)	-	C(4)		119.8(3)
C(7)	-	C(6)	-	C(5)		121.0(3)
C(9)	-	C(10)	-	C(5)		119.3(3)
C(8)	-	C(7)	-	C(6)		121.3(3)
C(14)	-	C(8)	-	C(7)		121.1(3)
C(14)	-	C(8)	-	C(9)		120.5(3)

TABLE 10

Valency Angles (degrees) and estimated standard deviations (cont.)

C(10)	-	C(9)	-	C(8)	122.2(3)
C(15)	-	C(14)	-	C(8)	115.9(4)
C(13)	-	C(12)	-	C(11)	118.6(3)
C(14)	-	C(13)	-	C(12)	108.8(3)
C(19)	-	C(13)	-	C(12)	111.4(3)
C(17)	-	C(13)	-	C(14)	97.2(3)
C(15)	-	C(14)	-	C(13)	104.6(3)
C(19)	-	C(13)	-	C(17)	111.3(3)
C(16)	-	C(15)	-	C(14)	106.7(3)
O(3)	-	H(02)	-	O(2)	135(?)
O(3)	-	H(03)	-	O(2)*	175(?)

* O(2) co-ordinates transposed by the symmetry operation $1-x, -\frac{1}{2}+y, \frac{5}{2} - z$.

The average H - $C(sp^3)$ - H valency angle is 106°

The average H - $C(sp^3)$ - $C(sp^3)$ valency angle is 109°

The average H - $C(sp^2)$ - $C(sp^2)$ valency angle is 119°

TABLE 11

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-lactone

Intramolecular bonded distances (Å) and estimated standard deviations.

Bond	Distance (MoKα)	Distance (CuKα)
Br - C(4)	1.894(10)	1.911(28)
O(1) - C(3)	1.364(16)	1.401(42)
O(1) - C(18)	1.422(10)	1.472(29)
O(2) - C(11)	1.369(12)	1.363(36)
O(2) - C(17)	1.473(10)	1.498(29)
O(3) - C(20)	1.200(12)	1.194(38)
O(4) - C(11)	1.202(10)	1.215(29)
C(1) - C(2)	1.366(20)	1.387(57)
C(1) - C(10)	1.419(9)	1.481(29)
C(2) - C(3)	1.413(15)	1.376(42)
C(3) - C(4)	1.380(9)	1.405(28)
C(4) - C(5)	1.406(16)	1.382(41)
C(5) - C(6)	1.429(9)	1.464(29)
C(5) - C(10)	1.431(13)	1.424(38)
C(6) - C(7)	1.347(18)	1.401(54)
C(7) - C(8)	1.430(14)	1.422(40)
C(8) - C(9)	1.377(9)	1.406(29)
C(8) - C(14)	1.512(16)	1.531(32)
C(9) - C(10)	1.412(16)	1.393(32)
C(11) - C(12)	1.511(17)	1.517(52)
C(12) - C(13)	1.525(10)	1.553(28)
C(12) - C(14)	1.574(13)	1.496(38)
C(12) - C(19)	1.537(15)	1.587(43)
C(13) - C(17)	1.513(15)	1.548(43)
C(14) - C(15)	1.550(14)	1.583(40)

TABLE 11

Intramolecular bonded distances (Å) and estimated standard deviations (cont.)

Bond	Distance (MoKα)	Distance (CuKα)
C(15) - C(16)	1.550(12)	1.615(38)
C(16) - C(17)	1.538(13)	1.482(39)
C(17) - C(20)	1.531(13)	1.552(40)
C(20) - C(21)	1.484(22)	1.493(69)

TABLE 11 (cont.)

Intramolecular bonded distances (Å) and estimated standard deviations for the hydrogen bonds (MoKα)

C(1)	-	H(1)	1.04(11)	C(16)	-	H(16B)	0.92(8)
C(2)	-	H(2)	0.99(6)	C(18)	-	H(18A)	0.89(12)
C(6)	-	H(6)	1.00(9)	C(18)	-	H(18B)	1.02(11)
C(7)	-	H(7)	0.98(7)	C(18)	-	H(18C)	1.24(13)
C(9)	-	H(9)	0.96(7)	C(19)	-	H(19A)	1.05(10)
C(13)	-	H(13A)	0.94(8)	C(19)	-	H(19B)	0.99(12)
C(13)	-	H(13B)	0.95(9)	C(19)	-	H(19C)	0.99(10)
C(14)	-	H(14)	0.98(5)	C(21)	-	H(21A)	1.13(11)
C(15)	-	H(15A)	0.94(10)	C(21)	-	H(21B)	1.09(11)
C(15)	-	H(15B)	1.03(9)	C(21)	-	H(21C)	0.75(11)
C(16)	-	H(16A)	1.10(11)				

TABLE 12

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-lactone

Valency Angles (degrees) and estimated standard deviations.

C(3)	-	C(4)	-	Br	117.2(5)
C(10)	-	C(1)	-	C(2)	121.7(5)
C(3)	-	C(2)	-	C(1)	120.4(5)
C(9)	-	C(10)	-	C(1)	121.8(9)
C(4)	-	C(3)	-	C(2)	118.6(7)
O(1)	-	C(3)	-	C(4)	118.0(9)
C(18)	-	O(1)	-	C(3)	118.7(5)
C(10)	-	C(5)	-	C(4)	118.0(5)
C(7)	-	C(6)	-	C(5)	121.4(9)
C(8)	-	C(7)	-	C(6)	122.6(5)
C(14)	-	C(8)	-	C(7)	118.4(6)
C(10)	-	C(9)	-	C(8)	122.3(9)
C(12)	-	C(14)	-	C(8)	112.7(6)
O(4)	-	C(11)	-	C(12)	129.9(5)
C(14)	-	C(12)	-	C(11)	105.3(7)
C(17)	-	O(2)	-	C(11)	107.3(7)
C(19)	-	C(12)	-	C(13)	114.5(7)
C(17)	-	C(13)	-	C(12)	99.6(7)
C(16)	-	C(17)	-	C(13)	111.0(6)
O(2)	-	C(17)	-	C(13)	103.7(4)
C(16)	-	C(15)	-	C(14)	115.6(5)
O(2)	-	C(17)	-	C(16)	107.8(5)
O(2)	-	C(17)	-	C(20)	110.2(6)
C(21)	-	C(20)	-	C(17)	118.8(8)
O(3)	-	C(20)	-	C(21)	123.8(6)
C(5)	-	C(4)	-	Br	119.8(3)
C(5)	-	C(10)	-	C(1)	118.3(9)

TABLE 12

Valency Angles (degrees) and estimated standard deviations (cont.)

O(1)	-	C(3)	-	C(2)	123.4(6)
C(5)	-	C(4)	-	C(3)	122.9(9)
C(6)	-	C(5)	-	C(4)	125.1(5)
C(10)	-	C(5)	-	C(6)	116.9(9)
C(9)	-	C(10)	-	C(5)	119.8(6)
C(9)	-	C(8)	-	C(7)	116.9(6)
C(14)	-	C(8)	-	C(9)	124.7(9)
C(15)	-	C(14)	-	C(8)	114.8(5)
O(2)	-	C(11)	-	C(12)	109.8(4)
C(13)	-	C(12)	-	C(11)	101.1(5)
C(19)	-	C(12)	-	C(11)	111.0(5)
O(4)	-	C(11)	-	O(2)	120.2(7)
C(14)	-	C(12)	-	C(13)	110.4(6)
C(19)	-	C(12)	-	C(14)	113.4(7)
C(15)	-	C(14)	-	C(12)	110.2(7)
C(20)	-	C(17)	-	C(13)	113.1(5)
C(17)	-	C(16)	-	C(15)	110.4(5)
C(20)	-	C(17)	-	C(16)	110.7(5)
O(3)	-	C(20)	-	C(17)	117.4(8)

The average H - $C(sp^3)$ - H valency angle is 112°

The average H - $C(sp^3)$ - $C(sp^3)$ valency angle is 106°

The average H - $C(sp^2)$ - $C(sp^2)$ valency angle is 119°

TABLE 13

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-ether

Intramolecular bonded distances and estimated standard deviations (Å)

Br	-	C(4)	1.92(2)	C(7)	-	C(8)	1.45(3)
O(1)	-	C(3)	1.34(3)	C(8)	-	C(9)	1.40(1)
O(1)	-	C(18)	1.44(2)	C(8)	-	C(14)	1.49(3)
O(2)	-	C(11)	1.46(2)	C(9)	-	C(10)	1.40(3)
O(2)	-	C(17)	1.48(2)	C(11)	-	C(12)	1.53(3)
O(3)	-	C(20)	1.21(2)	C(12)	-	C(13)	1.55(2)
C(1)	-	C(2)	1.35(3)	C(12)	-	C(14)	1.53(3)
C(1)	-	C(10)	1.44(1)	C(12)	-	C(19)	1.58(3)
C(2)	-	C(3)	1.40(3)	C(13)	-	C(17)	1.53(3)
C(3)	-	C(4)	1.40(1)	C(14)	-	C(15)	1.59(3)
C(4)	-	C(5)	1.37(3)	C(15)	-	C(16)	1.60(2)
C(5)	-	C(6)	1.44(1)	C(16)	-	C(17)	1.43(2)
C(5)	-	C(10)	1.43(2)	C(17)	-	C(20)	1.61(2)
C(6)	-	C(7)	1.32(3)	C(20)	-	C(21)	1.46(4)

TABLE 14

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-ether

Valency Angles (degrees) and estimated standard deviations (degrees)

C(3)	-	C(4)	-	Br	115.5(10)
C(18)	-	O(1)	-	C(3)	119.8(10)
C(4)	-	C(3)	-	O(1)	118.5(8)
C(12)	-	C(11)	-	O(2)	106.4(14)
C(16)	-	C(17)	-	O(2)	110.6(13)
C(17)	-	C(20)	-	O(3)	114.3(20)
C(10)	-	C(1)	-	C(2)	122.3(9)
C(5)	-	O(10)	-	C(1)	116.6(18)
C(4)	-	C(3)	-	C(2)	116.9(13)
C(6)	-	C(5)	-	C(4)	125.5(9)
C(10)	-	C(5)	-	C(6)	115.3(18)
C(9)	-	C(10)	-	C(5)	121.2(11)
C(9)	-	C(8)	-	C(7)	114.4(12)
C(14)	-	C(8)	-	C(9)	126.0(18)
C(12)	-	C(14)	-	C(8)	115.0(13)
C(13)	-	C(12)	-	C(11)	99.6(10)
C(19)	-	C(12)	-	C(11)	110.5(11)
C(19)	-	C(12)	-	C(13)	112.5(14)
C(19)	-	C(12)	-	C(14)	112.0(15)
C(16)	-	C(17)	-	C(13)	113.6(13)
C(16)	-	C(15)	-	C(14)	111.4(11)
C(20)	-	C(17)	-	C(16)	114.1(12)
C(5)	-	C(4)	-	Br	120.7(5)
C(2)	-	C(3)	-	O(1)	124.5(9)
C(17)	-	O(2)	-	C(11)	107.3(13)
C(13)	-	C(17)	-	O(2)	103.1(12)
C(20)	-	C(17)	-	O(2)	106.8(14)

TABLE 14

Valency Angles (degrees) and estimated standard deviations (degrees) (cont.)

C(21)	-	C(20)	-	O(3)	125.4(23)
C(3)	-	C(2)	-	C(1)	121.2(10)
C(9)	-	C(10)	-	C(1)	122.2(18)
C(5)	-	C(4)	-	C(3)	123.8(18)
C(10)	-	C(5)	-	C(4)	119.1(9)
C(7)	-	C(6)	-	C(5)	122.2(18)
C(8)	-	C(7)	-	C(6)	123.8(10)
C(14)	-	C(8)	-	C(7)	119.6(12)
C(10)	-	C(9)	-	C(8)	122.9(18)
C(15)	-	C(14)	-	C(8)	111.9(11)
C(14)	-	C(12)	-	C(11)	110.7(14)
C(14)	-	C(12)	-	C(13)	110.9(11)
C(17)	-	C(13)	-	C(12)	98.9(14)
C(15)	-	C(14)	-	C(12)	112.4(15)
C(20)	-	C(17)	-	C(13)	107.9(11)
C(17)	-	C(16)	-	C(15)	112.1(10)
C(21)	-	C(20)	-	C(17)	120.2(12)

TABLE 15

2-(6'-methoxy-2'-naphthyl)-1-methyl
-5-hydroxy-cyclopentane-1-ethanol

Torsion Angles (degrees)

C(18)	O(1)	C(3)	C(2)	180
C(18)	O(1)	C(3)	C(4)	-3
C(10)	C(1)	C(2)	C(3)	-3
C(2)	C(1)	C(10)	C(5)	3
C(2)	C(1)	C(10)	C(9)	-180
C(1)	C(2)	C(3)	O(1)	-180
C(1)	C(2)	C(3)	C(4)	2
O(1)	C(3)	C(4)	C(5)	-179
C(2)	C(3)	C(4)	C(5)	-1
C(3)	C(4)	C(5)	C(6)	178
C(3)	C(4)	C(5)	C(10)	1
C(4)	C(5)	C(6)	C(7)	180
C(10)	C(5)	C(6)	C(7)	-4
C(4)	C(5)	C(10)	C(1)	-2
C(4)	C(5)	C(10)	C(9)	-179
C(6)	C(5)	C(10)	C(1)	-178
C(6)	C(5)	C(10)	C(9)	4
C(5)	C(6)	C(7)	C(8)	2
C(6)	C(7)	C(8)	C(9)	0
C(7)	C(8)	C(9)	C(10)	1
C(14)	C(8)	C(9)	C(10)	178
C(7)	C(8)	C(14)	C(13)	-83
C(7)	C(8)	C(14)	C(15)	42
C(9)	C(8)	C(14)	C(13)	100
C(9)	C(8)	C(14)	C(15)	-135

TABLE 15 (cont.)

Torsion Angles (degrees) (cont.)

C(8)	C(9)	C(10)	C(1)	-180
C(8)	C(9)	C(10)	C(5)	-3
O(2)	C(11)	C(12)	C(13)	-79
C(11)	C(12)	C(13)	C(14)	176
C(11)	C(12)	C(13)	C(17)	68
C(11)	C(12)	C(13)	C(19)	-60
C(12)	C(13)	C(14)	C(8)	50
C(12)	C(13)	C(14)	C(15)	-80
C(17)	C(13)	C(14)	C(8)	170
C(17)	C(13)	C(14)	C(15)	40
C(19)	C(13)	C(14)	C(8)	-73
C(19)	C(13)	C(14)	C(15)	156
C(12)	C(13)	C(17)	O(3)	-52
C(12)	C(13)	C(17)	C(16)	72
C(14)	C(13)	C(17)	O(3)	-167
C(14)	C(13)	C(17)	C(16)	-43
C(19)	C(13)	C(17)	O(3)	76
C(19)	C(13)	C(17)	C(16)	-160
C(8)	C(14)	C(15)	C(16)	-156
C(13)	C(14)	C(15)	C(16)	-25
C(14)	C(15)	C(16)	C(17)	-2
C(15)	C(16)	C(17)	O(3)	157
C(15)	C(16)	C(17)	C(13)	29

The sign convention used for the torsion angles is such that the sign is negative if an anticlockwise rotation is required of Atom (1) to eclipse Atom (4) whilst looking down the (2) - (3) bond.

The average standard deviation of the torsion angles is 0.6°.

TABLE 16

2-(6'-methoxy-2'-naphthyl)-1-methyl-5-hydroxy-cyclopentane-1-ethanol

Mean Plane Calculations

	Atoms in plane	Atoms out of plane	Deviation (Å)
(1)	C(14)		0.01
	C(15)		-0.01
	C(16)		0.01
	C(17)		-0.01
		C(13)	0.69
		C(12)	2.23
		C(19)	0.30
		O(3)	0.54
		C(8)	0.54
(2)	C(11)		-0.06
	O(2)		0.05
	C(17)		-0.05
	C(13)		0.06
		C(12)	0.70
		O(3)	-0.66
		H(03)	1.84
		C(14))	1.08
		O(16)	1.35
(3)	C(1)		0.00
	C(2)		0.03
	C(3)		-0.01
	C(4)		-0.01
	C(5)		-0.02
	C(6)		0.02
	C(7)		0.01
	C(8)		0.00
	C(9)		-0.01
	C(10)		0.01

TABLE 17

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-lactone

Torsion Angles (degrees)

C(10)	C(1)	C(2)	C(3)	-1
C(2)	C(1)	C(10)	C(5)	-1
C(2)	C(1)	C(10)	C(9)	180
C(1)	C(2)	C(3)	C(4)	1
C(1)	C(2)	C(3)	O(1)	180
C(2)	C(3)	C(4)	Br	178
C(2)	C(3)	C(4)	C(5)	0
O(1)	C(3)	C(4)	Br	0
O(1)	C(3)	C(4)	C(5)	-178
C(2)	C(3)	O(1)	C(18)	6
C(4)	C(3)	O(1)	C(18)	-175
Br	C(4)	C(5)	C(6)	-1
Br	C(4)	C(5)	C(10)	-180
C(3)	C(4)	C(5)	C(6)	177
C(3)	C(4)	C(5)	C(10)	-1
C(4)	C(5)	C(6)	C(7)	179
C(10)	C(5)	C(6)	C(7)	-2
C(4)	C(5)	C(10)	C(1)	2
C(4)	C(5)	C(10)	C(9)	-179
C(6)	C(5)	C(10)	C(1)	-177
C(6)	C(5)	C(10)	C(9)	3
C(5)	C(6)	C(7)	C(8)	0
C(6)	C(7)	C(8)	C(9)	2
C(6)	C(7)	C(8)	C(14)	-177
C(7)	C(8)	C(9)	C(10)	-2

TABLE 17

Torsion Angles (degrees) (cont.)

C(14)	C(8)	C(9)	C(10)	178
C(7)	C(8)	C(14)	C(12)	-90
C(7)	C(8)	C(14)	C(15)	143
C(9)	C(8)	C(14)	C(12)	90
C(9)	C(8)	C(14)	C(15)	-37
C(8)	C(9)	C(10)	C(1)	179
C(8)	C(9)	C(10)	C(5)	-1
O(2)	C(11)	C(12)	C(13)	-24
O(2)	C(11)	C(12)	C(14)	91
O(2)	C(11)	C(12)	C(19)	-146
O(4)	C(11)	C(12)	C(13)	158
O(4)	C(11)	C(12)	C(14)	-87
O(4)	C(11)	C(12)	C(19)	36
C(12)	C(11)	O(2)	C(17)	-2
O(4)	C(11)	O(2)	C(17)	176
C(11)	C(12)	C(13)	C(17)	39
C(14)	C(12)	C(13)	C(17)	-73
C(19)	C(12)	C(13)	C(17)	158
C(11)	C(12)	C(14)	C(8)	179
C(11)	C(12)	C(14)	C(15)	-52
C(13)	C(12)	C(14)	C(8)	-73
C(13)	C(12)	C(14)	C(15)	57
C(19)	C(12)	C(14)	C(8)	57
C(19)	C(12)	C(14)	C(15)	-173

TABLE 17

Torsion Angles (degrees) (cont.)

C(12)	C(13)	C(17)	C(16)	74
C(12)	C(13)	C(17)	C(20)	-161
C(12)	C(13)	C(17)	O(2)	-41
C(8)	C(14)	C(15)	C(16)	90
C(12)	C(14)	C(15)	C(16)	-38
C(14)	C(15)	C(16)	C(17)	39
C(15)	C(16)	C(17)	C(13)	-59
C(15)	C(16)	C(17)	C(20)	175
C(15)	C(16)	C(17)	O(2)	54
C(13)	C(17)	C(20)	C(21)	114
C(13)	C(17)	C(20)	O(3)	-64
C(16)	C(17)	C(20)	C(21)	-121
C(16)	C(17)	C(20)	O(3)	61
O(2)	C(17)	C(20)	C(21)	-1
O(2)	C(17)	C(20)	O(3)	-180
C(13)	C(17)	O(2)	C(11)	28
C(16)	C(17)	O(2)	C(11)	-90
C(20)	C(17)	O(2)	C(11)	150

The sign convention used for the torsion angles is such that the sign is negative if an anticlockwise rotation is required of Atom (1) to eclipse Atom (4) whilst looking down the (2) - (3) bond.

The average standard deviation of the torsion angles is 1.1°.

TABLE 18

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-lactone

Mean Plane Calculations

	Atoms in plane	Atoms out of plane	Deviation (Å)
(1)	C(12)		0.01
	C(14)		0.00
	C(16)		0.00
	C(17)		-0.01
		C(13)	0.88
		C(15)	-0.48
		O(2)	-1.36
		C(11)	-1.37
		C(20)	0.35
		C(8)	1.30
		C(19)	0.31
(2)	O(2)		-0.01
	C(11)		0.01
	C(12)		-0.01
	C(17)		0.01
		O(4)	0.08
		C(13)	-0.65
		C(14)	1.50
		C(16)	1.48
		C(19)	-0.80
		C(20)	-0.74

TABLE 18

Mean Plane Calculations (cont.)

	Atoms in plane	Atoms out of plane	Deviation (Å)
(3)	C(1)		-0.02
	C(2)		-0.03
	C(3)		0.01
	C(4)		0.03
	C(5)		0.01
	C(6)		-0.03
	C(7)		-0.03
	C(8)		0.02
	C(9)		0.02
	C(10)		0.01

The angle between the perpendiculars of planes (1) and (2) is 74.4 degrees.

TABLE 19

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-ether

Torsion Angles (degrees)

C(18)	O(1)	C(3)	C(2)	7
C(18)	O(1)	C(3)	C(4)	-176
C(17)	O(2)	C(11)	C(12)	5
C(11)	O(2)	C(17)	C(13)	26
C(11)	O(2)	C(17)	C(16)	-96
C(11)	O(2)	C(17)	C(20)	139
C(10)	C(1)	C(2)	C(3)	-2
C(2)	C(1)	C(10)	C(5)	1
C(2)	C(1)	C(10)	C(9)	-180
C(1)	C(2)	C(3)	O(1)	179
C(1)	C(2)	C(3)	C(4)	2
O(1)	C(3)	C(4)	Br	4
O(1)	C(3)	C(4)	C(5)	-179
C(2)	C(3)	C(4)	Br	-179
C(2)	C(3)	C(4)	C(5)	-1
Br	C(4)	C(5)	C(6)	-5
Br	C(4)	C(5)	C(10)	179
C(3)	C(4)	C(5)	C(6)	178
C(3)	C(4)	C(5)	C(10)	1
C(4)	C(5)	C(6)	C(7)	-178
C(10)	C(5)	C(6)	C(7)	-1
C(4)	C(5)	C(10)	C(1)	0
C(4)	C(5)	C(10)	C(9)	180
C(6)	C(5)	C(10)	C(1)	-178

TABLE 19

Torsion Angles (degrees) (contd.)

C(6)	C(5)	C(10)	C(9)	3
C(5)	C(6)	C(7)	C(8)	-1
C(6)	C(7)	C(8)	C(9)	1
C(6)	C(7)	C(8)	C(14)	-179
C(7)	C(8)	C(9)	C(10)	1
C(14)	C(8)	C(9)	C(10)	-180
C(7)	C(8)	C(14)	C(12)	-95
C(7)	C(8)	C(14)	C(15)	135
C(9)	C(8)	C(14)	C(12)	86
C(9)	C(8)	C(14)	C(15)	-44
C(8)	C(9)	C(10)	C(1)	178
C(8)	C(9)	C(10)	C(5)	-3
O(2)	C(11)	C(12)	C(13)	-33
O(2)	C(11)	C(12)	C(14)	84
O(2)	C(11)	C(12)	C(19)	-152
C(11)	C(12)	C(13)	C(17)	47
C(14)	C(12)	C(13)	C(17)	-70
C(19)	C(12)	C(13)	C(17)	164
C(11)	C(12)	C(14)	C(8)	177
C(11)	C(12)	C(14)	C(15)	-53
C(13)	C(12)	C(14)	C(8)	-73
C(13)	C(12)	C(14)	C(15)	56
C(19)	C(12)	C(14)	C(8)	53
C(19)	C(12)	C(14)	C(15)	-177

TABLE 19

Torsion Angles (degrees) (contd.)

C(12)	C(13)	C(17)	O(2)	-45
C(12)	C(13)	C(17)	C(16)	74
C(12)	C(13)	C(17)	C(20)	-158
C(8)	C(14)	C(15)	C(16)	95
C(12)	C(14)	C(15)	C(16)	-36
C(14)	C(15)	C(16)	C(17)	38
C(15)	C(16)	C(17)	O(2)	54
C(15)	C(16)	C(17)	C(13)	-61
C(15)	C(16)	C(17)	C(20)	175
O(2)	C(17)	C(20)	O(3)	165
O(2)	C(17)	C(20)	C(21)	-11
C(13)	C(17)	C(20)	O(3)	-85

The sign convention used for the torsion angles is such that the sign is negative if an anticlockwise rotation is required of Atom (1) to eclipse Atom (4) whilst looking down the (2) - (3) bond.

The average standard deviation of the torsion angles is 2.6°.

TABLE 20

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-ether

Mean Plane Calculations

	Atoms in plane	Atoms out of plane	Deviation (Å)
(1)	C(14)		-0.01
	C(12)		0.01
	C(17)		-0.01
	C(16)		0.01
		C(13)	0.88
		C(15)	-0.51
		C(19)	0.44
		C(8)	1.25
		C(20)	0.37
		O(2)	-1.36
		C(11)	-1.35
(2)	O(2)		-0.03
	C(11)		0.03
	C(12)		-0.02
	C(17)		0.02
		C(13)	0.74
		C(14)	-1.46
		C(16)	-1.30
		C(19)	0.73
		C(20)	0.98

TABLE 20

Mean Plane Calculations (contd.)

	Atoms in plane	Atoms out of plane	Deviation (Å)
(3)	C(1)		-0.01
	C(2)		-0.03
	C(3)		0.00
	C(4)		0.01
	C(5)		0.03
	C(6)		-0.01
	C(7)		-0.03
	C(8)		0.00
	C(9)		0.02
	C(10)		0.01

The angle between the perpendiculars of planes (1) and (2) is 70.1 degrees.

TABLE 21

2-(6'-methoxy-2'-naphthyl)-1-methyl
-5-hydroxy-cyclopentane-1-ethanol

Intermolecular contacts (Å) of less than 4 Å.

C(7)	$C(19)_{I}$	3.887	C(16)	$C(9)_{IV}$	3.976
O(1)	$O(1)_{II}$	3.254	C(16)	$C(10)_{IV}$	3.932
O(1)	$C(18)_{II}$	3.485	C(17)	$C(5)_{IV}$	3.827
O(1)	$C(1)_{III}$	3.379	C(17)	$C(6)_{IV}$	3.803
O(1)	$C(2)_{III}$	3.885	C(6)	$C(18)_{V}$	3.811
C(3)	$C(1)_{III}$	3.795	C(7)	$C(18)_{V}$	3.848
C(3)	$C(2)_{III}$	3.860	C(15)	$C(4)_{V}$	3.967
C(18)	$C(1)_{III}$	3.585	C(15)	$C(6)_{V}$	3.934
O(3)	$C(12)_{IV}$	3.912	O(2)	$O(3)_{VI}$	2.669
C(9)	$O(1)_{IV}$	3.677	O(2)	$C(17)_{VI}$	3.473
C(9)	$C(3)_{IV}$	3.972	O(2)	$C(19)_{VI}$	3.800
C(14)	$C(2)_{IV}$	3.960	C(11)	$O(3)_{VI}$	3.436
C(14)	$C(3)_{IV}$	3.939	C(12)	$O(3)_{VI}$	3.724
C(15)	$C(1)_{IV}$	3.915	O(16)	$O(2)_{VI}$	3.477
C(15)	$C(10)_{IV}$	3.967	C(16)	$C(11)_{VI}$	3.999

The subscripts refer to the following transformations of the atomic co-ordinates:

(I)	$x, 1+y, z$	(IV)	$x, \frac{1}{2}-y, \frac{1}{2}+z$
(II)	$-x, 1-y, 1-z$	(V)	$x, \frac{3}{2}-y, \frac{1}{2}+z$
(III)	$-x, \frac{1}{2}+y, \frac{3}{2}-z$	(VI)	$1-x, \frac{1}{2}+y, \frac{5}{2}-z$

TABLE 22

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-lactone

Intermolecular contacts (Å) of less than 4 Å

Br	$C(18)_{I}$	3.92	C(1)	$C(6)_{VI}$	3.89
O(4)	$C(16)_{I}$	3.63	C(2)	$C(6)_{VI}$	3.76
C(19)	$C(1)_{I}$	3.96	C(2)	$C(7)_{VI}$	3.90
C(11)	$C(18)_{II}$	3.97	C(3)	$C(6)_{VI}$	3.88
O(2)	$C(18)_{II}$	3.83	C(3)	$C(7)_{VI}$	3.74
O(4)	$C(18)_{II}$	3.35	C(3)	$C(8)_{VI}$	3.82
Br	$O(2)_{III}$	3.70	C(4)	$C(5)_{VI}$	3.84
O(1)	$C(20)_{III}$	3.99	C(4)	$C(9)_{VI}$	3.80
O(1)	$C(21)_{III}$	3.60	C(4)	$C(10)_{VI}$	3.69
C(4)	$C(21)_{IV}$	3.63	C(5)	$C(5)_{VI}$	3.72
C(5)	$C(21)_{IV}$	3.77	C(5)	$C(10)_{VI}$	3.82
C(6)	$O(3)_{IV}$	3.80	C(7)	$O(1)_{VI}$	3.90
C(7)	$O(3)_{IV}$	3.92	C(8)	$O(1)_{VI}$	3.69
C(9)	$C(13)_{IV}$	3.88	C(14)	$C(18)_{VI}$	3.89
C(13)	$C(13)_{IV}$	3.63	C(14)	$O(1)_{VI}$	3.80
C(19)	$O(3)_{IV}$	3.79	C(15)	$C(18)_{VI}$	3.92
C(2)	$O(3)_{V}$	3.34	C(15)	$O(1)_{VI}$	3.60
C(1)	$O(3)_{V}$	3.50	C(6)	$C(6)_{VII}$	3.73
Br	$C(9)_{VI}$	3.77	C(6)	$C(7)_{VII}$	3.89

The subscripts refer to the following transformations of the atomic co-ordinates:

(I)	x, y, 1+z	(V)	-x, 1-y, -1-z
(II)	x, 1+y, 1+z	(VI)	1-x, 1-y, 1-z
(III)	x,-1+y, z	(VII)	1-x, 1-y, 1-z
(IV)	-x, 1-y, -z		

TABLE 23

2-(6'-methoxy-5'-bromo-2'-naphthyl)
-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-ether

Intermolecular contacts (Å) of less than 4 Å

Br	$C(18)_{I}$	3.91	Br	$C(9)_{VII}$	3.76
C(11)	$O(3)_{I}$	3.83	O(1)	$C(8)_{VII}$	3.83
Br	$O(2)_{II}$	3.70	O(1)	$C(14)_{VII}$	3.96
Br	$C(21)_{II}$	3.94	O(1)	$C(15)_{VII}$	3.56
O(1)	$O(3)_{II}$	3.94	C(1)	$C(6)_{VII}$	3.90
O(1)	$C(20)_{II}$	3.91	C(2)	$C(6)_{VII}$	3.82
O(1)	$C(21)_{II}$	3.80	C(2)	$C(7)_{VII}$	3.94
C(18)	$O(3)_{II}$	3.92	C(3)	$C(6)_{VII}$	3.95
O(2)	$C(18)_{III}$	3.50	C(3)	$C(7)_{VII}$	3.80
C(11)	$C(18)_{III}$	3.73	C(3)	$C(8)_{VII}$	3.90
O(3)	$C(19)_{IV}$	3.94	C(4)	$C(5)_{VII}$	3.92
C(3)	$C(21)_{IV}$	3.92	C(4)	$C(9)_{VII}$	3.86
C(4)	$C(21)_{IV}$	3.50	C(4)	$C(10)_{VII}$	3.78
C(5)	$C(21)_{IV}$	3.64	C(5)	$C(5)_{VII}$	3.74
C(9)	$C(13)_{IV}$	3.92	C(5)	$C(10)_{VII}$	3.84
C(13)	$C(13)_{IV}$	3.71	C(15)	$C(18)_{VII}$	3.89
C(19)	$C(19)_{V}$	3.95	C(6)	$C(6)_{VIII}$	3.72
O(3)	$C(1)_{VI}$	3.58	C(6)	$C(7)_{VIII}$	3.86
O(3)	$C(2)_{VI}$	3.40			

The subscripts refer to the following transformations of the atomic co-ordinates:

(I)	x, y, z - 1	(V)	- x, 1 - y, 1 - z
(II)	x, y - 1, z	(VI)	- x, 1 - y, - 1 - z
(III)	x, 1 + y, 1 + z	(VII)	1 - x, 1 - y, - z
(IV)	- x, 1 - y, - z	(VIII)	1 - x, 1 - y, 1 - z

2-(6'-methoxy-2'-naphthyl)-1-methyl-5-hydroxy-cyclopentane-ethanol

Table 24 Structure factor listings ($|F_o|$ and $|F_c|$ x 10)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	Fc	H	K	L	FO	FC	H	K	L	Fo	FC
21	2	1	32	32	19	1	-6	47	48	17	5	-1	30	33	17	0	6	68	69	16	2	-1	29	30
21	2	0	57	55	19	0	0	40	39	17	5	-2	42	44	17	0	4	35	41	16	2	-2	36	40
21	0	0	33	22	19	0	-6	57	59	17	5	-4	39	30	17	0	-2	69	87	16	2	-3	144	148
20	3	3	57	60	18	5	2	42	32	17	4	5	43	44	17	0	-4	64	71	16	2	-4	155	163
20	3	1	50	52	18	5	1	62	55	17	4	2	31	7	16	6	2	36	40	16	2	-8	40	36
20	3	-5	42	55	18	5	-3	43	32	17	4	-2	53	52	16	6	-2	47	40	16	2	-10	55	57
20	2	3	52	65	18	4	5	36	31	17	4	-4	33	33	16	5	0	32	31	16	2	-11	44	38
20	2	-4	32	20	18	4	2	36	29	17	4	-8	38	37	16	5	-1	29	12	16	1	5	124	133
20	2	-5	89	109	18	4	0	32	11	17	3	5	32	32	16	5	-2	36	24	16	1	4	31	22
20	2	-6	70	83	18	4	-1	39	32	17	3	3	84	90	16	5	-7	31	2	16	1	3	57	57
20	1	1	33	35	18	4	-2	41	38	17	3	2	43	48	16	4	6	68	73	16	1	0	93	95
20	1	-3	31	30	18	4	-3	30	40	17	3	1	31	28	16	4	-1	61	67	16	1	-2	29	20
20	1	-4	59	67	18	4	-6	37	34	17	3	0	38	40	16	4	-3	53	55	16	1	-8	41	36
20	1	-5	37	35	18	3	3	59	68	17	3	-3	107	112	16	4	-4	39	37	16	1	-9	44	45
20	1	-6	49	60	18	3	2	43	50	17	3	-5	85	85	16	4	-7	53	59	16	1	-10	41	43
20	1	-7	30	20	18	3	-4	92	97	17	2	9	67	72	16	3	5	37	31	16	1	-12	36	33
20	0	2	65	66	18	3	-5	55	52	17	2	8	44	44	16	3	4	56	63	16	0	6	30	19
20	0	0	69	78	18	2	4	59	54	17	2	4	131	136	16	3	3	75	73	16	0	4	44	44
19	3	3	64	73	18	2	3	73	86	17	2	3	92	96	16	3	2	32	44	16	0	2	104	108
19	3	2	32	44	18	2	2	63	57	17	2	2	73	77	16	3	1	39	28	16	0	-2	54	56
19	3	-4	33	32	18	2	-9	31	36	17	2	1	42	36	16	3	0	35	44	16	0	-4	34	37
19	3	-5	64	77	18	2	-4	98	99	17	2	0	34	28	16	3	-1	41	34	16	0	-6	54	51
19	2	4	33	32	18	2	-3	102	111	17	2	-2	50	51	16	3	-2	49	47	15	6	2	36	31
19	2	3	62	60	18	2	-5	70	70	17	2	-5	76	77	16	3	-3	82	82	15	6	-1	45	58
19	2	2	61	65	18	1	8	40	46	17	2	-6	34	35	16	3	-4	82	80	15	6	-2	42	37
19	2	-3	38	32	18	1	4	87	86	17	2	-10	50	56	16	3	-7	59	62	15	6	-3	30	20
19	2	-4	59	67	18	1	3	36	27	17	1	9	35	39	16	3	-8	64	63	15	6	-4	34	26
19	2	-5	34	39	18	1	1	29	26	17	1	4	50	59	16	3	-9	52	59	15	6	-5	52	46
19	2	-6	44	45	18	1	-3	74	87	17	1	3	42	39	16	3	-10	49	50	15	5	6	31	38
19	2	-8	34	23	18	1	-4	59	66	17	1	2	50	51	16	2	6	53	55	15	5	2	65	63
19	1	4	40	42	18	1	-5	79	94	17	1	1	28	4	16	2	5	93	101	15	5	-1	58	52
19	1	3	50	55	18	1	-6	30	29	17	1	-2	56	71	16	2	4	49	56	15	5	-5	38	39
19	1	2	77	88	18	0	4	78	84	17	1	-4	116	120	16	2	3	53	50	15	5	-7	38	48
19	1	1	54	50	18	0	2	36	40	17	1	-5	48	52	16	2	1	56	55	15	4	5	70	68
19	1	-5	44	43	18	0	-10	70	78	17	1	-9	39	41	16	2	0	31	31	15	4	4	32	23

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
15	4	1	60	64	15	1	-4	53	48	14	3	11	40	33	14	1	-2	77	77	13	4	0	137	133
15	4	-4	32	36	15	1	-7	45	43	14	3	7	54	58	14	1	-3	85	82	13	4	-1	82	75
15	4	-8	68	64	15	1	-9	62	70	14	3	6	66	70	14	1	-5	46	56	13	4	-2	91	102
15	4	-9	32	26	15	0	8	39	41	14	3	5	89	99	14	1	-6	52	60	13	4	-3	38	28
15	3	9	34	24	15	0	6	56	58	14	3	3	58	62	14	1	-7	35	21	13	4	-4	48	43
15	3	7	37	31	15	0	4	111	109	14	3	1	109	115	14	1	-9	49	51	13	4	-7	122	115
15	3	5	78	84	15	0	2	101	105	14	3	-1	136	133	14	0	10	30	23	13	4	-8	70	78
15	3	-2	58	68	15	0	0	64	53	14	3	-2	202	197	14	0	8	33	37	13	3	8	35	35
15	3	-4	101	106	15	0	-2	221	234	14	3	-3	137	132	14	0	6	330	336	13	3	6	83	84
15	3	-7	32	42	15	0	-4	43	39	14	3	-5	68	69	14	0	4	31	40	13	3	5	57	51
15	2	10	46	37	15	0	-6	39	40	14	3	-6	45	44	14	0	2	113	121	13	3	4	67	77
15	2	8	40	45	15	0	-12	44	35	14	3	-7	81	94	14	0	0	128	124	13	3	3	54	54
15	2	6	35	37	14	7	-2	36	15	14	2	11	51	51	14	0	-2	280	286	13	3	1	129	134
15	2	5	94	103	14	7	-3	60	52	14	2	10	49	48	14	0	-6	68	74	13	3	0	43	39
15	2	4	41	36	14	6	3	66	58	14	2	8	52	50	14	0	-8	199	203	13	3	-1	151	146
15	2	3	61	76	14	6	2	57	57	14	2	5	110	124	13	7	4	37	40	13	3	-3	208	212
15	2	2	53	59	14	6	1	41	38	14	2	4	165	180	13	7	1	71	63	13	3	-5	64	61
15	2	1	65	75	14	6	-2	40	38	14	2	2	29	35	13	7	-2	79	74	13	3	-7	103	110
15	2	0	69	71	14	6	-4	36	38	14	2	1	58	57	13	7	-3	65	61	13	3	-8	84	90
15	2	-1	41	41	14	6	-5	61	58	14	2	0	49	47	13	6	4	33	35	13	2	7	53	55
15	2	-2	32	9	14	5	2	49	45	14	2	-1	58	58	13	5	7	72	81	13	2	6	46	50
15	2	-3	68	69	14	5	-1	38	41	14	2	-2	76	75	13	5	3	32	29	13	2	5	53	57
15	2	-4	79	90	14	5	-3	38	43	14	2	-3	38	38	13	5	2	39	44	13	2	3	74	67
15	2	-5	35	39	14	5	-5	33	23	14	2	-4	61	66	13	5	1	73	62	13	2	2	66	65
15	2	-6	37	47	14	5	-7	66	77	14	2	-5	39	32	13	5	0	34	27	13	2	-1	44	47
15	1	10	38	29	14	4	8	41	40	14	2	-6	37	50	13	5	-1	47	44	13	2	-2	32	16
15	1	7	32	32	14	4	6	37	39	14	2	-9	30	28	13	5	-2	34	16	13	2	-3	98	103
15	1	6	55	49	14	4	3	58	59	14	2	-10	44	41	13	5	-3	30	24	13	2	-4	57	63
15	1	5	109	106	14	4	2	33	44	14	2	-13	32	3	13	5	-7	40	45	13	2	-5	42	37
15	1	4	256	267	14	4	1	130	133	14	1	10	31	29	13	5	-8	36	27	13	2	-6	40	49
15	1	2	41	38	14	4	-2	96	93	14	1	7	29	12	13	4	7	94	104	13	2	-8	81	87
15	1	1	56	71	14	4	-3	138	151	14	1	4	53	58	13	4	6	42	27	13	2	-9	57	56
15	1	0	85	90	14	4	-6	74	82	14	1	3	70	80	13	4	4	40	37	13	2	-13	40	33
15	1	-2	77	89	14	4	-7	52	66	14	1	0	44	43	13	4	3	63	74	13	1	12	58	54
15	1	-3	31	35	14	4	-11	33	16	14	1	-1	190	193	13	4	1	43	47	13	1	8	36	38

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
13	1	7	57	56	12	5	-1	135	130	12	2	11	30	11	12	1	-14	51	55	11	5	0	98	93
13	1	6	196	201	12	5	-2	72	64	12	2	8	44	45	12	0	10	30	41	11	5	-1	100	95
13	1	5	147	140	12	5	-3	41	31	12	2	7	64	68	12	0	6	157	163	11	5	-2	73	69
13	1	4	112	120	12	5	-9	36	47	12	2	6	62	67	12	0	4	115	125	11	5	-3	32	30
13	1	3	54	55	12	4	7	61	62	12	2	5	127	122	12	0	2	179	188	11	5	-4	40	36
13	1	-2	217	215	12	4	6	33	44	12	2	4	98	104	12	0	0	292	286	11	5	-5	40	40
13	1	-4	97	103	12	4	5	101	113	12	2	2	45	51	12	0	-2	136	142	11	5	-6	35	32
13	1	-6	54	61	12	4	3	43	41	12	2	-1	69	75	12	0	-4	77	51	11	5	-7	55	61
13	1	-7	78	78	12	4	2	32	31	12	2	-2	140	142	12	0	-6	311	310	11	5	-12	33	21
13	1	-8	107	107	12	4	1	95	89	12	2	-3	66	70	12	0	-8	65	60	11	4	11	31	22
13	1	-9	45	43	12	4	0	47	51	12	2	-4	29	37	12	0	-10	61	61	11	4	8	51	58
13	1	-14	35	26	12	4	-1	135	135	12	2	-5	88	90	12	0	-14	77	84	11	4	7	29	21
13	0	6	165	163	12	4	-2	78	66	12	2	-6	242	261	11	8	0	48	46	11	4	5	49	49
13	0	4	84	83	12	4	-4	62	62	12	2	-7	39	38	11	8	-1	49	43	11	4	2	59	62
13	0	0	39	44	12	4	-5	40	28	12	2	-9	30	6	11	7	4	32	9	11	4	0	206	209
13	0	-2	268	275	12	4	-6	69	78	12	2	-10	54	54	11	7	3	46	36	11	4	-2	202	202
13	0	-4	72	70	12	4	-7	29	38	12	2	-12	42	42	11	7	2	85	84	11	4	-3	30	27
13	0	-6	84	93	12	4	-8	75	80	12	2	-14	31	35	11	7	1	50	43	11	4	-5	65	70
13	0	-8	39	33	12	4	-9	71	71	12	1	13	30	19	11	7	-1	36	23	11	4	-6	113	121
13	0	-10	86	73	12	3	12	36	37	12	1	8	58	54	11	7	-2	68	51	11	4	-7	60	62
13	0	-14	60	60	12	3	11	30	32	12	1	7	223	236	11	7	-4	63	49	11	4	-8	47	50
12	7	5	32	3	12	3	8	36	32	12	1	6	34	30	11	7	-6	40	31	11	4	-10	35	20
12	7	4	35	35	12	3	6	85	100	12	1	5	131	138	11	6	8	33	28	11	4	-11	32	30
12	7	3	54	51	12	3	2	36	32	12	1	4	102	103	11	6	7	50	61	11	3	12	39	33
12	7	-1	35	23	12	3	0	59	55	12	1	3	54	49	11	6	2	44	43	11	3	10	30	24
12	7	-2	38	30	12	3	-1	101	102	12	1	2	70	74	11	6	1	41	29	11	3	9	31	30
12	6	7	33	42	12	3	-2	153	156	12	1	0	262	254	11	6	0	57	56	11	3	8	44	40
12	6	3	34	35	12	3	-3	60	52	12	1	-1	94	92	11	6	-1	37	31	11	3	5	127	139
12	6	1	84	74	12	3	-5	126	130	12	1	-2	66	60	11	6	-4	51	50	11	3	1	129	119
12	6	-2	53	45	12	3	-6	131	139	12	1	-3	80	75	11	6	-5	48	41	11	3	-2	117	120
12	6	-3	40	34	12	3	-7	61	67	12	1	-4	166	171	11	6	-6	35	15	11	3	-3	130	137
12	5	6	68	72	12	3	-8	74	79	12	1	-5	83	91	11	5	10	38	19	11	3	-4	50	61
12	5	5	44	47	12	3	-9	43	44	12	1	-7	97	96	11	5	5	32	43	11	3	-5	31	42
12	5	1	43	43	12	3	-10	48	47	12	1	-8	89	96	11	5	4	29	15	11	3	-6	121	123
12	5	0	54	56	12	3	-12	36	34	12	1	-12	33	33	11	5	3	35	37	11	3	-8	67	66

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
11	3	-13	77	81	11	1	-6	124	123	10	6	-10	53	51	10	3	4	111	114	10	1	8	298	306
11	3	-14	42	32	11	1	-7	88	87	10	5	9	35	29	10	3	3	151	150	10	1	7	95	96
11	2	12	67	62	11	1	-8	88	81	10	5	7	44	55	10	3	2	134	129	10	1	5	157	153
11	2	10	45	46	11	1	-10	66	75	10	5	5	121	131	10	3	1	130	134	10	1	4	49	52
11	2	8	83	93	11	1	-12	78	75	10	5	3	54	52	10	3	0	115	119	10	1	3	79	75
11	2	7	62	67	11	1	-13	35	43	10	5	1	29	25	10	3	-1	85	77	10	1	1	107	99
11	2	6	67	63	11	0	14	65	64	10	5	0	46	47	10	3	-2	66	69	10	1	0	30	14
11	2	5	94	96	11	0	12	54	47	10	5	-1	204	204	10	3	-3	46	55	10	1	-1	104	114
11	2	4	63	65	11	0	10	44	41	10	5	-2	95	88	10	3	-4	273	262	10	1	-2	168	181
11	2	2	75	77	11	0	8	61	50	10	5	-3	67	72	10	3	-5	209	214	10	1	-3	88	101
11	2	1	120	123	11	0	6	302	302	10	5	-4	87	86	10	3	-8	42	39	10	1	-4	83	82
11	2	0	101	116	11	0	4	278	284	10	5	-5	60	62	10	3	-9	47	50	10	1	-5	89	97
11	2	-2	73	71	11	0	2	174	171	10	5	-7	41	43	10	3	-10	41	31	10	1	-6	52	46
11	2	-4	95	94	11	0	0	411	402	10	5	-11	45	45	10	3	-13	34	24	10	1	-8	33	31
11	2	-5	111	107	11	0	-2	314	314	10	4	12	32	27	10	2	13	32	19	10	1	-9	63	65
11	2	-6	88	91	11	0	-4	97	96	10	4	11	38	23	10	2	10	69	75	10	1	-10	66	76
11	2	-7	79	77	11	0	-6	300	305	10	4	9	49	55	10	2	9	42	36	10	1	-12	48	64
11	2	-8	43	53	11	0	-8	86	78	10	4	8	38	39	10	2	8	65	66	10	1	-13	118	112
11	2	-10	90	92	11	0	-12	45	54	10	4	7	157	176	10	2	7	70	79	10	0	14	62	49
11	2	-13	58	60	11	0	-14	52	51	10	4	5	42	45	10	2	6	180	177	10	0	8	355	353
11	1	14	57	57	10	8	2	42	38	10	4	4	95	104	10	2	5	61	62	10	0	6	105	107
11	1	9	41	43	10	8	1	44	40	10	4	3	89	82	10	2	4	28	21	10	0	4	80	86
11	1	8	43	48	10	8	-1	34	27	10	4	2	90	87	10	2	2	260	249	10	0	2	235	245
11	1	7	173	169	10	8	-2	44	32	10	4	1	52	57	10	2	-2	261	264	10	0	0	497	478
11	1	6	134	138	10	8	-3	36	6	10	4	0	199	188	10	2	-5	185	177	10	0	-2	112	100
11	1	5	65	65	10	7	4	36	30	10	4	-1	174	167	10	2	-6	118	99	10	0	-4	130	132
11	1	4	154	152	10	7	2	53	47	10	4	-2	37	25	10	2	-7	39	30	10	0	-6	123	114
11	1	3	101	105	10	7	-1	74	66	10	4	-3	50	50	10	2	-8	72	77	10	0	-8	32	36
11	1	2	56	57	10	7	-3	30	32	10	4	-5	76	81	10	2	-10	33	40	10	0	-10	47	59
11	1	1	138	135	10	7	-5	32	18	10	4	-7	33	37	10	2	-11	53	72	10	0	-12	76	77
11	1	0	146	151	10	7	-8	57	43	10	3	9	41	47	10	2	-12	79	86	10	0	-14	98	100
11	1	-1	269	267	10	6	5	31	23	10	3	8	76	77	10	2	-13	92	89	9	8	1	36	21
11	1	-2	79	86	10	6	1	35	37	10	3	7	38	31	10	2	-14	32	27	9	8	0	47	37
11	1	-4	173	178	10	6	-3	53	53	10	3	6	54	60	10	1	12	32	6	9	8	-1	62	57
11	1	-5	89	90	10	6	-4	86	83	10	3	5	85	81	10	1	10	49	37	9	8	-3	48	46

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
9	8	-4	35	26	9	4	6	127	136	9	2	5	55	54	9	1	-12	62	66	8	5	6	33	32
9	7	3	89	84	9	4	4	50	51	9	2	4	62	53	9	0	8	416	410	8	5	5	79	75
9	7	1	36	22	9	4	2	133	126	9	2	3	43	47	9	0	6	220	224	8	5	4	173	176
9	7	-1	55	48	9	4	0	84	82	9	2	2	122	111	9	0	4	84	69	8	5	3	39	42
9	7	-2	31	24	9	4	-1	212	210	9	2	1	168	153	9	0	2	122	108	8	5	1	350	341
9	7	-4	66	71	9	4	-2	94	82	9	2	0	133	127	9	0	0	253	231	8	5	0	238	229
9	7	-8	32	36	9	4	-3	38	39	9	2	-1	77	70	9	0	-2	366	356	8	5	-1	117	118
9	7	-9	42	42	9	4	-5	96	88	9	2	-2	110	115	9	0	-6	138	137	8	5	-2	53	52
9	6	4	45	40	9	4	-6	36	46	9	2	-4	93	93	9	0	-10	96	100	8	5	-5	29	35
9	6	3	121	110	9	4	-9	69	62	9	2	-5	67	72	9	0	-12	43	46	8	5	-7	50	72
9	6	2	52	45	9	4	-10	54	48	9	2	-6	156	142	8	8	5	32	36	8	4	11	37	38
9	6	1	149	152	9	4	-13	60	59	9	2	-7	52	37	8	8	3	40	36	8	4	9	34	30
9	6	0	35	28	9	3	13	30	26	9	2	-10	70	66	8	8	2	45	34	8	4	8	48	55
9	6	-1	39	37	9	3	9	30	37	9	2	-11	56	68	8	8	1	38	31	8	4	7	94	110
9	6	-3	55	50	9	3	8	137	141	9	2	-12	45	48	8	8	0	45	43	8	4	6	51	60
9	6	-6	53	61	9	3	7	147	155	9	2	-13	32	16	8	8	-3	41	44	8	4	5	42	46
9	6	-7	53	62	9	3	5	108	126	9	2	-14	43	37	8	8	-5	32	17	8	4	4	63	56
9	6	-8	30	21	9	3	4	112	121	9	1	10	98	106	8	7	4	30	7	8	4	2	38	36
9	6	-11	42	44	9	3	3	49	60	9	1	9	37	25	8	7	3	30	8	8	4	1	133	144
9	5	8	34	38	9	3	2	154	135	9	1	8	169	176	8	7	2	76	68	8	4	0	64	69
9	5	7	46	59	9	3	1	171	162	9	1	7	251	261	8	7	1	30	34	8	4	-1	86	90
9	5	6	57	57	9	3	-1	139	133	9	1	6	128	126	8	7	0	69	65	8	4	-2	194	173
9	5	5	32	42	9	3	-3	114	115	9	1	5	75	70	8	7	-5	34	32	8	4	-3	62	60
9	5	4	75	70	9	3	-4	124	120	9	1	4	33	43	8	7	-9	44	37	8	4	-5	34	15
9	5	1	52	49	9	3	-5	365	358	9	1	3	102	90	8	6	6	39	43	8	4	-6	45	31
9	5	-1	54	52	9	3	-6	205	216	9	1	1	48	41	8	6	4	64	64	8	4	-7	114	111
9	5	-4	49	46	9	3	-7	44	41	9	1	0	111	110	8	6	3	88	85	8	4	-11	33	40
9	5	-5	49	43	9	3	-10	66	84	9	1	-1	97	96	8	6	1	68	58	8	3	9	69	62
9	5	-6	36	48	9	3	-11	95	95	9	1	-2	56	67	8	6	0	170	158	8	3	7	43	42
9	5	-11	34	26	9	3	-12	63	61	9	1	-4	151	146	8	6	-1	113	113	8	3	6	51	45
9	5	-12	40	47	9	2	14	39	33	9	1	-5	157	160	8	6	-3	54	42	8	3	4	148	155
9	4	13	63	56	9	2	11	47	48	9	1	-6	93	78	8	6	-7	54	60	8	3	3	66	45
9	4	10	38	29	9	2	8	101	103	9	1	-7	127	125	8	6	-11	34	27	8	3	1	123	121
9	4	9	66	79	9	2	7	67	69	9	1	-10	83	97	8	5	8	64	71	8	3	0	125	139
9	4	8	35	30	9	2	6	120	129	9	1	-11	30	33	8	5	7	41	52	8	3	-2	57	66

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
8	3	-3	106	104	8	2	-14	30	24	7	8	-3	33	35	7	4	9	45	45	7	2	1	42	42
8	3	-4	110	99	8	1	12	30	35	7	8	-4	33	14	7	4	7	69	67	7	2	0	153	146
8	3	-5	46	43	8	1	10	95	103	7	7	7	45	65	7	4	3	82	71	7	2	-1	175	158
8	3	-6	29	35	8	1	9	211	224	7	7	4	115	120	7	4	1	52	42	7	2	-3	66	75
8	3	-7	38	39	8	1	5	111	107	7	7	2	88	80	7	4	0	302	296	7	2	-4	528	515
8	3	-8	36	48	8	1	4	29	22	7	7	-6	34	39	7	4	-1	132	127	7	2	-5	164	164
8	3	-9	50	46	8	1	3	116	104	7	6	9	44	51	7	4	-2	37	33	7	2	-6	37	33
8	3	-10	57	60	8	1	2	509	480	7	6	5	56	47	7	4	-3	35	14	7	2	-7	71	78
8	3	-11	93	103	8	1	-1	309	305	7	6	4	125	123	7	4	-4	153	145	7	2	-8	45	45
8	3	-12	61	65	8	1	-2	36	31	7	6	3	108	105	7	4	-5	97	91	7	2	-10	46	55
8	3	-13	40	25	8	1	-3	275	244	7	6	2	76	77	7	4	-6	124	120	7	2	-11	97	92
8	2	15	30	25	8	1	-4	446	430	7	6	1	166	150	7	4	-7	46	49	7	2	-12	42	39
8	2	12	44	37	8	1	-5	208	211	7	6	0	96	88	7	4	-8	65	79	7	2	-13	65	60
8	2	11	88	90	8	1	-6	67	49	7	6	-1	170	153	7	4	-9	36	45	7	1	15	46	37
8	2	10	55	63	8	1	-7	40	41	7	6	-2	107	91	7	3	10	76	87	7	1	14	34	21
8	2	9	116	117	8	1	-8	51	52	7	6	-3	138	130	7	3	8	42	49	7	1	12	51	50
8	2	8	44	48	8	1	-9	48	47	7	6	-5	59	55	7	3	7	116	116	7	1	10	41	40
8	2	6	147	142	8	1	-10	42	39	7	6	-10	39	35	7	3	5	36	40	7	1	9	159	163
8	2	4	164	165	8	1	-12	72	69	7	6	-11	36	43	7	3	4	44	41	7	1	8	128	126
8	2	3	381	359	8	1	-13	46	47	7	5	6	62	69	7	3	3	229	223	7	1	7	144	145
8	2	2	216	200	8	0	14	33	27	7	5	5	98	103	7	3	2	125	120	7	1	6	53	41
8	2	1	331	318	8	0	8	327	340	7	5	3	32	36	7	3	1	150	138	7	1	4	124	124
8	2	0	61	45	8	0	6	185	173	7	5	2	126	120	7	3	0	103	108	7	1	3	173	169
8	2	-1	92	77	8	0	4	259	250	7	5	1	240	241	7	3	-1	71	84	7	1	2	106	94
8	2	-2	110	112	8	0	2	79	83	7	5	0	92	86	7	3	-2	180	170	7	1	1	716	709
8	2	-3	259	247	8	0	0	266	266	7	5	-2	145	139	7	3	-3	125	109	7	1	0	134	124
8	2	-4	350	354	8	0	-2	305	289	7	5	-3	183	189	7	3	-5	28	20	7	1	-1	257	249
8	2	-5	258	256	8	0	-4	241	252	7	5	-4	105	109	7	3	-15	41	37	7	1	-2	241	249
8	2	-7	73	80	8	0	-6	30	27	7	5	-6	80	82	7	2	11	75	75	7	1	-3	416	394
8	2	-8	91	97	8	0	-10	67	75	7	5	-8	32	36	7	2	10	157	165	7	1	-4	36	43
8	2	-9	46	56	8	0	-16	44	31	7	5	-9	56	56	7	2	9	154	162	7	1	-5	42	53
8	2	-10	111	121	7	8	2	59	52	7	5	-10	62	68	7	2	8	112	116	7	1	-6	160	151
8	2	-11	120	125	7	8	1	33	33	7	4	12	46	32	7	2	7	84	91	7	1	-7	139	132
8	2	-12	145	135	7	8	0	64	58	7	4	11	47	50	7	2	3	100	83	7	1	-9	96	96
8	2	-13	33	19	7	8	-1	30	24	7	4	10	32	38	7	2	2	159	154	7	1	-10	88	85

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	Fc	H	K	L	FO	Fc	H	K	L	FO	FC	H	K	L	FO	FC
7	1	-11	53	59	6	5	1	200	185	6	3	6	54	50	6	2	-8	86	93	6	0	-4	105	94
7	1	-12	80	78	6	5	0	92	87	6	3	5	48	32	6	2	-11	147	149	6	0	-6	86	100
7	1	-13	46	46	6	5	-2	221	194	6	3	4	112	105	6	2	-12	79	75	6	0	-8	131	122
7	0	12	51	42	6	5	-3	46	36	6	3	3	228	221	6	2	-13	48	39	6	0	-10	198	205
7	0	10	42	41	6	5	-4	86	77	6	3	2	104	99	6	2	-14	42	42	6	0	-12	90	82
7	0	8	136	132	6	5	-5	35	34	6	3	1	259	245	6	1	14	58	56	5	8	-3	45	37
7	0	6	487	462	6	5	-6	108	119	6	3	0	199	197	6	1	10	235	238	5	8	-4	31	28
7	0	4	118	98	6	5	-7	45	47	6	3	-1	31	28	6	1	9	148	150	5	8	-6	48	42
7	0	2	198	175	6	5	-8	96	101	6	3	-2	342	316	6	1	8	64	80	5	7	6	32	35
7	0	0	333	332	6	5	-9	74	81	6	3	-3	255	243	6	1	7	106	108	5	7	3	70	78
7	0	-2	480	467	6	4	13	39	32	6	3	-4	94	82	6	1	6	40	39	5	7	2	91	88
7	0	-4	333	331	6	4	11	74	76	6	3	-5	58	53	6	1	5	107	93	5	7	1	49	45
7	0	-6	53	50	6	4	9	105	112	6	3	-6	84	76	6	1	4	206	203	5	7	-2	71	70
7	0	-8	126	109	6	4	8	47	58	6	3	-7	69	67	6	1	3	91	99	5	7	-7	42	47
7	0	-12	58	56	6	4	7	39	41	6	3	-8	38	39	6	1	2	135	118	5	7	-10	48	54
7	0	-14	63	56	6	4	6	57	55	6	3	-9	122	133	6	1	1	151	136	5	6	12	56	50
6	8	5	37	40	6	4	5	120	121	6	3	-10	60	56	6	1	0	350	327	5	6	11	36	25
6	8	4	39	32	6	4	4	120	121	6	3	-11	34	28	6	1	-1	317	297	5	6	8	31	34
6	8	1	32	33	6	4	3	57	49	6	3	-12	43	44	6	1	-3	469	443	5	6	6	58	68
6	8	-3	49	38	6	4	2	97	101	6	2	14	31	22	6	1	-4	362	340	5	6	5	225	230
6	7	7	57	56	6	4	1	127	118	6	2	13	46	43	6	1	-5	54	41	5	6	4	39	51
6	7	-2	45	33	6	4	0	97	89	6	2	10	85	93	6	1	-6	45	47	5	6	3	116	124
6	7	-3	60	52	6	4	-1	35	36	6	2	9	155	159	6	1	-7	207	191	5	6	0	62	62
6	7	-5	38	35	6	4	-2	271	257	6	2	8	58	64	6	1	-8	39	40	5	6	-1	88	77
6	6	8	61	68	6	4	-3	50	54	6	2	7	126	130	6	1	-9	110	114	5	6	-2	76	78
6	6	6	46	56	6	4	-5	51	51	6	2	6	133	134	6	1	-10	54	73	5	6	-3	61	58
6	6	2	88	82	6	4	-6	131	142	6	2	5	55	49	6	1	-12	92	89	5	6	-5	97	104
6	6	0	87	90	6	4	-7	57	73	6	2	4	528	504	6	0	16	33	21	5	6	-6	84	86
6	6	-1	58	47	6	4	-8	33	43	6	2	3	366	346	6	0	10	104	90	5	6	-9	50	57
6	6	-2	73	66	6	4	-10	44	40	6	2	-1	46	29	6	0	8	215	216	5	5	13	33	27
6	6	-3	34	33	6	4	-12	35	50	6	2	-2	367	338	6	0	6	49	39	5	5	10	41	31
6	6	-5	58	69	6	3	15	38	31	6	2	-3	866	885	6	0	4	38	30	5	5	9	54	56
6	6	-6	106	118	6	3	11	89	84	6	2	-4	433	429	6	0	2	501	473	5	5	8	28	29
6	5	3	52	53	6	3	9	148	159	6	2	-5	42	27	6	0	0	441	429	5	5	7	63	67
6	5	2	218	215	6	3	7	35	50	6	2	-6	138	136	6	0	-2	253	239	5	5	5	83	90

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	5	4	133	141	5	3	2	96	85	5	1	16	36	27	4	8	-6	54	58	4	5	-6	84	98
5	5	3	43	46	5	3	1	265	248	5	1	13	35	33	4	7	8	41	41	4	5	-7	126	143
5	5	2	39	46	5	3	0	136	121	5	1	11	126	123	4	7	5	31	22	4	5	-10	31	52
5	5	1	42	40	5	3	-1	71	69	5	1	10	77	81	4	7	4	55	51	4	4	13	35	35
5	5	0	164	150	5	3	-2	246	236	5	1	9	201	206	4	7	2	87	91	4	4	11	33	26
5	5	-1	108	86	5	3	-3	501	476	5	1	8	34	36	4	7	1	53	52	4	4	10	38	37
5	5	-2	44	27	5	3	-4	66	75	5	1	6	74	70	4	7	-5	40	36	4	4	7	44	47
5	5	-3	133	119	5	3	-6	110	89	5	1	5	64	77	4	7	-6	37	36	4	4	6	79	80
5	5	-4	68	67	5	3	-7	237	240	5	1	4	247	235	4	7	-7	35	48	4	4	5	45	41
5	5	-6	63	72	5	3	-8	42	30	5	1	3	226	228	4	7	-8	33	34	4	4	4	27	22
5	5	-7	100	112	5	3	-9	217	229	5	1	2	117	115	4	7	-10	39	42	4	4	3	63	61
5	5	-8	60	74	5	3	-10	176	184	5	1	1	247	235	4	6	11	32	18	4	4	2	226	207
5	4	11	30	24	5	2	15	46	44	5	1	0	391	376	4	6	10	66	70	4	4	1	130	134
5	4	10	54	52	5	2	14	30	30	5	1	-1	282	267	4	6	8	37	40	4	4	0	141	122
5	4	9	50	57	5	2	11	43	57	5	1	-2	178	171	4	6	6	45	46	4	4	-1	267	231
5	4	8	128	136	5	2	10	33	18	5	1	-3	179	152	4	6	5	35	21	4	4	-2	147	148
5	4	5	31	19	5	2	9	58	69	5	1	-4	280	266	4	6	4	125	136	4	4	-3	152	143
5	4	4	66	62	5	2	8	49	55	5	1	-5	34	37	4	6	3	171	166	4	4	-4	36	38
5	4	3	30	32	5	2	7	150	135	5	1	-6	52	36	4	6	2	252	254	4	4	-5	119	117
5	4	2	56	57	5	2	5	97	86	5	1	-7	93	88	4	6	1	108	116	4	4	-7	145	152
5	4	1	107	98	5	2	4	95	100	5	1	-8	103	103	4	6	0	39	40	4	4	-9	130	138
5	4	0	191	178	5	2	2	283	263	5	1	-9	97	112	4	6	-1	114	102	4	4	-11	63	66
5	4	-1	50	44	5	2	1	54	52	5	1	-10	134	120	4	6	-3	40	38	4	4	-14	63	59
5	4	-2	37	30	5	2	0	29	41	5	1	-15	38	32	4	6	-4	84	83	4	4	-15	38	41
5	4	-3	139	123	5	2	-1	192	183	5	0	12	72	84	4	6	-6	67	64	4	3	11	188	198
5	4	-5	65	67	5	2	-2	219	204	5	0	2	86	74	4	5	9	53	49	4	3	10	117	109
5	4	-6	79	80	5	2	-3	53	61	5	0	0	566	563	4	5	8	68	77	4	3	9	28	33
5	4	-7	107	126	5	2	-4	582	569	5	0	-2	394	379	4	5	7	116	122	4	3	7	56	75
5	4	-9	54	55	5	2	-5	99	98	5	0	-4	245	228	4	5	6	121	131	4	3	6	48	52
5	4	-10	137	150	5	2	-7	60	58	5	0	-8	85	92	4	5	5	53	55	4	3	5	59	53
5	3	10	100	109	5	2	-9	83	74	4	9	1	37	35	4	5	3	87	84	4	3	4	147	136
5	3	9	103	113	5	2	-10	114	109	4	9	-2	31	11	4	5	2	163	159	4	3	3	165	162
5	3	5	55	59	5	2	-12	42	44	4	8	6	35	28	4	5	1	64	61	4	3	2	43	41
5	3	4	270	254	5	2	-13	53	43	4	8	-3	29	12	4	5	0	174	170	4	3	1	219	203
5	3	3	66	73	5	2	-15	40	24	4	8	-4	41	28	4	5	-5	100	106	4	3	0	64	54

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	3	-1	330	293	4	2	-12	34	24	3	9	1	46	32	3	6	-6	50	57	3	4	-9	66	82
4	3	-2	42	39	4	2	-13	31	34	3	9	-1	36	35	3	6	-11	32	26	3	3	15	58	48
4	3	-3	106	89	4	2	-14	57	50	3	8	7	32	29	3	5	13	45	31	3	3	14	46	38
4	3	-4	79	74	4	1	13	51	39	3	8	6	51	48	3	5	10	49	46	3	3	11	39	45
4	3	-5	112	117	4	1	12	86	82	3	8	4	31	46	3	5	8	48	51	3	3	9	126	127
4	3	-6	97	95	4	1	9	58	51	3	8	1	86	90	3	5	7	77	80	3	3	8	114	112
4	3	-7	97	96	4	1	4	71	59	3	8	-2	30	9	3	5	6	180	178	3	3	7	146	151
4	3	-8	74	60	4	1	3	368	356	3	8	-3	39	36	3	5	5	41	35	3	3	6	55	64
4	3	-9	78	72	4	1	2	173	165	3	8	-6	34	29	3	5	4	39	43	3	3	5	197	208
4	3	-10	167	176	4	1	1	318	302	3	8	-7	31	38	3	5	1	107	106	3	3	4	34	34
4	3	-11	79	77	4	1	0	85	75	3	8	-8	31	34	3	5	0	51	42	3	3	3	152	140
4	3	-15	37	15	4	1	-1	777	840	3	7	9	38	28	3	5	-1	431	384	3	3	2	79	84
4	3	-16	44	36	4	1	-3	575	556	3	7	8	56	63	3	5	-2	155	139	3	3	1	118	107
4	2	14	42	24	4	1	-4	82	85	3	7	7	43	47	3	5	-3	74	74	3	3	-1	240	229
4	2	12	61	48	4	1	-5	118	125	3	7	5	44	38	3	5	-5	64	81	3	3	-2	260	231
4	2	11	100	109	4	1	-7	83	82	3	7	4	90	104	3	5	-6	89	101	3	3	-3	300	304
4	2	10	48	41	4	1	-8	84	81	3	7	2	69	76	3	5	-9	71	84	3	3	-4	172	162
4	2	8	208	206	4	1	-9	207	208	3	7	-4	40	43	3	5	-10	50	55	3	3	-5	164	175
4	2	7	98	101	4	1	-13	105	96	3	7	-7	30	25	3	5	-11	38	38	3	3	-6	61	72
4	2	6	190	182	4	1	-14	30	9	3	7	-8	32	41	3	4	11	35	25	3	3	-7	96	96
4	2	5	302	302	4	1	-16	54	36	3	7	-11	52	45	3	4	10	37	47	3	3	-8	62	73
4	2	4	227	208	4	0	16	38	26	3	6	11	42	44	3	4	8	82	77	3	3	-9	210	215
4	2	3	348	322	4	0	14	46	33	3	6	10	45	44	3	4	7	152	150	3	3	-10	96	100
4	2	2	123	118	4	0	12	91	92	3	6	7	51	64	3	4	6	155	162	3	3	-11	64	62
4	2	-1	427	394	4	0	10	55	49	3	6	6	115	120	3	4	5	29	28	3	3	-13	88	82
4	2	-2	147	135	4	0	8	62	69	3	6	5	53	61	3	4	4	83	81	3	2	16	45	29
4	2	-3	275	261	4	0	6	58	53	3	6	4	45	45	3	4	3	135	130	3	2	13	63	62
4	2	-4	210	228	4	0	4	230	215	3	6	3	133	131	3	4	2	84	84	3	2	12	124	129
4	2	-5	44	48	4	0	2	540	512	3	6	1	116	121	3	4	1	155	145	3	2	11	198	205
4	2	-6	56	59	4	0	0	261	250	3	6	0	30	3	3	4	0	96	75	3	2	10	256	265
4	2	-7	143	154	4	0	-4	347	333	3	6	-1	151	135	3	4	-2	92	53	3	2	8	143	125
4	2	-8	52	45	4	0	-6	288	267	3	6	-2	55	50	3	4	-3	38	26	3	2	7	80	90
4	2	-9	240	236	4	0	-8	55	56	3	6	-3	130	124	3	4	-6	66	80	3	2	5	269	252
4	2	-10	209	205	4	0	-10	208	181	3	6	-4	48	43	3	4	-7	145	160	3	2	4	253	244
4	2	-11	75	75	4	0	-16	61	45	3	6	-5	50	53	3	4	-8	161	183	3	2	3	184	182

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	2	2	28	32	3	1	-7	26	31	2	7	2	61	70	2	4	15	34	29	2	3	-3	545	588
3	2	1	208	189	3	1	-8	92	103	2	7	1	44	49	2	4	11	42	43	2	3	-5	61	73
3	2	0	485	459	3	1	-9	30	31	2	7	0	64	57	2	4	10	77	75	2	3	-6	100	96
3	2	-1	265	245	3	1	-10	55	63	2	7	-1	66	67	2	4	9	81	85	2	3	-7	31	35
3	2	-2	694	700	3	1	-11	100	102	2	7	-3	64	61	2	4	8	39	40	2	3	-8	55	60
3	2	-3	112	116	3	1	-12	67	74	2	7	-5	78	86	2	4	7	282	277	2	3	-9	60	68
3	2	-4	268	265	3	1	-13	35	32	2	6	8	42	43	2	4	5	102	87	2	3	-11	59	67
3	2	-5	91	89	3	1	-14	57	47	2	6	6	36	40	2	4	4	208	213	2	3	-12	71	75
3	2	-6	163	149	3	0	16	30	17	2	6	4	149	161	2	4	2	184	175	2	3	-14	79	72
3	2	-7	144	155	3	0	12	68	60	2	6	3	113	119	2	4	1	101	98	2	3	-16	42	36
3	2	-8	115	122	3	0	10	90	93	2	6	1	110	124	2	4	0	211	199	2	2	12	90	87
3	2	-9	109	104	3	0	8	323	296	2	6	0	62	53	2	4	-1	87	75	2	2	11	146	151
3	2	-10	150	165	3	0	6	61	45	2	6	-1	35	29	2	4	-2	67	66	2	2	10	90	89
3	2	-11	55	47	3	0	4	834	857	2	6	-2	47	45	2	4	-3	59	67	2	2	9	57	54
3	2	-12	89	83	3	0	2	385	366	2	6	-3	74	66	2	4	-5	33	39	2	2	8	105	104
3	2	-13	95	85	3	0	0	215	202	2	6	-5	60	78	2	4	-6	114	123	2	2	7	109	110
3	2	-16	66	59	3	0	-2	240	227	2	6	-6	50	54	2	4	-9	132	139	2	2	6	32	25
3	1	14	38	14	3	0	-4	820	798	2	5	11	54	63	2	4	-11	42	33	2	2	5	118	114
3	1	13	30	11	3	0	-6	449	444	2	5	10	41	43	2	4	-13	69	66	2	2	4	213	223
3	1	12	29	23	3	0	-14	152	129	2	5	9	47	51	2	4	-14	46	45	2	2	3	178	177
3	1	10	251	241	2	9	2	31	41	2	5	8	118	123	2	3	14	42	41	2	2	2	91	81
3	1	9	99	96	2	9	-3	32	9	2	5	7	101	112	2	3	12	88	85	2	2	1	139	132
3	1	8	122	119	2	8	5	41	36	2	5	6	62	62	2	3	11	104	103	2	2	0	695	663
3	1	6	220	195	2	8	3	69	72	2	5	4	69	69	2	3	10	106	114	2	2	-1	595	565
3	1	5	274	266	2	8	2	36	37	2	5	3	112	119	2	3	8	90	91	2	2	-2	329	340
3	1	4	33	35	2	8	1	60	71	2	5	1	31	27	2	3	7	238	240	2	2	-3	107	99
3	1	3	172	167	2	8	-1	34	8	2	5	0	66	56	2	3	6	102	103	2	2	-4	226	238
3	1	2	429	422	2	8	-3	31	21	2	5	-1	185	163	2	3	5	387	389	2	2	-5	78	61
3	1	1	235	237	2	8	-4	34	31	2	5	-3	85	86	2	3	4	246	236	2	2	-6	110	120
3	1	0	374	352	2	8	-5	56	61	2	5	-4	51	47	2	3	3	77	66	2	2	-7	70	76
3	1	-2	620	655	2	7	10	35	20	2	5	-5	31	24	2	3	2	24	36	2	2	-8	189	200
3	1	-3	585	597	2	7	9	38	32	2	5	-6	62	64	2	3	1	201	183	2	2	-9	67	70
3	1	-4	60	56	2	7	8	48	52	2	5	-7	65	79	2	3	0	305	285	2	2	-11	58	56
3	1	-5	58	58	2	7	4	68	85	2	5	-8	65	78	2	3	-1	247	223	2	2	-13	45	47
3	1	-6	57	38	2	7	3	82	98	2	5	-11	45	37	2	3	-2	482	475	2	2	-14	54	53

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	2	-15	31	16	1	9	-4	31	24	1	5	-5	75	102	1	3	0	288	265	1	2	-8	151	151
2	2	-16	70	55	1	8	8	47	44	1	5	-8	107	126	1	3	-1	321	280	1	2	-10	28	24
2	1	7	125	118	1	8	3	38	58	1	5	-11	35	40	1	3	-2	261	278	1	2	-11	54	55
2	1	6	526	489	1	8	-2	69	58	1	4	14	58	51	1	3	-3	293	334	1	2	-12	151	158
2	1	4	38	40	1	8	-3	74	70	1	4	13	69	65	1	3	-4	147	160	1	2	-13	29	21
2	1	3	127	119	1	8	-6	57	75	1	4	11	35	44	1	3	-5	243	295	1	1	15	40	28
2	1	2	67	52	1	7	9	64	71	1	4	10	33	31	1	3	-6	107	119	1	1	13	125	117
2	1	0	514	477	1	7	7	31	21	1	4	9	45	48	1	3	-7	163	182	1	1	12	119	105
2	1	-2	232	229	1	7	6	52	54	1	4	8	74	75	1	3	-8	176	197	1	1	11	88	86
2	1	-3	64	55	1	7	5	58	56	1	4	7	84	93	1	3	-10	113	125	1	1	10	99	96
2	1	-4	53	73	1	7	4	74	97	1	4	6	155	169	1	3	-12	67	75	1	1	8	30	28
2	1	-5	63	59	1	7	2	42	46	1	4	5	33	25	1	3	-14	50	56	1	1	7	64	64
2	1	-6	234	231	1	7	0	38	45	1	4	4	76	72	1	3	-15	46	31	1	1	6	247	253
2	1	-7	85	80	1	7	-2	34	10	1	4	3	83	78	1	3	-16	61	53	1	1	5	217	220
2	1	-8	31	21	1	7	-6	73	94	1	4	2	227	241	1	2	16	35	33	1	1	4	359	364
2	1	-9	78	69	1	7	-9	43	54	1	4	1	131	128	1	2	13	31	26	1	1	3	502	502
2	1	-10	150	154	1	6	9	52	53	1	4	0	72	57	1	2	12	31	30	1	1	2	839	998
2	1	-13	31	34	1	6	8	69	78	1	4	-1	393	356	1	2	11	83	85	1	1	1	166	159
2	1	-14	100	90	1	6	7	124	151	1	4	-2	125	113	1	2	10	56	54	1	1	-1	617	725
2	0	14	29	28	1	6	5	34	32	1	4	-3	163	185	1	2	9	35	35	1	1	-2	542	597
2	0	12	112	98	1	6	4	34	24	1	4	-8	285	312	1	2	8	140	135	1	1	-3	158	161
2	0	10	80	72	1	6	3	38	55	1	4	-10	78	77	1	2	7	32	28	1	1	-4	381	397
2	0	8	152	164	1	6	1	35	42	1	4	-12	29	13	1	2	6	252	246	1	1	-5	69	69
2	0	6	883	862	1	6	-2	95	96	1	4	-13	52	46	1	2	5	65	66	1	1	-6	77	74
2	0	4	252	246	1	6	-3	43	48	1	3	13	82	81	1	2	4	193	181	1	1	-7	335	335
2	0	2	77	74	1	5	13	42	25	1	3	12	60	64	1	2	2	308	307	1	1	-8	236	219
2	0	0	338	334	1	5	7	220	240	1	3	9	66	72	1	2	1	159	160	1	1	-9	86	80
2	0	-2	704	769	1	5	6	92	102	1	3	8	106	110	1	2	0	502	464	1	1	-10	144	138
2	0	-4	567	548	1	5	5	32	44	1	3	7	96	108	1	2	-1	170	162	1	1	-12	35	45
2	0	-6	351	334	1	5	3	91	103	1	3	6	101	111	1	2	-2	127	141	1	1	-13	103	94
2	0	-8	680	646	1	5	2	141	157	1	3	5	55	67	1	2	-3	199	224	1	1	-14	37	36
2	0	-10	117	102	1	5	0	85	82	1	3	4	99	111	1	2	-4	232	243	1	1	-15	39	27
2	0	-12	75	79	1	5	-1	255	232	1	3	3	183	181	1	2	-5	129	138	1	0	14	60	50
1	9	1	42	55	1	5	-2	28	27	1	3	2	259	260	1	2	-6	118	130	1	0	12	60	52
1	9	-3	39	30	1	5	-3	78	83	1	3	1	27	15	1	2	-7	27	29	1	0	10	127	129

Table 24 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	0	8	195	182	0	4	6	34	46	0	1	5	338	335										
1	0	6	115	114	0	4	5	122	121	0	1	4	157	162										
1	0	4	283	297	0	4	4	108	116	0	1	3	70	76										
1	0	0	293	280	0	4	3	201	230	0	1	2	414	448										
1	0	-2	396	377	0	4	2	66	77	0	1	1	290	322										
1	0	-4	399	364	0	4	1	300	289	0	0	14	40	28										
1	0	-8	60	61	0	4	0	232	248	0	0	10	231	221										
1	0	-10	74	83	0	3	14	37	37	0	0	8	117	104										
1	0	-12	64	64	0	3	13	67	73	0	0	6	155	148										
1	0	-14	101	84	0	3	12	82	80	0	0	4	39	31										
1	0	-16	42	38	0	3	11	122	131	0	0	2	601	646										
0	8	4	34	46	0	3	9	116	118															
0	7	11	34	45	0	3	8	145	149															
0	7	8	31	18	0	3	7	75	82															
0	7	4	65	88	0	3	6	162	157															
0	7	3	65	81	0	3	5	203	208															
0	7	2	56	59	0	3	4	187	185															
0	6	10	41	40	0	3	3	205	234															
0	6	9	53	61	0	3	2	135	158															
0	6	7	32	46	0	3	1	521	545															
0	6	5	44	51	0	2	16	54	47															
0	6	4	72	94	0	2	13	53	46															
0	6	0	91	102	0	2	10	155	157															
0	5	7	29	34	0	2	6	25	40															
0	5	6	37	44	0	2	5	65	74															
0	5	5	106	137	0	2	3	341	371															
0	5	4	77	83	0	2	2	30	33															
0	5	3	101	113	0	2	1	235	261															
0	5	2	67	75	0	2	0	413	439															
0	5	1	40	40	0	1	16	34	28															
0	4	12	74	72	0	1	14	56	44															
0	4	11	55	62	0	1	11	31	32															
0	4	9	143	162	0	1	10	34	32															
0	4	8	81	102	0	1	7	236	232															
0	4	7	53	55	0	1	6	378	376															

2-(6'-methoxy-5'-bromo-2'-naphthyl)-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-lactone

Table 25 Structure factor listings ($|F_o|$ and $|F_c|$ x 10)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
15	-7	-1	77	76	14	-11	1	67	39	13	-7	-5	86	100	13	-14	0	94	76	12	-8	1	149	151
15	-7	-4	92	88	14	-11	0	122	128	13	-7	-7	80	103	13	-14	-2	87	83	12	-8	0	100	111
15	-9	-1	74	74	14	-11	-1	104	103	13	-8	-1	121	120	12	-1	-1	68	9	12	-8	-1	57	49
15	-9	-2	73	82	14	-11	-2	78	88	13	-8	-2	139	128	12	-1	-5	76	79	12	-8	-2	122	161
15	-9	-4	58	69	14	-11	-3	101	97	13	-8	-4	64	68	12	-2	-2	57	21	12	-8	-3	57	48
15	-9	-5	68	62	14	-11	-4	63	71	13	-8	-5	104	95	12	-2	-3	56	64	12	-8	-5	69	69
15	-10	-4	77	63	14	-11	-5	81	88	13	-9	3	77	96	12	-2	-4	55	54	12	-9	2	138	143
15	-11	0	77	77	14	-12	1	92	90	13	-9	2	88	71	12	-3	0	87	84	12	-9	1	60	62
15	-11	-2	96	105	14	-12	-1	118	127	13	-9	1	77	81	12	-3	-1	93	81	12	-9	0	168	173
15	-11	-4	90	100	14	-12	-5	81	89	13	-9	0	98	104	12	-3	-3	86	84	12	-9	-1	191	198
15	-13	-2	68	70	14	-13	0	90	101	13	-9	-1	70	80	12	-3	-5	77	82	12	-9	-2	60	26
15	-13	-3	62	60	14	-13	-1	90	80	13	-9	-2	72	91	12	-3	-6	75	70	12	-9	-3	137	140
14	-3	-4	56	64	14	-13	-3	97	109	13	-9	-3	72	132	12	-4	-2	91	93	12	-9	-4	156	159
14	-4	-3	57	61	14	-14	1	84	87	13	-9	-4	119	35	12	-4	-4	126	136	12	-9	-6	120	133
14	-5	0	59	42	14	-14	-1	82	70	13	-9	-5	69	80	12	-4	-5	108	107	12	-9	-7	121	116
14	-5	-2	82	91	14	-14	-2	112	115	13	-9	-6	73	108	12	-4	-7	79	71	12	-10	4	97	114
14	-5	-5	62	37	13	-1	-5	60	58	13	-10	1	67	59	12	-5	3	79	73	12	-10	3	109	121
14	-6	-4	57	35	13	-2	-1	57	35	13	-10	0	98	95	12	-5	-3	77	73	12	-10	1	85	85
14	-6	-6	75	65	13	-3	0	62	54	13	-10	-1	62	71	12	-5	-6	87	93	12	-10	-1	60	56
14	-7	1	93	95	13	-3	-6	57	8	13	-10	-2	136	155	12	-5	-7	57	74	12	-10	-2	135	157
14	-7	0	85	88	13	-4	0	72	59	13	-10	-3	80	62	12	-6	1	123	128	12	-10	-3	129	136
14	-7	-2	115	125	13	-4	-1	57	59	13	-10	-4	71	78	12	-6	-1	127	140	12	-10	-4	58	56
14	-7	-3	85	88	13	-4	-4	98	95	13	-11	0	81	80	12	-6	-2	141	161	12	-10	-5	54	21
14	-8	-1	77	75	13	-4	-7	74	85	13	-11	-3	90	99	12	-6	-3	111	93	12	-10	-6	75	81
14	-8	-2	59	63	13	-5	-1	56	41	13	-11	-4	86	76	12	-6	-4	81	91	12	-11	4	99	93
14	-9	1	86	87	13	-5	-5	73	83	13	-11	-6	67	73	12	-6	-5	114	123	12	-11	2	130	139
14	-9	-1	85	96	13	-6	0	76	63	13	-12	2	59	57	12	-6	-7	120	124	12	-11	1	145	144
14	-9	-2	170	182	13	-6	-1	67	64	13	-12	1	154	152	12	-6	-8	85	77	12	-11	-1	108	101
14	-9	-3	73	93	13	-6	-4	65	81	13	-12	0	90	97	12	-7	3	70	60	12	-11	-3	111	134
14	-10	2	102	91	13	-6	-5	59	37	13	-12	-5	97	84	12	-7	2	89	79	12	-11	-4	213	223
14	-10	1	101	73	13	-6	-7	150	156	13	-13	2	122	111	12	-7	0	100	95	12	-11	-5	71	56
14	-10	0	57	48	13	-7	0	64	78	13	-13	-1	114	125	12	-7	-1	107	111	12	-11	-6	66	72
14	-10	-4	125	139	13	-7	-1	59	47	13	-13	-4	119	121	12	-7	-7	121	115	12	-12	3	134	126
14	-10	-5	101	110	13	-7	-2	60	71	13	-14	2	100	74	12	-8	4	66	61	12	-12	2	105	99
14	-11	2	65	46	13	-7	-3	107	113	13	-14	1	144	146	12	-8	3	58	60	12	-12	1	64	67

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
12	-12	0	176	178	11	-2	-3	55	46	11	-7	1	74	67	11	-11	-2	151	161	10	0	-8	84	78
12	-12	-2	120	145	11	-2	-4	56	68	11	-7	0	57	58	11	-12	3	67	69	10	-1	2	74	79
12	-12	-3	115	100	11	-3	3	79	65	11	-7	-1	178	178	11	-12	2	55	64	10	-1	-1	72	91
12	-12	-5	67	68	11	-3	0	124	126	11	-7	-2	129	129	11	-12	0	143	145	10	-1	-3	86	106
12	-12	-6	116	112	11	-3	-1	137	140	11	-7	-4	167	163	11	-12	-1	140	147	10	-1	-4	98	96
12	-13	2	190	185	11	-3	-3	73	83	11	-7	-5	72	50	11	-12	-3	174	183	10	-1	-6	82	99
12	-13	1	104	107	11	-3	-4	113	116	11	-7	-6	136	139	11	-12	-4	163	153	10	-1	-7	108	110
12	-13	-1	130	125	11	-3	-6	96	106	11	-7	-7	175	177	11	-12	-6	126	119	10	-2	4	69	60
12	-13	-2	137	141	11	-3	-7	56	45	11	-8	5	59	44	11	-13	4	80	82	10	-2	3	64	81
12	-13	-4	70	83	11	-4	4	98	97	11	-8	3	85	86	11	-13	3	99	93	10	-2	1	63	65
12	-13	-5	74	74	11	-4	2	63	66	11	-8	1	82	82	11	-13	-2	108	107	10	-2	0	106	110
12	-13	-6	69	60	11	-4	1	102	98	11	-8	0	156	152	11	-13	-5	60	62	10	-2	-2	133	136
12	-14	0	134	127	11	-4	0	68	61	11	-8	-3	132	132	11	-14	3	104	99	10	-2	-3	130	131
12	-14	-2	77	81	11	-4	-2	111	127	11	-8	-5	62	74	11	-14	2	135	126	10	-2	-4	53	44
12	-14	-3	130	123	11	-4	-5	105	107	11	-8	-8	74	53	11	-14	1	75	79	10	-2	-5	149	151
12	-14	-4	58	61	11	-4	-8	72	76	11	-9	4	130	120	11	-14	0	87	100	10	-2	-6	73	72
12	-14	-5	106	105	11	-5	2	103	98	11	-9	3	104	93	11	-14	-1	115	111	10	-2	-8	81	84
12	-15	2	96	91	11	-5	0	122	139	11	-9	-2	103	117	11	-14	-3	136	155	10	-3	2	80	81
12	-15	1	107	104	11	-5	-1	127	126	11	-9	-4	162	173	11	-14	-4	122	124	10	-3	1	135	133
12	-15	-1	134	137	11	-5	-2	103	96	11	-9	-5	153	154	11	-15	3	62	69	10	-3	-1	66	90
12	-15	-2	162	166	11	-5	-3	99	115	11	-9	-7	125	132	11	-15	1	107	112	10	-3	-2	60	50
12	-16	0	69	74	11	-5	-4	124	113	11	-10	5	73	78	11	-15	0	133	147	10	-3	-4	141	149
12	-16	-1	104	94	11	-5	-7	68	58	11	-10	3	134	126	11	-15	-2	103	95	10	-3	-5	53	57
12	-16	-3	92	86	11	-6	4	63	66	11	-10	0	107	107	11	-15	-3	81	87	10	-3	-7	118	119
11	3	-5	59	42	11	-6	3	92	91	11	-10	-1	61	63	11	-16	2	104	107	10	-4	4	60	45
11	1	-2	56	58	11	-6	1	82	79	11	-10	-3	174	194	11	-16	1	58	60	10	-4	3	130	126
11	1	-3	103	104	11	-6	0	185	184	11	-10	-4	150	145	10	3	-1	56	31	10	-4	2	56	49
11	0	-4	71	80	11	-6	-1	77	69	11	-10	-6	113	105	10	2	-2	58	41	10	-4	1	86	83
11	0	-6	61	57	11	-6	-3	60	58	11	-10	-7	65	57	10	2	-3	62	62	10	-4	0	118	115
11	-1	2	89	77	11	-6	-4	66	51	11	-11	4	98	89	10	1	-1	76	72	10	-4	-2	224	237
11	-1	-4	69	79	11	-6	-5	176	168	11	-11	3	68	51	10	1	-2	84	80	10	-4	-3	156	156
11	-1	-6	147	150	11	-6	-6	125	127	11	-11	2	95	90	10	1	-3	208	219	10	-4	-5	158	147
11	-2	2	110	112	11	-6	-8	62	64	11	-11	1	298	299	10	1	-4	100	119	10	-4	-6	150	151
11	-2	1	74	83	11	-7	4	59	59	11	-11	0	129	138	10	0	1	84	73	10	-4	-9	63	47
11	-2	-2	107	123	11	-7	2	133	124	11	-11	-1	120	138	10	0	-5	70	69	10	-5	4	78	74

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
10	-5	2	88	100	10	-8	-4	205	205	10	-11	-7	59	50	10	-16	2	76	86	9	-1	-7	110	101
10	-5	1	156	148	10	-8	-5	65	52	10	-12	5	128	122	10	-16	1	121	132	9	-1	-8	57	63
10	-5	-1	211	219	10	-8	-6	150	157	10	-12	4	62	68	10	-16	-2	101	106	9	-2	5	84	71
10	-5	-2	171	171	10	-8	-7	61	76	10	-12	3	93	85	10	-17	0	124	127	9	-2	4	55	42
10	-5	-3	117	109	10	-9	4	126	125	10	-12	2	153	155	10	-17	-1	96	92	9	-2	3	203	206
10	-5	-4	232	239	10	-9	3	142	151	10	-12	1	73	65	9	4	-2	61	57	9	-2	2	72	67
10	-5	-5	107	104	10	-9	2	67	77	10	-12	0	80	78	9	3	0	82	82	9	-2	1	83	83
10	-5	-8	74	61	10	-9	1	181	187	10	-12	-1	214	228	9	3	-1	86	106	9	-2	0	134	139
10	-5	-9	58	49	10	-9	0	54	55	10	-12	-2	118	104	9	3	-2	57	52	9	-2	-1	94	102
10	-6	5	113	109	10	-9	-1	208	214	10	-12	-3	71	83	9	3	-4	63	62	9	-2	-3	228	229
10	-6	3	61	80	10	-9	-2	209	236	10	-12	-4	152	154	9	2	-3	75	67	9	-2	-4	145	142
10	-6	2	118	112	10	-9	-3	110	115	10	-12	-5	76	68	9	2	-5	93	93	9	-2	-5	102	98
10	-6	0	78	72	10	-9	-5	87	86	10	-12	-6	68	65	9	2	-6	64	40	9	-2	-6	190	187
10	-6	-3	108	112	10	-9	-6	109	111	10	-12	-7	153	152	9	1	2	64	59	9	-2	-7	70	53
10	-6	-4	142	139	10	-9	-7	88	88	10	-13	4	78	86	9	1	1	69	58	9	-2	-9	131	134
10	-6	-6	346	346	10	-9	-8	95	89	10	-13	3	195	195	9	1	-1	143	165	9	-3	3	57	62
10	-6	-7	174	169	10	-10	5	109	104	10	-13	2	159	151	9	1	-2	140	153	9	-3	1	198	211
10	-6	-8	57	59	10	-10	3	157	162	10	-13	1	141	146	9	1	-4	107	102	9	-3	0	303	296
10	-7	4	119	122	10	-10	2	152	150	10	-13	0	158	158	9	1	-5	80	77	9	-3	-2	117	120
10	-7	2	139	136	10	-10	1	58	44	10	-13	-2	59	62	9	1	-7	79	81	9	-3	-3	68	64
10	-7	1	181	182	10	-10	0	221	226	10	-13	-3	100	100	9	0	1	74	76	9	-3	-4	86	89
10	-7	-1	291	299	10	-10	-1	218	232	10	-13	-5	86	86	9	0	0	87	91	9	-3	-5	117	113
10	-7	-2	302	339	10	-10	-2	106	106	10	-14	4	110	105	9	0	-2	74	70	9	-4	5	147	144
10	-7	-3	57	56	10	-10	-3	84	80	10	-14	3	105	104	9	0	-3	75	89	9	-4	4	108	100
10	-7	-4	142	142	10	-10	-4	213	213	10	-14	2	176	177	9	0	-4	66	63	9	-4	3	125	127
10	-7	-6	129	125	10	-10	-6	77	82	10	-14	1	91	93	9	0	-5	83	87	9	-4	2	118	122
10	-7	-7	73	60	10	-10	-7	109	108	10	-14	-1	155	164	9	0	-6	70	57	9	-4	1	197	199
10	-7	-8	85	82	10	-11	4	98	99	10	-14	-2	154	161	9	0	-8	56	55	9	-4	0	292	296
10	-8	5	79	90	10	-11	3	187	178	10	-14	-4	89	95	9	-1	4	68	73	9	-4	-1	200	208
10	-8	4	72	53	10	-11	1	139	134	10	-14	-5	169	161	9	-1	1	126	129	9	-4	-3	300	302
10	-8	3	70	61	10	-11	0	164	159	10	-15	3	59	47	9	-1	-1	93	96	9	-4	-4	193	191
10	-8	2	133	125	10	-11	-2	190	214	10	-15	2	76	72	9	-1	-2	123	133	9	-4	-6	143	158
10	-8	0	247	250	10	-11	-3	156	160	10	-15	0	125	132	9	-1	-4	121	116	9	-4	-7	129	129
10	-8	-1	202	195	10	-11	-5	136	137	10	-15	-1	61	58	9	-1	-5	120	122	9	-5	5	58	37
10	-8	-3	233	231	10	-11	-6	73	72	10	-15	-3	119	120	9	-1	-6	59	36	9	-5	4	74	96

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	Fc	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
9	-5	3	82	81	9	-8	3	78	78	9	-11	3	101	104	9	-15	3	68	73	8	1	-7	107	102
9	-5	1	194	191	9	-8	2	222	220	9	-11	2	240	237	9	-15	2	121	113	8	1	-8	111	98
9	-5	0	353	350	9	-8	1	338	331	9	-11	1	282	284	9	-15	0	103	93	8	0	2	132	127
9	-5	-2	143	155	9	-8	-1	182	188	9	-11	0	157	158	9	-15	-1	126	137	8	0	0	156	159
9	-5	-3	102	109	9	-8	-2	140	149	9	-11	-1	156	161	9	-15	-3	57	62	8	0	-2	290	303
9	-5	-4	129	132	9	-8	-4	245	244	9	-11	-2	147	173	9	-15	-4	96	104	8	0	-3	152	157
9	-5	-5	195	188	9	-8	-5	80	61	9	-11	-3	375	403	9	-16	3	99	100	8	0	-4	113	114
9	-5	-6	78	63	9	-8	-6	112	114	9	-11	-4	89	92	9	-16	1	124	130	8	0	-5	98	98
9	-5	-8	104	101	9	-8	-7	78	72	9	-11	-5	55	67	9	-16	0	86	77	8	0	-7	61	53
9	-6	5	139	144	9	-9	6	85	103	9	-11	-6	111	103	9	-16	-2	83	83	8	0	-9	63	50
9	-6	3	82	98	9	-9	5	57	42	9	-12	5	89	97	9	-17	1	105	99	8	-1	4	105	100
9	-6	2	187	178	9	-9	3	130	128	9	-12	4	123	127	9	-17	-1	96	95	8	-1	3	199	194
9	-6	1	59	54	9	-9	2	125	134	9	-12	3	88	93	8	6	-1	59	12	8	-1	2	77	71
9	-6	-1	245	239	9	-9	1	71	76	9	-12	2	203	202	8	6	-3	59	38	8	-1	1	103	96
9	-6	-2	117	102	9	-9	0	309	310	9	-12	1	186	185	8	6	-5	78	57	8	-1	0	105	101
9	-6	-3	64	64	9	-9	-1	203	214	9	-12	0	54	40	8	6	-6	60	56	8	-1	-2	198	211
9	-6	-4	240	238	9	-9	-2	215	229	9	-12	-1	136	137	8	4	-3	70	78	8	-1	-3	131	139
9	-6	-5	89	78	9	-9	-3	149	149	9	-12	-2	75	57	8	4	-6	102	100	8	-1	-4	143	143
9	-6	-6	106	122	9	-9	-5	75	78	9	-12	-4	68	68	8	3	1	78	85	8	-1	-5	268	265
9	-6	-7	142	140	9	-9	-6	154	154	9	-12	-5	125	111	8	3	-2	70	73	8	-1	-7	88	94
9	-6	-9	56	59	9	-9	-8	100	97	9	-12	-7	74	81	8	3	-4	69	70	8	-1	-8	144	157
9	-7	5	62	21	9	-10	5	149	140	9	-13	5	134	134	8	3	-5	76	57	8	-2	3	143	144
9	-7	4	128	133	9	-10	4	249	247	9	-13	3	131	132	8	3	-7	58	70	8	-2	2	187	186
9	-7	3	165	163	9	-10	2	260	257	9	-13	2	220	221	8	2	2	62	66	8	-2	0	148	164
9	-7	1	283	276	9	-10	1	139	136	9	-13	0	194	199	8	2	0	73	73	8	-2	-1	179	193
9	-7	0	265	272	9	-10	0	236	254	9	-13	-1	144	141	8	2	-2	81	92	8	-2	-2	159	154
9	-7	-1	132	122	9	-10	-1	172	186	9	-13	-3	175	179	8	2	-3	60	61	8	-2	-3	102	106
9	-7	-2	270	289	9	-10	-2	135	138	9	-13	-4	117	114	8	2	-6	123	124	8	-2	-4	181	172
9	-7	-3	124	120	9	-10	-3	55	31	9	-14	4	88	97	8	1	3	55	47	8	-2	-5	117	118
9	-7	-4	120	127	9	-10	-4	120	122	9	-14	3	60	66	8	1	0	54	49	8	-2	-6	111	112
9	-7	-5	234	230	9	-10	-5	146	148	9	-14	1	142	144	8	1	-1	88	74	8	-2	-7	153	156
9	-7	-6	117	116	9	-10	-7	68	55	9	-14	0	107	118	8	1	-2	295	312	8	-2	-8	54	8
9	-7	-8	89	83	9	-10	-8	58	13	9	-14	-2	143	139	8	1	-3	246	249	8	-2	-9	82	89
9	-8	5	111	114	9	-11	6	128	135	9	-14	-3	94	94	8	1	-4	133	124	8	-3	3	110	105
9	-8	4	110	109	9	-11	5	120	125	9	-14	-5	74	86	8	1	-5	94	99	8	-3	2	92	85

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	Fc	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
8	-3	1	121	123	8	-5	-6	215	215	8	-8	-3	108	104	8	-11	-2	116	121	8	-16	3	91	94
8	-3	0	224	230	8	-5	-9	115	117	8	-8	-4	60	40	8	-11	-3	172	183	8	-16	2	87	90
8	-3	-1	66	70	8	-6	6	85	94	8	-8	-7	92	105	8	-11	-4	109	110	8	-16	0	96	87
8	-3	-2	245	241	8	-6	5	61	82	8	-8	-8	142	154	8	-11	-6	108	104	8	-16	-2	60	57
8	-3	-3	104	103	8	-6	4	225	231	8	-9	6	57	48	8	-12	4	128	134	8	-16	-3	121	96
8	-3	-5	169	172	8	-6	2	217	219	8	-9	5	169	179	8	-12	3	170	174	8	-17	1	110	104
8	-3	-6	58	38	8	-6	1	162	154	8	-9	4	85	92	8	-12	1	210	221	7	6	1	66	50
8	-3	-7	61	45	8	-6	0	83	90	8	-9	3	110	94	8	-12	0	132	132	7	6	0	102	104
8	-3	-8	103	107	8	-6	-1	255	262	8	-9	2	181	174	8	-12	-2	156	156	7	6	-3	72	74
8	-3	-9	58	70	8	-6	-2	72	39	8	-9	1	190	193	8	-12	-3	125	142	7	6	-4	86	69
8	-4	5	62	63	8	-6	-4	137	133	8	-9	0	424	436	8	-12	-4	101	99	7	5	1	59	42
8	-4	4	180	186	8	-6	-5	121	122	8	-9	-1	295	303	8	-12	-5	141	139	7	5	0	77	63
8	-4	2	280	277	8	-6	-6	130	132	8	-9	-3	265	273	8	-12	-6	121	113	7	5	-2	77	79
8	-4	1	136	137	8	-6	-7	153	148	8	-9	-4	183	180	8	-13	5	125	113	7	5	-4	87	82
8	-4	0	231	242	8	-6	-8	108	104	8	-9	-5	112	117	8	-13	4	108	105	7	5	-5	123	123
8	-4	-1	284	297	8	-7	6	144	146	8	-9	-6	135	134	8	-13	3	70	70	7	5	-7	75	80
8	-4	-2	260	262	8	-7	5	91	98	8	-9	-7	125	126	8	-13	2	162	160	7	4	4	61	50
8	-4	-3	108	106	8	-7	3	188	190	8	-9	-8	62	56	8	-13	1	159	158	7	4	0	101	97
8	-4	-4	212	196	8	-7	2	172	169	8	-10	5	73	75	8	-13	0	58	66	7	4	-1	101	91
8	-4	-5	120	110	8	-7	1	141	143	8	-10	4	244	242	8	-13	-1	228	239	7	4	-6	59	57
8	-4	-6	127	131	8	-7	0	246	261	8	-10	3	147	142	8	-13	-2	111	100	7	4	-7	104	105
8	-4	-7	186	193	8	-7	-1	286	286	8	-10	2	95	98	8	-13	-4	135	138	7	4	-8	115	104
8	-4	-8	60	68	8	-7	-3	421	425	8	-10	1	133	130	8	-13	-6	97	103	7	3	4	99	91
8	-4	-9	80	95	8	-7	-4	165	157	8	-10	-1	57	52	8	-14	4	108	105	7	3	1	174	176
8	-5	6	103	100	8	-7	-5	429	429	8	-10	-2	253	273	8	-14	3	204	203	7	3	0	140	149
8	-5	4	71	67	8	-7	-6	398	399	8	-10	-3	175	184	8	-14	2	86	87	7	3	-2	114	115
8	-5	3	171	175	8	-8	6	61	68	8	-10	-5	290	292	8	-14	1	65	65	7	3	-4	81	74
8	-5	2	79	86	8	-8	5	74	79	8	-10	-7	57	47	8	-14	0	119	105	7	3	-5	147	152
8	-5	1	77	90	8	-8	4	168	162	8	-10	-8	82	99	8	-14	-2	92	70	7	3	-6	60	72
8	-5	0	231	227	8	-8	3	58	46	8	-11	5	117	121	8	-14	-3	113	110	7	3	-7	106	112
8	-5	-1	73	70	8	-8	2	136	134	8	-11	3	115	114	8	-15	2	131	129	7	3	-8	136	139
8	-5	-2	162	151	8	-8	1	182	171	8	-11	2	157	160	8	-15	1	99	98	7	2	3	57	52
8	-5	-3	368	349	8	-8	0	134	132	8	-11	1	150	157	8	-15	-1	146	147	7	2	2	60	69
8	-5	-4	99	83	8	-8	-1	155	167	8	-11	0	148	150	8	-15	-2	85	88	7	2	0	111	126
8	-5	-5	153	152	8	-8	-2	183	194	8	-11	-1	259	283	8	-15	-4	137	129	7	2	-1	158	172

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
7	2	-2	163	161	7	-1	-9	72	84	7	-4	-3	114	107	7	-7	1	238	236	7	-10	3	222	221
7	2	-4	77	102	7	-2	5	134	131	7	-4	-4	270	268	7	-7	0	394	398	7	-10	2	180	182
7	2	-5	72	74	7	-2	4	99	97	7	-4	-5	289	286	7	-7	-1	437	464	7	-10	1	273	275
7	2	-6	90	88	7	-2	3	57	46	7	-4	-6	79	72	7	-7	-2	329	318	7	-10	0	410	422
7	2	-7	68	73	7	-2	2	235	238	7	-4	-8	138	144	7	-7	-3	355	343	7	-10	-1	80	71
7	1	3	54	36	7	-2	1	316	311	7	-5	6	97	111	7	-7	-4	348	330	7	-10	-2	161	165
7	1	1	54	58	7	-2	0	102	113	7	-5	5	144	149	7	-7	-5	52	38	7	-10	-3	207	209
7	1	0	174	178	7	-2	-1	227	237	7	-5	3	135	135	7	-7	-6	149	151	7	-10	-4	97	88
7	1	-2	242	243	7	-2	-2	132	147	7	-5	2	100	92	7	-7	-7	68	52	7	-10	-5	111	100
7	1	-3	285	293	7	-2	-4	296	289	7	-5	1	49	46	7	-8	7	63	75	7	-10	-6	141	152
7	1	-4	69	68	7	-2	-5	241	235	7	-5	0	262	251	7	-8	6	117	130	7	-11	5	141	140
7	1	-5	213	222	7	-2	-6	54	63	7	-5	-1	353	359	7	-8	4	109	93	7	-11	4	203	205
7	1	-6	119	117	7	-2	-7	131	132	7	-5	-2	173	146	7	-8	3	250	249	7	-11	2	151	146
7	1	-8	71	65	7	-2	-8	114	130	7	-5	-3	508	489	7	-8	1	186	190	7	-11	0	111	118
7	1	-9	67	83	7	-3	6	116	115	7	-5	-4	330	323	7	-8	0	425	423	7	-11	-1	145	149
7	0	5	89	71	7	-3	4	149	154	7	-5	-5	137	126	7	-8	-2	211	224	7	-11	-2	198	222
7	0	3	58	60	7	-3	3	172	168	7	-5	-6	92	80	7	-8	-3	153	156	7	-11	-3	124	130
7	0	2	256	261	7	-3	2	162	164	7	-5	-9	76	72	7	-8	-4	98	98	7	-11	-4	80	84
7	0	1	231	235	7	-3	-1	278	283	7	-6	7	144	162	7	-8	-6	152	151	7	-11	-5	69	66
7	0	-1	160	186	7	-3	-2	269	274	7	-6	6	149	153	7	-8	-8	85	107	7	-11	-7	56	59
7	0	-3	109	122	7	-3	-3	391	371	7	-6	4	198	198	7	-9	7	74	80	7	-12	6	171	172
7	0	-4	121	124	7	-3	-4	187	170	7	-6	3	237	233	7	-9	5	174	174	7	-12	5	143	138
7	0	-5	151	153	7	-3	-5	86	97	7	-6	1	388	383	7	-9	4	167	178	7	-12	3	172	167
7	0	-7	149	151	7	-3	-6	158	168	7	-6	0	222	219	7	-9	3	85	92	7	-12	2	306	303
7	-1	5	64	63	7	-3	-8	132	148	7	-6	-1	65	89	7	-9	2	434	424	7	-12	1	121	111
7	-1	3	159	151	7	-3	-9	63	68	7	-6	-2	179	214	7	-9	1	215	215	7	-12	0	245	252
7	-1	2	50	42	7	-4	7	61	61	7	-6	-5	271	259	7	-9	0	134	133	7	-12	-2	227	246
7	-1	0	196	210	7	-4	5	58	58	7	-6	-6	220	209	7	-9	-1	285	299	7	-12	-3	201	203
7	-1	-1	141	146	7	-4	4	128	120	7	-6	-7	62	61	7	-9	-2	148	154	7	-12	-4	61	62
7	-1	-2	119	125	7	-4	3	167	169	7	-6	-8	152	155	7	-9	-3	104	104	7	-12	-5	70	66
7	-1	-3	337	336	7	-4	2	118	107	7	-7	6	95	94	7	-9	-4	208	207	7	-12	-6	100	98
7	-1	-4	68	58	7	-4	1	628	620	7	-7	5	128	129	7	-9	-7	99	98	7	-13	4	198	194
7	-1	-5	248	252	7	-4	0	222	221	7	-7	4	91	87	7	-10	6	150	143	7	-13	3	112	114
7	-1	-6	174	186	7	-4	-1	253	252	7	-7	3	121	130	7	-10	5	110	111	7	-13	2	98	101
7	-1	-8	61	83	7	-4	-2	344	336	7	-7	2	301	291	7	-10	4	71	50	7	-13	1	220	223

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
7	-13	0	109	122	6	6	-4	96	101	6	1	5	82	82	6	-1	-9	78	86	6	-4	-2	171	174
7	-13	-2	169	162	6	6	-5	83	81	6	1	3	121	119	6	-2	6	150	143	6	-4	-3	259	252
7	-13	-3	60	63	6	5	-2	71	68	6	1	2	59	50	6	-2	5	79	71	6	-4	-5	316	307
7	-13	-5	80	58	6	5	-3	142	143	6	1	1	106	108	6	-2	4	404	412	6	-4	-6	251	250
7	-14	5	100	104	6	5	-5	106	118	6	1	0	185	193	6	-2	3	244	249	6	-4	-7	57	43
7	-14	3	193	193	6	5	-6	82	95	6	1	-1	96	102	6	-2	2	118	107	6	-4	-8	120	107
7	-14	2	99	106	6	4	4	84	76	6	1	-2	48	41	6	-2	1	246	257	6	-4	-9	125	145
7	-14	0	107	104	6	4	2	84	94	6	1	-3	94	97	6	-2	0	179	170	6	-5	7	96	97
7	-14	-1	77	74	6	4	1	93	88	6	1	-4	226	232	6	-2	-1	316	314	6	-5	5	288	288
7	-14	-3	102	93	6	4	-1	144	156	6	1	-5	128	126	6	-2	-2	243	233	6	-5	4	130	132
7	-14	-4	91	101	6	4	-2	61	71	6	1	-6	205	210	6	-2	-3	184	181	6	-5	3	195	196
7	-15	4	71	59	6	4	-7	97	107	6	1	-7	84	88	6	-2	-4	241	219	6	-5	2	346	339
7	-15	3	98	86	6	4	-8	108	111	6	1	-9	65	72	6	-2	-5	229	214	6	-5	1	209	199
7	-15	2	66	59	6	3	5	61	27	6	0	4	201	200	6	-2	-6	122	126	6	-5	0	78	76
7	-15	1	169	175	6	3	4	67	75	6	0	3	196	202	6	-2	-7	86	80	6	-5	-1	313	347
7	-15	-1	59	58	6	3	3	114	126	6	0	1	305	313	6	-2	-8	193	192	6	-5	-2	155	167
7	-15	-2	103	104	6	3	2	94	87	6	0	0	129	127	6	-2	-9	98	112	6	-5	-4	264	256
7	-15	-4	61	47	6	3	1	83	81	6	0	-1	396	396	6	-3	7	83	93	6	-5	-5	52	43
7	-16	3	81	72	6	3	0	150	159	6	0	-2	582	574	6	-3	1	266	243	6	-5	-6	62	70
7	-16	2	116	105	6	3	-2	131	134	6	0	-4	122	122	6	-3	-1	476	493	6	-5	-7	197	207
7	-16	1	98	100	6	3	-3	177	185	6	0	-6	73	52	6	-3	-2	403	353	6	-6	7	66	52
7	-16	-1	116	113	6	3	-4	141	150	6	0	-7	143	146	6	-3	-3	112	116	6	-6	6	142	149
7	-16	-2	63	60	6	3	-5	130	127	6	0	-8	149	156	6	-3	-4	273	266	6	-6	5	119	124
7	-17	1	71	56	6	3	-6	136	134	6	-1	5	85	87	6	-3	-6	223	228	6	-6	4	86	74
6	9	-5	63	55	6	3	-8	79	93	6	-1	4	150	141	6	-3	-7	133	130	6	-6	3	323	310
6	8	1	66	66	6	2	4	98	107	6	-1	3	58	52	6	-3	-8	97	99	6	-6	2	261	253
6	8	-1	58	53	6	2	3	116	110	6	-1	2	111	107	6	-3	-9	76	81	6	-6	1	127	126
6	8	-3	81	60	6	2	1	139	144	6	-1	1	76	75	6	-4	6	159	158	6	-6	0	245	246
6	8	-4	61	66	6	2	0	53	55	6	-1	0	107	117	6	-4	5	131	141	6	-6	-1	324	339
6	6	2	56	69	6	2	-1	67	77	6	-1	-2	239	215	6	-4	4	78	81	6	-6	-2	340	331
6	6	1	76	73	6	2	-2	223	236	6	-1	-3	138	135	6	-4	3	266	270	6	-6	-3	264	260
6	6	0	78	77	6	2	-4	79	83	6	-1	-4	335	323	6	-4	2	54	57	6	-6	-5	342	336
6	6	-1	172	177	6	2	-5	51	48	6	-1	-5	173	156	6	-4	1	372	356	6	-6	-6	150	148
6	6	-2	61	69	6	2	-7	168	173	6	-1	-6	278	281	6	-4	0	296	281	6	-6	-7	66	62
6	6	-3	71	46	6	2	-8	109	113	6	-1	-7	150	145	6	-4	-1	60	62	6	-6	-8	94	100

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
6	-6	-9	81	78	6	-9	-7	125	128	6	-13	5	69	46	5	7	-6	90	96	5	2	2	108	93
6	-7	7	108	102	6	-9	-8	123	126	6	-13	4	105	104	5	7	-8	69	57	5	2	1	213	219
6	-7	5	200	203	6	-10	7	63	46	6	-13	3	173	168	5	6	1	134	133	5	2	0	124	141
6	-7	4	230	235	6	-10	6	140	140	6	-13	1	137	143	5	6	0	61	78	5	2	-1	66	68
6	-7	2	158	149	6	-10	5	240	243	6	-13	0	131	127	5	6	-1	111	100	5	2	-2	76	89
6	-7	1	311	300	6	-10	3	163	154	6	-13	-1	55	30	5	6	-5	153	158	5	2	-3	57	58
6	-7	-2	237	246	6	-10	1	250	255	6	-13	-2	165	158	5	6	-8	71	65	5	2	-4	203	203
6	-7	-4	286	289	6	-10	0	335	349	6	-13	-3	63	69	5	5	3	72	79	5	2	-5	192	194
6	-7	-5	458	446	6	-10	-1	164	181	6	-13	-5	74	67	5	5	0	72	71	5	2	-6	75	64
6	-7	-7	145	154	6	-10	-2	62	65	6	-14	5	118	111	5	5	-3	149	152	5	2	-7	68	87
6	-7	-8	60	60	6	-10	-3	188	186	6	-14	4	87	89	5	5	-4	131	139	5	2	-8	108	112
6	-8	6	165	163	6	-10	-4	133	142	6	-14	2	119	118	5	5	-6	105	109	5	2	-9	72	59
6	-8	5	147	159	6	-10	-6	133	128	6	-14	1	81	62	5	5	-7	91	85	5	1	5	118	123
6	-8	4	93	100	6	-11	5	56	60	6	-14	0	62	63	5	5	-9	98	88	5	1	2	113	111
6	-8	3	284	278	6	-11	4	202	193	6	-14	-1	141	135	5	4	3	70	60	5	1	0	137	154
6	-8	2	192	189	6	-11	3	246	254	6	-14	-2	87	92	5	4	1	146	149	5	1	-1	615	636
6	-8	0	272	273	6	-11	2	121	125	6	-14	-4	87	65	5	4	0	64	65	5	1	-2	402	397
6	-8	-1	203	212	6	-11	0	172	170	6	-15	3	86	85	5	4	-1	103	109	5	1	-3	186	183
6	-8	-2	189	189	6	-11	-1	126	118	6	-15	1	119	114	5	4	-2	140	148	5	1	-4	403	397
6	-8	-3	346	345	6	-11	-2	274	305	6	-15	0	159	151	5	4	-3	76	84	5	1	-5	122	114
6	-8	-4	166	170	6	-11	-3	122	138	6	-15	-2	87	86	5	4	-4	300	298	5	1	-6	172	174
6	-8	-5	206	200	6	-11	-4	153	167	6	-15	-3	82	74	5	4	-5	204	206	5	1	-7	143	137
6	-8	-6	100	109	6	-11	-5	84	81	6	-16	2	67	64	5	3	5	76	89	5	1	-9	78	78
6	-8	-7	70	81	6	-12	6	86	89	6	-16	-1	67	45	5	3	3	118	123	5	0	7	92	86
6	-9	7	111	116	6	-12	5	146	139	6	-16	-2	99	94	5	3	2	97	105	5	0	6	84	65
6	-9	6	66	56	6	-12	4	83	77	5	10	-3	73	41	5	3	1	70	74	5	0	5	55	67
6	-9	4	226	211	6	-12	3	65	71	5	9	-3	63	36	5	3	0	154	163	5	0	4	93	90
6	-9	3	231	231	6	-12	2	205	204	5	9	-5	84	72	5	3	-1	245	243	5	0	3	172	172
6	-9	1	382	380	6	-12	1	57	64	5	9	-6	100	94	5	3	-3	198	209	5	0	2	191	194
6	-9	0	265	274	6	-12	0	215	230	5	8	2	112	104	5	3	-4	308	307	5	0	1	277	276
6	-9	-1	173	187	6	-12	-1	228	229	5	8	1	117	116	5	3	-5	102	114	5	0	0	344	349
6	-9	-2	244	248	6	-12	-3	88	90	5	8	-1	56	52	5	3	-6	170	166	5	0	-1	385	369
6	-9	-3	95	86	6	-12	-4	200	197	5	7	2	56	50	5	3	-7	235	235	5	0	-2	762	744
6	-9	-4	169	175	6	-12	-6	76	60	5	7	1	85	87	5	3	-9	112	115	5	0	-3	344	313
6	-9	-5	257	256	6	-13	6	101	91	5	7	-5	94	84	5	2	3	115	114	5	0	-4	62	61

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	0	-5	86	86	5	-3	4	256	251	5	-5	-6	82	80	5	-8	7	81	68	5	-10	-4	134	140
5	0	-6	95	96	5	-3	3	121	118	5	-5	-7	169	171	5	-8	6	55	42	5	-10	-5	125	117
5	0	-7	68	76	5	-3	2	322	304	5	-5	-8	146	150	5	-8	5	230	231	5	-10	-6	69	44
5	0	-8	161	167	5	-3	1	756	737	5	-6	8	91	106	5	-8	3	302	298	5	-10	-7	84	86
5	0	-9	77	83	5	-3	-1	184	177	5	-6	7	104	120	5	-8	2	491	489	5	-11	6	143	146
5	-1	5	90	79	5	-3	-2	472	444	5	-6	6	83	67	5	-8	1	64	60	5	-11	5	88	79
5	-1	4	179	181	5	-3	-4	302	296	5	-6	5	201	203	5	-8	0	252	258	5	-11	4	104	92
5	-1	2	333	327	5	-3	-5	174	175	5	-6	4	81	93	5	-8	-1	425	446	5	-11	3	323	329
5	-1	1	242	244	5	-3	-7	227	234	5	-6	3	143	137	5	-8	-2	98	105	5	-11	2	148	159
5	-1	-1	45	23	5	-3	-8	167	176	5	-6	2	427	423	5	-8	-3	123	118	5	-11	1	226	233
5	-1	-2	229	223	5	-4	6	140	147	5	-6	0	427	433	5	-8	-7	116	120	5	-11	0	210	216
5	-1	-3	97	94	5	-4	5	65	56	5	-6	-1	126	156	5	-8	-8	66	64	5	-11	-1	64	67
5	-1	-4	398	377	5	-4	3	253	250	5	-6	-2	169	138	5	-9	7	88	75	5	-11	-2	151	144
5	-1	-5	299	284	5	-4	2	181	190	5	-6	-3	334	328	5	-9	6	151	156	5	-11	-3	157	163
5	-1	-6	126	122	5	-4	0	549	556	5	-6	-4	350	349	5	-9	5	166	179	5	-11	-5	69	63
5	-1	-7	161	170	5	-4	-1	142	150	5	-6	-5	172	175	5	-9	4	76	55	5	-12	7	98	112
5	-1	-8	73	83	5	-4	-2	295	270	5	-6	-7	137	144	5	-9	3	281	290	5	-12	5	120	119
5	-1	-10	75	87	5	-4	-3	431	405	5	-6	-9	63	62	5	-9	2	121	113	5	-12	4	129	148
5	-2	6	160	167	5	-4	-4	279	264	5	-7	8	105	94	5	-9	1	488	504	5	-12	2	99	101
5	-2	5	54	49	5	-4	-6	209	203	5	-7	7	197	201	5	-9	0	330	354	5	-12	1	239	250
5	-2	4	237	236	5	-4	-9	113	113	5	-7	6	140	152	5	-9	-2	266	284	5	-12	0	93	96
5	-2	3	226	226	5	-5	8	72	75	5	-7	4	188	191	5	-9	-3	234	242	5	-12	-1	152	162
5	-2	2	75	94	5	-5	7	94	99	5	-7	3	191	190	5	-9	-4	72	73	5	-12	-2	184	192
5	-2	1	268	260	5	-5	6	133	143	5	-7	2	200	208	5	-9	-5	219	212	5	-12	-4	136	125
5	-2	0	603	579	5	-5	5	68	74	5	-7	1	320	323	5	-9	-6	112	118	5	-12	-5	110	102
5	-2	-1	170	184	5	-5	4	329	342	5	-7	0	348	362	5	-9	-7	57	54	5	-13	6	84	79
5	-2	-2	735	677	5	-5	3	166	174	5	-7	-1	53	72	5	-9	-8	95	101	5	-13	5	72	70
5	-2	-3	446	412	5	-5	2	557	531	5	-7	-2	239	261	5	-10	7	89	88	5	-13	4	56	43
5	-2	-4	117	122	5	-5	1	559	551	5	-7	-3	264	266	5	-10	5	207	212	5	-13	3	201	202
5	-2	-5	146	157	5	-5	0	145	160	5	-7	-4	194	186	5	-10	4	91	93	5	-13	2	125	138
5	-2	-6	214	215	5	-5	-1	516	527	5	-7	-5	493	495	5	-10	3	297	296	5	-13	0	138	126
5	-2	-8	72	82	5	-5	-2	532	503	5	-7	-6	126	125	5	-10	2	202	195	5	-13	-3	104	118
5	-2	-9	113	117	5	-5	-3	129	134	5	-7	-7	96	92	5	-10	1	131	150	5	-14	5	107	117
5	-3	8	76	75	5	-5	-4	222	220	5	-7	-8	81	91	5	-10	-1	185	192	5	-14	4	223	213
5	-3	7	65	71	5	-5	-5	154	157	5	-8	8	66	61	5	-10	-2	199	217	5	-14	3	134	137

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	-14	2	95	88	4	6	-2	216	222	4	3	-3	89	89	4	0	5	96	90	4	-2	0	147	144
5	-14	1	102	98	4	6	-3	152	164	4	3	-5	226	243	4	0	4	65	56	4	-2	-1	1010	980
5	-14	0	76	70	4	6	-5	100	91	4	3	-6	157	153	4	0	3	326	318	4	-2	-3	562	526
5	-14	-2	86	84	4	6	-6	99	100	4	3	-7	335	337	4	0	2	240	246	4	-2	-4	602	558
5	-15	4	66	47	4	6	-8	88	89	4	3	-8	134	139	4	0	0	181	168	4	-2	-5	114	105
5	-15	3	85	85	4	5	5	68	55	4	3	-9	69	77	4	0	-1	536	552	4	-2	-6	258	258
5	-15	2	115	117	4	5	3	103	107	4	2	6	70	68	4	0	-2	238	215	4	-2	-7	166	179
5	-15	0	119	108	4	5	2	185	183	4	2	4	119	121	4	0	-3	347	334	4	-2	-9	65	61
5	-15	-1	106	91	4	5	0	158	153	4	2	3	235	236	4	0	-4	284	281	4	-3	7	166	177
5	-15	-3	103	96	4	5	-1	192	202	4	2	2	58	40	4	0	-5	170	150	4	-3	5	261	263
5	-16	3	101	77	4	5	-2	125	141	4	2	1	194	201	4	0	-6	283	295	4	-3	4	367	373
4	11	-3	94	76	4	5	-3	54	36	4	2	0	230	251	4	0	-7	134	145	4	-3	3	240	234
4	11	-4	87	98	4	5	-4	178	177	4	2	-1	79	84	4	0	-9	84	103	4	-3	2	432	407
4	10	-2	67	64	4	5	-5	78	85	4	2	-2	246	219	4	-1	7	111	114	4	-3	1	124	101
4	10	-4	80	76	4	5	-6	101	102	4	2	-3	242	254	4	-1	6	122	126	4	-3	-1	167	152
4	9	0	59	64	4	5	-7	82	85	4	2	-5	211	207	4	-1	5	191	184	4	-3	-2	494	458
4	9	-3	65	62	4	5	-9	103	105	4	2	-6	106	112	4	-1	4	316	324	4	-3	-3	298	283
4	9	-4	68	75	4	4	6	67	59	4	2	-9	61	76	4	-1	3	231	244	4	-3	-4	69	50
4	9	-6	70	69	4	4	5	111	106	4	1	7	83	79	4	-1	2	54	60	4	-3	-5	397	397
4	9	-7	71	60	4	4	3	104	98	4	1	6	55	60	4	-1	1	290	296	4	-3	-6	102	106
4	8	3	76	48	4	4	2	78	77	4	1	5	136	140	4	-1	0	150	128	4	-3	-7	104	111
4	8	1	61	47	4	4	1	155	156	4	1	4	234	249	4	-1	-1	343	327	4	-3	-8	190	203
4	8	-2	137	135	4	4	0	214	228	4	1	3	158	165	4	-1	-2	117	78	4	-4	8	91	97
4	8	-3	70	77	4	4	-2	238	242	4	1	2	179	190	4	-1	-3	80	78	4	-4	7	112	119
4	8	-7	58	40	4	4	-3	108	123	4	1	1	362	368	4	-1	-4	234	239	4	-4	5	184	186
4	8	-8	62	52	4	4	-4	159	158	4	1	0	212	234	4	-1	-5	156	162	4	-4	4	160	156
4	7	3	58	57	4	4	-5	222	224	4	1	-1	495	508	4	-1	-6	103	114	4	-4	3	195	179
4	7	2	103	102	4	4	-6	121	131	4	1	-2	408	411	4	-1	-7	132	139	4	-4	2	557	529
4	7	0	117	118	4	4	-7	104	105	4	1	-3	105	93	4	-1	-8	110	105	4	-4	1	374	365
4	7	-1	100	95	4	3	5	122	135	4	1	-4	287	284	4	-2	7	81	70	4	-4	0	507	487
4	7	-4	106	106	4	3	4	139	142	4	1	-5	217	227	4	-2	6	85	88	4	-4	-1	393	395
4	7	-6	90	88	4	3	2	257	266	4	1	-7	231	242	4	-2	5	340	349	4	-4	-2	351	320
4	7	-7	79	72	4	3	1	279	300	4	1	-8	92	102	4	-2	4	152	172	4	-4	-3	351	333
4	6	1	80	71	4	3	-1	211	223	4	1	-10	62	76	4	-2	3	311	298	4	-4	-4	193	192
4	6	0	122	130	4	3	-2	343	347	4	0	6	93	96	4	-2	2	407	392	4	-4	-5	85	80

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	-4	-6	93	88	4	-7	1	216	212	4	-10	4	290	290	4	-13	-2	64	60	3	7	-4	159	151
4	-5	7	119	118	4	-7	0	611	625	4	-10	3	116	120	4	-13	-3	65	75	3	7	-5	91	97
4	-5	6	195	198	4	-7	-1	123	130	4	-10	2	298	300	4	-14	4	92	97	3	7	-6	67	59
4	-5	5	129	136	4	-7	-2	331	334	4	-10	1	330	339	4	-14	3	103	102	3	7	-7	114	108
4	-5	4	224	213	4	-7	-3	285	284	4	-10	0	74	70	4	-14	1	107	99	3	6	0	203	206
4	-5	3	287	302	4	-7	-4	140	137	4	-10	-1	145	143	4	-14	0	87	95	3	6	-1	151	158
4	-5	2	90	71	4	-7	-5	88	90	4	-10	-2	132	128	4	-14	-3	84	70	3	6	-2	115	122
4	-5	1	248	242	4	-7	-6	155	161	4	-10	-4	132	139	4	-15	4	56	39	3	6	-3	273	288
4	-5	0	696	699	4	-8	7	124	125	4	-10	-5	116	128	4	-15	3	57	32	3	6	-4	144	150
4	-5	-2	768	744	4	-8	5	215	213	4	-10	-7	93	77	4	-15	2	97	85	3	6	-6	135	128
4	-5	-3	436	423	4	-8	4	350	353	4	-11	6	124	123	4	-15	1	82	77	3	6	-8	87	94
4	-5	-4	99	88	4	-8	3	157	168	4	-11	5	205	200	4	-15	-1	94	89	3	5	4	73	78
4	-5	-5	275	275	4	-8	2	231	226	4	-11	4	61	70	4	-16	1	81	66	3	5	3	123	111
4	-5	-6	138	146	4	-8	1	329	339	4	-11	3	59	27	3	11	-3	57	42	3	5	2	160	171
4	-5	-8	123	128	4	-8	0	198	203	4	-11	0	203	214	3	10	2	57	27	3	5	1	206	226
4	-6	8	103	103	4	-8	-1	253	278	4	-11	-1	282	296	3	10	0	64	56	3	5	-1	191	201
4	-6	7	179	199	4	-8	-2	253	260	4	-11	-2	115	126	3	10	-2	74	72	3	5	-2	133	141
4	-6	5	282	280	4	-8	-3	94	86	4	-11	-3	96	100	3	10	-3	70	77	3	5	-3	116	90
4	-6	4	225	227	4	-8	-4	348	356	4	-11	-4	101	110	3	10	-5	125	119	3	5	-4	302	283
4	-6	3	85	72	4	-8	-5	83	86	4	-11	-5	70	59	3	9	-3	57	69	3	5	-5	170	166
4	-6	2	169	168	4	-8	-6	53	42	4	-12	7	140	141	3	9	-4	81	80	3	5	-7	85	93
4	-6	1	398	397	4	-8	-7	78	83	4	-12	6	137	143	3	9	-7	66	60	3	4	5	179	171
4	-6	-1	81	28	4	-9	8	67	81	4	-12	4	123	121	3	8	3	96	106	3	4	2	136	151
4	-6	-2	372	360	4	-9	6	182	169	4	-12	3	186	190	3	8	2	88	99	3	4	0	211	222
4	-6	-3	68	54	4	-9	5	135	146	4	-12	1	150	144	3	8	1	66	58	3	4	-1	205	223
4	-6	-4	227	230	4	-9	3	88	84	4	-12	0	59	59	3	8	0	102	102	3	4	-2	159	160
4	-6	-5	245	250	4	-9	2	264	268	4	-12	-1	93	109	3	8	-2	169	169	3	4	-3	284	284
4	-6	-6	97	98	4	-9	0	248	263	4	-12	-2	156	160	3	8	-3	184	192	3	4	-4	260	267
4	-6	-7	109	109	4	-9	-1	222	240	4	-12	-5	138	136	3	8	-5	83	93	3	4	-5	96	93
4	-7	7	80	90	4	-9	-2	137	134	4	-13	5	111	103	3	8	-6	98	95	3	4	-6	193	184
4	-7	6	208	213	4	-9	-3	73	67	4	-13	4	101	95	3	7	4	58	56	3	4	-7	119	122
4	-7	5	124	127	4	-9	-6	107	112	4	-13	3	91	90	3	7	3	73	65	3	4	-8	106	114
4	-7	4	59	56	4	-9	-7	87	90	4	-13	2	154	144	3	7	2	132	130	3	4	-9	112	119
4	-7	3	308	309	4	-10	7	140	131	4	-13	0	119	118	3	7	1	128	133	3	3	7	95	103
4	-7	2	75	80	4	-10	6	125	137	4	-13	-1	128	113	3	7	0	56	53	3	3	4	125	123

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	3	3	127	144	3	1	-5	317	308	3	-1	-8	117	120	3	-4	5	174	171	3	-6	1	349	353
3	3	2	109	109	3	1	-6	225	228	3	-1	-9	104	114	3	-4	4	383	383	3	-6	-1	246	238
3	3	1	268	276	3	1	-7	60	64	3	-2	7	132	138	3	-4	3	68	47	3	-6	-2	159	168
3	3	0	46	54	3	1	-8	208	221	3	-2	6	104	117	3	-4	2	861	817	3	-6	-3	129	134
3	3	-1	169	170	3	1	-9	107	110	3	-2	5	359	364	3	-4	1	536	510	3	-6	-4	64	54
3	3	-2	384	379	3	0	7	91	84	3	-2	4	384	393	3	-4	-1	227	242	3	-6	-5	218	232
3	3	-4	149	145	3	0	6	68	74	3	-2	3	214	200	3	-4	-2	88	87	3	-6	-7	89	90
3	3	-5	246	235	3	0	5	61	60	3	-2	2	841	825	3	-4	-3	76	74	3	-6	-8	132	135
3	3	-6	124	142	3	0	4	240	239	3	-2	1	419	420	3	-4	-4	269	267	3	-7	8	158	160
3	3	-7	59	43	3	0	3	164	151	3	-2	-1	528	487	3	-4	-5	267	270	3	-7	7	99	106
3	3	-8	177	187	3	0	2	438	428	3	-2	-2	598	572	3	-4	-7	246	245	3	-7	6	143	139
3	2	6	75	75	3	0	1	299	307	3	-2	-3	291	253	3	-4	-8	106	120	3	-7	5	190	191
3	2	5	174	174	3	0	0	805	830	3	-2	-4	529	480	3	-4	-9	56	7	3	-7	3	395	386
3	2	4	89	90	3	0	-1	1210	1308	3	-2	-5	169	173	3	-5	8	110	125	3	-7	2	397	384
3	2	3	138	135	3	0	-2	386	373	3	-2	-6	70	71	3	-5	6	110	112	3	-7	0	117	127
3	2	2	380	381	3	0	-3	285	261	3	-2	-7	349	366	3	-5	5	147	150	3	-7	-1	179	199
3	2	1	61	75	3	0	-4	125	109	3	-2	-8	110	129	3	-5	4	122	115	3	-7	-2	47	25
3	2	0	376	394	3	0	-6	187	182	3	-3	8	105	107	3	-5	3	441	422	3	-7	-3	459	459
3	2	-1	281	304	3	0	-7	157	151	3	-3	7	112	102	3	-5	2	606	583	3	-7	-4	401	401
3	2	-2	200	175	3	0	-8	76	84	3	-3	5	157	156	3	-5	1	254	240	3	-7	-5	147	147
3	2	-3	347	331	3	0	-9	90	98	3	-3	4	111	97	3	-5	0	350	353	3	-7	-6	186	185
3	2	-4	332	320	3	-1	7	68	70	3	-3	3	340	347	3	-5	-1	506	522	3	-8	7	133	135
3	2	-6	319	316	3	-1	6	197	202	3	-3	2	322	306	3	-5	-2	226	197	3	-8	6	142	152
3	2	-7	96	97	3	-1	5	152	163	3	-3	1	53	36	3	-5	-3	512	503	3	-8	4	298	308
3	2	-9	104	110	3	-1	3	269	266	3	-3	0	754	751	3	-5	-4	296	294	3	-8	3	302	302
3	1	7	78	91	3	-1	2	77	70	3	-3	-1	154	149	3	-5	-5	103	100	3	-8	2	57	42
3	1	6	123	136	3	-1	1	469	438	3	-3	-2	199	169	3	-5	-6	176	174	3	-8	1	280	293
3	1	5	126	136	3	-1	0	74	78	3	-3	-3	326	308	3	-5	-7	122	128	3	-8	0	198	218
3	1	4	124	120	3	-1	-1	826	796	3	-3	-4	250	244	3	-5	-9	82	82	3	-8	-1	119	124
3	1	1	410	408	3	-1	-2	299	272	3	-3	-5	213	219	3	-6	7	158	170	3	-8	-2	336	344
3	1	0	203	220	3	-1	-3	532	494	3	-3	-6	136	142	3	-6	6	130	140	3	-8	-3	122	123
3	1	-1	85	104	3	-1	-4	280	257	3	-3	-8	83	88	3	-6	5	103	81	3	-8	-4	266	259
3	1	-2	410	377	3	-1	-5	151	152	3	-3	-9	94	91	3	-6	4	420	417	3	-8	-5	195	198
3	1	-3	383	355	3	-1	-6	272	265	3	-4	7	146	158	3	-6	3	58	70	3	-8	-6	56	76
3	1	-4	204	187	3	-1	-7	73	64	3	-4	6	284	306	3	-6	2	96	78	3	-9	8	84	96

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	-9	7	58	68	3	-11	-6	67	42	2	10	-4	89	102	2	6	-7	146	154	2	3	-6	380	404
3	-9	6	62	49	3	-12	6	107	109	2	10	-5	70	60	2	5	7	58	49	2	3	-7	242	257
3	-9	5	120	107	3	-12	4	121	116	2	10	-6	75	85	2	5	6	90	97	2	3	-8	99	91
3	-9	3	132	120	3	-12	3	172	178	2	9	-1	119	111	2	5	4	158	160	2	2	7	60	56
3	-9	2	246	255	3	-12	1	118	118	2	9	-2	61	70	2	5	3	227	235	2	2	5	271	274
3	-9	1	338	361	3	-12	0	74	70	2	9	-3	73	54	2	5	1	261	272	2	2	4	318	328
3	-9	0	120	116	3	-12	-2	109	93	2	9	-4	86	74	2	5	0	253	268	2	2	2	690	673
3	-9	-1	191	205	3	-12	-3	95	106	2	9	-5	82	93	2	5	-1	146	130	2	2	1	383	403
3	-9	-2	116	128	3	-12	-4	71	70	2	9	-8	102	104	2	5	-2	354	352	2	2	0	65	81
3	-9	-4	113	118	3	-13	5	91	86	2	8	3	204	202	2	5	-3	286	293	2	2	-1	473	470
3	-9	-5	67	77	3	-13	4	131	136	2	8	2	251	249	2	5	-4	55	49	2	2	-2	80	89
3	-9	-6	97	84	3	-13	3	65	42	2	8	0	194	197	2	5	-5	250	249	2	2	-4	415	409
3	-9	-7	103	117	3	-13	2	137	128	2	8	-1	116	131	2	5	-6	168	189	2	2	-5	125	129
3	-10	8	63	52	3	-13	1	121	132	2	8	-3	145	152	2	5	-7	53	59	2	2	-6	303	295
3	-10	7	96	75	3	-13	-1	164	157	2	8	-4	118	139	2	5	-8	105	99	2	2	-7	204	212
3	-10	6	225	239	3	-13	-2	126	114	2	8	-5	72	78	2	4	5	79	82	2	1	8	70	83
3	-10	5	84	94	3	-13	-4	70	63	2	8	-6	137	137	2	4	4	92	104	2	1	6	115	117
3	-10	4	202	200	3	-14	5	100	101	2	8	-7	85	93	2	4	3	70	60	2	1	4	154	144
3	-10	3	276	282	3	-14	3	80	83	2	7	4	80	80	2	4	2	177	166	2	1	3	176	147
3	-10	2	298	308	3	-14	2	101	93	2	7	1	101	107	2	4	1	122	149	2	1	2	58	38
3	-10	1	314	327	3	-14	0	79	80	2	7	0	110	124	2	4	-1	405	409	2	1	0	605	647
3	-10	0	96	102	3	-14	-1	72	65	2	7	-2	212	208	2	4	-2	196	209	2	1	-2	159	139
3	-10	-1	85	89	3	-15	4	89	81	2	7	-4	96	88	2	4	-3	284	270	2	1	-3	686	654
3	-10	-2	228	222	3	-15	-1	66	52	2	7	-5	223	228	2	4	-4	422	414	2	1	-4	234	233
3	-10	-3	211	209	2	12	-2	67	53	2	7	-6	82	91	2	4	-5	107	123	2	1	-5	280	272
3	-10	-5	79	83	2	12	-5	73	69	2	7	-7	91	79	2	4	-6	121	128	2	1	-6	186	192
3	-10	-6	59	66	2	11	2	64	56	2	7	-8	89	99	2	4	-9	76	76	2	1	-7	127	134
3	-11	6	55	57	2	11	0	58	50	2	6	3	165	171	2	3	6	164	178	2	1	-8	95	103
3	-11	5	160	160	2	11	-1	110	104	2	6	2	108	111	2	3	4	214	215	2	1	-9	121	129
3	-11	4	97	107	2	11	-2	80	78	2	6	0	222	217	2	3	3	206	217	2	0	8	75	75
3	-11	3	113	121	2	11	-3	83	68	2	6	-1	156	179	2	3	1	299	293	2	0	7	141	140
3	-11	1	234	246	2	10	1	66	48	2	6	-2	105	116	2	3	0	349	370	2	0	5	302	303
3	-11	-1	274	283	2	10	0	89	89	2	6	-3	183	174	2	3	-2	193	181	2	0	4	459	461
3	-11	-2	204	209	2	10	-1	109	107	2	6	-4	210	211	2	3	-3	468	447	2	0	3	257	266
3	-11	-4	122	126	2	10	-3	181	177	2	6	-6	134	136	2	3	-5	162	153	2	0	2	341	317

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	0	1	828	829	2	-2	-5	379	383	2	-4	-9	57	64	2	-7	0	228	212	2	-10	8	59	70
2	0	0	848	888	2	-2	-6	132	150	2	-5	8	103	118	2	-7	-1	313	323	2	-10	6	118	119
2	0	-1	690	674	2	-2	-7	53	62	2	-5	7	92	117	2	-7	-2	334	353	2	-10	5	131	131
2	0	-2	522	474	2	-2	-8	140	155	2	-5	6	130	117	2	-7	-3	223	220	2	-10	3	242	241
2	0	-3	64	40	2	-3	8	118	132	2	-5	5	283	289	2	-7	-4	472	479	2	-10	2	204	214
2	0	-4	76	71	2	-3	6	354	352	2	-5	4	76	87	2	-7	-5	58	65	2	-10	1	121	118
2	0	-5	198	209	2	-3	5	341	348	2	-5	3	220	180	2	-7	-6	96	89	2	-10	0	257	257
2	0	-7	116	118	2	-3	4	71	89	2	-5	2	637	609	2	-7	-7	105	98	2	-10	-1	116	120
2	0	-8	89	103	2	-3	3	346	317	2	-5	1	100	108	2	-8	7	69	53	2	-10	-3	133	138
2	-1	8	90	90	2	-3	2	407	387	2	-5	0	133	133	2	-8	6	176	172	2	-10	-4	74	72
2	-1	6	181	175	2	-3	1	165	173	2	-5	-1	817	836	2	-8	5	86	92	2	-10	-6	81	85
2	-1	5	291	298	2	-3	0	710	743	2	-5	-2	418	414	2	-8	4	84	82	2	-11	7	136	131
2	-1	3	381	373	2	-3	-1	660	663	2	-5	-3	94	90	2	-8	3	257	257	2	-11	6	59	79
2	-1	2	281	273	2	-3	-2	219	209	2	-5	-4	267	273	2	-8	2	121	131	2	-11	5	81	71
2	-1	1	508	497	2	-3	-3	439	400	2	-5	-6	64	45	2	-8	1	365	368	2	-11	4	159	167
2	-1	0	616	599	2	-3	-6	204	198	2	-5	-7	110	131	2	-8	0	360	383	2	-11	2	120	95
2	-1	-1	926	923	2	-3	-7	93	94	2	-6	9	100	103	2	-8	-1	182	202	2	-11	1	148	140
2	-1	-2	210	183	2	-3	-9	72	73	2	-6	8	81	102	2	-8	-2	51	46	2	-11	0	171	181
2	-1	-3	592	547	2	-4	9	91	103	2	-6	7	86	89	2	-8	-3	78	56	2	-11	-4	90	78
2	-1	-4	260	262	2	-4	7	113	97	2	-6	6	263	276	2	-8	-4	84	87	2	-11	-5	94	91
2	-1	-5	244	232	2	-4	6	122	128	2	-6	5	150	166	2	-8	-6	99	91	2	-12	6	61	64
2	-1	-6	226	227	2	-4	5	102	119	2	-6	4	152	144	2	-8	-7	69	75	2	-12	5	114	136
2	-1	-8	77	78	2	-4	4	223	201	2	-6	3	271	276	2	-9	8	80	83	2	-12	2	139	133
2	-1	-9	99	96	2	-4	3	602	576	2	-6	1	578	562	2	-9	7	147	155	2	-12	0	127	130
2	-2	9	78	62	2	-4	2	257	252	2	-6	0	305	324	2	-9	6	77	90	2	-12	-1	82	96
2	-2	7	160	166	2	-4	1	281	264	2	-6	-1	384	353	2	-9	5	127	123	2	-12	-3	74	70
2	-2	5	170	164	2	-4	0	689	740	2	-6	-2	223	221	2	-9	4	274	285	2	-13	6	60	76
2	-2	4	347	346	2	-4	-1	557	554	2	-6	-4	120	139	2	-9	2	176	173	2	-13	4	80	81
2	-2	3	314	314	2	-4	-2	400	398	2	-6	-6	118	125	2	-9	1	345	362	2	-13	3	114	121
2	-2	2	50	59	2	-4	-3	319	316	2	-7	8	211	211	2	-9	0	83	95	2	-13	1	87	84
2	-2	1	478	452	2	-4	-4	301	276	2	-7	7	136	147	2	-9	-1	93	96	2	-13	-2	89	72
2	-2	-1	83	67	2	-4	-5	204	192	2	-7	5	221	219	2	-9	-2	127	126	2	-14	5	131	135
2	-2	-2	708	675	2	-4	-6	80	74	2	-7	4	256	264	2	-9	-3	108	108	2	-14	4	95	91
2	-2	-3	232	226	2	-4	-7	112	106	2	-7	2	327	327	2	-9	-4	110	105	2	-14	2	79	74
2	-2	-4	193	200	2	-4	-8	95	89	2	-7	1	423	439	2	-9	-5	69	67	1	13	0	57	51

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	Fc	H	K	L	FO	Fc	H	K	L	FO	FC	H	K	L	FO	FC
1	13	-4	63	59	1	7	6	84	95	1	5	-3	540	505	1	3	-6	396	390	1	1	-9	79	84
1	12	2	67	42	1	7	5	84	79	1	5	-4	314	319	1	3	-7	125	133	1	0	9	78	80
1	12	0	80	78	1	7	4	95	88	1	5	-5	151	134	1	3	-9	104	118	1	0	7	101	100
1	12	-6	67	50	1	7	3	139	144	1	5	-6	184	180	1	2	8	67	56	1	0	6	253	258
1	11	3	77	44	1	7	1	149	144	1	5	-8	153	161	1	2	7	77	57	1	0	4	245	240
1	11	-2	135	126	1	7	0	106	104	1	5	-9	92	94	1	2	6	189	197	1	0	3	460	470
1	11	-3	145	137	1	7	-2	226	219	1	4	8	88	63	1	2	4	275	273	1	0	1	686	689
1	11	-5	117	111	1	7	-3	156	169	1	4	7	95	85	1	2	3	259	270	1	0	0	497	546
1	11	-7	80	39	1	7	-5	108	87	1	4	6	120	128	1	2	2	215	196	1	0	-1	396	359
1	10	3	67	36	1	7	-6	80	99	1	4	5	120	136	1	2	1	493	500	1	0	-2	637	608
1	10	2	56	59	1	7	-8	148	142	1	4	4	206	207	1	2	0	232	261	1	0	-3	325	329
1	10	1	74	78	1	7	-9	128	136	1	4	3	64	79	1	2	-2	201	196	1	0	-4	216	190
1	10	-1	83	76	1	6	7	61	52	1	4	2	233	208	1	2	-3	69	80	1	0	-5	418	412
1	10	-3	94	82	1	6	4	73	73	1	4	1	319	334	1	2	-4	269	242	1	0	-6	196	210
1	10	-4	113	111	1	6	2	250	251	1	4	0	102	112	1	2	-5	277	268	1	0	-8	145	144
1	10	-7	67	60	1	6	1	254	271	1	4	-1	139	124	1	2	-6	183	193	1	0	-9	60	64
1	9	3	82	77	1	6	0	78	84	1	4	-2	46	26	1	2	-7	241	242	1	-1	8	147	144
1	9	1	100	88	1	6	-1	198	200	1	4	-3	503	437	1	2	-8	155	170	1	-1	7	151	150
1	9	0	76	79	1	6	-2	146	165	1	4	-4	183	159	1	2	-9	60	54	1	-1	5	369	369
1	9	-1	76	74	1	6	-3	130	113	1	4	-5	194	195	1	1	8	119	122	1	-1	4	215	229
1	9	-2	221	220	1	6	-4	151	148	1	4	-6	89	91	1	1	7	77	88	1	-1	3	172	140
1	9	-3	99	96	1	6	-5	89	103	1	4	-7	62	59	1	1	6	95	86	1	-1	2	726	698
1	9	-4	75	63	1	6	-6	115	110	1	4	-8	173	180	1	1	5	194	193	1	-1	1	177	147
1	9	-5	106	101	1	6	-7	178	178	1	3	8	84	92	1	1	4	125	138	1	-1	0	199	163
1	9	-7	60	50	1	6	-8	97	108	1	3	6	231	230	1	1	3	473	461	1	-1	-1	312	281
1	9	-8	78	71	1	6	-9	83	67	1	3	5	145	147	1	1	2	370	367	1	-1	-2	61	66
1	8	4	62	73	1	5	6	95	93	1	3	3	464	451	1	1	1	175	199	1	-1	-3	108	95
1	8	2	142	141	1	5	5	75	90	1	3	2	430	431	1	1	0	95	97	1	-1	-4	254	247
1	8	1	158	168	1	5	4	112	108	1	3	1	58	48	1	1	-1	127	118	1	-1	-5	130	126
1	8	0	66	60	1	5	3	155	159	1	3	0	615	657	1	1	-2	268	238	1	-1	-6	206	209
1	8	-1	230	234	1	5	2	238	246	1	3	-1	181	183	1	1	-3	299	280	1	-1	-7	226	244
1	8	-2	125	145	1	5	1	197	183	1	3	-2	157	156	1	1	-4	453	439	1	-2	8	68	75
1	8	-4	231	229	1	5	0	522	531	1	3	-3	403	370	1	1	-5	113	101	1	-2	7	73	71
1	8	-6	92	80	1	5	-1	255	273	1	3	-4	281	279	1	1	-6	220	214	1	-2	6	185	195
1	8	-7	137	143	1	5	-2	56	33	1	3	-5	193	172	1	1	-7	169	181	1	-2	5	348	367

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	-2	4	231	211	1	-4	1	194	177	1	-6	-4	88	94	1	-9	-1	147	131	1	-13	0	99	90
1	-2	3	319	301	1	-4	0	384	415	1	-6	-6	123	119	1	-9	-2	186	191	1	-13	-1	72	54
1	-2	2	70	51	1	-4	-1	187	188	1	-6	-7	56	28	1	-9	-4	57	33	1	-13	-2	65	23
1	-2	1	340	316	1	-4	-2	382	358	1	-6	-8	62	23	1	-9	-5	82	86	1	-14	4	94	84
1	-2	-1	340	313	1	-4	-3	493	487	1	-7	7	159	161	1	-10	8	90	82	0	13	1	65	44
1	-2	-2	620	597	1	-4	-4	118	120	1	-7	6	165	183	1	-10	7	64	86	0	13	-2	81	66
1	-2	-3	825	789	1	-4	-6	106	111	1	-7	5	55	43	1	-10	5	120	111	0	13	-5	89	74
1	-2	-4	258	244	1	-4	-8	56	54	1	-7	4	245	239	1	-10	4	87	97	0	12	2	70	56
1	-2	-5	332	319	1	-5	8	89	79	1	-7	3	216	226	1	-10	3	104	106	0	12	0	55	30
1	-2	-6	151	166	1	-5	7	254	263	1	-7	2	50	60	1	-10	2	345	357	0	12	-1	91	77
1	-2	-7	136	149	1	-5	6	80	91	1	-7	1	135	153	1	-10	1	100	106	0	12	-3	80	61
1	-2	-8	99	110	1	-5	5	291	277	1	-7	0	88	111	1	-10	0	183	176	0	12	-4	81	93
1	-3	8	118	129	1	-5	4	224	234	1	-7	-1	228	232	1	-10	-1	167	168	0	12	-6	60	50
1	-3	7	231	250	1	-5	3	284	242	1	-7	-2	354	360	1	-10	-2	85	88	0	11	1	119	104
1	-3	6	259	253	1	-5	2	92	95	1	-7	-3	208	214	1	-10	-4	111	101	0	11	0	94	95
1	-3	5	596	596	1	-5	1	296	319	1	-7	-4	191	193	1	-11	7	110	88	0	11	-2	105	95
1	-3	4	236	227	1	-5	0	115	104	1	-7	-5	144	151	1	-11	6	136	143	0	11	-3	92	92
1	-3	3	188	167	1	-5	-1	271	274	1	-7	-7	111	107	1	-11	4	75	62	0	11	-5	106	106
1	-3	2	154	142	1	-5	-2	453	455	1	-8	8	96	95	1	-11	3	88	72	0	11	-6	123	130
1	-3	1	211	221	1	-5	-3	145	141	1	-8	6	147	134	1	-11	2	99	91	0	10	4	89	83
1	-3	0	50	43	1	-5	-4	301	305	1	-8	5	172	177	1	-11	1	67	70	0	10	1	98	105
1	-3	-1	385	378	1	-5	-5	185	193	1	-8	4	50	25	1	-11	0	121	132	0	10	-1	135	133
1	-3	-2	420	415	1	-5	-6	55	36	1	-8	3	143	143	1	-11	-1	91	101	0	10	-2	167	178
1	-3	-3	253	226	1	-5	-7	133	124	1	-8	2	273	289	1	-11	-2	90	77	0	10	-4	127	127
1	-3	-4	309	299	1	-5	-8	61	64	1	-8	1	62	63	1	-11	-3	78	95	0	10	-5	100	116
1	-3	-5	207	210	1	-6	9	83	95	1	-8	0	167	175	1	-12	7	77	80	0	10	-6	56	49
1	-3	-6	284	298	1	-6	8	128	142	1	-8	-1	238	254	1	-12	5	75	69	0	10	-7	133	129
1	-3	-7	208	214	1	-6	6	219	226	1	-8	-3	195	193	1	-12	4	169	179	0	10	-8	72	78
1	-4	9	105	110	1	-6	5	167	171	1	-8	-4	163	171	1	-12	2	117	110	0	9	6	72	69
1	-4	8	59	100	1	-6	3	500	492	1	-9	7	143	143	1	-12	1	79	81	0	9	3	115	101
1	-4	7	100	113	1	-6	2	323	311	1	-9	6	122	150	1	-12	0	125	116	0	9	1	127	118
1	-4	6	84	71	1	-6	0	300	319	1	-9	4	189	194	1	-12	-1	156	146	0	9	0	173	175
1	-4	5	209	211	1	-6	-1	166	180	1	-9	3	183	181	1	-13	4	66	55	0	9	-1	70	75
1	-4	3	762	731	1	-6	-2	164	152	1	-9	1	68	68	1	-13	3	60	72	0	9	-2	157	145
1	-4	2	573	548	1	-6	-3	217	210	1	-9	0	105	105	1	-13	1	68	65	0	9	-3	268	273

Table 25 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	9	-5	92	79	0	6	-3	162	170	0	3	8	74	71	0	1	6	62	58					
0	9	-6	104	114	0	6	-4	211	209	0	3	7	113	120	0	1	5	293	290					
0	8	4	128	126	0	6	-5	305	313	0	3	6	95	87	0	1	4	195	208					
0	8	3	266	279	0	6	-6	106	116	0	3	5	267	273	0	1	3	464	406					
0	8	1	204	212	0	6	-7	84	75	0	3	4	310	322	0	1	2	467	457					
0	8	-1	313	312	0	6	-8	90	94	0	3	3	125	109	0	1	1	58	34					
0	8	-2	257	272	0	5	8	60	62	0	3	2	332	342	0	1	0	79	105					
0	8	-3	75	86	0	5	6	94	86	0	3	1	273	304	0	1	-1	323	311					
0	8	-4	189	180	0	5	5	217	214	0	3	0	553	584	0	1	-2	686	697					
0	8	-5	271	292	0	5	3	96	97	0	3	-1	913	959	0	1	-3	310	276					
0	8	-7	92	85	0	5	2	261	273	0	3	-2	153	158	0	1	-4	294	276					
0	8	-8	102	119	0	5	1	54	96	0	3	-3	332	310	0	1	-5	166	172					
0	7	6	82	85	0	5	0	194	207	0	3	-4	491	493	0	1	-6	101	90					
0	7	5	142	139	0	5	-1	645	659	0	3	-5	161	182	0	1	-7	118	117					
0	7	4	209	201	0	5	-2	194	210	0	3	-6	74	60	0	1	-8	116	125					
0	7	3	377	381	0	5	-3	244	224	0	3	-7	85	90	0	0	9	93	92					
0	7	2	89	100	0	5	-4	458	459	0	3	-8	85	87	0	0	8	83	83					
0	7	-1	68	84	0	5	-6	187	183	0	3	-9	91	100	0	0	6	175	177					
0	7	-2	62	83	0	5	-7	135	152	0	2	9	82	80	0	0	5	164	173					
0	7	-3	256	259	0	5	-9	91	88	0	2	7	115	116	0	0	4	180	173					
0	7	-4	115	126	0	4	7	110	112	0	2	6	136	138	0	0	3	382	366					
0	7	-5	62	48	0	4	6	119	126	0	2	5	76	88	0	0	2	429	425					
0	7	-6	155	157	0	4	4	193	193	0	2	4	75	67	0	0	1	816	853					
0	7	-7	109	114	0	4	3	95	113	0	2	3	248	247										
0	7	-8	102	101	0	4	2	59	55	0	2	2	336	349										
0	7	-9	111	124	0	4	1	394	406	0	2	1	592	591										
0	6	7	68	71	0	4	0	90	13	0	2	-1	301	310										
0	6	6	60	53	0	4	-1	123	110	0	2	-2	660	634										
0	6	4	57	38	0	4	-2	738	703	0	2	-3	564	558										
0	6	3	196	210	0	4	-3	236	251	0	2	-4	107	131										
0	6	2	73	73	0	4	-4	152	133	0	2	-5	320	319										
0	6	1	307	319	0	4	-5	228	227	0	2	-6	347	363										
0	6	0	289	308	0	4	-6	153	168	0	2	-8	132	138										
0	6	-1	382	375	0	4	-8	135	139	0	1	8	86	93										
0	6	-2	468	472	0	4	-9	64	67	0	1	7	187	196										

2-(6'-methoxy-5'-bromo-2'-naphthyl)-1-methyl-5-carboxymethyl-cyclohexane-1,6,5-ether

Table 26 Structure factor listings ($|F_o|$ and $|F_c|$ x 10)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	-12	1	73	79	0	-4	-4	206	205	0	1	-5	298	288	0	5	-3	293	297	0	10	-1	145	149
0	-11	-1	97	84	0	-4	-3	136	138	0	1	-4	232	253	0	5	-2	275	223	0	10	0	68	72
0	-10	-3	62	37	0	-4	-2	150	145	0	1	-3	112	39	0	5	-1	534	537	0	10	1	84	66
0	-10	-2	77	58	0	-4	-1	394	398	0	1	0	137	162	0	5	0	345	346	0	11	-7	83	79
0	-10	-1	74	66	0	-4	7	84	77	0	1	1	263	176	0	6	-9	90	103	0	11	-6	132	129
0	-10	8	97	120	0	-3	-6	166	185	0	1	3	532	483	0	6	-6	212	215	0	11	-5	101	104
0	-9	-1	126	142	0	-3	-5	223	230	0	1	8	67	77	0	6	-5	257	254	0	11	-3	125	130
0	-9	0	129	136	0	-3	-4	172	172	0	2	-6	313	335	0	6	-4	93	106	0	11	-2	96	99
0	-9	6	115	114	0	-3	-3	165	171	0	2	-5	216	217	0	6	-3	158	159	0	11	0	77	67
0	-8	-3	126	108	0	-3	-2	368	370	0	2	-4	329	296	0	6	-2	508	507	0	12	2	64	47
0	-8	-1	177	189	0	-3	-1	195	198	0	2	-3	591	511	0	6	-1	462	467	0	13	-3	68	71
0	-8	3	87	95	0	-3	0	680	677	0	2	-2	577	533	0	6	0	218	218	0	13	-2	84	68
0	-8	6	115	123	0	-3	3	215	186	0	2	-1	262	213	0	6	5	95	99	1	-13	-1	86	71
0	-8	8	179	198	0	-2	-8	78	87	0	2	2	142	127	0	7	-6	133	140	1	-13	0	118	105
0	-7	-4	240	241	0	-2	-7	151	174	0	2	4	175	172	0	7	-5	72	60	1	-13	3	83	76
0	-7	-3	440	450	0	-2	-5	156	155	0	2	6	67	68	0	7	-3	231	233	1	-13	4	86	95
0	-7	-2	97	102	0	-2	-3	161	140	0	3	-8	161	174	0	7	5	70	59	1	-12	-1	107	111
0	-7	-1	112	140	0	-2	-1	634	611	0	3	-7	107	120	0	8	-5	302	309	1	-12	0	65	67
0	-7	4	146	154	0	-2	7	141	149	0	3	-6	136	135	0	8	-4	197	197	1	-12	1	81	88
0	-7	7	151	161	0	-1	-6	176	187	0	3	-5	256	236	0	8	-2	269	277	1	-12	2	108	127
0	-7	9	70	66	0	-1	-5	355	362	0	3	-4	453	426	0	8	-1	327	335	1	-12	4	154	157
0	-6	-4	57	44	0	-1	-4	176	152	0	3	-2	184	180	0	8	2	55	36	1	-12	5	98	99
0	-6	-3	65	56	0	-1	-2	665	661	0	3	-1	966	956	0	8	5	63	65	1	-11	-4	71	54
0	-6	-2	80	86	0	-1	1	352	331	0	4	-9	117	131	0	9	-7	82	78	1	-11	-3	101	117
0	-6	-1	323	340	0	-1	8	151	166	0	4	-6	281	297	0	9	-4	57	48	1	-11	-1	165	170
0	-6	8	102	116	0	-1	9	72	84	0	4	-5	72	66	0	9	-3	220	212	1	-11	0	134	130
0	-5	-7	85	78	0	0	-4	55	38	0	4	-4	90	65	0	9	-2	205	200	1	-11	1	64	61
0	-5	-6	110	114	0	0	-3	147	119	0	4	-3	270	279	0	9	-1	81	86	1	-11	2	104	102
0	-5	-5	139	136	0	0	1	900	984	0	4	-2	686	621	0	9	1	128	142	1	-11	4	125	124
0	-5	-4	90	77	0	0	2	404	436	0	4	-1	300	299	0	9	3	106	114	1	-11	6	157	161
0	-5	-3	203	202	0	0	6	112	106	0	4	0	86	26	0	9	4	63	88	1	-11	7	130	147
0	-5	-2	178	180	0	0	7	170	192	0	4	7	90	92	0	10	-7	107	110	1	-10	-4	71	73
0	-5	6	101	105	0	0	8	71	56	0	5	-7	147	158	0	10	-5	129	133	1	-10	-2	104	88
0	-5	8	126	137	0	0	9	80	94	0	5	-5	120	116	0	10	-4	148	146	1	-10	-1	166	176
0	-4	-5	117	118	0	1	-6	123	119	0	5	-4	517	505	0	10	-2	125	121	1	-10	0	165	164

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	-10	1	147	150	1	-7	4	277	287	1	-4	-7	96	111	1	-2	-5	81	85	1	0	1	826	791
1	-10	2	355	374	1	-7	5	169	181	1	-4	-6	122	140	1	-2	-4	315	314	1	0	2	64	105
1	-10	3	146	168	1	-7	7	118	135	1	-4	-5	93	91	1	-2	-3	917	853	1	0	3	251	222
1	-10	4	69	53	1	-7	8	109	128	1	-4	-4	296	287	1	-2	-2	458	466	1	0	4	330	340
1	-10	5	111	119	1	-6	-7	93	119	1	-4	-3	332	335	1	-2	0	138	129	1	0	5	125	134
1	-9	-6	103	112	1	-6	-6	68	61	1	-4	-2	306	283	1	-2	1	281	265	1	0	6	167	166
1	-9	-3	57	67	1	-6	-5	101	98	1	-4	-1	296	263	1	-2	2	262	227	1	0	7	137	145
1	-9	-2	93	82	1	-6	-4	165	163	1	-4	0	338	352	1	-2	3	344	303	1	0	8	97	118
1	-9	0	99	104	1	-6	-3	74	82	1	-4	1	353	383	1	-2	4	298	294	1	1	-8	82	98
1	-9	1	59	70	1	-6	-1	278	289	1	-4	2	519	503	1	-2	6	155	156	1	1	-7	179	190
1	-9	2	70	63	1	-6	0	286	296	1	-4	3	694	650	1	-2	7	165	186	1	1	-6	111	103
1	-9	3	190	193	1	-6	1	146	162	1	-4	4	73	90	1	-2	8	73	108	1	1	-5	160	156
1	-9	4	229	238	1	-6	2	340	312	1	-4	5	62	78	1	-1	-7	98	109	1	1	-4	465	474
1	-9	5	93	103	1	-6	3	511	503	1	-4	6	197	190	1	-1	-6	109	113	1	1	-3	288	306
1	-9	6	89	91	1	-6	4	108	121	1	-4	7	70	88	1	-1	-5	341	331	1	1	-2	77	32
1	-9	7	133	155	1	-6	5	72	78	1	-4	9	90	113	1	-1	-4	201	191	1	1	-1	164	150
1	-8	-4	153	154	1	-6	6	186	196	1	-3	-7	105	104	1	-1	-3	63	27	1	1	0	107	65
1	-8	-3	162	177	1	-6	7	98	89	1	-3	-6	100	108	1	-1	-2	356	338	1	1	1	87	66
1	-8	-2	136	124	1	-6	9	78	93	1	-3	-5	174	172	1	-1	-1	266	216	1	1	2	276	255
1	-8	-1	270	264	1	-5	-8	69	82	1	-3	-4	293	285	1	-1	1	115	84	1	1	3	537	522
1	-8	0	201	228	1	-5	-5	164	174	1	-3	-3	137	116	1	-1	2	605	574	1	1	4	107	109
1	-8	1	105	106	1	-5	-4	182	194	1	-3	-2	428	407	1	-1	3	477	435	1	1	5	137	141
1	-8	2	258	258	1	-5	-3	298	291	1	-3	-1	477	450	1	-1	4	147	153	1	1	6	209	231
1	-8	3	252	264	1	-5	-2	465	445	1	-3	0	37	38	1	-1	5	241	238	1	2	-9	100	97
1	-8	4	115	123	1	-5	-1	261	280	1	-3	1	117	108	1	-1	6	114	132	1	2	-8	112	132
1	-8	5	158	164	1	-5	0	125	114	1	-3	2	349	324	1	-1	8	66	75	1	2	-6	283	294
1	-8	6	199	207	1	-5	1	293	257	1	-3	3	332	334	1	0	-8	95	103	1	2	-5	415	418
1	-8	7	70	87	1	-5	2	272	283	1	-3	4	215	179	1	0	-7	117	127	1	2	-4	78	89
1	-7	-5	154	163	1	-5	3	446	416	1	-3	5	665	689	1	0	-6	240	254	1	2	-3	253	238
1	-7	-3	265	262	1	-5	4	261	256	1	-3	6	233	233	1	0	-5	346	349	1	2	-2	313	281
1	-7	-2	321	324	1	-5	5	426	426	1	-3	7	159	169	1	0	-4	67	67	1	2	-1	208	125
1	-7	-1	112	128	1	-5	6	73	57	1	-3	8	97	113	1	0	-3	510	468	1	2	0	153	154
1	-7	1	187	193	1	-5	7	234	255	1	-2	-9	75	72	1	0	-2	668	628	1	2	1	437	456
1	-7	2	117	141	1	-5	8	122	149	1	-2	-7	216	220	1	0	-1	304	273	1	2	2	337	337
1	-7	3	114	112	1	-5	9	76	92	1	-2	-6	285	304	1	0	0	421	466	1	2	4	254	237

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	2	5	75	81	1	5	-1	288	303	1	8	-1	179	158	2	-13	6	66	81	2	-8	-4	173	179
1	2	8	114	123	1	5	0	470	482	1	8	0	122	119	2	-12	-1	99	118	2	-8	-3	101	113
1	3	-8	68	62	1	5	1	244	265	1	8	1	83	85	2	-12	0	113	126	2	-8	-1	216	223
1	3	-7	185	194	1	5	2	65	40	1	8	2	136	139	2	-12	2	133	127	2	-8	0	376	404
1	3	-6	263	275	1	5	3	136	132	1	8	5	71	59	2	-12	5	84	84	2	-8	1	290	297
1	3	-5	139	150	1	5	4	129	126	1	9	-6	74	76	2	-12	6	96	100	2	-8	2	82	73
1	3	-4	395	398	1	5	6	84	106	1	9	-5	78	95	2	-11	-5	67	64	2	-8	3	209	219
1	3	-3	432	372	1	6	-8	168	181	1	9	-3	91	84	2	-11	-1	93	94	2	-8	4	120	112
1	3	-2	187	103	1	6	-7	190	191	1	9	-2	210	207	2	-11	1	115	122	2	-8	6	213	222
1	3	-1	316	296	1	6	-5	149	159	1	9	-1	90	94	2	-11	2	157	150	2	-8	7	159	174
1	3	0	471	497	1	6	-4	102	117	1	9	0	81	80	2	-11	4	153	167	2	-8	8	78	101
1	3	1	222	215	1	6	-3	56	61	1	9	1	112	112	2	-11	5	118	120	2	-6	0	271	301
1	3	2	361	359	1	6	-2	140	138	1	10	-7	85	79	2	-11	7	114	138	2	-6	1	471	494
1	3	3	364	372	1	6	-1	180	202	1	10	-5	64	71	2	-10	-4	100	89	2	-6	2	76	73
1	3	4	201	226	1	6	1	176	195	1	10	-4	126	114	2	-10	-3	141	128	2	-6	3	167	175
1	3	5	187	199	1	6	2	238	252	1	10	-3	103	102	2	-10	-1	120	103	2	-6	4	206	209
1	3	6	252	255	1	6	3	117	137	1	10	-1	71	73	2	-10	0	257	275	2	-6	6	167	179
1	4	-9	104	101	1	6	5	72	91	1	10	0	59	56	2	-10	1	86	92	2	-6	7	194	219
1	4	-8	165	198	1	6	6	69	64	1	10	2	67	53	2	-10	2	259	265	2	-6	8	65	68
1	4	-5	314	305	1	7	-9	132	148	1	11	-5	109	117	2	-10	3	204	212	2	-5	-5	74	62
1	4	-4	84	94	1	7	-6	141	141	1	11	-3	170	178	2	-10	5	77	80	2	-5	-4	271	270
1	4	-3	287	277	1	7	-5	55	48	1	11	-2	133	138	2	-10	6	153	164	2	-5	-3	107	118
1	4	-2	151	100	1	7	-4	139	140	1	12	-4	66	30	2	-10	7	85	99	2	-5	-2	579	582
1	4	-1	162	173	1	7	-3	168	174	1	12	-1	78	60	2	-9	-5	76	75	2	-5	-1	754	765
1	4	0	139	124	1	7	-2	158	173	1	12	0	109	110	2	-9	-2	96	91	2	-5	0	111	123
1	4	1	149	145	1	7	0	131	135	1	13	-5	89	86	2	-9	-1	72	73	2	-5	1	156	163
1	4	2	354	383	1	7	1	180	189	2	-14	1	88	84	2	-9	0	193	199	2	-5	2	627	584
1	4	3	68	86	1	7	2	91	120	2	-14	2	86	81	2	-9	1	272	264	2	-5	3	354	328
1	4	4	106	92	1	7	3	97	89	2	-14	3	69	47	2	-9	2	199	209	2	-5	5	343	362
1	5	-9	81	76	1	7	4	101	109	2	-14	4	80	74	2	-9	4	223	221	2	-5	6	239	263
1	5	-6	156	168	1	8	-8	112	103	2	-14	5	74	82	2	-9	5	181	190	2	-5	9	92	124
1	5	-5	120	128	1	8	-7	166	176	2	-13	-2	77	77	2	-9	7	105	114	2	-4	-6	110	103
1	5	-4	387	369	1	8	-5	88	96	2	-13	1	100	98	2	-9	8	107	140	2	-4	-5	133	137
1	5	-3	652	628	1	8	-4	236	237	2	-13	3	102	103	2	-8	-7	79	86	2	-4	-4	81	62
1	5	-2	77	66	1	8	-2	184	178	2	-13	4	124	129	2	-8	-6	98	100	2	-4	-3	242	233

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	-4	-2	384	383	2	-2	2	164	150	2	1	-9	91	98	2	3	0	354	360	2	6	-5	82	58
2	-4	-1	357	325	2	-2	3	249	215	2	1	-7	166	167	2	3	1	423	448	2	6	-4	226	203
2	-4	0	622	643	2	-2	4	342	347	2	1	-6	183	197	2	3	2	74	66	2	6	-3	189	180
2	-4	1	285	352	2	-2	5	438	460	2	1	-5	137	162	2	3	3	176	177	2	6	-1	193	192
2	-4	2	277	288	2	-2	6	105	111	2	1	-4	230	209	2	3	4	227	239	2	6	0	262	290
2	-4	3	438	418	2	-2	7	108	121	2	1	-3	689	652	2	3	5	67	71	2	6	1	64	61
2	-4	4	278	271	2	-2	8	106	121	2	1	-2	146	100	2	3	6	83	100	2	6	2	108	143
2	-4	5	176	192	2	-1	-8	74	82	2	1	0	748	760	2	4	-8	63	83	2	6	3	158	157
2	-4	6	118	127	2	-1	-7	91	92	2	1	1	87	69	2	4	-5	206	188	2	6	6	66	62
2	-4	7	140	159	2	-1	-6	58	65	2	1	2	249	235	2	4	-4	386	369	2	7	-8	69	78
2	-4	8	135	152	2	-1	-5	51	57	2	1	3	88	69	2	4	-3	218	222	2	7	-6	153	142
2	-3	-8	93	110	2	-1	-4	275	266	2	1	4	355	366	2	4	-2	174	172	2	7	-5	240	239
2	-3	-7	133	153	2	-1	-3	473	436	2	1	5	167	178	2	4	-1	388	383	2	7	-4	65	69
2	-3	-6	80	82	2	-1	-2	162	136	2	1	7	87	106	2	4	0	130	135	2	7	-3	87	81
2	-3	-5	158	168	2	-1	1	453	372	2	2	-9	93	103	2	4	1	57	69	2	7	-2	183	179
2	-3	-4	151	153	2	-1	2	184	199	2	2	-8	80	107	2	4	2	110	123	2	7	-1	54	65
2	-3	-3	221	210	2	-1	3	441	446	2	2	-6	59	80	2	4	3	178	208	2	7	0	60	56
2	-3	-2	312	256	2	-1	4	194	204	2	2	-5	193	175	2	4	4	91	89	2	7	2	97	123
2	-3	-1	747	802	2	-1	6	95	108	2	2	-4	337	318	2	4	6	73	77	2	7	3	137	159
2	-3	0	533	607	2	-1	7	104	122	2	2	-3	59	40	2	5	-9	77	86	2	8	-7	139	134
2	-3	1	77	58	2	0	-9	72	99	2	2	-2	122	134	2	5	-8	84	93	2	8	-6	133	132
2	-3	2	452	408	2	0	-8	150	167	2	2	-1	463	486	2	5	-7	59	47	2	8	-5	56	40
2	-3	3	432	411	2	0	-6	253	262	2	2	0	71	110	2	5	-6	213	210	2	8	-4	127	119
2	-3	4	108	115	2	0	-5	246	228	2	2	1	438	424	2	5	-5	213	211	2	8	-3	203	201
2	-3	5	282	299	2	0	-3	115	137	2	2	2	568	554	2	5	-3	317	326	2	8	-1	93	114
2	-3	6	302	324	2	0	-2	482	411	2	2	3	118	119	2	5	-2	478	478	2	8	0	164	166
2	-3	7	91	102	2	0	0	802	896	2	2	4	126	121	2	5	-1	156	141	2	8	1	60	46
2	-3	8	79	68	2	0	1	842	753	2	2	5	147	151	2	5	0	186	209	2	8	3	149	156
2	-2	-8	123	135	2	0	2	485	498	2	2	6	140	143	2	5	1	249	250	2	9	-8	112	114
2	-2	-6	238	257	2	0	3	259	261	2	3	-7	297	297	2	5	2	53	57	2	9	-5	118	119
2	-2	-5	367	370	2	0	4	390	377	2	3	-6	457	472	2	5	3	95	99	2	9	-4	78	92
2	-2	-4	115	142	2	0	5	290	315	2	3	-5	55	62	2	5	4	68	77	2	9	-1	137	151
2	-2	-3	392	369	2	0	6	132	136	2	3	-4	90	101	2	6	-8	88	77	2	10	-6	76	74
2	-2	-2	666	600	2	0	7	68	70	2	3	-3	466	432	2	6	-7	174	178	2	10	-5	62	47
2	-2	1	507	440	2	0	8	75	94	2	3	-2	377	388	2	6	-6	66	82	2	10	-4	77	97

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	10	-3	195	183	3	-10	-4	101	97	3	-8	7	150	160	3	-5	-1	488	505	3	-2	-8	125	131
2	10	-2	60	61	3	-10	-3	173	170	3	-8	8	151	177	3	-5	0	427	496	3	-2	-7	286	305
2	10	-1	67	58	3	-10	-2	152	137	3	-7	-6	60	51	3	-5	1	246	251	3	-2	-5	351	334
2	11	-2	76	63	3	-10	0	73	66	3	-7	-5	188	176	3	-5	2	462	407	3	-2	-4	334	332
2	11	-1	84	79	3	-10	1	360	383	3	-7	-3	305	305	3	-5	3	473	461	3	-2	-3	209	227
2	12	-2	67	63	3	-10	2	234	242	3	-7	-1	217	218	3	-5	4	190	208	3	-2	-2	616	562
3	-15	4	109	108	3	-10	3	334	334	3	-7	0	81	122	3	-5	6	213	209	3	-2	1	340	302
3	-14	-2	67	41	3	-10	4	245	252	3	-7	1	84	74	3	-5	7	123	142	3	-2	2	778	704
3	-14	-1	86	85	3	-10	6	175	185	3	-7	2	480	476	3	-4	-9	69	72	3	-2	3	333	327
3	-14	0	98	82	3	-10	7	117	129	3	-7	3	493	500	3	-4	-8	99	110	3	-2	5	294	303
3	-14	2	85	80	3	-9	-5	113	121	3	-7	4	168	176	3	-4	-7	92	88	3	-2	6	69	79
3	-14	3	103	104	3	-9	-4	128	131	3	-7	5	122	129	3	-4	-6	70	53	3	-1	-9	100	109
3	-14	5	65	79	3	-9	-3	84	71	3	-7	6	192	204	3	-4	-5	307	312	3	-1	-5	168	180
3	-13	-2	114	109	3	-9	-2	197	202	3	-7	8	79	82	3	-4	-4	150	155	3	-1	-4	524	448
3	-13	-1	123	124	3	-9	-1	221	229	3	-6	-8	86	97	3	-4	-3	130	86	3	-1	-3	561	496
3	-13	1	131	135	3	-9	0	83	99	3	-6	-6	163	168	3	-4	-2	106	97	3	-1	-2	165	208
3	-13	2	124	142	3	-9	1	325	317	3	-6	-5	119	127	3	-4	-1	136	188	3	-1	0	133	201
3	-13	4	145	134	3	-9	2	256	248	3	-6	-4	102	82	3	-4	1	609	585	3	-1	1	683	588
3	-13	5	153	161	3	-9	3	252	256	3	-6	-3	346	313	3	-4	2	968	929	3	-1	2	202	230
3	-12	-4	101	90	3	-9	4	108	114	3	-6	-2	89	85	3	-4	3	263	251	3	-1	3	96	103
3	-12	0	93	93	3	-9	5	110	121	3	-6	-1	294	280	3	-4	4	315	297	3	-1	4	177	164
3	-12	1	104	108	3	-9	6	141	156	3	-6	0	75	86	3	-4	5	114	100	3	-1	5	60	59
3	-12	3	202	193	3	-8	-7	80	100	3	-6	1	338	337	3	-4	6	164	151	3	-1	8	71	78
3	-12	4	158	170	3	-8	-6	134	129	3	-6	2	300	318	3	-4	8	83	112	3	0	-8	137	143
3	-12	6	87	88	3	-8	-5	103	107	3	-6	3	87	88	3	-3	-7	182	202	3	0	-7	224	238
3	-12	7	79	93	3	-8	-4	76	59	3	-6	4	342	331	3	-3	-6	166	156	3	0	-5	141	119
3	-11	-4	64	55	3	-8	-3	123	112	3	-6	5	183	189	3	-3	-4	336	343	3	0	-4	143	121
3	-11	-3	68	47	3	-8	-2	312	335	3	-6	7	112	122	3	-3	-3	439	396	3	0	-2	329	289
3	-11	-2	242	231	3	-8	-1	72	80	3	-6	8	117	143	3	-3	-2	57	95	3	0	0	612	682
3	-11	-1	261	263	3	-8	0	223	210	3	-5	-7	151	150	3	-3	1	180	206	3	0	2	365	349
3	-11	1	234	238	3	-8	1	343	352	3	-5	-6	153	168	3	-3	3	154	163	3	0	3	151	126
3	-11	4	84	70	3	-8	2	71	82	3	-5	-5	95	82	3	-3	4	284	285	3	0	4	114	83
3	-11	5	185	191	3	-8	3	283	279	3	-5	-4	288	260	3	-3	5	255	277	3	0	5	161	168
3	-11	6	136	145	3	-8	4	304	317	3	-5	-3	510	521	3	-3	6	125	130	3	0	6	167	180
3	-10	-6	76	81	3	-8	5	82	99	3	-5	-2	95	78	3	-3	7	180	194	3	1	-8	131	132

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	1	-6	322	316	3	3	5	150	178	3	7	1	74	66	4	-13	5	122	120	4	-9	2	171	153
3	1	-5	330	334	3	4	-9	72	89	3	7	2	141	142	4	-12	-5	130	107	4	-9	3	117	107
3	1	-4	70	73	3	4	-7	134	146	3	7	3	102	110	4	-12	-3	70	65	4	-9	4	139	155
3	1	-3	484	432	3	4	-6	155	165	3	8	-6	103	101	4	-12	-2	80	107	4	-9	5	99	34
3	1	-2	268	228	3	4	-4	283	254	3	8	-5	81	69	4	-12	0	98	95	4	-9	6	180	193
3	1	-1	70	49	3	4	-3	258	237	3	8	-3	148	147	4	-12	1	126	138	4	-9	7	103	118
3	1	0	119	125	3	4	0	216	233	3	8	-2	173	179	4	-12	3	198	185	4	-8	-5	95	103
3	1	1	338	322	3	4	3	102	109	3	8	0	118	115	4	-12	4	150	163	4	-8	-4	283	295
3	1	2	252	264	3	4	5	70	57	3	8	1	81	69	4	-12	5	70	88	4	-8	-3	82	69
3	1	4	172	152	3	5	-9	96	88	3	8	3	75	64	4	-12	7	116	127	4	-8	-2	342	345
3	1	7	85	85	3	5	-8	98	102	3	9	-7	67	69	4	-11	-4	112	104	4	-8	-1	171	201
3	2	-8	84	79	3	5	-6	56	50	3	9	-5	71	55	4	-11	-3	111	109	4	-8	0	197	174
3	2	-7	120	122	3	5	-5	215	207	3	9	-4	84	66	4	-11	-2	177	182	4	-8	1	355	326
3	2	-6	167	158	3	5	-4	261	264	3	10	-5	102	96	4	-11	-1	283	293	4	-8	2	222	210
3	2	-5	93	74	3	5	-3	109	126	3	10	-3	62	53	4	-11	0	188	213	4	-8	5	287	287
3	2	-4	412	364	3	5	-2	127	123	3	10	-2	67	63	4	-11	5	177	175	4	-8	6	101	122
3	2	-3	252	233	3	5	-1	146	167	3	10	0	62	44	4	-11	6	202	203	4	-8	7	71	67
3	2	-2	68	62	3	5	1	174	160	3	11	-1	66	45	4	-10	-5	126	139	4	-7	-6	140	149
3	2	1	95	84	3	5	2	160	145	4	-16	1	73	65	4	-10	-2	97	116	4	-7	-5	62	45
3	2	2	234	197	3	5	4	90	97	4	-15	-1	90	88	4	-10	0	102	78	4	-7	-4	75	68
3	2	3	188	196	3	5	5	68	67	4	-15	1	85	75	4	-10	1	366	366	4	-7	-3	171	171
3	2	5	132	133	3	6	-9	72	90	4	-15	2	92	99	4	-10	2	347	363	4	-7	-2	267	300
3	2	6	81	81	3	6	-8	76	68	4	-15	5	106	52	4	-10	3	107	107	4	-7	-1	198	202
3	3	-9	112	139	3	6	-7	113	59	4	-14	-3	99	81	4	-10	4	328	316	4	-7	0	497	514
3	3	-8	179	190	3	6	-4	215	187	4	-14	0	89	91	4	-10	5	142	153	4	-7	1	288	330
3	3	-6	279	258	3	6	-3	227	219	4	-14	1	96	99	4	-10	7	112	120	4	-7	3	343	304
3	3	-5	280	257	3	6	-2	124	125	4	-14	3	77	79	4	-10	8	97	102	4	-7	4	245	246
3	3	-4	101	65	3	6	-1	151	141	4	-14	4	143	111	4	-9	-7	118	135	4	-7	6	149	155
3	3	-3	58	50	3	6	0	202	191	4	-14	6	115	113	4	-9	-6	71	74	4	-7	7	209	224
3	3	-2	311	306	3	6	1	114	137	4	-13	-2	64	58	4	-9	-5	70	43	4	-6	-8	83	91
3	3	-1	198	224	3	6	4	63	65	4	-13	-1	136	132	4	-9	-4	129	140	4	-6	-5	247	229
3	3	1	201	205	3	7	-8	88	87	4	-13	0	65	71	4	-9	-3	78	73	4	-6	-4	278	288
3	3	2	224	227	3	7	-7	91	93	4	-13	1	65	37	4	-9	-1	250	258	4	-6	-3	248	231
3	3	3	94	91	3	7	-5	106	94	4	-13	2	142	148	4	-9	0	245	275	4	-6	-2	454	420
3	3	4	163	163	3	7	-4	167	163	4	-13	3	110	108	4	-9	1	72	5	4	-6	-1	48	53

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	-6	1	271	227	4	-3	1	109	86	4	0	-3	363	367	4	2	4	164	176	4	6	-2	233	236
4	-6	2	192	199	4	-3	2	221	173	4	0	-2	143	121	4	2	5	74	81	4	6	-1	54	71
4	-6	3	45	70	4	-3	3	135	93	4	0	-1	400	500	4	3	-8	116	120	4	6	0	79	64
4	-6	5	340	340	4	-3	4	406	410	4	0	0	237	230	4	3	-7	277	285	4	6	1	69	65
4	-6	6	175	183	4	-3	5	417	413	4	0	1	41	58	4	3	-6	135	155	4	6	2	62	57
4	-6	8	78	102	4	-3	7	158	169	4	0	2	148	149	4	3	-5	289	276	4	7	-7	90	84
4	-5	-7	88	77	4	-2	-8	119	109	4	0	3	302	324	4	3	-4	138	116	4	7	-4	103	98
4	-5	-6	141	144	4	-2	-7	158	165	4	0	4	229	246	4	3	-3	130	109	4	7	-3	84	86
4	-5	-5	90	103	4	-2	-6	122	141	4	0	6	89	99	4	3	-2	296	268	4	7	-1	78	78
4	-5	-3	393	378	4	-2	-4	497	474	4	0	7	81	88	4	3	-1	282	294	4	7	0	107	102
4	-5	-2	677	696	4	-2	-3	523	532	4	1	-8	87	92	4	3	1	177	177	4	7	3	72	47
4	-5	1	205	206	4	-2	1	155	88	4	1	-7	76	83	4	3	2	227	234	4	8	-5	64	66
4	-5	2	159	167	4	-2	2	377	314	4	1	-5	250	236	4	3	3	143	162	4	8	-3	64	40
4	-5	3	307	279	4	-2	3	423	397	4	1	-4	255	266	4	3	5	146	145	4	8	-2	120	110
4	-5	4	310	297	4	-2	4	53	55	4	1	-3	99	87	4	4	-9	83	81	4	8	-1	90	101
4	-5	6	178	176	4	-2	5	107	101	4	1	-2	513	494	4	4	-7	257	249	4	8	1	74	63
4	-5	7	166	191	4	-2	6	139	149	4	1	-1	530	552	4	4	-6	160	160	4	8	2	69	68
4	-4	-8	151	115	4	-2	7	74	73	4	1	0	192	213	4	4	-5	137	136	4	9	-7	79	54
4	-4	-6	66	47	4	-1	-9	83	80	4	1	1	352	356	4	4	-4	122	138	4	9	-4	109	90
4	-4	-5	195	167	4	-1	-7	60	49	4	1	2	155	166	4	4	-3	169	174	4	9	-3	94	74
4	-4	-4	198	194	4	-1	-6	256	238	4	1	4	84	72	4	4	-2	285	286	4	10	-4	89	98
4	-4	-3	129	139	4	-1	-5	148	130	4	1	5	131	134	4	4	0	186	183	4	10	-3	77	60
4	-4	-2	332	325	4	-1	-4	70	109	4	2	-9	71	70	4	4	1	158	174	4	11	-4	122	129
4	-4	1	369	362	4	-1	-3	159	145	4	2	-8	81	50	4	5	-7	63	76	4	11	-3	78	86
4	-4	2	677	623	4	-1	-2	71	116	4	2	-7	235	200	4	5	-5	119	94	5	-16	3	75	82
4	-4	3	360	323	4	-1	0	113	149	4	2	-6	113	107	4	5	-4	223	209	5	-15	-1	118	103
4	-4	4	49	46	4	-1	1	449	420	4	2	-5	75	89	4	5	-2	145	118	5	-15	0	104	93
4	-4	5	99	29	4	-1	2	192	174	4	2	-4	76	59	4	5	-1	191	193	5	-15	1	62	42
4	-4	6	70	82	4	-1	3	55	54	4	2	-3	273	261	4	5	2	135	136	5	-15	2	165	121
4	-4	8	72	86	4	-1	4	244	242	4	2	-2	159	139	4	5	3	121	123	5	-15	3	121	131
4	-3	-9	72	51	4	-1	5	207	212	4	2	-1	135	112	4	6	-9	89	124	5	-14	-3	84	78
4	-3	-8	86	105	4	0	-8	85	71	4	2	0	225	248	4	6	-8	80	85	5	-14	-2	74	77
4	-3	-6	188	168	4	0	-7	191	181	4	2	1	314	326	4	6	-6	131	126	5	-14	1	127	130
4	-3	-5	288	282	4	0	-6	237	241	4	2	2	112	111	4	6	-5	96	88	5	-14	2	113	104
4	-3	-3	461	405	4	0	-4	347	341	4	2	3	150	144	4	6	-3	176	168	5	-14	3	95	88

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	-14	4	193	196	5	-10	1	149	142	5	-7	-2	210	247	5	-4	1	206	239	5	-1	4	65	45
5	-14	5	136	137	5	-10	2	284	303	5	-7	1	338	350	5	-4	2	73	58	5	-1	5	97	105
5	-13	-4	66	63	5	-10	3	351	363	5	-7	2	299	309	5	-4	3	302	260	5	-1	6	80	96
5	-13	-3	72	77	5	-10	4	72	69	5	-7	3	124	97	5	-4	4	183	197	5	0	-9	114	121
5	-13	0	116	113	5	-10	5	242	253	5	-7	4	287	287	5	-4	6	145	150	5	0	-8	83	98
5	-13	2	144	146	5	-10	6	138	150	5	-7	5	140	142	5	-4	7	78	101	5	0	-7	123	112
5	-13	3	228	230	5	-9	-6	125	111	5	-7	6	67	44	5	-3	-8	149	152	5	0	-6	245	218
5	-13	4	101	105	5	-9	-5	75	74	5	-7	7	216	229	5	-3	-7	203	209	5	0	-4	186	149
5	-13	6	113	124	5	-9	-4	75	74	5	-7	8	139	176	5	-3	-6	143	136	5	0	-3	262	265
5	-12	-5	108	104	5	-9	-3	248	249	5	-6	-7	172	166	5	-3	-4	206	215	5	0	0	262	262
5	-12	-4	75	52	5	-9	-2	203	221	5	-6	-5	404	377	5	-3	-3	99	91	5	0	1	267	275
5	-12	-2	226	219	5	-9	0	349	354	5	-6	-4	360	338	5	-3	1	458	463	5	0	2	67	73
5	-12	-1	165	180	5	-9	1	439	458	5	-6	-3	299	297	5	-3	2	384	376	5	0	3	151	139
5	-12	0	122	109	5	-9	3	193	176	5	-6	1	51	103	5	-3	4	92	61	5	0	4	75	74
5	-12	1	245	243	5	-9	4	79	72	5	-6	2	251	240	5	-3	5	66	76	5	1	-8	83	77
5	-12	2	140	156	5	-9	6	79	84	5	-6	3	169	145	5	-3	6	116	132	5	1	-7	96	75
5	-12	3	67	76	5	-9	7	128	144	5	-6	4	54	60	5	-3	8	70	86	5	1	-6	136	142
5	-12	4	105	101	5	-8	-8	85	104	5	-6	5	103	94	5	-2	-9	114	117	5	1	-5	130	107
5	-12	5	154	158	5	-8	-7	113	116	5	-6	6	156	175	5	-2	-7	117	119	5	1	-4	361	355
5	-11	-4	88	83	5	-8	-6	69	56	5	-5	-8	126	130	5	-2	-6	218	211	5	1	-3	147	163
5	-11	-3	106	118	5	-8	-5	153	138	5	-5	-6	88	72	5	-2	-5	55	82	5	1	-2	361	389
5	-11	-1	114	87	5	-8	-4	63	44	5	-5	-5	188	193	5	-2	-4	272	244	5	1	0	217	250
5	-11	0	191	206	5	-8	-2	191	162	5	-5	-3	170	141	5	-2	-3	260	319	5	1	1	56	65
5	-11	1	272	276	5	-8	-1	363	399	5	-5	1	544	599	5	-2	1	343	343	5	1	2	69	46
5	-11	2	105	110	5	-8	0	263	306	5	-5	2	577	529	5	-2	3	260	257	5	1	3	133	158
5	-11	3	258	260	5	-8	1	63	40	5	-5	3	91	62	5	-2	4	328	328	5	1	5	85	76
5	-11	4	102	116	5	-8	2	452	443	5	-5	4	362	352	5	-2	6	104	95	5	2	-9	92	103
5	-11	6	134	130	5	-8	3	316	316	5	-5	5	124	126	5	-1	-8	138	137	5	2	-8	109	105
5	-11	7	86	96	5	-8	5	218	212	5	-5	8	81	104	5	-1	-7	154	153	5	2	-6	185	183
5	-10	-7	71	80	5	-8	6	131	147	5	-4	-8	82	69	5	-1	-6	53	39	5	2	-5	148	143
5	-10	-5	140	137	5	-8	7	78	82	5	-4	-7	152	149	5	-1	-5	314	281	5	2	-4	72	95
5	-10	-4	118	116	5	-7	-6	135	125	5	-4	-6	106	106	5	-1	-4	353	362	5	2	-2	55	71
5	-10	-3	133	111	5	-7	-5	369	356	5	-4	-5	71	56	5	-1	-1	48	68	5	2	-1	59	92
5	-10	-2	213	201	5	-7	-4	114	113	5	-4	-4	429	400	5	-1	2	405	388	5	2	1	232	236
5	-10	-1	229	234	5	-7	-3	328	287	5	-4	-3	276	295	5	-1	3	128	155	5	2	2	146	144

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	2	4	58	51	5	8	2	88	79	6	-11	-2	265	286	6	-8	-4	69	76	6	-5	-7	87	105
5	3	-9	71	77	5	9	-6	80	84	6	-11	0	138	96	6	-8	-3	238	251	6	-5	-5	167	121
5	3	-7	204	197	5	9	-5	74	81	6	-11	2	109	80	6	-8	-2	118	137	6	-5	-4	173	163
5	3	-6	147	139	5	10	-1	72	47	6	-11	3	189	176	6	-8	-1	190	217	6	-5	1	207	184
5	3	-5	130	114	6	-16	-2	102	104	6	-11	4	245	225	6	-8	0	210	213	6	-5	2	298	298
5	3	-3	149	155	6	-16	2	89	84	6	-11	5	186	186	6	-8	1	55	76	6	-5	3	306	305
5	3	-1	181	179	6	-15	-3	81	75	6	-11	7	101	114	6	-8	2	160	144	6	-5	5	279	254
5	3	0	181	186	6	-15	0	172	173	6	-10	-5	100	78	6	-8	3	325	302	6	-5	6	82	91
5	3	2	62	59	6	-15	1	104	101	6	-10	-4	251	237	6	-8	4	182	183	6	-4	-9	100	98
5	3	3	110	115	6	-15	3	118	104	6	-10	-3	80	80	6	-8	6	155	146	6	-4	-7	133	122
5	4	-6	122	109	6	-15	4	107	122	6	-10	-2	108	86	6	-8	7	97	104	6	-4	-6	250	246
5	4	-5	185	179	6	-14	-2	132	121	6	-10	-1	185	193	6	-7	-5	465	436	6	-4	-5	250	257
5	4	-4	229	236	6	-14	-1	125	113	6	-10	0	269	284	6	-7	-4	323	312	6	-4	-4	66	41
5	4	-3	114	121	6	-14	2	109	121	6	-10	1	257	264	6	-7	-3	183	174	6	-4	1	405	441
5	4	-2	117	116	6	-14	5	134	132	6	-10	2	86	64	6	-7	-2	162	213	6	-4	2	150	153
5	4	-1	114	127	6	-14	6	89	100	6	-10	3	254	241	6	-7	0	44	36	6	-4	3	146	119
5	4	1	131	115	6	-13	-4	74	57	6	-10	4	80	81	6	-7	1	255	279	6	-4	4	132	108
5	5	-7	95	92	6	-13	-3	100	102	6	-10	5	201	187	6	-7	2	292	274	6	-4	5	69	51
5	5	-6	77	87	6	-13	-2	105	103	6	-10	6	154	156	6	-7	3	177	190	6	-4	6	87	81
5	5	-4	115	107	6	-13	0	138	125	6	-9	-6	68	72	6	-7	4	146	137	6	-4	7	112	121
5	5	-3	110	111	6	-13	1	113	122	6	-9	-5	186	187	6	-7	5	270	268	6	-3	-9	71	60
5	5	0	61	68	6	-13	3	163	143	6	-9	-4	126	141	6	-7	6	64	75	6	-3	-7	58	68
5	5	1	79	115	6	-13	4	147	145	6	-9	-3	134	130	6	-6	-7	135	128	6	-3	-6	106	123
5	6	-8	85	86	6	-13	5	60	51	6	-9	-2	218	225	6	-6	-6	129	125	6	-3	-5	80	45
5	6	-5	175	149	6	-12	-4	179	160	6	-9	-1	111	171	6	-6	-5	82	102	6	-3	-4	205	203
5	6	-4	146	142	6	-12	-2	93	69	6	-9	0	278	260	6	-6	-4	68	31	6	-3	-3	46	113
5	6	-2	58	58	6	-12	-1	213	218	6	-9	1	350	324	6	-6	-3	253	286	6	-3	1	176	148
5	6	-1	127	133	6	-12	0	208	226	6	-9	2	133	125	6	-6	0	180	283	6	-3	2	190	176
5	6	1	95	84	6	-12	1	81	50	6	-9	3	96	78	6	-6	1	112	121	6	-3	3	204	186
5	7	-6	84	98	6	-12	2	200	171	6	-9	4	171	160	6	-6	2	80	57	6	-3	4	224	234
5	7	-3	69	54	6	-12	3	151	167	6	-9	5	158	182	6	-6	3	247	215	6	-3	6	114	119
5	7	-1	62	51	6	-12	5	134	131	6	-9	7	70	58	6	-6	4	134	126	6	-2	-9	118	113
5	7	1	100	112	6	-12	6	121	134	6	-8	-8	119	130	6	-6	6	116	103	6	-2	-8	179	166
5	7	2	93	114	6	-11	-6	110	100	6	-8	-7	147	145	6	-6	7	122	118	6	-2	-6	165	149
5	8	1	100	100	6	-11	-3	112	119	6	-8	-6	64	69	6	-5	-8	80	83	6	-2	-5	186	176

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
6	-2	-4	100	139	6	1	-4	247	229	6	6	-4	129	117	7	-12	-6	69	48	7	-9	-5	101	85
6	-2	-3	133	203	6	1	-3	185	200	6	6	-1	120	114	7	-12	-4	83	75	7	-9	-4	103	98
6	-2	0	88	122	6	1	-1	102	80	6	6	0	68	67	7	-12	-3	153	146	7	-9	-2	171	196
6	-2	1	283	268	6	1	0	201	216	6	7	-5	67	50	7	-12	-2	144	174	7	-9	0	134	177
6	-2	2	110	120	6	1	1	123	122	6	8	-5	70	53	7	-12	-1	59	18	7	-9	1	194	197
6	-2	3	198	164	6	1	3	173	158	6	8	-3	76	50	7	-12	0	274	282	7	-9	2	409	388
6	-2	4	367	339	6	1	4	123	122	6	9	-5	70	62	7	-12	1	91	95	7	-9	3	180	184
6	-2	5	108	109	6	1	6	70	67	7	-16	-2	85	61	7	-12	2	298	266	7	-9	4	75	70
6	-1	-8	96	92	6	2	-8	109	107	7	-16	-1	135	108	7	-12	3	203	192	7	-9	5	167	165
6	-1	-7	158	157	6	2	-7	130	141	7	-16	1	81	69	7	-12	4	99	106	7	-9	6	106	114
6	-1	-6	179	182	6	2	-6	62	32	7	-16	2	88	102	7	-12	5	61	52	7	-8	-8	69	55
6	-1	-5	192	163	6	2	-5	125	102	7	-16	3	87	75	7	-12	6	176	174	7	-8	-6	158	142
6	-1	-4	365	350	6	2	-2	201	173	7	-15	-3	82	47	7	-11	-6	74	54	7	-8	-4	239	204
6	-1	-3	84	112	6	2	-1	85	85	7	-15	-2	79	69	7	-11	-5	106	92	7	-8	-3	151	155
6	-1	-2	108	146	6	2	1	55	38	7	-15	0	125	76	7	-11	-3	201	169	7	-8	-2	108	185
6	-1	-1	47	46	6	2	2	97	99	7	-15	1	186	179	7	-11	-2	246	252	7	-8	1	224	236
6	-1	0	73	81	6	3	-6	94	84	7	-15	3	85	62	7	-11	-1	116	116	7	-8	2	75	109
6	-1	1	149	172	6	3	-5	101	89	7	-15	4	86	100	7	-11	0	95	97	7	-8	3	186	155
6	-1	2	56	33	6	3	-4	172	156	7	-14	-4	108	101	7	-11	2	180	194	7	-8	4	188	180
6	-1	3	155	153	6	3	-3	273	271	7	-14	-3	79	63	7	-11	3	129	130	7	-7	-8	78	70
6	-1	4	73	68	6	3	-2	131	130	7	-14	-1	105	82	7	-11	4	162	156	7	-7	-7	77	75
6	-1	6	91	92	6	3	0	143	115	7	-14	0	79	87	7	-11	5	196	186	7	-7	-5	66	25
6	0	-8	103	114	6	3	1	90	76	7	-14	2	100	103	7	-11	6	92	96	7	-7	-4	287	276
6	0	-5	52	30	6	3	3	82	81	7	-14	5	98	87	7	-10	-4	116	95	7	-7	-3	177	256
6	0	-3	109	74	6	3	4	111	119	7	-13	-3	116	86	7	-10	-3	199	186	7	-7	1	72	77
6	0	-1	306	364	6	4	-8	146	144	7	-13	-2	163	145	7	-10	-2	82	83	7	-7	2	303	264
6	0	0	104	78	6	4	-7	129	126	7	-13	-3	119	86	7	-10	-1	82	75	7	-7	3	194	187
6	0	1	198	181	6	4	-1	128	128	7	-13	-2	163	145	7	-10	0	390	413	7	-7	5	113	111
6	0	3	107	87	6	4	1	90	81	7	-13	0	148	140	7	-10	1	286	309	7	-7	6	192	189
6	0	4	96	89	6	4	2	126	122	7	-13	1	210	204	7	-10	2	110	93	7	-7	7	113	119
6	0	5	83	82	6	5	-6	85	82	7	-13	2	145	144	7	-10	3	205	178	7	-6	-8	81	82
6	1	-8	79	59	6	5	-5	109	103	7	-13	3	75	48	7	-10	4	120	132	7	-6	-6	267	230
6	1	-7	148	135	6	5	-3	144	130	7	-13	4	170	159	7	-10	6	93	99	7	-6	-5	243	237
6	1	-6	130	128	6	5	-2	93	103	7	-13	5	101	108	7	-10	7	102	133	7	-6	-4	106	83
6	1	-5	89	90	6	6	-5	94	90	7	-13	6	88	82	7	-9	-8	98	104	7	-6	-3	49	88

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
7	-6	1	319	353	7	-2	-4	172	213	7	2	-5	97	81	8	-13	0	59	65	8	-9	-1	152	233
7	-6	2	101	131	7	-2	0	50	80	7	2	-4	79	79	8	-13	1	110	105	8	-9	0	299	398
7	-6	3	156	138	7	-2	1	272	253	7	2	-3	103	102	8	-13	2	165	149	8	-9	1	128	170
7	-6	4	206	180	7	-2	2	280	267	7	2	-2	116	106	8	-13	3	110	119	8	-9	2	119	103
7	-6	5	70	98	7	-2	5	123	127	7	2	-1	153	154	8	-13	5	109	92	8	-9	3	140	126
7	-5	-8	80	70	7	-1	-7	140	132	7	2	0	165	176	8	-13	6	68	63	8	-9	5	100	74
7	-5	-7	82	69	7	-1	-6	185	178	7	4	-8	113	115	8	-12	-6	151	136	8	-9	6	126	116
7	-5	-6	88	67	7	-1	-5	136	176	7	4	-7	145	138	8	-12	-5	64	55	8	-8	-8	133	139
7	-5	-5	238	192	7	-1	-4	66	39	7	4	-1	65	69	8	-12	-3	140	145	8	-8	-6	127	92
7	-5	-4	282	324	7	-1	-2	74	143	7	5	-5	112	116	8	-12	-2	130	146	8	-8	-5	149	129
7	-5	1	179	236	7	-1	0	198	200	7	5	-4	82	73	8	-12	0	130	110	8	-8	-4	97	99
7	-5	2	68	32	7	-1	1	129	132	7	5	-2	65	61	8	-12	1	218	239	8	-8	-3	120	152
7	-5	3	234	223	7	-1	2	76	89	7	6	-3	68	74	8	-12	3	145	124	8	-8	0	94	37
7	-5	4	73	89	7	-1	3	75	60	7	6	0	75	76	8	-12	4	169	161	8	-8	1	119	115
7	-5	5	129	136	7	-1	4	79	86	7	6	1	104	39	8	-12	5	74	92	8	-8	2	129	133
7	-5	6	132	128	7	0	-8	64	57	8	-17	1	117	102	8	-11	-5	136	99	8	-8	4	185	154
7	-4	-8	127	126	7	0	-7	105	86	8	-16	-1	83	70	8	-11	-4	142	137	8	-8	5	133	117
7	-4	-6	199	181	7	0	-5	234	225	8	-16	0	77	94	8	-11	-2	129	103	8	-7	-8	71	55
7	-4	-5	226	211	7	0	-4	94	108	8	-16	2	77	62	8	-11	-1	231	267	8	-7	-7	113	89
7	-4	1	515	525	7	0	-1	127	147	8	-16	3	109	114	8	-11	0	134	149	8	-7	-6	263	234
7	-4	2	252	225	7	0	0	147	157	8	-15	-2	117	107	8	-11	3	147	151	8	-7	-5	323	308
7	-4	3	71	48	7	0	1	146	123	8	-15	-1	108	102	8	-11	4	72	73	8	-7	0	90	159
7	-4	6	65	88	7	0	2	203	218	8	-15	0	93	43	8	-11	5	88	64	8	-7	1	95	123
7	-3	-6	136	129	7	1	-9	74	72	8	-15	1	110	111	8	-10	-6	107	87	8	-7	2	114	94
7	-3	-5	70	39	7	1	-7	114	104	8	-15	2	159	150	8	-10	-5	203	180	8	-7	3	193	164
7	-3	-4	139	187	7	1	-6	135	115	8	-15	3	107	109	8	-10	-3	228	229	8	-7	4	129	124
7	-3	0	93	164	7	1	-5	167	158	8	-14	-3	82	85	8	-10	-2	179	206	8	-7	6	176	166
7	-3	1	64	66	7	1	-4	89	123	8	-14	-1	88	82	8	-10	1	95	110	8	-6	-8	89	92
7	-3	3	189	178	7	1	-3	213	228	8	-14	0	117	103	8	-10	2	143	151	8	-6	-7	97	91
7	-3	4	160	160	7	1	-2	275	282	8	-14	1	104	108	8	-10	3	122	90	8	-6	-6	217	179
7	-2	-9	67	38	7	1	0	120	124	8	-14	3	186	173	8	-10	4	256	224	8	-6	-5	223	205
7	-2	-8	197	183	7	1	1	93	78	8	-14	4	140	150	8	-10	5	146	135	8	-6	1	118	108
7	-2	-7	92	74	7	1	4	70	68	8	-13	-4	134	117	8	-9	-7	115	99	8	-6	2	227	201
7	-2	-6	156	143	7	2	-7	96	82	8	-13	-2	125	102	8	-9	-6	64	69	8	-6	3	107	88
7	-2	-5	290	257	7	2	-6	61	72	8	-13	-1	221	211	8	-9	-3	185	242	8	-6	4	171	119

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
8	-6	5	125	103	8	-1	-4	70	99	9	-15	0	89	86	9	-10	-1	88	140	9	-6	5	98	67
8	-5	-7	82	53	8	-1	0	69	62	9	-15	2	112	98	9	-10	0	145	195	9	-6	6	87	81
8	-5	-6	143	117	8	-1	1	91	83	9	-15	3	108	97	9	-10	1	142	141	9	-5	-9	83	58
8	-5	-5	86	110	8	-1	3	75	53	9	-14	-3	127	97	9	-10	2	315	291	9	-5	-8	102	89
8	-5	-4	66	117	8	-1	4	83	64	9	-14	0	106	94	9	-10	4	190	156	9	-5	-7	97	63
8	-5	0	50	92	8	0	-8	68	41	9	-14	1	134	133	9	-10	5	142	133	9	-5	-6	147	113
8	-5	1	74	60	8	0	-5	144	135	9	-14	2	80	83	9	-10	6	72	65	9	-5	-5	91	112
8	-5	3	128	104	8	0	-4	147	141	9	-14	4	128	121	9	-9	-7	145	78	9	-5	0	118	176
8	-5	4	182	163	8	0	0	129	130	9	-13	-1	124	104	9	-9	-6	194	132	9	-5	1	142	146
8	-5	6	95	84	8	0	3	94	82	9	-13	0	162	159	9	-9	0	270	318	9	-5	4	98	96
8	-4	-5	109	108	8	1	-8	91	82	9	-13	2	196	148	9	-9	3	178	121	9	-5	5	106	106
8	-4	-4	96	161	8	1	-7	84	94	9	-13	3	138	109	9	-9	4	171	130	9	-4	-7	107	88
8	-4	1	63	29	8	1	-5	71	64	9	-12	-6	77	65	9	-9	6	96	54	9	-4	-6	130	124
8	-4	2	299	260	8	1	-4	71	82	9	-12	-5	112	99	9	-8	-8	101	61	9	-4	-5	76	48
8	-4	3	143	113	8	1	-3	158	146	9	-12	-2	88	71	9	-8	-5	108	61	9	-4	-4	88	133
8	-4	4	74	64	8	1	-2	233	243	9	-12	-1	75	82	9	-8	-4	180	229	9	-4	-3	85	183
8	-4	5	97	75	8	1	4	66	28	9	-12	1	237	213	9	-8	-1	69	138	9	-4	1	312	259
8	-3	-9	117	118	8	2	-6	85	79	9	-12	2	281	256	9	-8	1	271	181	9	-4	2	114	57
8	-3	-5	78	109	8	2	-4	86	82	9	-12	4	143	135	9	-8	2	291	189	9	-4	3	120	76
8	-3	-3	60	134	8	2	0	89	68	9	-12	5	174	162	9	-8	3	182	141	9	-4	4	141	91
8	-3	0	130	180	8	3	-8	78	61	9	-12	6	106	97	9	-8	5	110	72	9	-4	5	176	64
8	-2	-7	163	145	8	3	-4	58	69	9	-11	-7	74	50	9	-7	-7	95	46	9	-3	-6	111	56
8	-2	-6	72	71	8	3	1	93	79	9	-11	-6	68	49	9	-7	-6	283	180	9	-3	-5	94	83
8	-2	-5	129	124	8	3	2	79	69	9	-11	-4	133	120	9	-7	-5	114	116	9	-3	0	117	102
8	-2	-4	116	141	8	4	-6	101	93	9	-11	-3	268	296	9	-7	0	222	294	9	-3	1	206	134
8	-2	-2	51	119	8	4	-3	69	57	9	-11	-2	81	136	9	-7	1	349	289	9	-3	3	211	125
8	-2	-1	52	115	9	-17	-1	125	97	9	-11	-1	121	144	9	-7	2	74	85	9	-3	5	114	83
8	-2	0	66	91	9	-17	1	104	61	9	-11	0	96	108	9	-7	3	115	107	9	-2	-7	158	93
8	-2	2	184	156	9	-17	2	100	92	9	-11	1	191	177	9	-7	4	130	120	9	-2	-6	177	146
8	-2	3	272	244	9	-16	-3	108	77	9	-11	2	156	132	9	-7	5	67	88	9	-2	-4	119	114
8	-2	4	98	87	9	-16	0	67	79	9	-11	3	105	97	9	-6	-7	68	59	9	-2	-3	136	154
8	-1	-9	95	76	9	-16	1	113	106	9	-11	4	153	140	9	-6	-5	125	131	9	-2	0	140	103
8	-1	-8	92	100	9	-16	3	92	69	9	-11	6	94	99	9	-6	1	61	73	9	-2	1	141	120
8	-1	-6	74	57	9	-15	-4	73	73	9	-10	-5	160	137	9	-6	2	137	114	9	-2	3	218	134
8	-1	-5	199	187	9	-15	-1	125	111	9	-10	-2	74	103	9	-6	3	133	132	9	-2	4	71	63

Table 20 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
9	-1	-9	73	65	10	-15	-3	85	64	10	-10	-7	92	95	10	-3	-7	84	69	11	-12	-1	89	118
9	-1	-8	69	61	10	-15	-1	72	68	10	-10	-4	89	134	10	-3	2	111	74	11	-12	0	112	132
9	-1	-7	74	58	10	-15	0	117	112	10	-10	0	121	189	10	-2	-6	68	70	11	-12	3	72	76
9	-1	-6	78	44	10	-15	1	63	59	10	-10	2	117	94	10	-2	-5	84	107	11	-11	0	79	92
9	-1	-5	107	93	10	-15	3	101	63	10	-10	3	184	158	10	-2	-3	55	51	11	-11	1	192	204
9	-1	-4	65	66	10	-15	4	72	67	10	-10	5	85	59	10	-2	0	85	70	11	-11	2	95	78
9	-1	-2	71	124	10	-14	-5	138	111	10	-9	-6	97	85	10	-1	-1	90	87	11	-11	5	72	75
9	-1	-1	110	174	10	-14	-4	85	79	10	-9	-5	78	91	10	-1	0	127	69	11	-10	-7	85	66
9	-1	1	79	49	10	-14	-2	143	135	10	-9	1	132	148	10	-1	2	125	58	11	-10	-6	71	83
9	-1	2	62	43	10	-14	-1	154	162	10	-9	2	106	121	10	-1	3	101	54	11	-10	-4	60	90
9	0	-9	69	44	10	-14	2	201	187	10	-9	3	72	37	10	0	-8	107	66	11	-10	3	159	134
9	0	-7	70	59	10	-14	3	153	146	10	-9	4	148	108	10	0	-6	102	84	11	-10	4	132	97
9	0	-6	78	63	10	-14	4	75	57	10	-9	5	84	72	10	0	1	95	78	11	-9	-5	79	112
9	0	-4	63	34	10	-13	-3	109	106	10	-8	-7	104	88	10	1	-4	155	95	11	-9	0	60	106
9	0	-3	97	104	10	-13	0	126	133	10	-8	-6	74	72	10	1	-3	220	154	11	-9	1	120	119
9	0	-2	64	69	10	-13	1	124	140	10	-8	0	56	98	10	1	-1	101	71	11	-9	2	76	63
9	0	1	69	66	10	-13	2	81	68	10	-8	2	62	44	10	3	-7	103	31	11	-9	4	68	55
9	1	-7	88	63	10	-13	3	168	129	10	-8	3	74	64	11	-17	0	164	132	11	-9	5	81	77
9	1	-5	79	68	10	-13	4	117	101	10	-7	-8	81	68	11	-16	-2	69	46	11	-8	0	86	117
9	1	-2	64	95	10	-12	-5	110	101	10	-7	1	131	121	11	-16	2	105	91	11	-8	1	65	81
9	1	-1	156	170	10	-12	-4	92	82	10	-7	2	162	146	11	-15	-2	74	62	11	-8	4	106	74
9	2	-6	63	49	10	-12	-2	90	98	10	-7	4	99	62	11	-15	0	132	115	11	-7	-7	69	84
9	2	-5	87	73	10	-12	-1	152	207	10	-7	5	104	85	11	-15	1	123	111	11	-7	-2	83	100
9	2	-3	87	90	10	-12	0	83	95	10	-6	-7	135	115	11	-14	-4	110	105	11	-7	2	111	95
9	2	-2	61	60	10	-12	2	154	144	10	-6	-6	257	262	11	-14	-3	73	86	11	-7	3	68	71
9	3	-4	60	44	10	-12	3	165	166	10	-6	3	99	102	11	-14	-1	106	111	11	-6	-7	81	65
9	3	-1	66	65	10	-12	5	116	91	10	-6	4	88	86	11	-14	0	93	106	11	-6	-6	94	103
9	3	0	82	73	10	-11	-6	88	58	10	-5	-6	81	90	11	-14	2	109	83	11	-6	0	71	101
9	4	-5	64	29	10	-11	-5	84	91	10	-5	-5	71	77	11	-14	3	110	108	11	-6	1	71	76
10	-17	-1	124	96	10	-11	-3	110	188	10	-5	1	93	79	11	-13	0	65	64	11	-6	3	63	46
10	-17	0	102	99	10	-11	0	68	79	10	-5	2	119	100	11	-13	1	158	154	11	-6	4	95	89
10	-16	-3	133	70	10	-11	1	72	116	10	-4	-6	97	108	11	-13	2	108	89	11	-5	2	68	41
10	-16	-2	116	93	10	-11	3	99	67	10	-4	0	68	95	11	-13	4	80	55	11	-4	-5	60	53
10	-16	1	118	105	10	-11	4	106	100	10	-4	1	99	88	11	-12	-4	108	118	11	-4	1	97	72
10	-16	2	91	99	10	-11	5	74	64	10	-4	3	93	85	11	-12	-3	73	101	11	-4	2	77	62

Table 26 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC
11	-4	4	100	106	12	-7	0	72	85
11	-3	-4	68	78	12	-6	-8	82	53
11	-3	0	98	98	12	-6	1	66	80
11	-2	2	106	97	12	-6	2	78	66
11	-1	-6	76	85	12	-5	-7	76	72
11	0	-6	68	66	12	-4	-8	72	50
11	1	-3	71	81	12	-4	0	67	101
11	3	-5	115	41	12	0	-5	68	27
12	-15	-3	83	52	13	-16	-1	76	62
12	-15	-2	113	121	13	-16	0	97	84
12	-15	-1	88	109	13	-14	1	124	124
12	-15	1	78	70	13	-14	2	83	90
12	-15	2	90	81	13	-12	1	93	70
12	-14	-4	67	59	13	-9	2	84	73
12	-14	-3	76	113	13	-9	3	101	83
12	-14	0	91	91	13	-6	-7	70	112
12	-14	3	90	89	13	-5	-3	61	25
12	-13	-5	107	93	14	-14	1	81	57
12	-13	1	64	57	14	-12	2	72	69
12	-13	2	169	152	14	-11	0	79	102
12	-12	0	73	124					
12	-12	1	91	94					
12	-12	3	93	68					
12	-12	4	132	122					
12	-11	2	125	131					
12	-11	3	115	114					
12	-10	-6	73	87					
12	-10	1	91	89					
12	-10	4	94	66					
12	-9	-7	76	73					
12	-9	0	74	151					
12	-9	2	87	78					
12	-8	1	84	110					
12	-8	2	86	112					
12	-7	-7	102	79					

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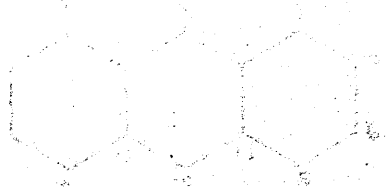


CHAPTER 3

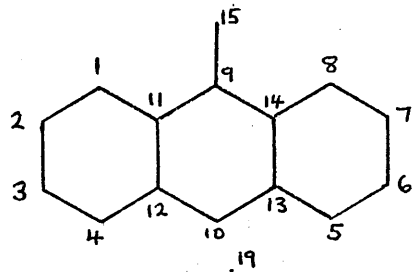
9-METHYLANTHRACENE

AND

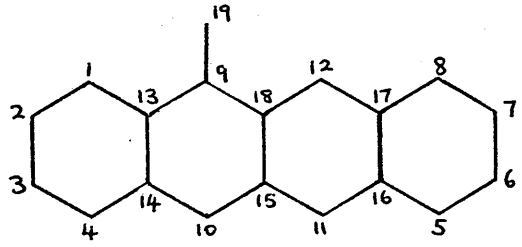
9-METHYLTETRACENE

3.1. Introduction

Following the structure determinations of the naphthalene compounds in chapter 2 it was decided to examine some higher order, polycyclic aromatic hydrocarbons. For this study crystals of 9-methylanthracene and 9-methyltetracene were made available by Professor E. Clar of Glasgow University.



9-methylanthracene



9-methyltetracene

The planar structure of anthracene[1,2] was conclusively established in 1933 by use of two-dimensional X-ray data. Later the structure was redetermined[3,4] by the triple Fourier series method and subsequently a detailed refinement using the same experimental data was carried out.[5,6] X-ray studies of anthracene[7] have also been made at 290°K and 95°K. A number of compounds containing anthracene moieties have been examined as many display carcinogenic activity, e.g. some methyl 1:2-benzathraquinones[8,9] and 5,6,dihydrodibenz/a,j/ anthracene[10]. The structure of 9-methyl anthracene had previously been obtained from two dimensional X-ray data and the results published[11].

This chapter deals with the complete redetermination of the structure of 9-methylanthracene by direct methods using diffractometer data. Although the unit cell dimensions in this study and in the previous structure determination are virtually identical the packing of the molecules in the crystal is different. The structure of 9-methyltetracene has not yet been solved and only information on the crystal data is given.

3.2.1. Experimental

Crystal data

9-methyltetracene

Molecular formula	$C_{19}H_{14}$
Molecular weight	242.3 a.m.u.
Crystal system	monoclinic
Space group	$P2_1/c$ (C_{2h}^2)
Cell dimensions	$\underline{a}$ = 10.794(2) Å
	$\underline{b}$ = 14.697(4) Å
	$\underline{c}$ = 7.980(2) Å
	β = 93.95(3)°
Cell volume (u)	1262.8 Å^3
Density (observed)	1.25 g.cm^{-3}
Density (calculated)	1.27 g.cm^{-3}
Molecules per unit cell (z)	4
Number of electrons per unit cell ($F_{(000)}$)	512
Linear absorption coefficient, μ (MoKα)	0.78 cm^{-1}

The crystal of 9-methyltetracene used in the analysis was red, translucent and rectangular in shape. The preliminary cell dimensions were obtained from rotation and Weissenberg films and the observed density was in agreement with 4 molecules per unit cell.

The crystal was transferred to the diffractometer and an orientation matrix was calculated. The reflections were scanned by 72 steps of 0.01° and each step of the scan was counted for 1 second. At the start and end of each scan a stationary crystal-stationary

counter background count was taken for 18 seconds. The reflections of the octants hkl and $h\bar{k}\bar{l}$ were collected out to $\theta \leqslant 27^{o}$. The stabilised X-ray generator was operated at 46kV and 16mA and the intensities were corrected for Lorentz and polarisation effects but not for absorption. During the data collection a slight movement of the crystal was detected but the intensities of the two standard reflection did not change by $> 3\sigma$. A total of 2756 independent structure amplitudes was obtained, of which 1643 had $I > 3\sigma(I)$.

3.3.1. Experimental

Crystal data

9-methylanthracene

Molecular formula	$C_{15}H_{12}$
Molecular weight	192.2 a.m.u.
Crystal system	monoclinic
Space group	$P2_1/c$ (C_{2h}^2)
Cell dimensions	$\underline{a}$ = 8.920(3) Å
	$\underline{b}$ = 14.641(4) Å
	$\underline{c}$ = 8.078(4) Å
	β = 96.47(3)°
Cell volume (u)	1048.3 Å^3
Density (observed)	1.24 g.cm^{-3}
Density (calculated)	1.22 g.cm^{-3}
Molecules per unit cell (z)	4
Number of electrons per unit cell ($F_{(000)}$)	408
Linear absorption coefficient, μ (MoKα)	0.74 cm^{-1}

The crystal of 9-methylanthracene used in the analysis was yellow, translucent and rectangular in shape. Oscillation, rotation and Weissenberg photographs were taken with Cu(Kα) radiation and the crystal system was shown to be monoclinic. The systematically absent reflections (h0l when l = 2n+1 and 0k0 when k = 2n+1) determined the space group to be $P2_1/c$. The observed density was in close agreement for the density calculated assuming 4 molecules per unit cell.

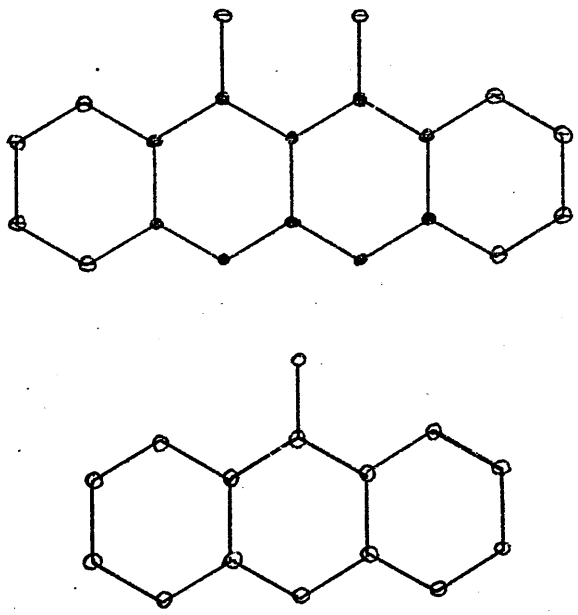
The crystal was transferred to the diffractometer and an orientation matrix was calculated. The reflections were scanned by 72 steps of 0.01° and each step of the scan was counted for 1 second. At the start and end of each scan a stationary crystal-stationary counter background count was taken for 18 seconds. The reflections of the octants $h\bar{k}l$ and $\bar{h}\bar{k}l$ were collected out to $\theta \leqslant 27^{\circ}$. The stabilised X-ray generator was operated at 46 kV and 16mA and the intensities were corrected for Lorentz and polarisation effects but not for absorption. A total of 2292 independent structure amplitudes was obtained, of which 1279 had $I > 3\sigma(I)$.

3.3.2. Structure analysis of 9-methylanthracene

Based on an overall temperature factor of 4.50 $Å^2$ 201 E values were calculated to be ≥ 1.75, and the Sigma two relationships were calculated. The three origin fixing phases (table 1) phased 97 of the 201 E values, so an assumed phase of a fourth reflection ($\bar{6}\ \bar{6}\ 2$) was used to generate a total of 142 phased E values. An E map generated with the phase of $\bar{6}\ \bar{6}\ 2$ as 0 was thought to yield the structure with the exception of the methyl carbon. In subsequent least-squares calculations four 'atoms' were found to be associated with high temperature factors ($B > 8.0$) and were therefore removed from further calculations. The remaining ten atoms, which were the highest E map peaks, resulted in a discrepency index of 0.32, and a difference map at this stage showed a number of peaks including the four E map peaks originally thought to be atom positions. The pseudo-homometric variant[12] now consisted of 18 peaks in a tetracene arrangement plus 2 extra peaks close to what appeared to be the 9 and 12 positions of tetracene. These 2 peaks were thought to arise from the methyl carbon so the actual position was taken to lie half way between them (Fig. 1). The atom positions of the remainder of the molecule were adjusted accordingly and all 15 carbon positions were shown to be correctly located by least squares and structure factor calculations. Only one of the four starting phases, ($6\ \bar{2}\ 3$) was shown to be 0, and as the phase of the structure invariant ($\bar{6}\ \bar{6}\ 2$) was originally phased incorrectly the E map clearly could not yield the correct solution. With the 4 correct phases in the starting set the phases of 142 E values were regenerated, and a subsequent E map yielded the correct solution.

Fig. 1

The E map peaks, difference map peaks and correct atomic positions of 9-methylanthracene



• = 10 highest E map peaks

⊖ = Difference map peaks

o = Actual atom positions

The example of the methyl carbon adjustment:

	x	y	z
Positions of the two pseudo	0.87	0.45	0.325
methyl carbons	0.65	0.45	0.125
Actual atom position	0.76	0.45	0.225

Table 1

9-METHYL ANTHRACENE

(a) Initial set of phases

Reflection	Parity	Initial Phase	Correct Phase	E
$\bar{7}$ $\bar{2}$ 3	U G U	0	π	5.68
$\bar{2}$ $\bar{1}$ 7	G U U	0	π	5.02
6 $\bar{2}$ 3	G G U	0	0	4.05
$\bar{6}$ $\bar{6}$ 2	G G G	0	π	4.36

(b) E statistics

Average value of	$\lvert E \rvert$	$\lvert E^2 \rvert$	$\lvert E^2-1 \rvert$
Found	0.67	0.98	1.18
Theoretical for centric	0.798	1.00	0.968
Theoretical for acentric	0.886	1.00	0.736

Percentage of values for	$E > 1.0$	$E > 2.0$	$E > 3.0$
Found	21.17	5.92	1.61
Theoretical for centric	31.73	4.55	0.27
Theoretical for acentric	36.79	1.83	0.01

Isotropic refinement of the carbon atoms converged at R = 0.157 and after one cycle of least-squares calculating with the atoms refining anisotropically, all the hydrogen positions were located from a difference Fourier map. With the hydrogens included in the structure factor calculation R was 0.096, and after allowing the hydrogens to refine isotropically R converged to 0.091.

A unit weighting scheme was employed in the least-squares calculations, and all the computing was carried out on the Univac 1108 computer at the National Engineering Laboratory, East Kilbride.

3.4. Discussion

The positions of the molecules in the crystal differ from those previously obtained from the two-dimensional data. Figure 2 is a general view of the molecule, and the packing of the molecules in the crystal is shown in Figure 3. A packing diagram obtained from the atom co-ordinates of the two-dimensional data is shown for comparison (Figure 4). As the unit cell dimensions in both studies are very similar it can be concluded that either the four molecules of the unit cell are capable of packing in two different orientations, or that the structure obtained from the limited two-dimensional data is incorrect.

The molecular parameters and positional standard deviations are given in tables 3 and 4, and the molecular geometry is shown in tables 5, 6, 7, 8 and 9. Table 2 compares the bond lengths obtained in this study to 9-nitroanthracene[13], and to anthracene itself. There is no significant difference between the lengths of chemically equivalent bonds, nor is there any significant difference between the bonds which would be chemically equivalent if the methyl group was absent. This is also found for 9-nitroanthracene and hence an average of the relevant bond lengths has been made for direct comparison with this compound and with anthracene. The average bond length in the anthracene moiety is 1.403 Å which is intermediate between the $C(sp^3)$ - $C(sp^3)$ single bond of 1.537 Å and the $C(sp^2)$ = $C(sp^2)$ double bond of 1.335 Å[14]. The average bond length in anthracene[6] is 1.404 Å, in anthrone[15] 1.407 Å, in 9:10-dihydro-1:2:5:6-dibenzanthracene[16] 1.401 Å and 1.39 Å in the anthracene moiety of the previous structure determination of the molecule. The C(9) - C(15) bond length of 1.503 Å is in good agreement with the average $C(sp^3)$ - C_6H_5 bond length of 1.505 Å

Fig. 2

A general view of the molecule

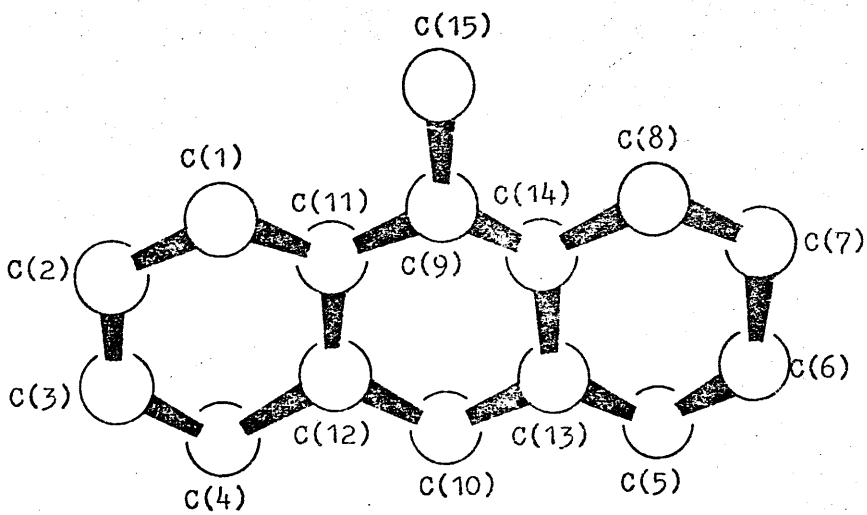


Fig. 3

The crystal structure of 9-methylanthracene, viewed down the c axis.

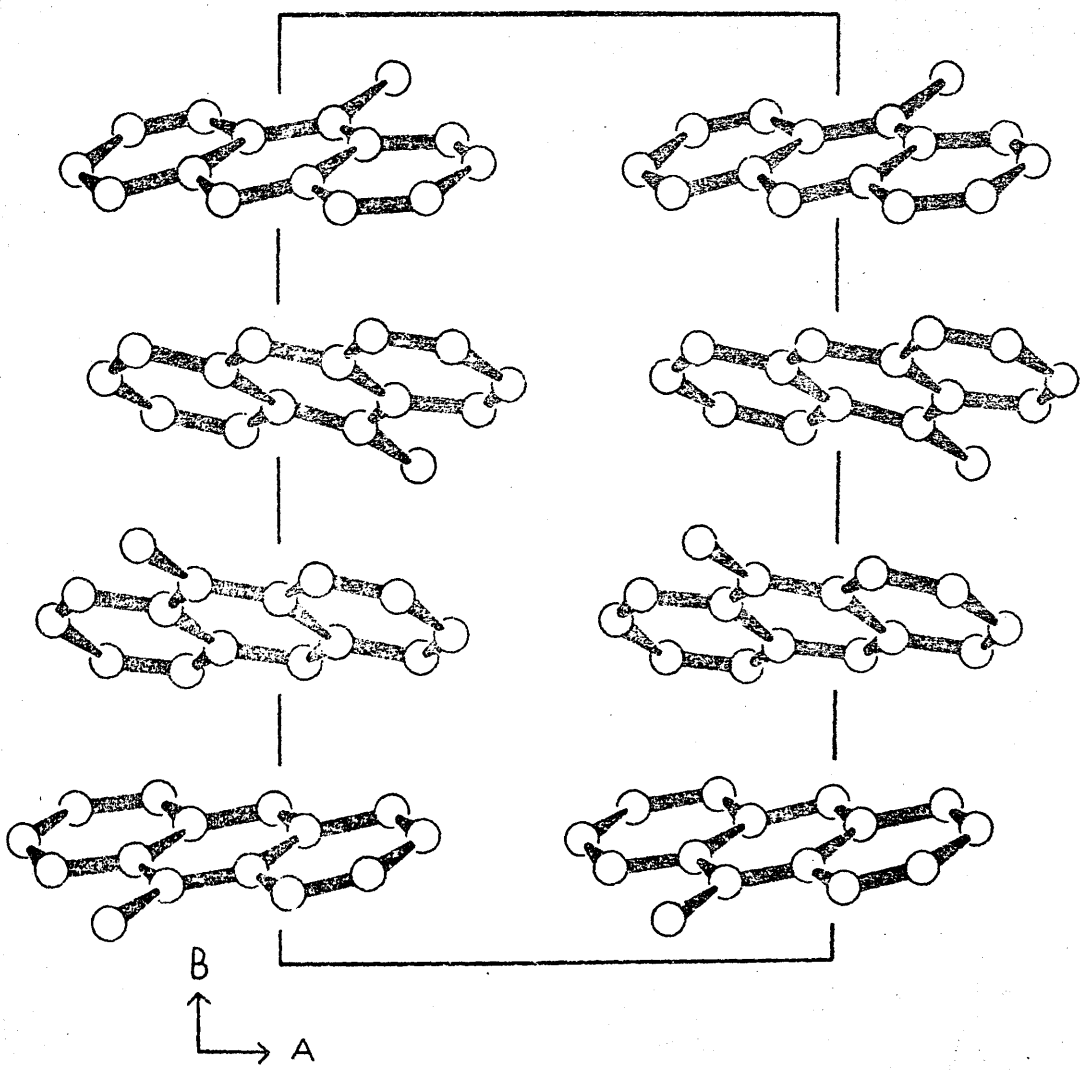
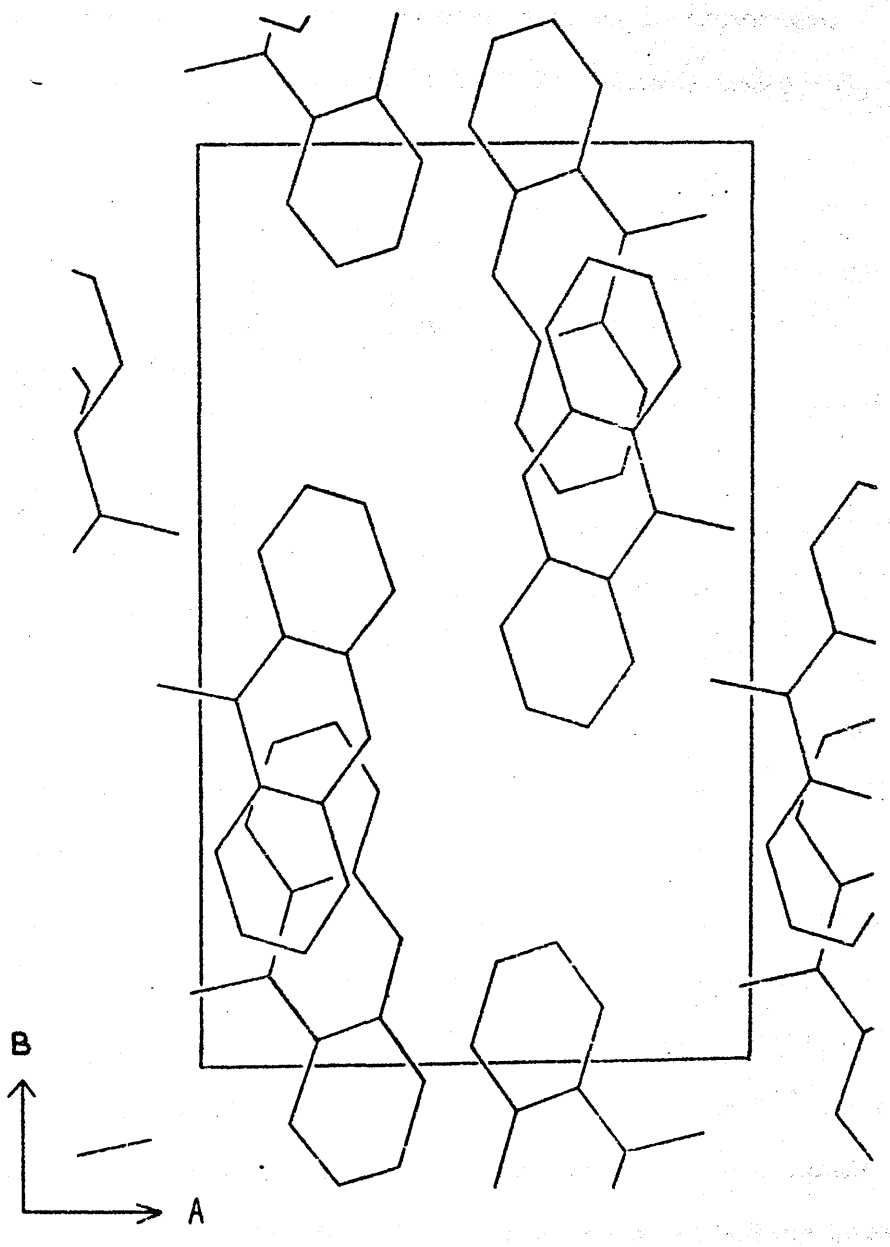


Fig. 4

The crystal structure of 9-methylanthracene (obtained from two-dimensional data) viewed down the c axis.

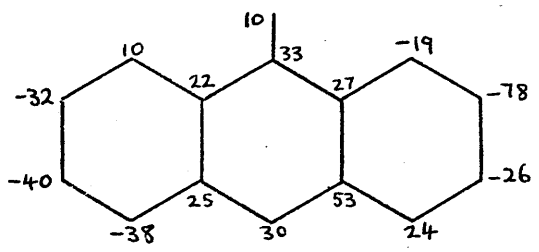


quoted by Sutton et al[14].

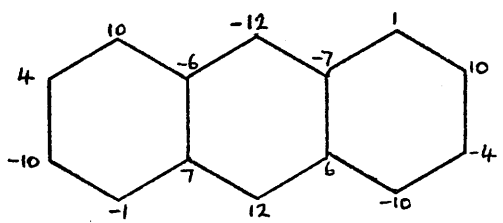
The molecule is almost planar but there are significant deviations from the mean plane; the equation of the plane through the molecule is

$$0.2427X + 0.8985Y - 0.3659Z = 6.9485 \qquad (17)$$

where X, Y and Z are orthogonalised co-ordinates in angstroms. Here the greatest deviation from the plane is by C(7), -0.078Å and C(13), 0.053Å.



Atom deviations from the plane (Å x 10^{-3}) for 9-methyl anthracene.



Atom deviations from the plane (Å x 10^{-3}) for anthracene[6]

The molecule is distorted from planarity to a greater extent than in anthracene where the maximum deviation from the molecular plane is 0.012 Å. 9-cyanoanthracene[18] is reported to be deformed from planarity in a similar way to anthracene. The maximum deviation from the anthracene plane in 9-anthraldehyde[19] is 0.06 Å and 0.012 Å in 9-nitroanthracene. In phenanthrene[20] the greatest deviation from the molecular plane is 0.040 Å and in 9:10 dihydroanthracene[21] the molecule is bent about the 9-10 bond with each planar half of the molecule inclined to each other by 145°. For 9-methyl anthracene out-of-plane bending is present with the six atoms C(2), C(3), C(4), C(6), C(7) and C(8) lying

below the plane and the remaining atoms lying above the plane. The magnitude of the largest torsion angle, $|4^{\circ}|$, is found at C(6) - C(5) - C(13) - C(10).

There are two short contacts between the peri-substituents and the methyl hydrogens, H(8) - H(15B) is 1.97(9) Å and H(1) - H(15A) is 2.15(8) Å. The in-plane bending here is evident in the valency angles C(1) - C(11) - C(9) $\angle 123.9^{\circ}\rangle$ and C(9) - C(14) - C(8) $\angle 124.4^{\circ}\rangle$:- these angles are significantly larger than the corresponding valency angles C(5) - C(13) - C(10) $\angle 121.7^{\circ}\rangle$ and C(4) - C(12) - C(10) $\angle 122.0^{\circ}\rangle$. There is also a significant decrease in the average bond length, aa', (table 2) of 0.029 Å compared to that found in anthracene. Also in anthracene the average bond length, e, is 1.431 Å and in 9-methylanthracene this bond is 1.456 Å, however, it is not possible to say that this difference is necessarily significant, for $\Delta = 2.4\sigma$.

The overcrowding of the peri-substituents in 9-methylanthracene has therefore been relieved by a combination of in-plane and out-of-plane deformations. This effect is more prominant in 1,8-dichloro-9-methylanthracene[22] where the two valency angles C(1) - C(11) - C(9) and C(9) - C(14) - C(8) are 5.6° larger than the valency angles C(5) - C(13) - C(10) and C(4) - C(12) - C(10). Although peri-interaction in naphthalene derivatives has been widely discussed in the literature[23] there is a scarcity of information on these interactions for anthracene compounds. The structure of 1,8-dihydroxyanthraquinone[24] has been published, but the standard deviations are approximately 0.04 Å in the bond lengths and 2° in the valency angles.

The average carbon-hydrogen bond length found for 9-methylanthracene in this study is 0.95 Å. The intermolecular separations are all normal van der Waal contacts.

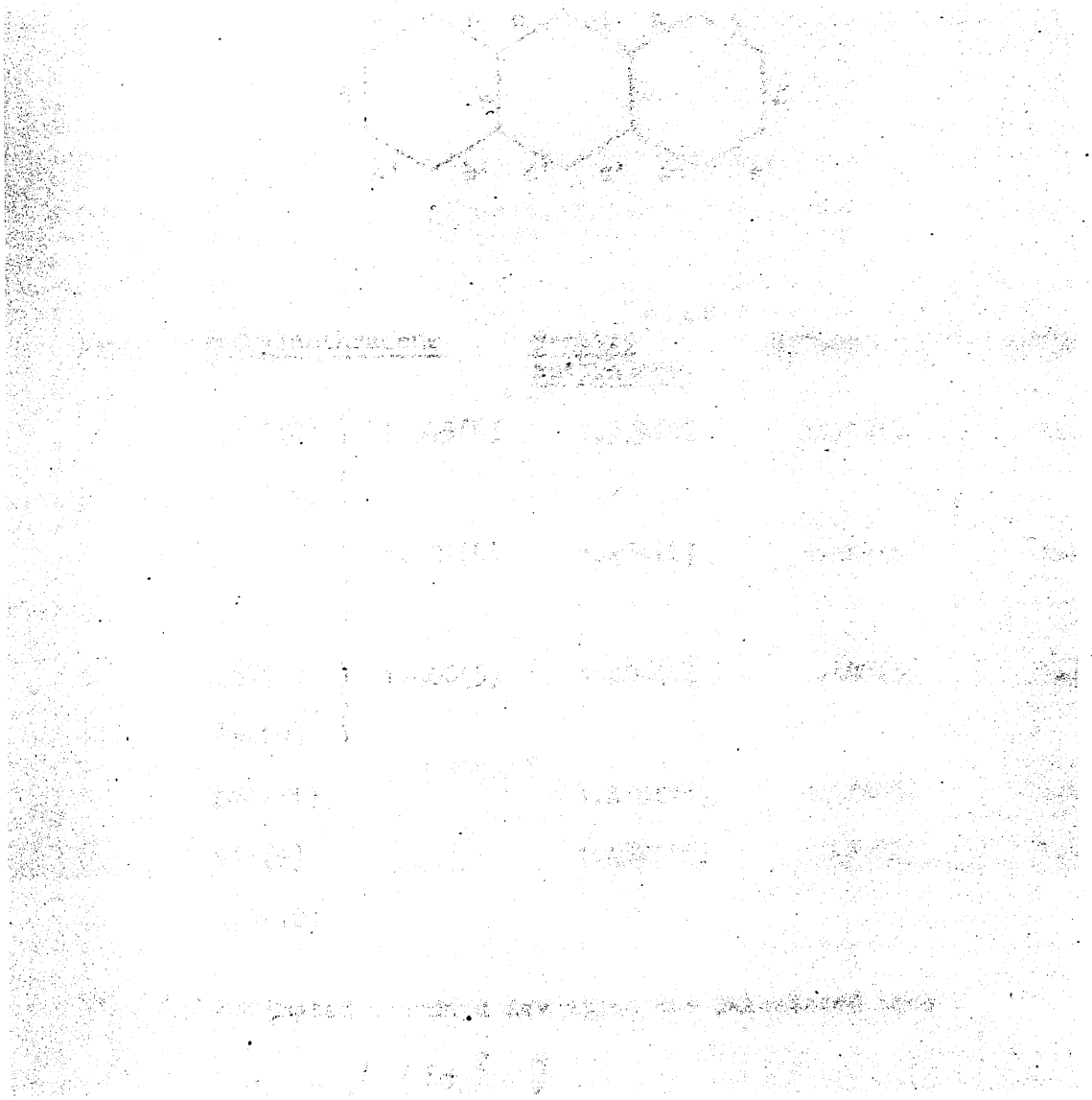
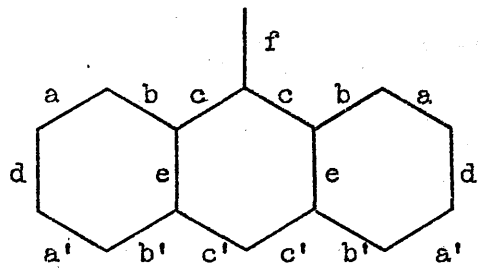


Table 2

A comparison of the bond lengths in 9-methylanthracene, 9-nitroanthracene and anthracene.



Bond	9-methylanthracene		9-nitro anthracene[13]	anthracene[7]	anthracene[6]
a	1.340(10)	1.345(6)	1.399(8)	1.374(5)	1.364(4)
a'	1.350(11)				
b	1.434(9)	1.429(5)	1.434(8)	1.442(5)	1.431(3)
b'	1.423(9)				
c	1.407(9)	1.400(5)	1.400(8)	1.402(5)	1.396(3)
c'	1.392(9)				
d	1.426(11)		1.413(11)	1.416(5)	1.417(6)
e	1.456(9)		1.437(11)	1.431(5)	1.434(4)
f	1.503(10)				

The mean estimated standard deviation was calculated from

$$\sigma_i = \sqrt{\left(\frac{\Sigma\sigma_n^2}{n(n-1)}\right)}$$

TABLE 3

9-Methylanthracene

Fractional Atomic co-ordinates and positional standard deviations

Atom	x	y	z
C(1)	1.1009(8)	0.4208(5)	0.3038(9)
C(2)	1.2492(8)	0.4024(5)	0.3424(10)
C(3)	1.3316(8)	0.3594(5)	0.2223(10)
C(4)	1.2623(7)	0.3351(5)	0.0731(9)
C(5)	0.8053(8)	0.3188(4)	-0.3279(8)
C(6)	0.6543(8)	0.3301(5)	-0.3686(9)
C(7)	0.5676(8)	0.3691(5)	-0.2489(9)
C(8)	0.6339(7)	0.3979(5)	-0.1025(9)
C(9)	0.8643(7)	0.4140(4)	0.1062(8)
C(10)	1.0332(7)	0.3295(4)	-0.1288(8)
C(11)	1.0200(7)	0.3975(4)	0.1478(8)
C(12)	1.1050(7)	0.3543(4)	0.0250(8)
C(13)	0.8791(7)	0.3461(4)	-0.1730(8)
C(14)	0.7934(6)	0.3877(4)	-0.0501(8)
C(15)	0.7746(8)	0.4572(5)	0.2322(8)
H(1)	1.0472(61)	0.4545(37)	0.3885(66)
H(2)	1.3040(67)	0.4304(42)	0.4334(74)
H(3)	1.4270(79)	0.3319(49)	0.2459(91)
H(4)	1.3125(60)	0.3039(38)	-0.0237(69)
H(5)	0.8675(61)	0.2907(38)	-0.3968(71)
H(6)	0.6105(69)	0.3061(42)	-0.4906(81)
H(7)	0.4753(80)	0.3690(49)	-0.2548(90)
H(8)	0.5821(56)	0.4205(35)	-0.0088(65)

TABLE 3

Fractional Atomic co-ordinates and positional standard deviations (cont.)

Atom	x	y	z
H(10)	1.0977(54)	0.2950(34)	-0.2050(61)
H(15A)	0.8229(77)	0.4990(48)	0.3000(84)
H(15B)	0.6920(78)	0.4898(48)	0.1764(86)
H(15C)	0.7487(74)	0.4210(47)	0.3012(85)

TABLE 4

Anisotropic thermal parameters for the carbon atoms ($\times 10^4$)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
C(1)	151(11)	55(4)	211(15)	2(10)	-4(19)	-1(12)
C(2)	171(12)	76(5)	215(16)	-32(13)	-90(22)	-5(14)
C(3)	118(10)	76(5)	275(18)	-15(12)	-54(21)	29(16)
C(4)	106(9)	65(4)	218(15)	-4(10)	45(18)	9(13)
C(5)	159(11)	49(3)	183(13)	10(10)	-4(18)	-16(11)
C(6)	176(12)	62(4)	207(16)	-10(12)	-99(22)	4(13)
C(7)	132(10)	74(5)	215(14)	10(11)	-49(19)	17(13)
C(8)	113(9)	57(4)	208(14)	27(9)	48(18)	16(12)
C(9)	118(9)	40(3)	177(12)	3(8)	54(16)	6(10)
C(10)	119(9)	45(3)	181(13)	5(9)	59(16)	2(10)
C(11)	125(9)	40(3)	148(11)	-7(9)	38(16)	13(10)
C(12)	102(8)	44(3)	195(13)	-7(8)	24(16)	19(10)
C(13)	129(9)	36(3)	167(12)	2(8)	37(16)	10(9)
C(14)	109(8)	36(3)	174(12)	4(8)	35(15)	25(9)
C(15)	143(10)	71(5)	205(12)	22(11)	105(18)	-18(13)

Anisotropic temperature factors were employed in the form:

$$T = \exp\left[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)\right]$$

TABLE 4 (contd.)

Isotropic thermal parameters for the hydrogen atoms

H(1)	1.98	H(7)	4.76
H(2)	3.25	H(8)	1.25
H(3)	5.57	H(10)	1.24
H(4)	2.52	H(15A)	7.91
H(5)	2.42	H(15B)	4.55
H(6)	4.11	H(15C)	5.38

The average standard deviation of the isotropic temperature factors is 1.3 $\mathring{A}^2$

TABLE 5

Intramolecular bonded distances and estimated standard deviations (Å)

C(1)	-	C(2)	1.351(11)	C(11)	-	C(12)	1.458(9)
C(1)	-	C(11)	1.421(9)	C(13)	-	C(14)	1.453(9)
C(2)	-	C(3)	1.428(11)	C(1)	-	H(1)	1.01(6)
C(3)	-	C(4)	1.339(11)	C(2)	-	H(2)	0.93(6)
C(4)	-	C(12)	1.441(10)	C(3)	-	H(3)	0.94(8)
C(5)	-	C(6)	1.360(11)	C(4)	-	H(4)	1.05(6)
C(5)	-	C(13)	1.405(9)	C(5)	-	H(5)	0.93(6)
C(6)	-	C(7)	1.424(11)	C(6)	-	H(6)	1.08(6)
C(7)	-	C(8)	1.329(10)	C(7)	-	H(7)	0.82(8)
C(8)	-	C(14)	1.446(9)	C(8)	-	H(8)	0.99(5)
C(9)	-	C(11)	1.413(9)	C(10)	-	H(10)	1.02(5)
C(9)	-	C(14)	1.401(9)	C(15)	-	H(15A)	0.90(7)
C(9)	-	C(15)	1.503(10)	C(15)	-	H(15B)	0.95(7)
C(10)	-	C(12)	1.381(9)	C(15)	-	H(15C)	0.82(7)
C(10)	-	C(13)	1.402(9)				

TABLE 6

Valency angles (degrees) and estimated standard deviations

C(11)	-	C(1)	-	C(2)	122.9(5)
C(3)	-	C(2)	-	C(1)	119.8(6)
C(9)	-	C(11)	-	C(1)	123.9(5)
C(12)	-	C(11)	-	C(1)	117.1(5)
C(4)	-	C(3)	-	C(2)	120.5(5)
C(12)	-	C(4)	-	C(3)	121.8(5)
C(10)	-	C(12)	-	C(4)	122.0(4)
C(11)	-	C(12)	-	C(4)	117.8(5)
C(13)	-	C(5)	-	C(6)	122.2(5)
C(7)	-	C(6)	-	C(5)	118.9(5)
C(10)	-	C(13)	-	C(5)	121.7(5)
C(14)	-	C(13)	-	C(5)	119.9(5)
C(8)	-	C(7)	-	C(6)	120.7(5)
C(14)	-	C(8)	-	C(7)	123.5(5)
C(9)	-	C(14)	-	C(8)	124.4(4)
C(13)	-	C(14)	-	C(8)	114.8(5)
C(14)	-	C(9)	-	C(11)	119.9(4)
C(15)	-	C(9)	-	C(11)	119.7(5)
C(12)	-	C(11)	-	C(9)	119.0(4)
C(15)	-	C(9)	-	C(14)	120.3(5)
C(13)	-	C(14)	-	C(9)	120.8(5)
C(13)	-	C(10)	-	C(12)	121.7(5)
C(11)	-	C(12)	-	C(10)	120.1(5)
C(14)	-	C(13)	-	C(10)	118.4(4)

TABLE 7

Torsion Angles (degrees)

C(11)	-	C(1)	-	C(2)	-	C(3)		1
C(2)	-	C(1)	-	C(11)	-	C(9)		178
C(2)	-	C(1)	-	C(11)	-	C(12)		-2
C(1)	-	C(2)	-	C(3)	-	C(4)		-2
C(2)	-	C(3)	-	C(4)	-	C(12)		2
C(3)	-	C(4)	-	C(12)	-	C(10)		180
C(3)	-	C(4)	-	C(12)	-	C(11)		-3
C(13)	-	C(5)	-	C(6)	-	C(7)		-1
C(6)	-	C(5)	-	C(13)	-	C(10)		176
C(6)	-	C(5)	-	C(13)	-	C(14)		0
C(5)	-	C(6)	-	C(7)	-	C(8)		3
C(6)	-	C(7)	-	C(8)	-	C(14)		-3
C(7)	-	C(8)	-	C(14)	-	C(9)		-177
C(7)	-	C(8)	-	C(14)	-	C(13)		2
C(14)	-	C(9)	-	C(11)	-	C(1)		-179
C(14)	-	C(9)	-	C(11)	-	C(12)		1
C(15)	-	C(9)	-	C(11)	-	C(1)		-1
C(15)	-	C(9)	-	C(11)	-	C(12)		179
C(11)	-	C(9)	-	C(14)	-	C(8)		177
C(11)	-	C(9)	-	C(14)	-	C(13)		-2
C(15)	-	C(9)	-	C(14)	-	C(8)		-1
C(15)	-	C(9)	-	C(14)	-	C(13)		180
C(13)	-	C(10)	-	C(12)	-	C(4)		178

TABLE 7

Torsion Angles (degrees) (cont.)

C(13)	-	C(10)	-	C(12)	-	C(11)		1
C(12)	-	C(10)	-	C(13)	-	C(5)		-178
C(12)	-	C(10)	-	C(13)	-	C(14)		-2
C(1)	-	C(11)	-	C(12)	-	C(4)		2
C(1)	-	C(11)	-	C(12)	-	C(10)		180
C(9)	-	C(11)	-	C(12)	-	C(4)		-178
C(9)	-	C(11)	-	C(12)	-	C(10)		0
C(5)	-	C(13)	-	C(14)	-	C(8)		0
C(5)	-	C(13)	-	C(14)	-	C(9)		179
C(10)	-	C(13)	-	C(14)	-	C(8)		-177
C(10)	-	C(13)	-	C(14)	-	C(9)		3

The sign convention used for the torsion angles is such that the sign is negative if an anticlockwise rotation is required of atom (1) to eclipse atom (4) whilst looking down the (2) - (3) bond.

The average standard deviation of the torsion angles is 0.8°.

TABLE 8

Mean Plane Calculations

	Atoms in plane	Atoms out of plane	Deviation (Å)
(1)	C(1)		0.01
	C(2)		-0.03
	C(3)		-0.04
	C(4)		-0.04
	C(5)		0.02
	C(6)		-0.03
	C(7)		-0.08
	C(8)		-0.02
	C(9)		0.03
	C(10)		0.03
	C(11)		0.02
	C(12)		0.02
	C(13)		0.05
	C(14)		0.03
	C(15)		0.01

TABLE 9

Intermolecular contacts (Å) of less than 4 Å

C(6)	$C(15)_{I}$	3.97	C(11)	$C(5)_{IV}$	3.72
C(4)	$C(8)_{II}$	3.86	C(11)	$C(10)_{IV}$	3.78
C(7)	$C(15)_{III}$	3.99	C(12)	$C(5)_{IV}$	3.96
C(1)	$C(10)_{IV}$	3.76	C(12)	$C(10)_{IV}$	3.98
C(2)	$C(4)_{IV}$	3.94	C(13)	$C(5)_{IV}$	3.80
C(2)	$C(10)_{IV}$	3.92	C(14)	$C(5)_{IV}$	3.51
C(8)	$C(6)_{IV}$	3.83	C(14)	$C(6)_{IV}$	3.77
C(9)	$C(5)_{IV}$	3.50	C(3)	$C(7)_{V}$	3.95
C(10)	$C(5)_{IV}$	3.98			

The subscripts refer to the following transformations of the atomic co-ordinates:

(I) x, y, 1+z

(II) 1+x, y, z

(III) 1-x, 1-y, -z

(IV) x, $\frac{1}{2}$-y, $\frac{1}{2}$+z

(V) 1+x, $\frac{1}{2}$-y, $\frac{1}{2}$+z

Table 10 — 9-Methylanthracene
Structure factor listings ($|F_o|$ and $|F_c|$ x 10)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
10	0	2	29	36	8	-1	1	74	84	7	-1	7	58	46	7	-9	0	21	22	6	-3	1	54	58
10	-1	3	43	44	8	-1	0	51	53	7	-1	5	26	24	7	-10	3	39	41	6	-3	0	48	46
10	-2	3	17	22	8	-2	2	31	31	7	-1	4	46	44	7	-10	2	74	76	6	-4	7	31	22
10	-3	3	54	57	8	-2	1	80	91	7	-1	2	42	38	7	-10	1	61	70	6	-4	5	26	24
10	-4	3	20	18	8	-2	0	24	28	7	-1	1	29	26	7	-11	4	18	9	6	-4	4	81	75
10	-4	2	23	24	8	-3	2	17	18	7	-2	7	27	26	7	-11	3	43	50	6	-4	3	173	170
10	-5	3	18	18	8	-3	1	110	123	7	-2	3	34	36	7	-11	2	56	51	6	-4	2	64	66
10	-5	2	18	8	8	-4	6	55	55	7	-2	2	75	78	7	-11	1	44	46	6	-4	1	33	35
10	-8	0	19	14	8	-4	4	44	42	7	-2	1	54	58	7	-11	0	17	11	6	-5	7	35	32
9	0	4	63	65	8	-4	3	36	42	7	-3	7	41	25	7	-12	3	17	13	6	-5	6	20	10
9	0	2	53	56	8	-4	2	51	52	7	-3	6	42	36	7	-12	2	48	41	6	-5	4	48	44
9	0	0	116	140	8	-4	1	39	45	7	-3	2	71	76	7	-12	1	85	85	6	-5	3	225	229
9	-1	5	49	51	8	-4	0	47	57	7	-3	1	38	44	7	-12	0	23	30	6	-5	2	116	119
9	-1	1	22	27	8	-5	4	23	25	7	-4	7	25	19	7	-13	2	34	36	6	-5	1	41	42
9	-1	0	31	36	8	-6	2	40	46	7	-4	4	57	53	7	-13	1	63	69	6	-6	5	21	22
9	-3	5	42	49	8	-6	0	33	41	7	-4	3	63	62	7	-14	1	24	28	6	-6	4	21	24
9	-4	4	36	39	8	-7	5	26	26	7	-4	2	65	59	7	-14	0	33	34	6	-6	3	115	112
9	-4	2	24	17	8	-7	2	30	36	7	-4	0	22	16	6	0	8	68	40	6	-6	2	116	117
9	-4	0	71	78	8	-7	1	24	25	7	-5	6	37	27	6	0	4	180	171	6	-6	1	28	28
9	-5	4	17	11	8	-7	0	31	40	7	-5	3	42	40	6	0	0	45	49	6	-7	3	32	38
9	-5	0	39	48	8	-8	4	20	27	7	-5	2	123	126	6	-1	8	31	25	6	-8	3	93	90
9	-6	1	17	11	8	-8	2	30	35	7	-5	1	34	33	6	-1	7	17	14	6	-8	2	79	80
9	-7	3	20	14	8	-8	1	52	60	7	-6	6	18	20	6	-1	5	38	39	6	-9	5	22	20
9	-8	3	17	23	8	-8	0	17	18	7	-6	2	150	160	6	-1	4	153	150	6	-9	3	94	93
9	-8	1	18	7	8	-9	2	20	15	7	-9	1	79	81	6	-1	3	210	210	6	-9	2	97	92
9	-8	0	29	24	8	-9	1	52	53	7	-7	3	50	51	6	-1	1	40	36	6	-10	3	32	35
9	-9	2	19	4	8	-9	0	21	16	7	-7	2	118	120	6	-1	0	60	59	6	-10	2	70	73
9	-10	0	21	27	8	-10	2	20	23	7	-7	1	19	12	6	-2	5	50	50	6	-10	0	50	52
9	-11	0	22	21	8	-11	1	30	37	7	-8	6	20	23	6	-2	3	292	288	6	-11	4	31	32
8	0	6	38	37	8	-11	0	25	25	7	-8	4	20	14	6	-2	2	51	49	6	-11	3	24	22
8	0	4	33	28	8	-12	1	53	55	7	-8	3	34	32	6	-2	0	41	46	6	-11	1	33	30
8	0	2	48	45	8	-12	0	44	49	7	-8	2	101	100	6	-3	5	23	24	6	-11	0	48	51
8	0	0	81	101	8	-13	0	47	51	7	-8	1	105	107	6	-3	4	112	111	6	-12	1	19	22
8	-1	5	25	25	7	0	6	21	27	7	-9	3	26	20	6	-3	3	26	15	6	-13	4	31	26
8	-1	3	20	22	7	0	4	63	63	7	-9	2	108	115	6	-3	2	46	42	6	-13	2	29	27

Table 10 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
6	-13	1	22	20	5	-5	5	103	106	5	-14	3	18	20	4	-4	0	134	129	4	-11	7	29	32
6	-14	3	36	32	5	-5	4	138	132	5	-14	1	46	46	4	-5	6	34	30	4	-11	6	43	43
6	-14	0	34	36	5	-5	3	77	76	5	-14	0	117	120	4	-5	5	164	167	4	-11	5	24	29
6	-15	0	38	41	5	-5	0	98	95	5	-15	1	35	35	4	-5	4	51	54	4	-11	2	20	17
5	0	8	25	17	5	-6	7	20	18	5	-16	0	31	29	4	-5	3	34	39	4	-11	1	35	41
5	0	4	156	142	5	-6	5	123	121	4	0	6	18	20	4	-5	1	242	235	4	-11	0	17	20
5	0	2	22	20	5	-6	4	49	50	4	0	4	54	50	4	-5	0	166	158	4	-12	5	25	26
5	0	0	39	33	5	-6	3	24	23	4	0	0	148	129	4	-6	6	162	175	4	-12	4	22	21
5	-1	8	26	18	5	-6	2	84	86	4	-1	6	25	24	4	-6	5	76	71	4	-12	3	24	23
5	-1	7	32	16	5	-6	1	18	18	4	-1	5	48	40	4	-6	4	19	12	4	-12	2	30	25
5	-1	6	34	31	5	-6	0	52	53	4	-1	4	20	25	4	-6	3	28	34	4	-12	1	37	40
5	-1	4	358	350	5	-7	6	35	28	4	-1	2	72	83	4	-6	2	71	74	4	-12	0	49	52
5	-1	3	77	77	5	-7	5	117	115	4	-1	1	191	169	4	-6	1	140	123	4	-13	6	34	40
5	-1	2	58	65	5	-7	4	21	19	4	-1	0	506	475	4	-7	6	75	73	4	-13	5	23	31
5	-1	1	42	51	5	-7	3	44	42	4	-2	9	24	16	4	-7	5	95	94	4	-13	4	28	21
5	-1	0	281	253	5	-7	2	42	44	4	-2	8	17	14	4	-7	2	52	46	4	-13	1	72	71
5	-2	8	18	7	5	-8	6	27	32	4	-2	6	81	74	4	-7	1	44	37	4	-14	4	35	34
5	-2	7	26	17	5	-8	5	37	32	4	-2	5	139	129	4	-8	6	35	38	4	-14	1	21	25
5	-2	6	21	13	5	-8	2	50	56	4	-2	4	22	18	4	-8	5	32	30	4	-14	0	98	102
5	-2	5	189	176	5	-9	5	61	62	4	-2	3	79	82	4	-8	3	33	34	4	-15	4	19	10
5	-2	4	45	42	5	-9	4	23	31	4	-2	2	62	68	4	-8	1	55	47	4	-16	2	19	14
5	-2	3	70	71	5	-9	0	139	139	4	-2	1	416	389	4	-8	0	19	18	4	-16	1	58	57
5	-2	2	52	51	5	-10	5	26	26	4	-2	0	55	61	4	-9	6	78	76	4	-16	0	28	29
5	-2	1	49	46	5	-10	4	22	19	4	-3	6	23	28	4	-9	5	113	119	4	-17	1	70	72
5	-2	0	43	38	5	-10	2	26	25	4	-3	5	104	103	4	-9	4	53	51	3	0	6	17	12
5	-3	6	21	19	5	-10	0	114	116	4	-3	3	22	26	4	-9	3	26	37	3	0	0	47	46
5	-3	5	177	172	5	-11	6	18	14	4	-3	2	26	33	4	-9	1	33	33	3	-1	6	76	76
5	-3	4	256	251	5	-11	0	49	47	4	-3	1	144	133	4	-9	0	26	21	3	-1	5	31	29
5	-3	3	53	55	5	-12	4	32	28	4	-3	0	319	304	4	-10	7	37	41	3	-1	3	74	80
5	-3	2	37	47	5	-12	3	19	14	4	-4	8	18	7	4	-10	6	116	122	3	-1	2	44	45
5	-3	0	124	101	5	-12	0	57	55	4	-4	6	21	22	4	-10	5	22	22	3	-1	1	269	256
5	-4	5	39	38	5	-13	4	64	62	4	-4	5	21	24	4	-10	4	20	21	3	-1	0	73	67
5	-4	4	96	96	5	-13	3	23	22	4	-4	3	46	48	4	-10	2	33	27	3	-2	7	129	130
5	-4	2	44	45	5	-13	1	48	46	4	-4	2	20	14	4	-10	1	45	44	3	-2	6	51	57
5	-4	1	37	35	5	-13	0	131	128	4	-4	1	64	50	4	-10	0	58	52	3	-2	5	65	60

Table 10 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	-2	4	34	29	3	-7	0	97	103	3	-15	0	38	38	2	-4	3	149	156	2	-11	3	23	22
3	-2	3	75	85	3	-8	6	25	33	3	-16	2	20	13	2	-4	2	151	136	2	-11	2	76	67
3	-2	2	35	38	3	-8	2	173	175	3	-17	3	17	9	2	-4	1	85	91	2	-11	1	30	28
3	-2	1	189	178	3	-8	1	36	41	3	-17	2	20	21	2	-5	8	45	60	2	-12	4	33	39
3	-2	0	120	103	3	-8	0	19	16	3	-17	1	31	33	2	-5	7	20	20	2	-12	3	94	100
3	-3	7	24	20	3	-9	7	48	59	3	-18	0	25	28	2	-5	2	45	35	2	-12	2	26	27
3	-3	6	43	53	3	-9	6	22	17	2	0	8	44	33	2	-5	1	46	49	2	-12	1	57	55
3	-3	3	26	13	3	-9	3	94	97	2	0	4	120	95	2	-6	9	18	26	2	-13	4	53	56
3	-3	2	46	38	3	-9	2	200	196	2	0	0	494	486	2	-6	8	27	32	2	-13	3	74	80
3	-3	1	64	63	3	-9	1	31	30	2	-1	8	77	85	2	-6	3	153	140	2	-13	2	28	31
3	-4	7	19	16	3	-10	7	53	57	2	-1	7	27	27	2	-6	2	211	191	2	-13	1	19	15
3	-4	3	48	57	3	-10	6	58	71	2	-1	5	28	25	2	-6	1	19	24	2	-14	4	31	30
3	-4	2	172	162	3	-10	5	20	23	2	-1	4	41	32	2	-6	0	53	42	2	-14	1	21	23
3	-4	1	155	155	3	-10	3	38	39	2	-1	3	148	144	2	-7	3	151	127	2	-14	0	42	40
3	-4	0	96	83	3	-10	2	21	28	2	-1	2	37	33	2	-7	1	45	40	2	-15	4	23	19
3	-5	7	25	32	3	-10	1	159	154	2	-1	1	217	201	2	-7	0	60	65	2	-15	3	19	14
3	-5	6	37	50	3	-10	0	25	20	2	-1	0	94	93	2	-7	2	236	215	2	-15	2	23	22
3	-5	4	47	45	3	-11	5	34	32	2	-2	8	32	31	2	-8	8	18	8	2	-16	4	20	23
3	-5	3	21	19	3	-11	3	31	35	2	-2	7	91	105	2	-8	6	23	29	2	-16	3	39	43
3	-5	2	319	320	3	-11	2	34	27	2	-2	6	22	13	2	-8	5	30	34	2	-17	3	36	34
3	-5	1	150	144	3	-11	1	134	126	2	-2	5	88	91	2	-8	4	24	29	2	-17	2	23	22
3	-5	0	151	159	3	-11	0	20	20	2	-2	4	51	43	2	-8	3	74	84	1	0	8	26	22
3	-6	8	19	22	3	-12	7	29	33	2	-2	3	356	335	2	-8	2	155	148	1	0	6	42	36
3	-6	6	95	116	3	-12	3	33	34	2	-2	2	238	223	2	-8	1	102	107	1	0	4	612	494
3	-6	5	46	48	3	-12	2	52	53	2	-2	1	300	300	2	-8	0	71	64	1	0	2	277	258
3	-6	4	26	25	3	-12	0	24	22	2	-2	0	86	93	2	-9	8	24	19	1	0	0	615	613
3	-6	3	19	19	3	-13	3	43	44	2	-3	8	44	57	2	-9	6	18	15	1	-1	5	31	23
3	-6	2	58	62	3	-13	2	61	54	2	-3	7	25	29	2	-9	4	25	25	1	-1	4	261	227
3	-6	1	242	223	3	-13	1	40	43	2	-3	5	28	32	2	-9	3	58	68	1	-1	3	249	235
3	-6	0	73	73	3	-13	0	26	21	2	-3	4	22	15	2	-9	2	98	88	1	-1	2	30	18
3	-7	7	21	25	3	-14	3	27	27	2	-3	3	281	281	2	-9	0	22	23	1	-1	1	197	194
3	-7	6	26	35	3	-14	1	54	54	2	-3	2	205	188	2	-10	6	27	26	1	-1	0	223	214
3	-7	4	30	30	3	-14	0	47	45	2	-3	1	189	191	2	-10	3	77	72	1	-2	9	27	31
3	-7	2	158	152	3	-15	5	18	1	2	-3	0	135	132	2	-10	2	67	55	1	-2	8	24	19
3	-7	1	84	73	3	-15	1	33	29	2	-4	8	18	17	2	-10	1	21	17	1	-2	6	24	22

Table 10 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	-2	5	50	60	1	-6	3	76	69	1	-12	1	22	17	0	-3	10	23	22	0	-8	4	96	97
1	-2	3	139	145	1	-6	2	37	41	1	-12	0	115	103	0	-3	6	38	56	0	-8	2	38	35
1	-2	2	38	39	1	-6	1	37	25	1	-13	3	50	46	0	-3	3	61	78	0	-8	1	221	195
1	-2	1	205	207	1	-6	0	45	51	1	-13	0	50	53	0	-3	2	156	189	0	-8	0	46	52
1	-2	0	70	74	1	-7	7	20	26	1	-14	4	71	68	0	-3	1	493	514	0	-9	8	17	11
1	-3	9	18	11	1	-7	4	24	28	1	-14	3	73	65	0	-4	5	171	238	0	-9	6	64	72
1	-3	8	19	12	1	-7	3	51	37	1	-15	4	81	79	0	-4	4	77	97	0	-9	5	40	33
1	-3	7	19	30	1	-7	2	26	29	1	-15	3	103	91	0	-4	3	41	52	0	-9	3	21	19
1	-3	6	24	26	1	-7	1	38	34	1	-15	0	64	56	0	-4	2	53	57	0	-9	2	26	21
1	-3	5	28	34	1	-7	0	54	47	1	-16	5	28	28	0	-4	1	827	845	0	-9	1	56	54
1	-3	4	63	53	1	-8	5	43	45	1	-16	3	46	47	0	-4	0	1394	1470	0	-10	5	91	92
1	-3	3	151	156	1	-8	4	18	22	1	-16	2	25	23	0	-5	7	17	23	0	-10	4	115	114
1	-3	2	29	46	1	-8	3	86	79	1	-16	1	21	15	0	-5	6	40	53	0	-10	2	58	52
1	-3	1	449	453	1	-8	2	41	38	1	-16	0	49	49	0	-5	5	91	102	0	-11	6	19	19
1	-3	0	165	161	1	-8	1	72	67	1	-17	3	31	28	0	-5	4	26	32	0	-11	5	119	114
1	-4	6	19	11	1	-8	0	136	123	1	-17	1	20	19	0	-5	2	83	75	0	-11	4	127	122
1	-4	5	69	91	1	-9	5	30	27	1	-17	0	19	22	0	-5	1	333	321	0	-11	3	39	38
1	-4	4	184	216	1	-9	4	19	11	1	-18	2	31	30	0	-6	9	18	7	0	-11	2	23	20
1	-4	3	213	243	1	-9	3	34	34	0	0	10	31	22	0	-6	7	23	40	0	-12	6	39	43
1	-4	2	64	61	1	-9	1	44	35	0	0	8	23	26	0	-6	6	37	36	0	-12	5	70	70
1	-4	1	159	155	1	-9	0	54	47	0	0	6	27	25	0	-6	5	94	120	0	-12	4	131	127
1	-4	0	153	142	1	-10	8	24	16	0	0	4	204	175	0	-6	4	22	34	0	-12	3	40	42
1	-5	8	26	29	1	-10	4	79	77	0	0	2	522	500	0	-6	3	63	67	0	-12	1	21	16
1	-5	6	22	31	1	-10	1	46	38	0	-1	9	22	20	0	-6	2	26	36	0	-12	0	158	148
1	-5	5	63	72	1	-11	8	24	18	0	-1	7	24	21	0	-6	1	57	64	0	-13	7	21	18
1	-5	4	151	161	1	-11	7	18	3	0	-1	5	60	80	0	-6	0	172	166	0	-13	6	23	21
1	-5	3	45	46	1	-11	5	18	17	0	-1	4	29	45	0	-7	9	23	22	0	-13	2	17	20
1	-5	2	102	107	1	-11	4	116	111	0	-1	3	43	78	0	-7	6	81	83	0	-13	1	22	24
1	-5	1	133	135	1	-11	3	48	44	0	-1	2	48	87	0	-7	5	104	118	0	-14	5	28	25
1	-5	0	107	101	1	-11	2	44	41	0	-2	6	32	49	0	-7	4	34	35	0	-14	4	75	71
1	-6	9	38	47	1	-11	1	51	46	0	-2	5	28	43	0	-7	3	61	64	0	-14	1	18	22
1	-6	7	28	37	1	-11	0	82	77	0	-2	4	38	60	0	-7	2	161	154	0	-14	0	76	69
1	-6	6	17	16	1	-12	5	33	31	0	-2	3	54	79	0	-7	1	197	184	0	-15	5	23	17
1	-6	5	38	41	1	-12	4	32	23	0	-2	2	113	153	0	-8	6	29	33	0	-15	4	92	83
1	-6	4	18	11	1	-12	3	37	37	0	-2	1	68	69	0	-8	5	222	237	0	-15	3	29	28

Table 10 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	-15	1	55	52	-1	-4	1	1063	1108	-1	-11	7	33	38	-2	-1	3	314	268	-2	-7	6	31	28
0	-16	4	36	33	-1	-5	7	34	44	-1	-11	6	61	73	-2	-1	2	331	311	-2	-7	5	19	13
0	-16	3	45	45	-1	-5	6	107	142	-1	-11	5	78	79	-2	-1	1	143	135	-2	-7	4	54	56
0	-16	2	19	4	-1	-5	5	33	43	-1	-11	4	22	22	-2	-2	8	18	15	-2	-7	3	175	165
0	-16	1	39	40	-1	-5	4	71	82	-1	-11	3	49	53	-2	-2	7	31	34	-2	-7	2	500	484
0	-16	0	77	72	-1	-5	3	18	12	-1	-11	2	192	182	-2	-2	6	43	37	-2	-7	1	107	97
0	-18	1	27	23	-1	-5	2	214	215	-1	-11	1	86	73	-2	-2	4	79	69	-2	-8	6	35	32
0	-18	0	22	17	-1	-5	1	179	174	-1	-12	6	26	29	-2	-2	3	96	85	-2	-8	5	43	46
-1	0	10	30	16	-1	-6	8	21	16	-1	-12	5	69	68	-2	-2	1	219	210	-2	-8	3	139	134
-1	0	6	295	248	-1	-6	6	54	68	-1	-12	3	74	71	-2	-3	8	68	63	-2	-8	1	160	158
-1	0	4	103	75	-1	-6	5	36	44	-1	-12	2	121	114	-2	-3	7	176	185	-2	-9	8	24	21
-1	0	2	114	107	-1	-6	2	180	189	-1	-12	1	112	99	-2	-3	6	55	60	-2	-9	7	22	20
-1	-1	7	86	144	-1	-6	1	294	278	-1	-13	7	22	17	-2	-3	5	20	25	-2	-9	6	21	21
-1	-1	5	63	67	-1	-7	6	158	196	-1	-13	4	32	27	-2	-3	4	32	18	-2	-9	5	21	19
-1	-1	3	174	167	-1	-7	5	98	116	-1	-13	3	51	56	-2	-3	3	254	246	-2	-9	4	19	16
-1	-1	2	209	189	-1	-7	2	553	550	-1	-13	2	32	29	-2	-3	2	338	313	-2	-9	2	140	131
-1	-1	1	728	705	-1	-7	1	310	280	-1	-13	1	63	56	-2	-3	1	55	55	-2	-9	1	68	63
-1	-2	9	21	18	-1	-8	6	43	60	-1	-14	4	42	39	-2	-4	8	96	110	-2	-10	5	17	19
-1	-2	7	37	61	-1	-8	5	138	165	-1	-14	3	20	16	-2	-4	7	28	27	-2	-10	3	162	169
-1	-2	6	39	65	-1	-8	4	30	25	-1	-14	2	48	38	-2	-4	6	52	65	-2	-10	2	169	162
-1	-2	4	22	28	-1	-8	3	24	31	-1	-14	1	18	3	-2	-4	5	33	29	-2	-10	1	79	81
-1	-2	2	112	125	-1	-8	2	351	339	-1	-15	5	20	16	-2	-4	4	45	49	-2	-11	7	43	43
-1	-2	1	391	390	-1	-8	1	542	485	-1	-15	1	45	45	-2	-4	3	166	148	-2	-11	5	25	29
-1	-3	7	60	101	-1	-9	7	23	30	-1	-16	4	20	20	-2	-4	2	241	225	-2	-11	4	56	62
-1	-3	6	138	200	-1	-9	6	50	54	-1	-16	3	29	31	-2	-5	8	67	72	-2	-11	3	248	245
-1	-3	5	29	39	-1	-9	5	67	74	-1	-17	4	17	4	-2	-5	7	73	87	-2	-11	2	189	175
-1	-3	4	80	101	-1	-9	4	40	37	-1	-17	3	25	22	-2	-5	6	86	95	-2	-11	1	62	58
-1	-3	3	51	65	-1	-9	2	166	163	-2	0	8	208	164	-2	-5	3	123	117	-2	-12	3	115	122
-1	-3	2	309	339	-1	-9	1	65	67	-2	0	6	106	95	-2	-5	2	366	343	-2	-12	2	50	53
-1	-3	1	1126	1207	-1	-10	5	23	19	-2	0	2	265	251	-2	-5	1	67	65	-2	-12	1	65	62
-1	-4	7	26	28	-1	-10	4	33	35	-2	-1	9	30	20	-2	-6	5	53	58	-2	-13	6	18	7
-1	-4	6	131	213	-1	-10	3	18	20	-2	-1	7	304	249	-2	-6	2	272	264	-2	-13	1	33	39
-1	-4	5	76	115	-1	-10	2	130	130	-2	-1	6	37	23	-2	-6	1	49	52	-2	-14	4	38	39
-1	-4	3	118	146	-1	-10	1	113	99	-2	-1	5	59	44	-2	-7	8	46	52	-2	-14	3	100	102
-1	-4	2	305	318	-1	-11	8	17	8	-2	-1	4	27	31	-2	-7	7	32	39	-2	-14	2	20	23

Table 10 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-2	-14	1	18	17	-3	-4	4	159	153	-3	-11	2	20	13	-4	-3	7	19	14	-4	-9	1	47	45
-2	-15	6	19	16	-3	-4	3	138	129	-3	-11	1	53	43	-4	-3	6	24	20	-4	-10	8	23	13
-2	-15	4	66	71	-3	-4	2	83	76	-3	-12	7	35	27	-4	-3	5	148	137	-4	-10	6	36	36
-2	-15	3	91	94	-3	-4	1	102	110	-3	-12	5	18	9	-4	-3	4	146	146	-4	-10	5	79	85
-2	-15	2	23	23	-3	-5	8	36	36	-3	-12	3	60	59	-4	-3	3	75	67	-4	-11	6	36	40
-2	-16	4	39	42	-3	-5	6	34	33	-3	-12	2	22	24	-4	-3	2	83	87	-4	-11	5	31	35
-2	-16	3	56	59	-3	-5	4	28	30	-3	-12	1	18	16	-4	-3	1	75	72	-4	-12	4	23	23
-3	0	8	140	104	-3	-5	3	146	117	-3	-13	7	28	23	-4	-4	9	65	52	-4	-12	3	19	15
-3	0	4	402	352	-3	-5	2	158	149	-3	-13	3	37	32	-4	-4	5	37	46	-4	-12	2	19	24
-3	-1	7	17	16	-3	-5	1	42	38	-3	-13	2	20	15	-4	-4	4	99	91	-4	-13	4	52	50
-3	-1	5	86	61	-3	-6	9	41	42	-3	-14	4	83	97	-4	-4	3	73	72	-4	-13	3	31	22
-3	-1	4	162	134	-3	-6	8	30	35	-3	-14	3	44	44	-4	-4	2	57	57	-4	-13	1	20	11
-3	-1	3	460	411	-3	-6	7	21	16	-3	-15	5	29	33	-4	-4	1	57	67	-4	-14	4	29	33
-3	-1	2	17	19	-3	-6	4	102	102	-3	-15	4	74	78	-4	-5	9	46	37	-4	-14	3	25	24
-3	-1	1	236	230	-3	-6	3	129	128	-3	-15	3	21	35	-4	-5	6	36	30	-4	-15	4	24	29
-3	-2	8	52	42	-3	-6	2	19	8	-3	-16	4	23	22	-4	-5	3	40	32	-4	-15	1	29	28
-3	-2	7	44	38	-3	-6	1	62	62	-3	-16	3	50	47	-4	-5	1	52	50	-4	-16	3	19	20
-3	-2	6	36	28	-3	-7	9	33	38	-3	-16	2	19	7	-4	-6	5	130	132	-5	0	8	28	30
-3	-2	4	24	24	-3	-7	8	81	85	-3	-17	3	30	29	-4	-6	4	79	75	-5	0	6	59	40
-3	-2	3	362	318	-3	-7	5	47	47	-3	-17	2	22	17	-4	-6	3	47	50	-5	0	4	69	67
-3	-2	2	56	48	-3	-7	4	62	66	-3	-17	1	17	6	-4	-6	2	42	34	-5	0	2	47	44
-3	-2	1	100	96	-3	-7	2	89	85	-4	0	10	68	52	-4	-6	1	75	77	-5	-1	6	30	22
-3	-3	9	28	29	-3	-8	9	78	80	-4	0	4	86	81	-4	-7	8	22	18	-5	-1	5	20	16
-3	-3	8	84	76	-3	-8	3	67	52	-4	0	2	38	41	-4	-7	6	55	63	-5	-1	4	51	49
-3	-3	7	26	15	-3	-8	1	31	27	-4	-1	7	44	38	-4	-7	5	110	113	-5	-1	3	24	27
-3	-3	6	42	36	-3	-9	8	40	37	-4	-1	5	26	24	-4	-7	4	33	37	-5	-1	2	72	77
-3	-3	5	25	23	-3	-9	5	32	28	-4	-1	4	134	112	-4	-7	1	26	25	-5	-1	1	22	12
-3	-3	4	251	228	-3	-9	2	42	42	-4	-1	3	33	26	-4	-8	5	28	32	-5	-2	8	18	20
-3	-3	3	206	196	-3	-10	5	32	33	-4	-1	2	68	79	-4	-8	4	41	40	-5	-2	7	32	20
-3	-3	2	17	10	-3	-10	4	19	15	-4	-1	1	43	37	-4	-9	8	29	26	-5	-2	6	47	41
-3	-3	1	33	40	-3	-10	3	64	66	-4	-2	6	21	9	-4	-9	7	20	12	-5	-2	4	45	34
-3	-4	9	82	75	-3	-11	8	37	39	-4	-2	5	71	69	-4	-9	5	20	16	-5	-2	3	50	50
-3	-4	8	82	73	-3	-11	7	21	19	-4	-2	4	92	87	-4	-9	4	66	67	-5	-2	1	284	261
-3	-4	6	43	37	-3	-11	4	53	53	-4	-2	2	98	95	-4	-9	3	30	26	-5	-3	6	33	32
-3	-4	5	66	60	-3	-11	3	50	58	-4	-2	1	58	53	-4	-9	2	48	47	-5	-3	4	43	48

Table 10 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-5	-3	2	81	80	-5	-11	6	24	32	-6	-5	7	32	31	-7	0	2	56	58	-7	-8	7	18	14
-5	-3	1	158	145	-5	-11	4	19	14	-6	-5	6	22	15	-7	-1	8	42	38	-7	-8	2	30	32
-5	-4	9	17	11	-5	-11	1	61	64	-6	-5	4	64	69	-7	-1	4	130	128	-7	-8	1	34	31
-5	-4	7	18	18	-5	-12	5	24	25	-6	-5	3	30	29	-7	-1	3	97	101	-7	-9	3	43	39
-5	-4	6	20	15	-5	-12	3	19	12	-6	-5	2	109	118	-7	-1	2	94	97	-7	-9	2	22	25
-5	-4	5	24	26	-5	-12	2	23	26	-6	-5	1	164	161	-7	-2	7	36	40	-7	-9	1	26	36
-5	-4	2	25	20	-5	-12	1	24	28	-6	-6	7	32	28	-7	-2	6	20	27	-7	-10	3	33	31
-5	-4	1	35	25	-5	-13	6	21	22	-6	-6	6	51	51	-7	-2	5	23	32	-7	-10	2	36	39
-5	-5	8	19	14	-5	-13	5	25	21	-6	-6	4	18	10	-7	-2	4	66	61	-7	-12	3	19	24
-5	-5	6	67	61	-5	-13	4	18	16	-6	-6	2	328	326	-7	-2	3	379	387	-7	-12	1	20	18
-5	-5	5	18	22	-5	-13	2	20	21	-6	-6	1	147	156	-7	-2	2	108	110	-7	-13	4	34	32
-5	-5	3	30	32	-5	-13	1	74	70	-6	-7	4	23	28	-7	-2	1	19	18	-7	-14	3	43	45
-5	-5	2	51	44	-5	-14	3	21	14	-6	-7	3	37	37	-7	-3	6	18	15	-8	0	4	138	149
-5	-5	1	260	250	-5	-14	1	30	32	-6	-7	2	106	108	-7	-3	4	81	77	-8	0	2	27	21
-5	-6	5	92	97	-5	-16	3	20	18	-6	-7	1	142	142	-7	-3	3	142	145	-8	-1	5	30	28
-5	-6	4	22	20	-6	0	4	29	29	-6	-8	6	21	18	-7	-3	2	134	144	-8	-1	4	143	150
-5	-6	3	31	29	-6	-1	8	27	19	-6	-8	4	19	21	-7	-4	7	20	16	-8	-1	3	79	83
-5	-6	2	99	100	-6	-1	6	35	36	-6	-8	3	32	26	-7	-4	5	19	27	-8	-1	2	19	19
-5	-6	1	90	82	-6	-1	5	37	43	-6	-8	2	50	48	-7	-4	4	34	31	-8	-1	1	22	24
-5	-7	6	33	44	-6	-1	4	39	39	-6	-9	6	27	30	-7	-4	2	86	84	-8	-2	5	44	50
-5	-7	1	128	121	-6	-1	3	44	44	-6	-9	3	46	40	-7	-4	1	32	32	-8	-2	4	42	47
-5	-8	6	30	31	-6	-1	2	139	145	-6	-9	1	153	158	-7	-5	8	18	11	-8	-2	3	75	77
-5	-8	3	36	38	-6	-2	7	95	80	-6	-10	3	51	57	-7	-5	4	82	82	-8	-2	2	21	26
-5	-8	1	47	48	-6	-2	6	35	35	-6	-10	2	144	147	-7	-5	3	19	12	-8	-2	1	18	21
-5	-9	6	63	65	-6	-2	4	18	16	-6	-10	1	149	151	-7	-5	2	45	48	-8	-3	4	36	33
-5	-9	5	40	41	-6	-2	3	113	108	-6	-11	2	20	14	-7	-5	1	47	48	-8	-3	3	33	36
-5	-9	3	31	34	-6	-2	2	203	203	-6	-11	1	100	100	-7	-6	8	56	41	-8	-4	6	17	7
-5	-9	2	59	60	-6	-2	1	26	17	-6	-12	2	39	39	-7	-6	5	35	32	-8	-4	5	65	71
-5	-9	1	202	199	-6	-3	6	43	49	-6	-13	3	47	48	-7	-6	4	54	54	-8	-4	4	90	98
-5	-10	7	26	20	-6	-3	5	30	30	-6	-13	1	50	53	-7	-6	3	106	108	-8	-5	5	102	104
-5	-10	6	41	48	-6	-3	3	59	59	-6	-14	3	28	29	-7	-6	2	133	139	-8	-5	4	132	135
-5	-10	5	61	63	-6	-3	2	113	119	-6	-14	2	21	17	-7	-6	1	17	22	-8	-5	2	30	36
-5	-10	4	46	46	-6	-3	1	88	89	-6	-14	1	43	44	-7	-7	7	18	9	-8	-6	5	39	41
-5	-10	2	70	68	-6	-4	3	42	41	-7	0	6	32	31	-7	-7	3	53	56	-8	-6	4	80	89
-5	-10	1	82	88	-6	-5	8	23	17	-7	0	4	107	107	-7	-7	2	86	91	-8	-6	3	18	21

Table 10 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-8	-6	2	32	37	-9	-7	4	30	32															
-8	-7	4	28	29	-9	-7	1	28	31															
-8	-7	2	30	35	-9	-8	5	73	79															
-8	-8	5	54	56	-9	-8	2	18	23															
-8	-8	4	28	33	-9	-8	1	26	34															
-8	-8	3	21	16	-9	-9	1	29	35															
-8	-9	6	23	25	-9	-10	4	29	35															
-8	-9	5	74	79	-9	-10	2	19	21															
-8	-9	2	18	10	-10	-3	5	28	30															
-8	-10	4	54	60	-10	-3	3	27	24															
-8	-10	3	24	30	-10	-3	1	38	41															
-8	-11	4	46	42	-10	-4	2	28	31															
-8	-11	3	17	21	-10	-5	1	29	36															
-9	0	6	25	23	-10	-7	1	48	55															
-9	0	4	22	23	-10	-8	2	47	55															
-9	0	2	44	51	-11	0	2	40	41															
-9	-1	6	23	20	-11	-1	3	36	38															
-9	-1	3	18	15	-11	-3	3	32	28															
-9	-2	6	32	31	-11	-4	2	34	35															
-9	-2	5	17	0																				
-9	-2	3	28	33																				
-9	-2	2	17	18																				
-9	-3	6	33	32																				
-9	-3	5	35	38																				
-9	-3	4	18	22																				
-9	-4	5	59	63																				
-9	-4	3	20	18																				
-9	-4	1	67	82																				
-9	-5	5	57	66																				
-9	-5	4	17	21																				
-9	-5	1	37	41																				
-9	-6	6	35	36																				
-9	-6	5	24	24																				
-9	-6	4	22	30																				
-9	-7	5	33	28																				

3.5. References

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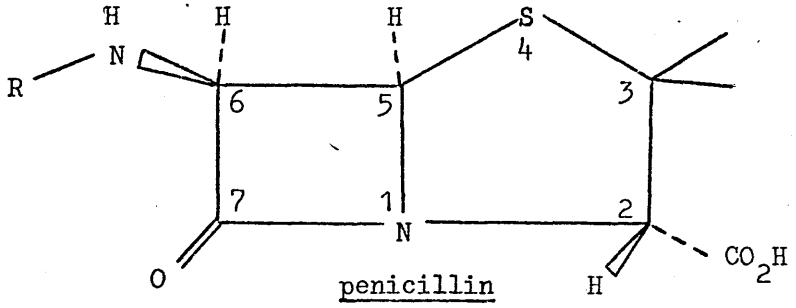
CHAPTER 4

6β-TRIMETHYLAMMONIO PENICILLANIC ACID HEMIHYDROIODIDE

4.1. Introduction

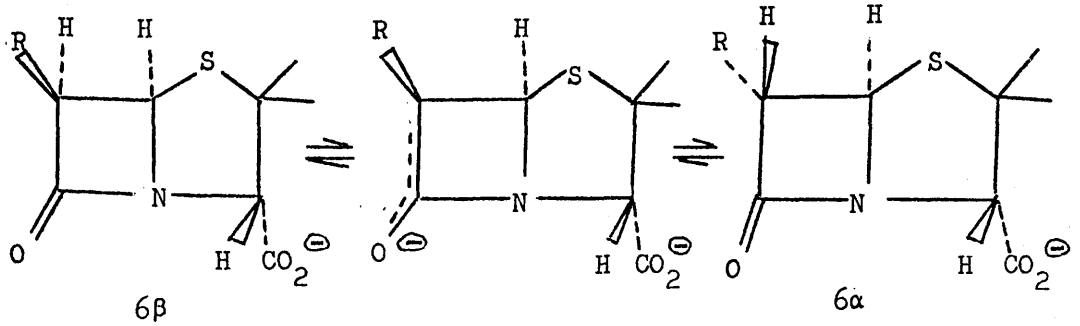
Penicillin was one of the first antibiotics studied[1] and it has been suggested that the molecule can be substituted for the D-alanyl-D-alanine residue[2-4] in the body. This effectively inhibits bacterial cell wall synthesis by interfering with the final cross-linking process.



penicillin

In 1945 the structure of the basic molecule was elucidated by chemical degradation and X-ray crystallographic analysis; sodium benzyl-penicillin[5] and rubidium benzylpenicillin[5] were the first crystal structures to be solved. Later Pitt[6] published the structure of potassium benzylpenicillin. Penicillin was first synthesised by Sheehan[7] and the first semi-synthetic penicillins were obtained by Doyle et al[8].

Recently a number of reactions, involving the epimerisation of penicillanic acid derivatives, have been studied.[9-14] For the equilibrium:-



(I) (II) (III)

where R = $\overset{+}{N}Me_3$, the ionisation from (I) to (II) in the presence of base is known to be faster[15] than from (III) to (II). However, this does not fully account for the overwhelming preponderance of the 6α epimer at equilibrium.[15,16]

The 6β epimer has been prepared as the crystalline hemihydroiodide[15,17] which can be written as $(R^+CO_2H\ \ ^-O_2CR^+)I^-$. The combination of carboxyl group ($-CO_2H$) and carboxylate anion ($-CO_2^-$) is well known in the acid salts of monobasic and dibasic carboxylic acids and can give rise to short, symmetrical hydrogen bonds. An X-ray study of the penicillanic acid hemihydroiodide crystal structure was undertaken to determine whether this provided another example of such a short hydrogen bond.

4.2. Experimental

Crystal data

Molecular formula	$(C_{11}H_{18}N_2O_3S)_2.HI$
Molecular weight	644.6 a.m.u.
Crystal system	monoclinic
Space group	C2 (C_2^3)
Cell dimensions	$\underline{a}$ = 19.44 Å
	$\underline{b}$ = 6.28 Å
	$\underline{c}$ = 11.33 Å
	$\underline{\beta}$ = 95.0°
Cell volume (u)	1376.5 $Å^3$
Density (observed)	1.55g.cm^{-3}
Density (calculated)	1.56g.cm^{-3}

Molecules per unit cell (Z)	2 x ($C_{22}H_{37}N_4O_6S_2I$)
Number of electrons per unit cell ($F_{(000)}$)	660
Linear absorption coefficient, μ(MoKα)	13.69 cm^{-1}

Rotation, Weissenberg and precession photographs taken with MoKα radiation showed the crystal system to be monoclinic. The systematically absent reflections(hkl when h+k = 2n + 1, h0l when h = 2n+1, 0k0 when k = 2n+1) for the optically active compound suggested the space group as C2 with two molecules per unit cell. The intensity data of layers h0l to h6l were recorded by means of equi-inclination Weissenberg photographs taken with Zr-filtered MoKα radiation. A Joyce-Loebl integrating microdensitometer was used to measure the intensities and the 1380 independent structure amplitudes obtained were corrected for Lorentz and polarisation effects.

4.3 Structure analysis

The iodine atom which lies on a two-fold axis was used to define the origin and the co-ordinates of the sulphur atom were found from a Fourier synthesis. A further Fourier synthesis based on the heavy-atom phases showed diminished pseudo-symmetry and fourteen further atoms were located. After two cycles of least-squares calculations the R factor was 0.241 and a Fourier difference map, at this stage, gave the co-ordinates of the two remaining carbon atoms. After two further cycles of isotropic refinement the R factor reduced to 0.151. Here the Weissenberg data were scaled to data collected about the l axis on the precession camera, and placed on an absolute overall scale. The iodine and sulphur atoms were allowed to refine with anisotropic temperature

factors and two further cycles of least-squares calculations lowered the R factor to 0.095. At this stage a small number of dubious reflections were checked and corrected if in error. Assuming the absolute configuration of the β epimer on a right handed set of axes, a further two cycles of least squares converged to R = 0.090. No hydrogen positions could be located from a Fourier difference map.

A unitary weighting scheme (w = 1) was employed in the least-squares calculations.

The computing was carried out at the Atlas Computer Laboratory, Chilton using the X-RAY-63 system and at Sussex University on the ICL 1905E computer.

4.4 Discussion

The molecular structure of the β-epimer is shown in Figure 1 and the crystal packing structure in Figure 2. The final atomic co-ordinates, standard deviations and temperature factors are given in Table 1. Tables 2, 3, 4 and 5 list the bond lengths, valency angles, torsion angles and mean plane calculations respectively.

The β-lactam ring has a buckled conformation, with the atom C(7) lying 0.31 Å above the plane defined by the C(5), N(1) and C(6) atoms. In phenoxymethylpenicillin[18] and benzylpenicillin the C(7) atom of the β-lactam ring is displaced by 0.15 Å. Also, the torsion angles in the β-lactam ring of the β-epimer are twice the magnitude of those for phenoxymethylpenicillin. The cephalosporins[20,21] also contain fused β-lactam rings and some properties of these rings are listed below.

Compound	Sum of angles around N(1)	C(7)-O(13) bond length (Å)	C(7)-N(1) bond length (Å)
Ampicillin[21]	339(1)°	1.198(7)	1.369(7)
Benzylpenicillin[6]	337(3)°	1.17(4)	1.34(4)
β-epimer	342(2)°	1.15(2)	1.41(2)
Cephaloglycine[21]	353(6)°	1.28(5)	1.48(5)
Cephaloridine[21]	350.7(8)°	1.214(8)	1.382(8)
Δ^2-Cephalosporins V[21]	359.3(8)°	1.223(7)	1.339(7)
Phenoxymethylpenicillin[18]	337(2)°	1.21(2)	1.46(2)

The thiazolidine ring of the β-epimer has an envelope conformation where C(2) is 0.47 Å below the plane containing the C(3), S(4), C(5) and N(1) atoms. In phenoxymethylpenicillin the corresponding atom is displaced by 0.51 Å and the valency angles in this ring agree to within 2° of the similar angles of the β-epimer. The N(1)-C(5) bond length of the β-epimer at 1.43 Å approximates to that found in benzylpenicillin (1.47(4) Å) but is shorter ($\Delta = 3\sigma$) than the 1.52 Å distance found in phenoxymethylpenicillin.

The carboxyl groups of the two penicillin moieties in the Zwitter ion are linked by a short crystallographically symmetrical hydrogen bond with O(12).....$O(12)_{II}$ 2.46 Å; this compares well with the "very short" hydrogen bonds found in the acid salts of some carboxylic acids.[22] Intermolecular hydrogen bonds involving 2-fold symmetry are found in sodium hydrogen diacetate[23] (O.....O = 2.44 Å) potassium hydrogen dianisate[24] (2.48 Å), potassium hydrogen succinate[25] (2.446 Å) and ammonium hydrogen glutarate[25] (2.460 Å). The carbon-oxygen bonds of the carboxy groups show that the C(10)-O(11) bond, 1.23 Å,

Figure 1

A general view of the molecular configuration.

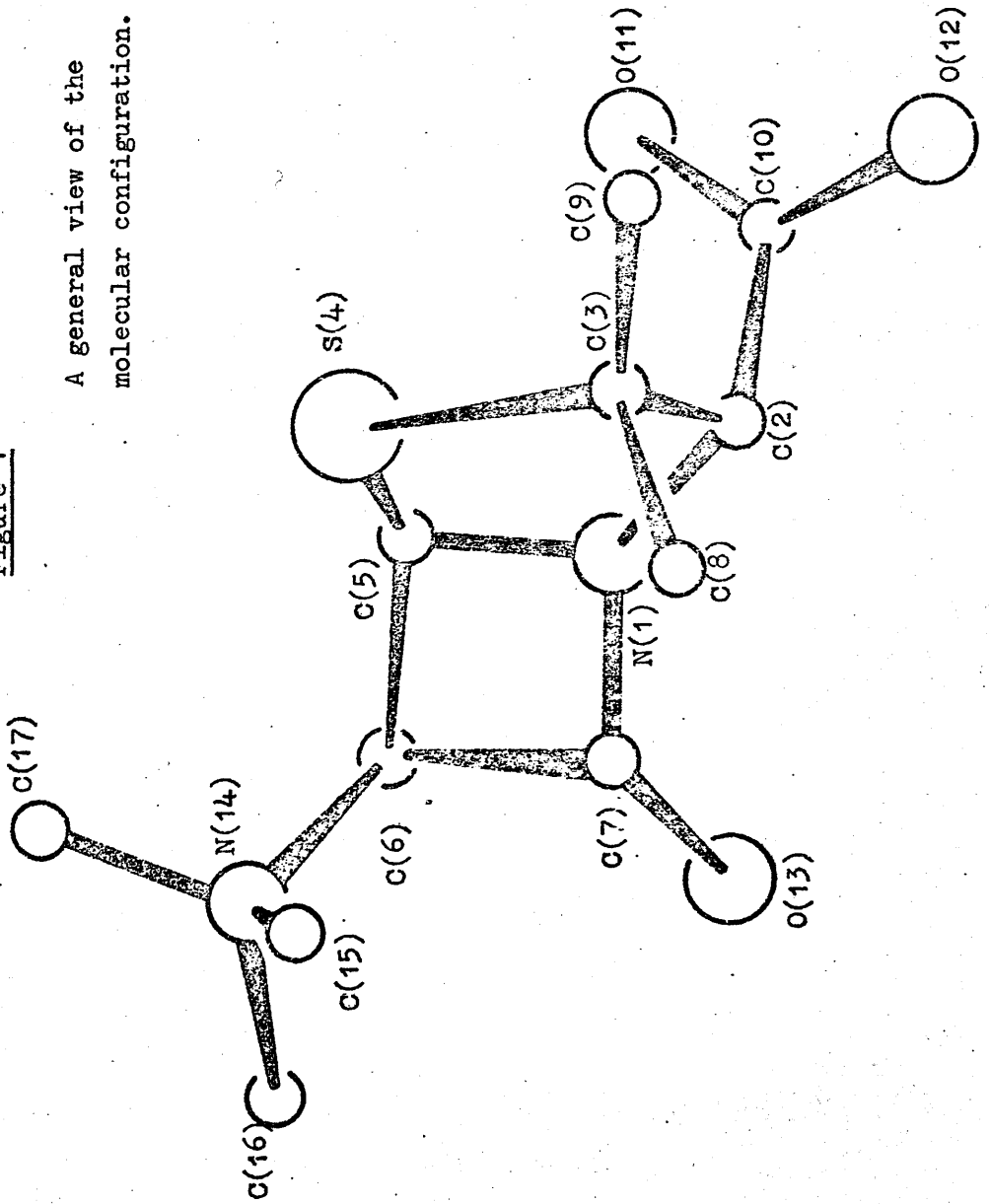
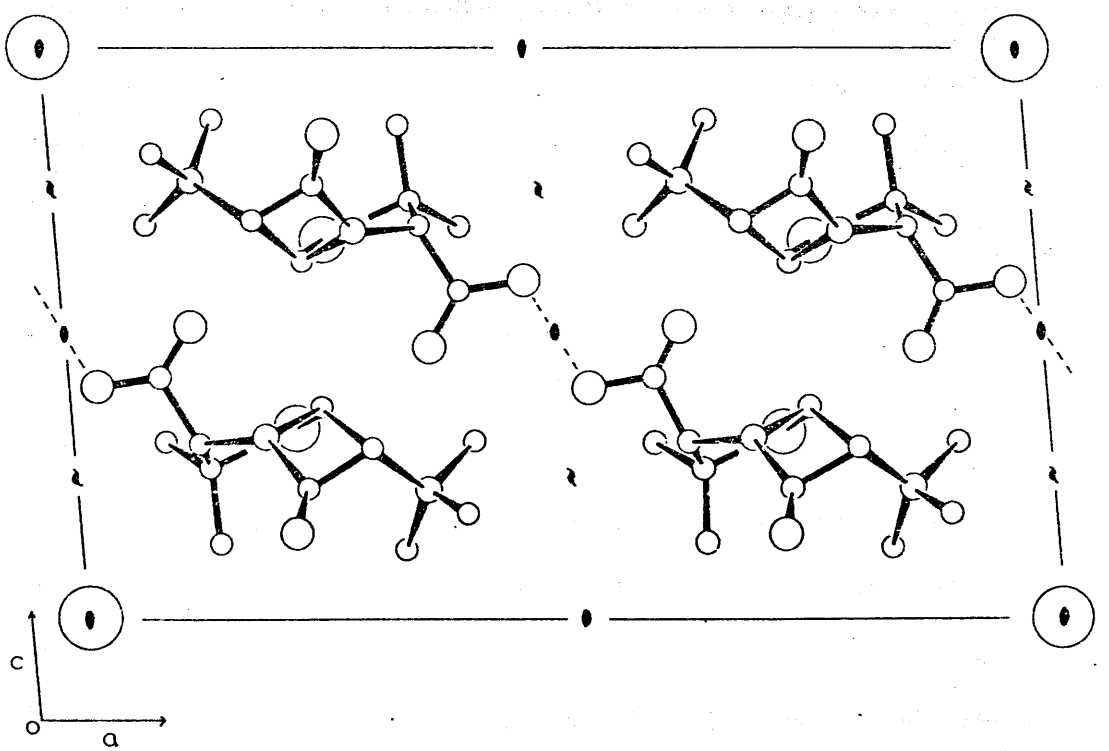


Figure 2



The crystal structure of 6β-trimethylammoniopenicillanic acid hemihydroiodide viewed along the '<u>b</u>' axis.

has more double bond character than the C(10)-O(12) bond, 1.30 Å. In phenoxymethylpenicillin there is an intermolecular hydrogen bond between one carboxyl oxygen and the amide oxygen; this oxygen-oxygen contact is 2.76 Å and the two carbon-oxygen bonds of the carboxy group are 1.21 Å and 1.35 Å. The Zwitterionic form of 6-[D(-) α -aminophenylacetamido] penicillanic acid[27] as the crystalline trihydrate exhibits intermolecular hydrogen bonding between both carboxyl oxygens. Here, as expected, the carbon-oxygen distances are approximately equal at 1.240 Å and 1.245 Å, so indicating a high degree of π-orbital resonance.

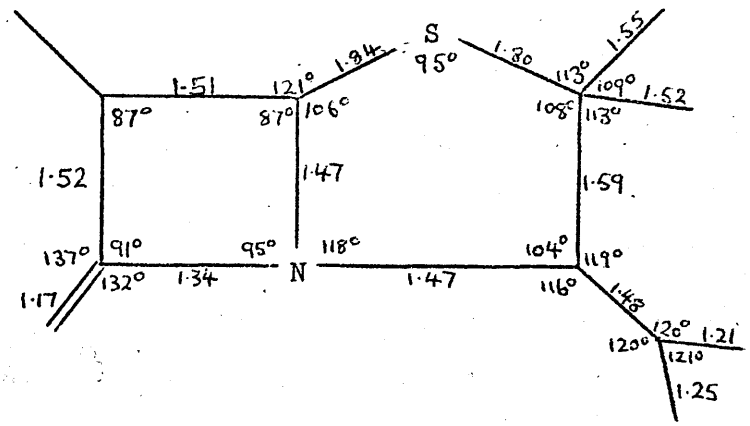
Assuming that the hydrogen atom lies half way between the two symmetry related oxygens of the carboxyl group for the β epimer, its co-ordinates are 0.0000, 0.1697, 0.0000.

The average nitrogen-carbon distance in the tri-methyl ammonium group is 1.50 Å which compares well to the average value of 1.48 Å quoted by Sutton et al[28] for 4-covalent nitrogen-carbon distances of this type. The intermolecular distances are given in table 6. Apart from the $O(12)....O(12)_{II}$ contact the distances are normal van der Waals interactions.

A comparison of the bond lengths and angles for benzylpenicillin, phenoxymethylpenicillin and the β-epimer is shown overleaf. In all three thiazolidine rings the largest valency angles is at the nitrogen atom and the smallest at the sulphur atom.

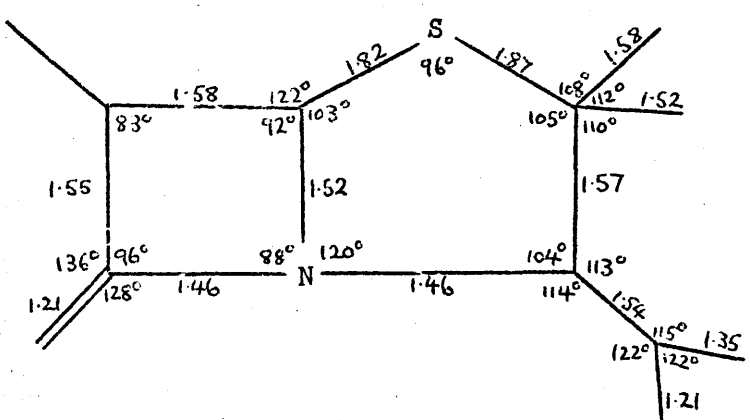
Bond lengths (Å) and angles in (a) benzyl penicillin,

(b) phenoxymethylpenicillin and (c) β-epimer



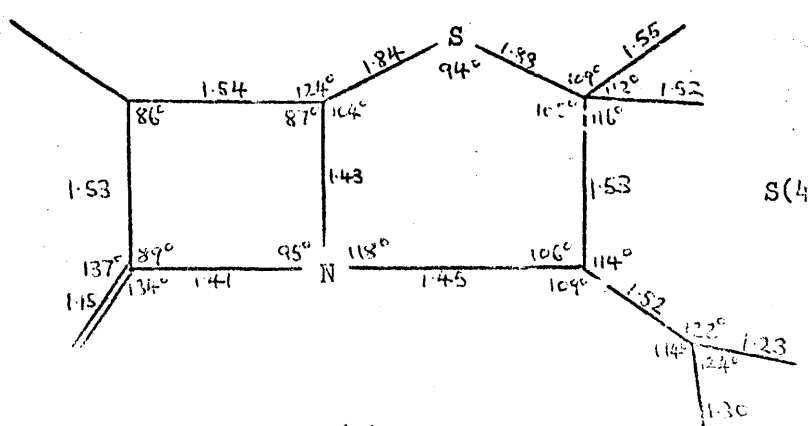
(a)

S(4)-C(3)-C(8) = 105°



(b)

S(4)-C(3)-C(8) = 109°



(c)

S(4)-C(3)-C(8) = 106°

Table 1

Fractional Atomic co-ordinates, positional standard deviations and temperature factors.

Atom	x	y	z	B
I	0.0000	0.0000	0.0000	⁄
N(1)	0.1971(6)	0.1151(23)	0.3210(10)	2.09
C(2)	0.1288(6)	0.2116(27)	0.3062(11)	1.75
C(3)	0.1401(7)	0.4404(25)	0.2650(12)	2.06
S(4)	0.2281(2)	0.5161(11)	0.3330(3)	⁄
C(5)	0.2534(7)	0.2413(27)	0.3725(12)	1.85
C(6)	0.3012(7)	0.1038(30)	0.3019(13)	2.19
C(7)	0.2353(6)	0.0201(43)	0.2350(11)	2.32
C(8)	0.0904(10)	0.6050(39)	0.3070(17)	3.80
C(9)	0.1409(8)	0.4441(30)	0.1283(14)	2.88
C(10)	0.0953(7)	0.1952(30)	0.4218(12)	2.05
O(11)	0.1283(6)	0.2162(25)	0.5183(11)	3.61
O(12)	0.0286(6)	0.1697(25)	0.4074(10)	3.30
O(13)	0.2208(6)	-0.0717(24)	0.1485(11)	3.86
N(14)	0.3568(6)	0.1914(24)	0.2304(10)	2.02
C(15)	0.3301(9)	0.3190(36)	0.1248(15)	3.12
C(16)	0.3950(7)	0.0069(63)	0.1843(13)	3.50
C(17)	0.4071(9)	0.3266(37)	0.3090(15)	3.21

⁄ for the iodine and sulphur atoms anisotropic temperature factors were employed.

The average standard deviation of the isotropic temperature factors is 0.25 Å^2.

Table 1(contd)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23} ($\times 10^4$)
I	13(0)	262(6)	95(2)	0	22(1)	0
S(4)	15(1)	42(10)	55(3)	3(7)	-4(2)	-2(14)

Anisotropic temperature factors were employed in the form

$$T = \exp[-(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{12}hk+b_{13}hl+b_{23}kl)]$$

Due to the space group symmetry requirements the iodine atom was given a multiplicity of 0.5 and the b_{12} and b_{23} temperature factors were fixed at 0.

Table 2

Intramolecular bonded distances and estimated standard deviations (Å)

N(1)	-	C(2)	1.45(2)	C(5)	-	C(6)	1.54(2)
N(1)	-	C(5)	1.43(2)	C(6)	-	C(7)	1.53(2)
N(1)	-	C(7)	1.41(2)	C(6)	-	N(14)	1.51(2)
C(2)	-	C(3)	1.53(2)	C(7)	-	O(13)	1.15(2)
C(2)	-	C(10)	1.52(2)	C(10)	-	O(11)	1.23(2)
C(3)	-	S(4)	1.88(1)	C(10)	-	O(12)	1.30(2)
C(3)	-	C(8)	1.52(3)	N(14)	-	C(15)	1.50(2)
C(3)	-	C(9)	1.55(2)	N(14)	-	C(16)	1.49(3)
S(4)	-	C(5)	1.84(2)	N(14)	-	C(17)	1.52(2)

Table 3

Valency angles (degrees) and estimated standard deviations

C(5)	-	N(1)	-	C(2)	118.2(11)
C(3)	-	C(2)	-	N(1)	105.8(11)
C(7)	-	N(1)	-	C(5)	95.0(10)
C(6)	-	C(5)	-	N(1)	87.3(10)
O(13)	-	C(7)	-	N(1)	134.3(9)
S(4)	-	C(3)	-	C(2)	105.2(9)
C(9)	-	C(3)	-	C(2)	109.4(10)
O(12)	-	C(10)	-	C(2)	113.5(8)
C(9)	-	C(3)	-	S(4)	108.5(7)
C(9)	-	C(3)	-	C(8)	111.5(12)
C(7)	-	C(6)	-	C(5)	86.1(10)
N(14)	-	C(6)	-	C(7)	118.0(9)
C(15)	-	N(14)	-	C(6)	114.2(10)
C(17)	-	N(14)	-	C(6)	110.1(10)
C(16)	-	N(14)	-	C(15)	106.5(14)
C(17)	-	N(14)	-	C(16)	108.8(11)
C(7)	-	N(1)	-	C(2)	128.8(9)
C(10)	-	C(2)	-	N(1)	109.2(10)
S(4)	-	C(5)	-	N(1)	104.0(11)
C(6)	-	C(7)	-	N(1)	88.9(10)
C(10)	-	C(2)	-	C(3)	114.2(9)
C(8)	-	C(3)	-	C(2)	115.5(11)
O(11)	-	C(10)	-	C(2)	122.1(9)
C(8)	-	C(3)	-	S(4)	106.3(9)
C(5)	-	S(4)	-	C(3)	94.4(8)

Table 3 (contd.)

C(6)	-	C(5)	-	S(4)	124.0(6)
N(14)	-	C(6)	-	C(5)	124.5(10)
O(13)	-	C(7)	-	C(6)	136.7(9)
C(16)	-	N(14)	-	C(6)	107.8(15)
O(12)	-	C(10)	-	O(11)	124.3(10)
C(17)	-	N(14)	-	C(15)	109.2(13)

Table 4

Torsion Angles (degrees)

C(5)	N(1)	C(2)	C(3)	40
C(5)	N(1)	C(2)	C(10)	-83
C(7)	N(1)	C(2)	C(3)	-84
C(7)	N(1)	C(2)	C(10)	153
C(2)	N(1)	C(5)	S(4)	-28
C(2)	N(1)	C(5)	C(6)	-152
C(7)	N(1)	C(5)	S(4)	111
C(7)	N(1)	C(5)	C(6)	-13
C(2)	N(1)	C(7)	C(6)	146
C(2)	N(1)	C(7)	O(13)	-31
C(5)	N(1)	C(7)	C(6)	13
C(5)	N(1)	C(7)	O(13)	-164
N(1)	C(2)	C(3)	S(4)	-30
N(1)	C(2)	C(3)	C(8)	-147
N(1)	C(2)	C(3)	C(9)	86
C(10)	C(2)	C(3)	S(4)	90
C(10)	C(2)	C(3)	C(8)	-27
C(10)	C(2)	C(3)	C(9)	-154
N(1)	C(2)	C(10)	O(11)	37
N(1)	C(2)	C(10)	O(12)	-146
C(3)	C(2)	C(10)	O(11)	-81
C(3)	C(2)	C(10)	O(12)	96
C(2)	C(3)	S(4)	C(5)	14
C(8)	C(3)	S(4)	C(5)	137
C(9)	C(3)	S(4)	C(5)	-103
C(3)	S(4)	C(5)	N(1)	6

Table 4 (contd.)

C(3)	S(4)	C(5)	C(6)	102
N(1)	C(5)	C(6)	C(7)	12
N(1)	C(5)	C(6)	N(14)	133
S(4)	C(5)	C(6)	C(7)	-93
S(4)	C(5)	C(6)	N(14)	28
C(5)	C(6)	C(7)	N(1)	-12
C(5)	C(6)	C(7)	O(13)	164
N(14)	C(6)	C(7)	N(1)	-139
N(14)	C(6)	C(7)	O(13)	37
C(5)	C(6)	N(14)	C(15)	-66
C(5)	C(6)	N(14)	C(16)	175
C(5)	C(6)	N(14)	C(17)	57
C(7)	C(6)	N(14)	C(15)	39
C(7)	C(6)	N(14)	C(16)	-79
C(7)	C(6)	N(14)	C(17)	163

The sign convention used for the torsion angles is such that the sign is negative if an anticlockwise rotation is required of Atom (1) to eclipse Atom (4) whilst looking down the (2) - (3) bond.

The average standard deviation of the torsion angles is 1.5°.

Table 5

Mean plane calculations

	Atoms in plane	Atoms out of plane	Deviation (Å)
(1)	N(1)		0.00
	C(5)		0.00
	C(6)		0.00
		S(4)	1.47
		C(2)	0.59
		C(7)	0.31
		O(13)	0.70
		N(14)	0.90
(2)	N(1)		-0.09
	C(5)		0.08
	C(6)		-0.07
	C(7)		0.08
(3)	S(4)		0.03
	C(3)		-0.03
	C(5)		-0.04
	N(1)		0.03
		C(2)	-0.47
		C(8)	-0.98
		C(9)	1.40
		C(10)	-1.97
(4)	S(4)		0.00
	C(5)		0.00
	N(1)		0.00
		C(2)	-0.60
		C(3)	-0.19
		C(8)	-1.20
		C(9)	1.19
		C(10)	-2.10

Table 6

The intermolecular contacts of less than 4 Å

C(3)	$O(13)_I$	3.73	C(8)	$C(17)_{III}$	3.83
S(4)	$N(1)_I$	3.81	I	$C(15)_{IV}$	3.87
S(4)	$C(6)_I$	3.98	O(12)	$C(17)_{IV}$	3.32
S(4)	$C(7)_I$	3.36	S(4)	$C(5)_V$	3.61
S(4)	$O(13)_I$	3.32	S(4)	$O(11)_V$	3.37
C(8)	$N(1)_I$	3.81	C(5)	$O(11)_V$	3.90
C(8)	$C(2)_I$	3.88	O(11)	$C(6)_V$	3.38
C(8)	$C(7)_I$	3.97	O(11)	$C(16)_V$	3.90
C(8)	$C(10)_I$	3.92	C(17)	$C(10)_V$	3.83
C(8)	$O(12)_I$	3.94	C(17)	$O(11)_V$	3.24
C(8)	$O(13)_I$	3.81	C(17)	$O(12)_V$	3.98
C(9)	$O(13)_I$	3.41	I	$C(15)_{VI}$	3.87
C(10)	$O(12)_{II}$	3.22	O(13)	$C(15)_{VI}$	3.24
O(11)	$O(12)_{II}$	3.25	C(15)	$C(9)_{VI}$	3.79
O(12)	$O(12)_{II}$	2.46	C(16)	$C(9)_{VI}$	3.57
C(8)	$C(16)_{III}$	3.98			

The subscripts refer to the following transformations of the atomic co-ordinates:

(I) $x, 1+y, z$ (IV) $-\frac{1}{2}+x, -\frac{1}{2}+y, z$

(II) $-x, y, 1-z$ (V) $\frac{1}{2}-x, \frac{1}{2}+y, 1-z$

(III) $-\frac{1}{2}+x, \frac{1}{2}+y, z$ (VI) $\frac{1}{2}-x, -\frac{1}{2}+y, -z$

Table 7 Structure factor listings ($|F_o|$ and $|F_c| \times 10$)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	0	4	631	593	6	0	3	172	160	8	0	-8	742	826	12	0	-2	524	485	16	0	3	186	216
2	0	6	183	193	6	0	4	895	1003	8	0	-9	138	185	12	0	-3	825	816	16	0	4	536	524
2	0	7	654	650	6	0	5	609	673	8	0	-11	346	377	12	0	-4	103	125	16	0	5	182	223
2	0	8	88	75	6	0	7	254	255	8	0	-12	230	258	12	0	-5	943	995	16	0	6	318	314
2	0	9	115	128	6	0	8	708	766	8	0	-14	127	92	12	0	-6	445	486	16	0	7	178	202
2	0	10	246	278	6	0	9	121	101	10	0	0	822	662	12	0	-7	117	151	16	0	10	200	226
2	0	11	361	405	6	0	10	128	98	10	0	1	103	101	12	0	-8	471	464	16	0	-1	424	402
2	0	14	154	165	6	0	11	248	287	10	0	2	782	732	12	0	-9	234	229	16	0	-2	766	710
2	0	-3	662	642	6	0	14	129	120	10	0	3	755	652	12	0	-11	282	309	16	0	-3	546	549
2	0	-4	1271	1415	6	0	-2	994	898	10	0	4	201	176	12	0	-14	161	163	16	0	-4	556	536
2	0	-5	851	903	6	0	-3	529	468	10	0	5	660	626	14	0	0	666	647	16	0	-5	213	271
2	0	-6	194	193	6	0	-4	511	602	10	0	6	636	689	14	0	1	386	384	16	0	-6	292	279
2	0	-7	525	599	6	0	-5	320	349	10	0	7	419	438	14	0	2	545	499	16	0	-8	579	536
2	0	-8	505	529	6	0	-6	493	450	10	0	9	150	167	14	0	3	328	360	16	0	-9	114	152
2	0	-10	548	596	6	0	-7	781	814	10	0	11	186	183	14	0	4	532	527	16	0	-10	118	140
2	0	-11	166	169	6	0	-8	283	326	10	0	12	123	157	14	0	5	156	133	16	0	-11	303	323
2	0	-12	158	121	6	0	-9	277	331	10	0	-2	496	515	14	0	6	332	327	18	0	0	192	230
4	0	3	1059	1095	6	0	-10	372	426	10	0	-3	963	905	14	0	8	325	299	18	0	1	335	310
4	0	4	427	346	6	0	-13	253	267	10	0	-4	787	811	14	0	9	217	203	18	0	2	398	446
4	0	5	482	502	6	0	-15	161	125	10	0	-6	530	568	14	0	-1	903	843	18	0	3	392	418
4	0	6	558	616	8	0	1	913	876	10	0	-7	615	648	14	0	-2	124	122	18	0	5	317	292
4	0	7	474	516	8	0	2	606	507	10	0	-9	226	260	14	0	-3	681	577	18	0	6	365	322
4	0	8	110	161	8	0	3	440	458	10	0	-10	603	626	14	0	-4	698	585	18	0	8	150	172
4	0	9	450	451	8	0	4	839	817	10	0	-13	151	168	14	0	-5	200	248	18	0	9	201	208
4	0	10	102	75	8	0	5	281	319	12	0	0	467	383	14	0	-6	511	515	18	0	-1	689	693
4	0	12	215	228	8	0	6	451	394	12	0	2	667	653	14	0	-7	392	439	18	0	-2	390	402
4	0	13	148	182	8	0	7	336	334	12	0	3	436	360	14	0	-8	235	280	18	0	-4	445	420
4	0	-4	254	250	8	0	8	136	152	12	0	4	638	590	14	0	-9	319	357	18	0	-5	283	311
4	0	-5	1359	1389	8	0	9	299	321	12	0	5	227	218	14	0	-10	161	191	18	0	-6	575	513
4	0	-6	701	715	8	0	10	315	349	12	0	6	97	41	14	0	-12	124	142	18	0	-7	318	313
4	0	-8	471	546	8	0	13	154	135	12	0	7	412	409	14	0	-13	205	192	18	0	-9	207	240
4	0	-9	318	327	8	0	-3	612	612	12	0	8	168	192	14	0	-15	198	163	18	0	-10	124	159
4	0	-12	238	260	8	0	-4	672	656	12	0	9	222	259	16	0	0	260	255	18	0	-11	181	165
4	0	-15	160	146	8	0	-5	825	868	12	0	10	164	141	16	0	1	559	506	20	0	0	245	270
6	0	0	317	345	8	0	-6	571	574	12	0	-1	375	308	16	0	2	323	318	20	0	1	520	497

Table 7 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
20	0	2	137	195	24	0	-2	305	334	29	1	-3	185	215	3	1	-11	175	163	7	1	-2	316	305
20	0	3	197	220	24	0	-3	153	230	29	1	-6	154	191	3	1	-12	250	268	7	1	-3	1382	1259
20	0	4	308	341	24	0	-4	219	261	1	1	7	527	597	3	1	-13	176	144	7	1	-4	1113	1041
20	0	5	238	247	24	0	-7	247	238	1	1	8	159	160	3	1	-15	138	109	7	1	-5	462	437
20	0	7	154	176	24	0	-8	233	255	1	1	9	311	340	5	1	1	1181	1149	7	1	-6	654	641
20	0	10	168	161	26	0	0	162	183	1	1	10	348	332	5	1	2	270	237	7	1	-7	470	483
20	0	-1	205	220	26	0	1	133	192	1	1	12	250	263	5	1	3	102	134	7	1	-9	321	324
20	0	-2	329	349	26	0	3	235	281	1	1	13	198	178	5	1	4	934	986	7	1	-10	395	431
20	0	-3	332	333	26	0	-1	131	171	1	1	-3	642	677	5	1	5	516	493	7	1	-11	160	171
20	0	-4	354	338	26	0	-2	162	189	1	1	-4	302	193	5	1	6	539	506	7	1	-12	208	168
20	0	-5	411	407	26	0	-3	132	205	1	1	-5	836	930	5	1	7	794	820	7	1	-13	179	163
20	0	-6	183	245	26	0	-4	133	187	1	1	-6	529	570	5	1	8	192	204	7	1	-14	133	81
20	0	-7	222	287	26	0	-5	165	220	1	1	-7	381	381	5	1	10	317	325	9	1	0	688	523
20	0	-8	150	198	26	0	-6	236	299	1	1	-8	498	547	5	1	13	181	173	9	1	1	1177	1059
20	0	-9	178	176	26	0	-7	138	125	1	1	-9	276	281	5	1	-3	943	869	9	1	2	798	732
20	0	-10	129	138	28	0	1	140	186	1	1	-10	255	267	5	1	-4	382	300	9	1	3	269	241
20	0	-11	231	210	28	0	-1	170	257	1	1	-11	222	195	5	1	-5	974	1022	9	1	4	855	829
22	0	0	498	498	28	0	-3	171	75	1	1	-13	152	127	5	1	-6	327	352	9	1	5	399	389
22	0	1	187	233	28	0	-4	172	214	1	1	-14	245	257	5	1	-7	238	209	9	1	6	263	259
22	0	3	226	257	28	0	-6	143	75	3	1	3	705	707	5	1	-8	648	704	9	1	7	562	596
22	0	4	174	191	28	0	-7	145	175	3	1	4	709	688	5	1	-9	321	352	9	1	8	397	389
22	0	6	204	235	30	0	0	180	225	3	1	5	733	806	5	1	-10	224	202	9	1	10	217	176
22	0	-1	165	220	0	0	4	327	386	3	1	6	253	212	5	1	-11	250	259	9	1	13	164	166
22	0	-2	165	190	0	0	6	835	989	3	1	7	245	243	5	1	-12	118	122	9	1	-1	804	668
22	0	-3	382	390	0	0	7	610	642	3	1	8	521	517	7	1	1	450	319	9	1	-2	963	825
22	0	-4	337	310	0	0	8	306	244	3	1	9	418	416	7	1	2	1453	1377	9	1	-3	472	327
22	0	-5	121	183	0	0	9	487	535	3	1	10	225	212	7	1	3	1093	1092	9	1	-4	588	579
22	0	-6	213	261	0	0	10	262	285	3	1	11	320	281	7	1	5	642	572	9	1	-5	802	822
22	0	-7	177	219	0	0	11	129	190	3	1	14	163	167	7	1	6	842	859	9	1	-6	430	423
22	0	-9	394	330	0	0	12	224	245	3	1	-4	696	808	7	1	8	141	126	9	1	-7	508	499
22	0	-12	174	187	1	1	3	1013	1019	3	1	-6	722	791	7	1	8	141	126	9	1	-8	552	532
24	0	1	154	179	1	1	4	1067	1126	3	1	-7	626	639	7	1	9	443	424	9	1	-9	147	165
24	0	2	311	319	1	1	5	466	491	3	1	-8	258	291	7	1	11	145	140	9	1	-10	234	217
24	0	5	133	142	1	1	6	378	331	3	1	-9	259	237	7	1	12	197	195	9	1	-11	201	206
24	0	-1	215	288	29	1	-2	150	148	3	1	-10	339	338	7	1	-1	687	609	9	1	-13	203	186

Table 7 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
9	1	-14	233	226	13	1	10	177	177	15	1	-12	210	197	19	1	-9	316	297	25	1	2	194	186
11	1	0	960	886	13	1	11	206	206	17	1	0	374	382	19	1	-11	168	181	25	1	3	139	153
11	1	1	244	182	13	1	14	147	154	17	1	1	412	430	19	1	-12	142	152	25	1	5	143	170
11	1	2	525	500	13	1	-1	933	812	17	1	2	558	538	21	1	0	169	186	25	1	-1	191	241
11	1	3	828	791	13	1	-2	692	586	17	1	3	203	205	21	1	2	422	437	25	1	-3	235	257
11	1	4	354	300	13	1	-3	410	372	17	1	4	175	198	21	1	3	263	263	25	1	-4	334	311
11	1	5	383	413	13	1	-4	617	538	17	1	5	388	337	21	1	5	340	326	25	1	-5	138	144
11	1	6	581	561	13	1	-5	746	700	17	1	8	379	359	21	1	6	161	151	25	1	-6	171	194
11	1	7	220	202	13	1	-6	366	325	17	1	-1	676	659	21	1	8	171	152	25	1	-7	174	196
11	1	8	172	129	13	1	-7	401	355	17	1	-2	312	216	21	1	-1	438	464	25	1	-9	180	181
11	1	9	479	500	13	1	-8	390	377	17	1	-3	235	223	21	1	-2	224	213	25	1	-12	157	126
11	1	10	170	165	13	1	-9	138	157	17	1	-4	907	829	21	1	-3	318	279	27	1	1	176	200
11	1	12	186	197	13	1	-10	250	230	17	1	-5	318	316	21	1	-4	537	488	27	1	4	148	140
11	1	15	150	139	13	1	-11	213	207	17	1	-6	194	195	21	1	-5	213	222	27	1	-1	142	194
11	1	-1	897	752	13	1	-12	128	120	17	1	-7	509	474	21	1	-6	178	199	27	1	-2	286	266
11	1	-2	529	505	13	1	-13	233	201	17	1	-8	266	269	21	1	-7	385	326	27	1	-4	144	182
11	1	-3	1179	1016	15	1	0	535	530	17	1	-10	270	288	21	1	-9	166	171	27	1	-5	205	236
11	1	-4	506	461	15	1	1	540	486	17	1	-11	162	150	21	1	-10	241	218	27	1	-8	186	177
11	1	-5	375	360	15	1	2	279	264	17	1	-13	174	178	21	1	-12	147	125	29	1	0	150	153
11	1	-6	534	490	15	1	3	563	534	19	1	0	403	389	21	1	-13	186	154	29	1	3	154	143
11	1	-7	434	427	15	1	4	429	408	19	1	1	457	460	23	1	0	220	256	0	2	3	908	1022
11	1	-8	399	417	15	1	5	395	392	19	1	2	161	154	23	1	1	385	376	0	2	4	479	509
11	1	-9	398	403	15	1	6	522	524	19	1	3	393	372	23	1	4	283	298	0	2	5	344	385
11	1	-10	160	172	15	1	9	217	206	19	1	4	290	294	23	1	7	174	191	0	2	6	801	802
11	1	-11	169	157	15	1	12	141	147	19	1	6	279	263	23	1	-2	412	400	0	2	-12	285	279
11	1	-12	217	221	15	1	-1	254	206	19	1	7	273	266	23	1	-3	202	225	0	2	-15	211	180
11	1	-15	175	137	15	1	-2	672	602	19	1	9	168	80	23	1	-5	320	333	0	2	7	393	367
13	1	0	446	413	15	1	-3	873	781	19	1	-1	273	270	23	1	-6	325	310	0	2	8	327	338
13	1	1	826	713	15	1	-4	223	197	19	1	-2	570	554	23	1	-7	166	175	0	2	9	404	444
13	1	2	709	587	15	1	-5	403	407	19	1	-3	491	431	23	1	-8	195	194	0	2	11	208	214
13	1	3	345	351	15	1	-6	822	752	19	1	-4	140	156	23	1	-9	141	137	0	2	12	271	279
13	1	4	716	649	15	1	-8	160	166	19	1	-5	348	326	23	1	-10	145	132	0	2	15	183	180
13	1	5	488	441	15	1	-9	353	365	19	1	-6	375	325	23	1	-11	148	152	2	2	3	675	756
13	1	7	363	380	15	1	-10	173	168	19	1	-7	172	167	23	1	-14	160	114	2	2	4	703	731
13	1	8	302	278	15	1	-11	202	181	19	1	-8	354	349	25	1	0	253	282	2	2	5	701	765

Table 7 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	2	6	406	423	8	2	9	261	280	16	2	4	436	497	4	2	-5	294	331	10	2	-6	550	553
2	2	7	347	401	8	2	10	174	161	16	2	5	208	216	4	2	-6	735	745	10	2	-7	389	389
2	2	8	575	632	10	2	0	707	660	16	2	7	315	344	4	2	-7	262	292	10	2	-8	154	143
2	2	9	186	234	10	2	1	244	251	16	2	10	176	194	4	2	-8	308	331	10	2	-9	399	370
2	2	10	256	258	10	2	2	613	650	18	2	0	584	589	4	2	-9	483	492	10	2	-10	310	334
2	2	11	298	328	10	2	3	484	470	18	2	2	292	311	4	2	-12	256	273	10	2	-13	244	237
2	2	14	176	148	10	2	4	325	312	18	2	3	322	335	4	2	-13	135	131	12	2	-1	387	353
4	2	2	506	477	10	2	5	550	595	18	2	5	271	274	4	2	-14	142	121	12	2	-2	766	718
4	2	4	659	651	10	2	6	360	373	18	2	6	208	244	6	2	-1	881	900	12	2	-3	447	463
4	2	5	230	146	10	2	8	408	435	20	2	1	437	478	6	2	-2	791	855	12	2	-4	745	721
4	2	6	630	695	10	2	11	251	277	20	2	2	255	312	6	2	-3	649	648	12	2	-5	476	501
4	2	7	271	242	12	2	0	492	476	20	2	4	296	318	6	2	-4	772	774	12	2	-6	331	370
4	2	8	177	163	12	2	1	977	945	20	2	5	135	145	6	2	-5	261	247	12	2	-7	231	254
4	2	9	548	559	12	2	2	328	358	20	2	7	202	214	6	2	-6	333	359	12	2	-8	362	372
4	2	10	273	252	12	2	3	372	369	22	2	0	327	375	6	2	-7	740	781	12	2	-9	147	184
4	2	11	151	190	12	2	4	583	587	22	2	2	166	196	6	2	-8	323	369	12	2	-10	125	121
4	2	12	226	244	12	2	5	167	186	22	2	3	324	362	6	2	-10	400	404	12	2	-11	245	244
4	2	13	137	177	12	2	6	292	314	24	2	1	175	223	6	2	-11	193	181	12	2	-12	168	167
6	2	0	362	337	12	2	7	244	243	24	2	2	176	222	6	2	-13	192	202	14	2	-1	709	724
6	2	2	1078	1047	12	2	9	200	194	24	2	4	149	178	6	2	-14	176	164	14	2	-2	376	370
6	2	3	617	659	12	2	10	265	311	26	2	0	260	315	8	2	-1	739	717	14	2	-3	456	451
6	2	5	812	864	14	2	0	628	653	26	2	3	154	195	8	2	-2	896	889	14	2	-4	473	503
6	2	6	186	167	14	2	1	143	127	2	2	-3	421	394	8	2	-3	506	580	14	2	-6	333	347
6	2	7	199	209	14	2	2	555	569	2	2	-4	783	850	8	2	-4	194	220	14	2	-7	553	537
6	2	8	375	402	14	2	3	558	615	2	2	-5	688	706	8	2	-5	825	802	14	2	-8	190	223
6	2	9	178	154	14	2	4	189	187	2	2	-6	265	289	8	2	-6	412	423	14	2	-9	197	213
6	2	11	346	342	14	2	5	451	439	2	2	-7	388	434	8	2	-7	298	308	14	2	-10	260	272
8	2	0	627	628	14	2	6	274	299	2	2	-8	341	345	8	2	-8	428	468	16	2	-1	342	371
8	2	1	1167	1117	14	2	7	149	146	2	2	-9	396	454	8	2	-9	386	399	16	2	-2	615	656
8	2	2	155	77	14	2	8	336	332	2	2	-10	348	362	8	2	-11	249	247	16	2	-3	257	279
8	2	3	722	663	14	2	9	162	162	2	2	-11	339	328	8	2	-12	293	288	16	2	-4	237	266
8	2	4	685	730	16	2	0	188	202	2	2	-13	135	144	10	2	-1	949	919	16	2	-5	638	631
8	2	5	217	229	16	2	1	519	564	4	2	-2	524	572	10	2	-3	464	469	16	2	-6	166	191
8	2	6	339	370	16	2	2	222	229	4	2	-3	708	735	10	2	-4	564	564	16	2	-7	322	309
8	2	7	521	527	16	2	3	227	260	4	2	-4	964	988	10	2	-5	506	488	16	2	-8	281	322

Table 7 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
16	2	-9	206	223	26	2	-6	219	249	3	3	5	593	474	5	3	-6	302	318	9	3	9	150	102
16	2	-11	172	164	26	2	-9	162	176	3	3	6	710	715	5	3	-7	325	281	9	3	10	210	175
16	2	-12	178	163	28	2	-7	164	238	3	3	8	466	390	5	3	-8	383	319	9	3	11	186	158
18	2	-1	285	319	0	2	-3	926	1022	3	3	9	411	411	5	3	-9	192	153	9	3	-1	450	476
18	2	-2	233	210	0	2	-4	479	509	3	3	10	206	199	5	3	-10	271	258	9	3	-2	751	741
18	2	-3	472	523	0	2	-5	352	385	3	3	11	205	146	5	3	-11	266	241	9	3	-3	260	238
18	2	-4	189	225	0	2	-6	801	802	3	3	14	128	100	5	3	-14	299	220	9	3	-4	497	432
18	2	-5	334	333	0	2	-7	408	367	3	3	-3	648	582	7	3	1	466	473	9	3	-5	605	622
18	2	-6	433	447	0	2	-8	342	338	3	3	-4	928	819	7	3	2	377	351	9	3	-6	297	262
18	2	-7	181	182	0	2	-9	404	444	3	3	-5	334	397	7	3	3	638	654	9	3	-7	476	461
18	2	-9	273	278	0	2	-10	113	155	3	3	-6	748	658	7	3	4	338	350	9	3	-8	465	454
18	2	-10	200	179	0	2	-11	190	214	3	3	-7	812	776	7	3	5	595	528	9	3	-9	175	157
18	2	-12	151	172	1	3	3	483	510	3	3	-8	153	146	7	3	6	550	518	9	3	-10	151	128
18	2	-13	156	167	1	3	4	1117	1041	3	3	-9	285	296	7	3	8	205	146	9	3	-11	178	166
20	2	-1	197	225	27	3	-2	137	197	3	3	-10	189	178	7	3	9	316	314	9	3	-13	152	120
20	2	-2	354	396	27	3	-5	198	214	3	3	-12	161	140	7	3	10	132	109	9	3	-14	184	143
20	2	-3	236	240	1	3	5	310	300	3	3	-13	147	96	7	3	11	181	109	11	3	1	361	346
20	2	-4	312	342	1	3	6	366	344	3	3	-16	170	136	7	3	12	191	140	11	3	2	353	369
20	2	-5	224	233	1	3	7	412	351	5	3	1	689	647	7	3	-1	604	566	11	3	3	699	730
20	2	-7	271	315	1	3	8	267	251	5	3	2	244	244	7	3	-2	669	615	11	3	4	276	301
20	2	-8	259	271	1	3	9	202	162	5	3	3	667	611	7	3	-3	1059	917	11	3	6	529	464
20	2	-10	208	216	1	3	10	314	260	5	3	4	816	734	7	3	-4	594	558	11	3	7	159	137
22	2	-1	249	290	1	3	13	242	207	5	3	5	248	258	7	3	-5	357	349	11	3	8	167	145
22	2	-3	285	302	1	3	-3	614	576	5	3	6	286	236	7	3	-6	427	475	11	3	9	175	130
22	2	-4	166	210	1	3	-4	346	316	5	3	7	650	534	7	3	-7	353	308	11	3	10	142	140
22	2	-5	194	227	1	3	-5	801	723	5	3	8	174	151	7	3	-9	566	485	11	3	11	149	111
22	2	-6	280	314	1	3	-6	452	410	5	3	9	140	133	7	3	-10	195	196	11	3	-1	206	209
22	2	-8	206	201	1	3	-7	244	32	5	3	10	325	249	7	3	-12	296	284	11	3	-2	587	587
22	2	-9	183	203	1	3	-8	533	501	5	3	11	112	121	9	3	1	1060	1012	11	3	-3	673	633
24	2	-1	245	297	1	3	-9	334	316	5	3	13	215	158	9	3	2	548	501	11	3	-4	250	253
24	2	-2	245	315	1	3	-10	123	133	5	3	-1	867	765	9	3	3	133	116	11	3	-5	261	211
24	2	-4	249	297	1	3	-11	395	323	5	3	-2	923	915	9	3	4	603	548	11	3	-6	678	681
24	2	-5	230	255	1	3	-12	113	73	5	3	-3	164	166	9	3	5	331	323	11	3	-7	330	292
24	2	-7	184	219	1	3	-14	126	135	5	3	-4	603	621	9	3	7	337	306	11	3	-8	187	179
26	2	-3	282	303	3	3	1	358	398	5	3	-5	850	772	9	3	8	410	383	11	3	-9	297	306

Table 7 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
11	3	-11	141	136	15	3	-4	205	213	19	3	7	304	252	25	3	8	103	91	6	4	10	144	136
11	3	-12	226	199	15	3	-5	351	346	19	3	-1	187	225	25	3	-1	206	225	6	4	11	152	169
11	3	-15	169	132	15	3	-6	307	310	19	3	-2	383	402	25	3	-3	185	202	8	4	0	813	910
13	3	1	183	216	15	3	-7	280	279	19	3	-3	386	407	25	3	-4	228	228	8	4	1	337	376
13	3	2	385	346	15	3	-8	205	184	19	3	-5	276	276	25	3	-7	168	199	8	4	3	480	545
13	3	3	272	290	15	3	-9	242	255	19	3	-6	314	335	25	3	-10	145	135	8	4	4	419	412
13	3	4	312	293	15	3	-10	187	156	19	3	-8	257	223	27	3	1	169	149	8	4	6	335	410
13	3	5	488	489	15	3	-11	151	131	19	3	-9	153	194	27	3	4	175	175	8	4	7	218	212
13	3	6	160	181	15	3	-12	203	191	19	3	-10	182	151	2	4	3	164	168	8	4	9	199	202
13	3	8	314	281	15	3	-13	133	87	21	3	1	142	155	22	4	-9	219	197	8	4	10	257	225
13	3	-1	712	710	15	3	-14	138	102	21	3	2	276	274	2	4	4	290	374	10	4	0	244	212
13	3	-2	542	522	17	3	1	337	338	21	3	3	119	116	2	4	5	311	351	10	4	1	247	248
13	3	-3	175	145	17	3	2	483	457	21	3	4	149	145	2	4	6	282	289	10	4	2	625	682
13	3	-4	671	704	17	3	3	105	107	21	3	5	264	257	2	4	7	419	434	10	4	3	202	199
13	3	-5	405	423	17	3	4	264	208	21	3	6	127	69	2	4	8	295	312	10	4	5	520	526
13	3	-7	369	358	17	3	5	323	314	21	3	8	164	176	2	4	11	179	174	10	4	6	153	133
13	3	-8	286	229	17	3	7	167	162	21	3	-1	356	370	4	4	1	426	540	10	4	8	311	339
13	3	-9	173	140	17	3	8	211	202	21	3	-3	201	193	4	4	2	349	436	10	4	11	197	209
13	3	-10	313	297	17	3	11	136	135	21	3	-4	332	354	4	4	3	553	700	12	4	0	441	412
13	3	-11	168	145	17	3	-1	235	275	21	3	-5	188	187	4	4	4	358	344	12	4	1	553	581
13	3	-12	124	90	17	3	-2	267	268	21	3	-6	192	176	4	4	5	169	209	12	4	2	255	256
13	3	-13	130	145	17	3	-3	305	310	21	3	-7	215	222	4	4	6	329	376	12	4	3	289	276
13	3	-14	165	109	17	3	-4	366	340	21	3	-8	201	207	4	4	7	141	141	12	4	4	335	326
15	3	1	346	372	17	3	-5	374	355	21	3	-9	159	143	4	4	8	175	169	12	4	5	180	150
15	3	2	203	227	17	3	-6	230	211	21	3	-10	164	158	4	4	9	264	271	12	4	6	188	194
15	3	3	427	418	17	3	-7	335	359	21	3	-13	145	139	4	4	11	149	122	12	4	7	260	284
15	3	5	244	237	17	3	-8	115	150	23	3	1	248	279	6	4	0	192	202	12	4	10	225	210
15	3	6	332	294	17	3	-9	119	122	23	3	4	129	152	6	4	1	378	396	14	4	0	372	338
15	3	7	209	160	17	3	-10	195	212	23	3	-2	261	281	6	4	2	627	673	14	4	1	211	205
15	3	9	242	216	17	3	-12	187	129	23	3	-3	195	191	6	4	3	253	264	14	4	2	439	425
15	3	10	126	127	17	3	-13	137	117	23	3	-5	178	264	6	4	4	427	517	14	4	3	360	379
15	3	12	136	114	19	3	1	172	179	23	3	-8	188	186	6	4	5	322	337	14	4	4	186	235
15	3	-1	147	138	19	3	3	286	286	23	3	-11	143	172	6	4	6	137	122	14	4	5	166	226
15	3	-2	331	356	19	3	4	281	295	25	3	2	187	184	6	4	7	208	201	14	4	6	141	165
15	3	-3	459	461	19	3	6	209	210	25	3	5	169	154	6	4	8	326	322	14	4	8	217	230

Table 7 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
16	4	0	244	240	4	4	-1	176	232	12	4	-5	536	534	20	4	-8	264	252	7	5	6	397	403
16	4	1	373	368	4	4	-2	303	373	12	4	-6	178	195	20	4	-11	222	179	7	5	8	153	161
16	4	2	164	167	4	4	-3	633	798	12	4	-8	351	369	22	4	-3	255	262	7	5	9	163	114
16	4	3	167	164	4	4	-4	285	292	12	4	-9	203	192	22	4	-6	206	218	9	5	0	176	187
16	4	4	298	314	4	4	-5	355	419	12	4	-11	249	207	1	5	3	356	427	9	5	1	178	147
16	4	5	177	157	4	4	-6	386	434	14	4	-1	371	407	21	5	-3	225	169	9	5	2	331	343
16	4	6	150	160	4	4	-8	294	278	14	4	-2	172	189	21	5	-4	186	151	9	5	3	300	244
16	4	7	219	210	4	4	-9	365	404	14	4	-3	348	342	1	5	4	467	578	9	5	4	288	332
18	4	0	399	405	6	4	-1	616	730	14	4	-4	389	387	1	5	5	267	297	9	5	5	236	205
18	4	2	143	143	6	4	-2	394	484	14	4	-5	183	97	1	5	7	549	585	9	5	7	241	245
18	4	3	373	371	6	4	-3	256	277	14	4	-6	285	276	1	5	10	280	275	9	5	8	161	119
18	4	6	194	227	6	4	-4	502	580	14	4	-7	340	318	3	5	0	279	407	11	5	0	512	470
20	4	1	303	310	6	4	-5	281	238	14	4	-8	177	146	3	5	2	363	453	11	5	1	267	224
20	4	2	243	260	6	4	-6	228	225	14	4	-9	260	256	3	5	3	288	377	11	5	3	341	349
20	4	4	158	145	6	4	-7	461	513	14	4	-10	247	233	3	5	4	162	167	11	5	4	196	183
20	4	5	230	252	6	4	-9	161	146	16	4	-1	160	146	3	5	5	520	564	11	5	6	285	268
22	4	0	254	282	6	4	-10	241	218	16	4	-2	491	465	3	5	6	430	381	11	5	9	248	240
22	4	3	262	239	8	4	-2	448	483	16	4	-3	230	219	3	5	7	251	226	13	5	1	239	281
24	4	1	172	145	8	4	-3	514	565	16	4	-4	213	218	3	5	8	176	149	13	5	2	345	358
24	4	2	212	218	8	4	-4	245	259	16	4	-5	366	360	3	5	9	327	318	13	5	4	299	272
0	4	2	269	387	8	4	-5	270	305	16	4	-6	174	157	5	5	0	199	245	13	5	5	269	261
0	4	3	442	561	8	4	-6	429	440	16	4	-7	179	155	5	5	1	620	735	13	5	8	176	155
0	4	4	269	333	8	4	-7	146	131	16	4	-8	371	346	5	5	2	234	233	15	5	0	332	320
0	4	5	388	431	8	4	-8	269	269	16	4	-11	168	195	5	5	3	173	134	15	5	1	149	176
0	4	6	441	512	8	4	-9	252	232	18	4	-1	298	288	5	5	4	473	523	15	5	3	291	291
0	4	8	292	298	10	4	-1	697	723	18	4	-3	317	317	5	5	5	253	251	15	5	6	297	297
0	4	9	313	305	10	4	-2	378	389	18	4	-4	323	271	5	5	6	204	208	17	5	1	198	194
2	4	-2	342	485	10	4	-4	612	631	18	4	-6	369	316	5	5	7	277	289	17	5	2	258	233
2	4	-3	266	341	10	4	-5	321	318	18	4	-7	219	226	5	5	8	210	176	17	5	5	248	257
2	4	-4	502	655	10	4	-6	168	171	18	4	-9	201	195	5	5	10	237	205	19	5	1	244	235
2	4	-5	259	295	10	4	-7	355	392	18	4	-10	240	189	7	5	0	558	565	19	5	3	218	237
2	4	-6	286	293	10	4	-8	209	172	20	4	-1	237	219	7	5	1	307	263	1	5	-3	261	270
2	4	-7	382	404	10	4	-10	292	272	20	4	-2	262	299	7	5	2	297	357	1	5	-5	432	452
2	4	-8	222	228	12	4	-2	492	487	20	4	-4	188	172	7	5	3	316	346	1	5	-6	304	325
2	4	-10	304	299	12	4	-3	454	423	20	4	-5	382	344	7	5	5	180	133	1	5	-7	159	168

Table 7 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	5	-8	262	261	11	5	-9	236	223	2	6	8	232	169	2	6	-2	145	186	16	6	-2	324	274
1	5	-9	151	104	13	5	-1	408	387	4	6	0	275	336	2	6	-3	136	160	18	6	-1	219	181
1	5	-10	161	146	13	5	-2	238	186	4	6	1	174	185	2	6	-4	181	181	18	6	-3	272	191
3	5	-3	314	390	13	5	-4	286	235	4	6	3	283	279	2	6	-5	270	278					
3	5	-4	364	387	13	5	-5	276	244	4	6	4	344	315	2	6	-7	346	300					
3	5	-5	220	201	13	5	-7	299	265	4	6	6	237	206	2	6	-9	245	190					
3	5	-6	241	185	13	5	-8	236	189	4	6	7	222	203	4	6	-2	273	285					
3	5	-7	293	280	15	5	-1	209	176	6	6	0	168	190	4	6	-3	426	467					
3	5	-10	228	193	15	5	-2	236	198	6	6	2	402	458	4	6	-6	229	214					
5	5	-1	233	314	15	5	-3	337	306	6	6	3	171	119	4	6	-9	349	226					
5	5	-2	398	467	15	5	-5	250	171	6	6	5	283	279	6	6	-1	454	522					
5	5	-4	196	169	15	5	-6	364	340	6	6	8	283	262	6	6	-2	197	147					
5	5	-5	550	569	17	5	-1	407	374	8	6	0	390	345	6	6	-4	306	274					
5	5	-8	406	355	17	5	-2	161	155	8	6	1	281	290	6	6	-5	270	200					
5	5	-11	298	263	17	5	-4	403	357	8	6	2	179	186	6	6	-7	220	190					
7	5	-1	154	138	17	5	-5	168	123	8	6	3	268	224	8	6	-1	258	252					
7	5	-2	237	225	19	5	-2	210	210	8	6	4	308	304	8	6	-2	224	202					
7	5	-3	439	461	19	5	-3	173	180	8	6	6	227	202	8	6	-3	407	325					
7	5	-4	139	146	19	5	-4	175	147	8	6	8	255	181	8	6	-5	235	210					
7	5	-6	495	498	19	5	-5	178	191	8	6	9	219	203	8	6	-6	280	217					
7	5	-7	277	231	21	5	-1	182	179	10	6	0	156	194	8	6	-7	230	88					
7	5	-9	293	246	21	5	-2	182	158	10	6	2	542	467	10	6	-1	441	354					
9	5	-1	416	428	0	6	1	92	208	10	6	5	323	309	10	6	-3	258	234					
9	5	-2	350	351	0	6	2	85	120	10	6	8	308	220	10	6	-4	361	279					
9	5	-4	590	544	18	6	-6	286	212	12	6	0	243	203	10	6	-5	217	99					
9	5	-5	355	309	0	6	3	276	320	12	6	1	351	306	10	6	-7	309	260					
9	5	-6	167	148	0	6	4	179	128	12	6	4	331	310	12	6	-2	370	273					
9	5	-7	204	187	0	6	5	227	209	12	6	7	344	296	12	6	-3	217	152					
9	5	-8	187	206	0	6	6	224	203	14	6	2	308	262	12	6	-4	182	160					
9	5	-10	239	220	0	6	9	316	269	14	6	3	199	193	12	6	-5	300	257					
11	5	-1	196	182	2	6	0	102	184	16	6	1	438	370	12	6	-8	304	222					
11	5	-2	251	193	2	6	1	248	338	16	6	4	219	238	14	6	-1	230	218					
11	5	-3	507	506	2	6	4	207	159	18	6	0	268	255	14	6	-3	304	262					
11	5	-6	369	319	2	6	5	275	265	18	6	3	323	269	14	6	-4	242	189					
11	5	-7	186	136	2	6	7	215	215	2	6	-1	112	147	14	6	-6	296	218					

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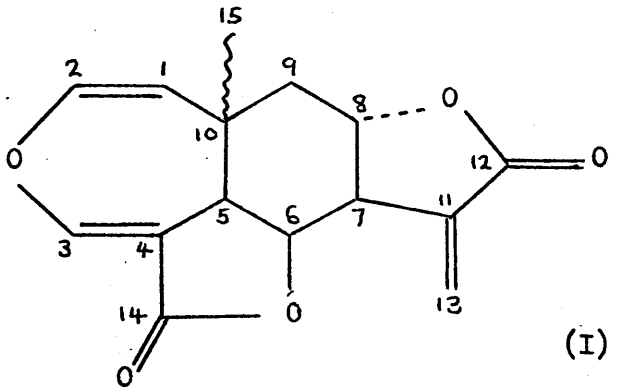
CHAPTER 5

THREE SESQUITERPENE-LACTONES

5.1 Introduction

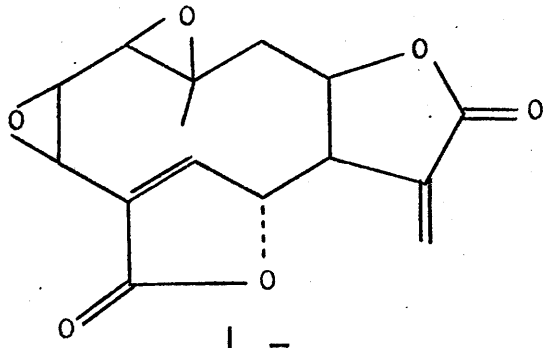
Many of the extracts of the genus Mikania (family compositae, tribe Eupatorieae Cass., subtribe Ageratinae Less) are known to have been used successfully in folk medicine. Werner Herz and his co-workers at Florida University have reported the isolation and partial structure determination of six lactones from Mikania scandens (L.) Willd[1] (climbing hempvine). Five of these belong to the germacrane type[2], some of which are known to exhibit tumor-inhibitory activity[3,4]. One of these, dihydromikanolide, formed crystals suitable for X-ray analysis as did the sixth lactone, miscandenin, a variant resulting from a germacradiene-elemadiene interconversion.

The structures of all six dilactones were suggested by U.V., I.R., and N.M.R. spectra; the correct stereochemistry of miscandenin was not fully determined with respect to the C(15) methyl group and the hydrogen attached to C5.

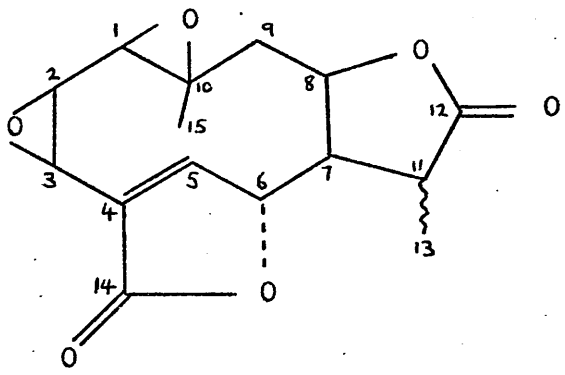


(I) Miscandenin

The extract, dihydromikanolide, may also be obtained by partial hydrogenation of the mikanolide extract:



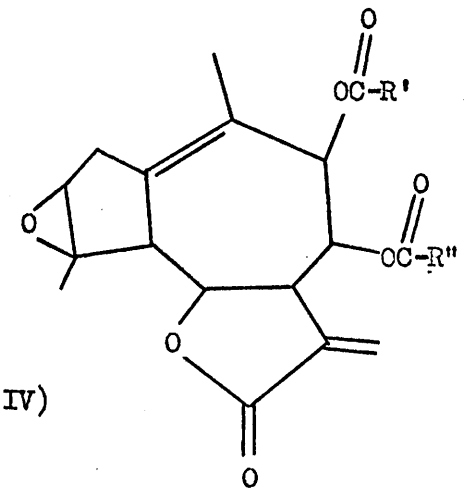
II Mikanolide



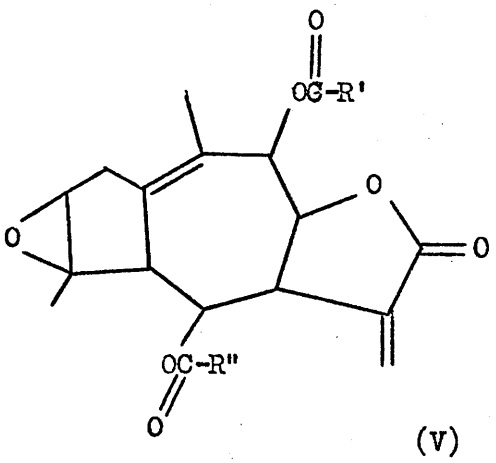
III Dihydromikanolide

The crystal structure of dihydromikanolide was examined to confirm the stereochemistry of the molecule, also the stereochemistry at C(11) was not known.

Crystals of a third sesquiterpene lactone, berlandin, were also supplied by Werner Herz. This lactone was thought to possess structure (IV) or (V), the stereochemistry being unknown.



(IV)



(V)

R',R" = $-CH_3$, $-C(CH_3)=C(H)CH_3$

The configuration of berlandin was shown to be (IV); the structures of the three compounds were determined by the application of non-centrosymmetric direct method procedures.

5.2.1 Experimental

Crystal data

Miscandenin

Molecular formula	$C_{15}H_{14}O_5$
Molecular weight	274.3 a.m.u.
Crystal system	orthorhombic
Space group	$P2_12_12_1$ (D_2^4)
Cell dimensions	$\underline{a}$ = 8.586(4) Å
	$\underline{b}$ = 14.918(5) Å
	$\underline{c}$ = 10.211(3) Å
Cell volume (u)	1307.8 $Å^3$
Density (observed)	1.37 $g.cm^{-3}$
Density (calculated)	1.39 $g.cm^{-3}$
Molecules per unit cell (Z)	4
Number of electrons per unit cell ($F_{(000)}$)	576
Linear absorption coefficient, μ(MoKα)	1.14 cm^{-1}

The crystal used for X-ray analysis was colourless, and rectangular in shape. Weissenberg and precession photographs of the crystal taken with CuKα and MoKα radiation respectively, determined the space group as $P2_12_12_1$. The axial systematically absent reflections are h00 when h = 2n+1, 0k0 when k = 2n+1 and 00l when l = 2n+1; the initial cell dimensions were obtained, and the observed density was found to be close to that calculated for four molecules per unit cell.

The cell dimensions were refined by least-squares analysis of the angular settings of 12 reflections measured on the diffractometer at $\theta(MoK\alpha)$ about 16°. The octant hkl was measured out to $\theta \leqslant 27^{\circ}$ by means of a $\theta-2\theta$ scan of 40 steps of 0.02° per second. Stationary crystal-stationary counter background counts were taken for 15 seconds at the start and end of each scan. The stabilised X-ray generator was operated at 44kV and 16mA and the intensities were corrected for Lorentz and polarization effects but not for absorption. A total of 1639 independent structure amplitudes was obtained, of which 1222 had $I > 2\sigma(I)$.

5.2.2 Structure analysis

Normalised structure factors were calculated for all the structure amplitudes based on an overall temperature factor of 3.65 Å, and this gave 184 E values greater than 1.5. Sigma 2 relationships were calculated and the initial set of phases consisted of three origin-determining phases,[5-7] a suitable enantiomorph and 2 further phases which were given values of $\pm\pi/4$, $\pm 3\pi/4$ (table 1). The 16 sets of starting phases were used to initiate tangent formula[8] calculations and the Karle R index[7] range was from 0.19 - 0.32. An E map generated from 184 E values based on the phases associated with the lowest R index yielded the correct solution. The initial values of the two variable phases were $3\pi/4$ for 7 4 5 and $3\pi/4$ for 3 12 1, although initial phases of $-3\pi/4$ and $-3\pi/4$ phased the 184 E values identically.

Two atoms of the 7-membered ring and the methyl carbon could not be located from the E map but the remaining carbon and oxygen atoms were found. An initial structure factor calculation gave a discrepency index (R) of 0.541, and after one cycle of least squares calculations a Fourier difference map revealed the missing atoms. Reflections for which $I \leqslant 2\sigma$ were now regarded as 'unobserved' and further removed from calculations. The atoms were allowed to refine isotropically to R = 0.144 using a unitary weighting scheme. Subsequent anisotropic refinement of the atoms converged at R = 0.104, and a difference Fourier map showed all the hydrogen positions. The hydrogens were refined isotropically and a final R value of 0.702 was obtained. The weighting scheme used for the last 4 cycles of least squares calculations was of the type $w=1/(1+((F_{obs} - F_B)/F_A)^2)$, where the final values of F_A and F_B were 4.44 and 9.48 respectively. An attempt was made to determine the absolute stereochemistry of the molecule using the anomalous dispersion corrections of oxygen and carbon quoted by Engel[9]. Structure factor calculations were made using these corrections for the molecule and its mirror image; the final R values obtained were R = 0.07022, R (weighted) = 0.06548 and R = 0.07022, R (weighted) = 0.06552. The difference in R (weighted) here has been shown by the Hamilton[10] significant test to be an insignificant demonstration of the correct absolute configuration. Hence the correct absolute configuration of the sesquiterpene, on a right handed set of axes, was assumed. The computing was carried out on the Univac 1108 computer at the National Engineering Laboratory, East Kilbride.

TABLE 1

MISCANDENIN

(a) Initial set of phases

Reflection				Phase	E
1	15	0	origin + enantiomorph	π/2 (fixed)	3.12
0	5	5		π/2 (fixed)	3.07
6	9	0		0 (fixed)	2.83
0	15	2		π/2 (fixed)	2.98
7	4	5		$\pm$ π/4, $\pm$ 3π/4	2.75
3	12	1		$\pm$ π/4, $\pm$ 3π/4	2.38

This starting set led to the mirror image of the correct absolute configuration.

(b) E statistics

Average value of	$\|E\|$	$\|E^2\|$	$\|E^2-1\|$
Found	0.847	1.00	0.806
Theoretical for centric	0.798	1.00	0.968
Theoretical for acentric	0.886	1.00	0.736
Percentage of values for:	$E > 1.0$	$E > 2.0$	$E > 3.0$
Found	35.68	3.30	0.18
Theoretical for centric	31.73	4.55	0.27
Theoretical for acentric	36.79	1.83	0.01

5.3.1 Experimental

Crystal data

Dihydromikanolide	
Molecular formula	$C_{15}H_{16}O_6$
Molecular weight	292.3 a.m.u.
Crystal system	monoclinic
Space group	$P2_1$ (C_2^2)
Cell dimensions	$\underline{a}$ = 10.451(6) Å
	$\underline{b}$ = 7.122(4) Å
	$\underline{c}$ = 9.233(5) Å
	$\underline{\beta}$ = 99.77(3)°
Cell volume (u)	677.3 Å^3
Density (observed)	1.40 g.cm^{-3}
Density (calculated)	1.43 g.cm^{-3}
Molecules per unit cell (z)	2
Number of electrons per unit cell ($F_{(000)}$)	308
Linear absorption coefficient, μ (MoKα)	1.20 cm^{-1}

The crystals of dihydromikanolide are colourless prisms which extinguish under polarised light. Preliminary cell dimensions were obtained from rotation and Weissenberg photographs taken with CuKα radiation. The space group was determined from the systematically absent reflections (0k0 when k = 2n+1) to be either $P2_1$ or $P2_1/m$. As the natural product, dihydromikanolide, is chiral it cannot crystallise in a centrosymmetric

space group hence $P2_1/m$ was rejected. The observed density indicated that there were 2 molecules per unit cell.

The cell dimensions were refined by least squares analysis of the angular settings of 12 reflections measured on the diffractometer at $\theta(MoK\alpha)$ about 16°. The quadrants hkl and $hk\bar{l}$ were measured out to $\theta \leqslant 30^\circ$ with a θ-2θ scan of 60 steps of 0.02° per second. Stationary crystal-stationary counter background counts were taken for 15 seconds at the start and end of each scan. The stabilised X-ray generator was operated at 40kV and 16mA and the intensities were corrected for Lorentz and polarisation effects but not for absorption. A total of 2116 independent structure amplitudes was obtained, of which 1486 had $I > 3\sigma(I)$.

5.3.2 Structure analysis

The 220 E values greater than 1.50 were calculated based on an overall temperature factor of 3.47 $\mathring{A}^2$ and the Sigma 2 relationships were generated. The three origin fixing phases (table 2) were given phases of 0 , the enantiomorph phase was initially $\pi/2$ and a further 3 phases were assigned $\pm \pi/2$. This gave 8 possible starting sets of 7 phases for tangent formula calculations resulting in a Karle R index range of 0.17 - 0.29. An E map was generated based on the phases obtained from the tangent formula calculation which gave the lowest Karle R index. The map showed clearly the atomic positions of all the oxygen and carbon atoms in the molecule.

An initial structure factor calculation gave a discrepancy index (R) of 0.356 and the reflections for which $I \leq 3\sigma I$ were now considered as 'unobserved' and removed from further calculations. The atoms were refined isotropically using a unit weighting scheme to R = 0.145. With the atoms refining anisotropically R fell to 0.100, and a difference Fourier map showed all the remaining hydrogen atom positions. Nine reflections with large $F_{(obs)}$ values and small $\frac{\sin\theta}{\lambda}$ values appeared to be effected by extinction and were removed from the calculations. Using values for the imaginary part of the anomalous dispersion for oxygen and carbon, quoted by Engel, an attempt was made to determine the absolute stereochemistry of the molecule. Structure factor calculations were made using these corrections for the molecule and its mirror image; the final R values obtained were R = 0.06205, R (weighted) = 0.07063 and R = 0.06207 and R(weighted) = 0.07064. The difference in R (weighted) is an insignificant demonstration of the correct absolute configuration. Therefore the normal absolute configuration of the sesquiterpene was assumed. The weighting scheme used for the last 4 cycles of least squares was of the type $w = 1/(1+((F_{obs} - F_B)/F_A)^2$, where the final values of F_A and F_B were 6.00 and 4.84 respectively. All computing was carried out on the Univac 1108 computer at the National Engineering Laboratory, East Kilbride.

TABLE 2

DIHYDROMIKANOLIDE

(a) Initial set of phases

Reflection				Phase	E
3	0	$\bar{7}$	origin	0 (fixed)	2.87
6	1	4	origin	0 (fixed)	2.74
0	4	1	origin	0 (fixed)	2.72
2	9	$\bar{5}$	enantiomorph	$\pi/2$	2.72
11	1	6		$\pm \pi/2$	2.32
14	1	$\bar{2}$		$\pm \pi/2$	2.18
2	1	$\bar{12}$		$\pm \pi/2$	2.16

(b) E statistics

Average value of	$\lvert E \rvert$	$\lvert E^2 \rvert$	$\lvert E^2-1 \rvert$
Found	0.869	1.00	0.756
Theoretical for centric	0.798	1.00	0.968
Theoretical for acentric	0.886	1.00	0.736

Percentage of values for	$E > 1.0$	$E > 2.0$	$E > 3.0$
Found	37.03	2.04	0.03
Theoretical for centric	31.73	4.55	0.27
Theoretical for acentric	36.79	1.83	0.01

5.4.1 Experimental

Crystal data

Berlandin

Molecular formula	$C_{22}H_{26}O_7$
Molecular weight	402.5 a.m.u.
Crystal system	orthorhombic
Space group	$P2_12_12_1$ (D_2^4)
Cell dimensions	$\underline{a}$ = 6.306(3) Å
	$\underline{b}$ = 37.040(11) Å
	$\underline{c}$ = 8.959(3) Å
Cell volume (u)	2092.8 $Å^3$
Density (observed)	1.27 $g.cm^{-3}$
Density (calculated)	1.28 $g.cm^{-3}$
Molecules per unit cell (z)	4
Number of electrons per unit cell $(F_{(000)})$	856
Linear absorption coefficient, $\mu(MoK_\alpha)$	1.02 cm^{-1}

The crystals of berlandin are large, colourless and rectangular in shape. The space group and initial cell dimensions were determined in the same way as miscandenin.

The cell dimensions were refined by least-squares analysis of the angular settings of 12 reflections measured on the diffractometer at θ ($MoK\alpha$) about 16°. A θ-2θ scan of 60 steps of 0.01° per second out to $\theta \leqslant 27°$ was employed and stationary crystal-stationary counter background counts were taken for 15 seconds at the start and end of each scan. The stabilised X-ray generator was operated at 36 kV and

12mA and the intensities were corrected for Lorentz and polarization effects but not for absorption. A total of 2649 independent structure amplitudes was obtained, of which 2240 had $I > 2\sigma(I)$.

5.4.2 Structure analysis

Based on an overall temperature factor of 4.61 $\mathring{A}^2$, 302 E values were calculated with values greater than 1.50. Sigma 2 relationships were derived and the initial set of phases consisted of 3 origin-determining phases, a suitable enantiomorph and 2 further phases which were given values of $\pm \pi/4$, $\pm 3\pi/4$ (table 3). This gave 16 sets of starting phases which were used to initiate tangent formula calculations and the Karle R index range was from 0.20 - 0.35. An E map generated from the phases of the 302 E values associated with the lowest Karle R index yielded the correct solution. The initial values of the 2 variable phases, which gave a Karle R index of 0.20, were $\pi/4$ for 3 21 3 and $-3\pi/4$ for 3 30 1. The next lowest Karle R index in the range of values was 0.27. From the initial E map 25 atoms including all the oxygens were located.

An initial structure factor calculation gave a discrepancy index (R) of 0.355 and the reflections for which $I \leq 2\sigma(I)$ were removed from further calculations. The remaining 4 atoms were located from a difference Fourier synthesis and all 29 atoms were allowed to refine isotropically. Isotropic refinement converged at R = 0.176 and when the atoms refined anisotropically R fell to 0.142. At this stage 14 reflections which were thought to be affected by extinction were removed from the calculations and R fell to 0.102.

TABLE 3

BERLANDIN

(a) Initial set of phases

Reflection				Phase	E
1	37	0	origin	π/2 (fixed)	4.32
0	3	9	+	π/2 (fixed)	2.83
6	0	3	+	π/2 (fixed)	2.14
0	29	8	enantiomorph	π/2 (fixed)	2.09
3	21	3		± π/4, ± 3π/4	2.97
3	30	1		± π/4, ± 3π/4	2.79

This starting set led to the mirror image of the correct absolute configuration.

(b) E statistics

Average value of	$\|E\|$	$\|E^2\|$	$\|E^2-1\|$
Found	0.857	1.00	0.803
Theoretical for centric	0.798	1.00	0.968
Theoretical for acentric	0.886	1.00	0.736

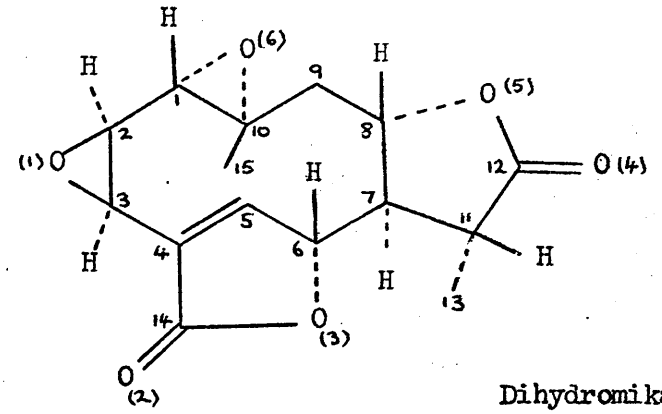
Percentage of values for	E > 1.0	E > 2.0	E > 3.0
Found	35.90	2.40	0.06
Theoretical for centric	31.73	4.55	0.27
Theoretical for acentric	36.79	1.83	0.01

A difference Fourier synthesis based on data with $\frac{\sin\theta}{\lambda} \leqslant 0.5$ showed 17 hydrogen positions. With the hydrogens as fixed-atom contributors R fell to 0.086 and 6 more hydrogens were found from a difference synthesis. R now fell to 0.082 but the remaining 3 methyl hydrogens attached to C(22) could not be located from a subsequent difference synthesis. The located hydrogens were allowed to refine isotropically and a final R value of 0.079 was obtained. A unit weighting scheme was used. The absolute configuration of the molecule was not determined by use of anomalous dispersion corrections (both R values were identical) so the correct absolute configuration of the sesquiterpene was assumed. The computing was carried out on the Univac 1108 computer at the National Engineering Laboratory, East Kilbride.

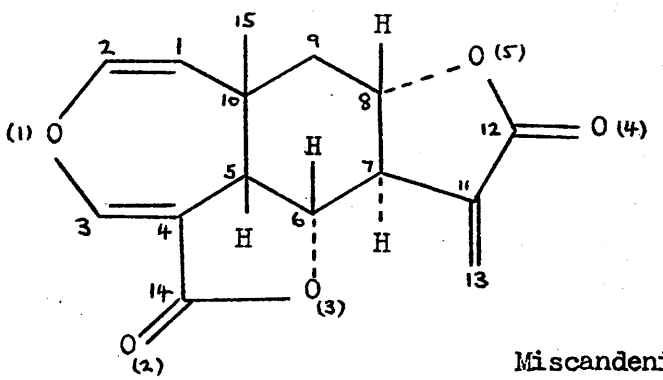
5.5 Discussion

The molecular structures of the 3 sesquiterpenes are shown in Figures 1, 2 and 3 and the molecular packing of the 3 molecules is shown in Figures 4, 5 and 6. The final co-ordinates, with their standard deviations and thermal parameters for dihydromikanolide, miscandenin and berlandin are listed in tables 7 and 8, 9 and 10, and 11 and 12, respectively. Similarly the bond lengths and valency angles are listed in tables 13 and 14, 15 and 16, and 17 and 18. The torsion angles and mean plane calculations are listed in tables 19 and 20, 21 and 22, 23 and 24; tables 25, 26 and 27 list the intermolecular contacts.

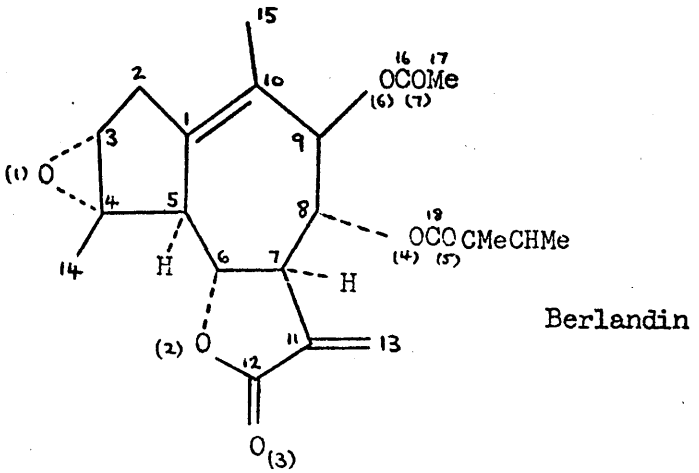
Diagrams of the stereochemistry of the 3 molecules are shown below:



Dihydromikanolide



Miscandenin



Berlandin

Fig. 1

A general view of the Dihydromikanolide molecule

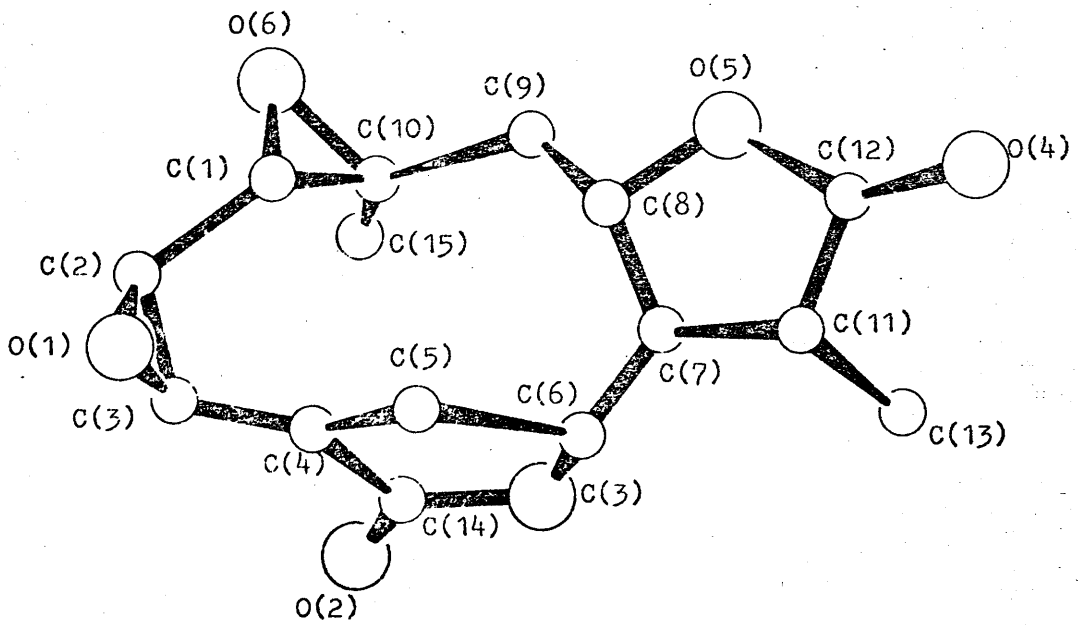


Fig. 2

A general view of the Miscandenin molecule

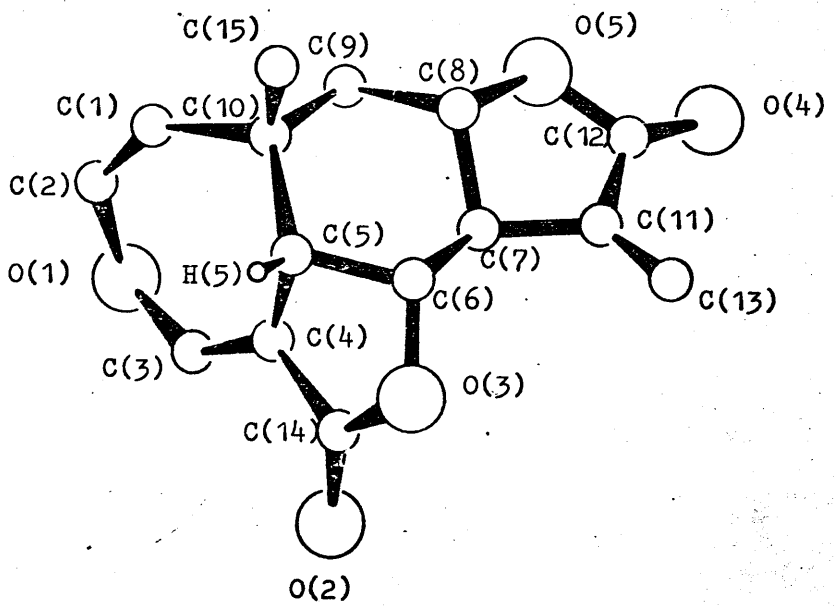
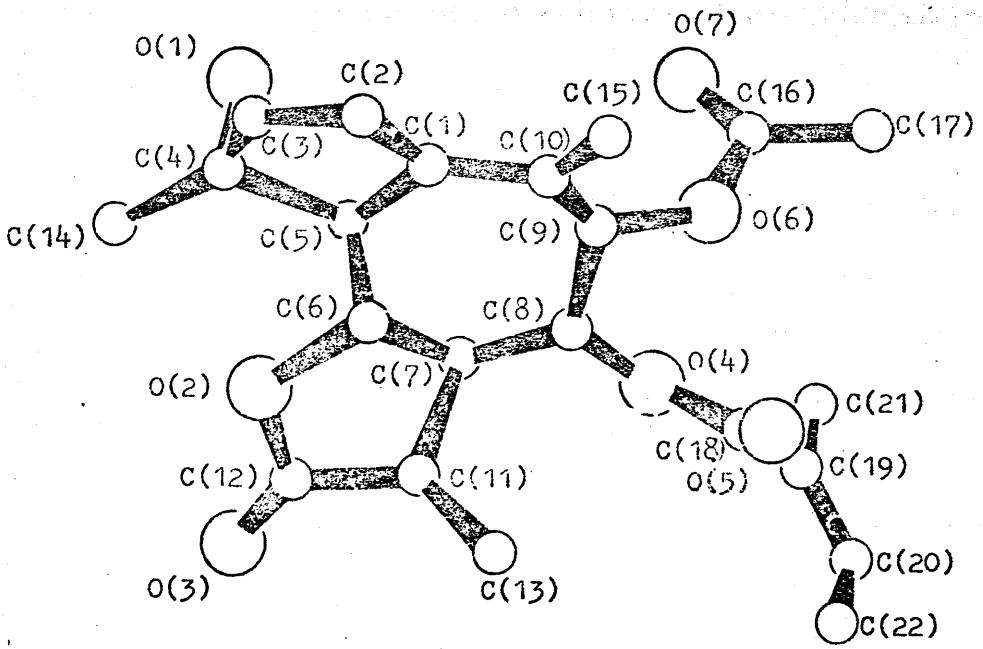


Fig. 3

A general view of the Berlandin molecule

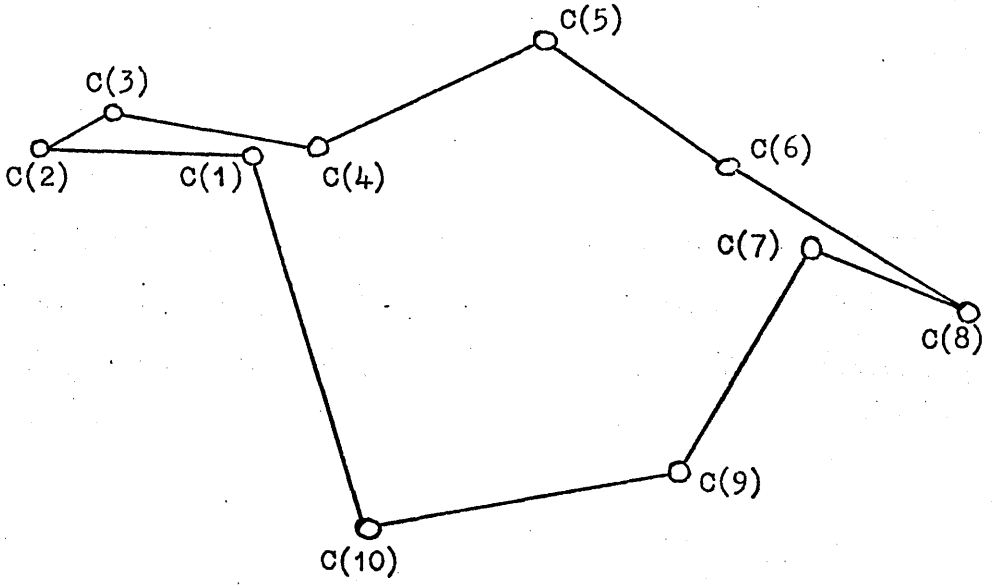


The two epoxide groups on the ten-membered ring in dihydromikanolide are in the anti-position to each other. Also the C(13) methyl group lies below the plane of the lactone ring as shown.

In miscandenin C(15) and H(5) are syn to each other and the remaining basic stereochemical features of the molecule were obtained by this analysis.

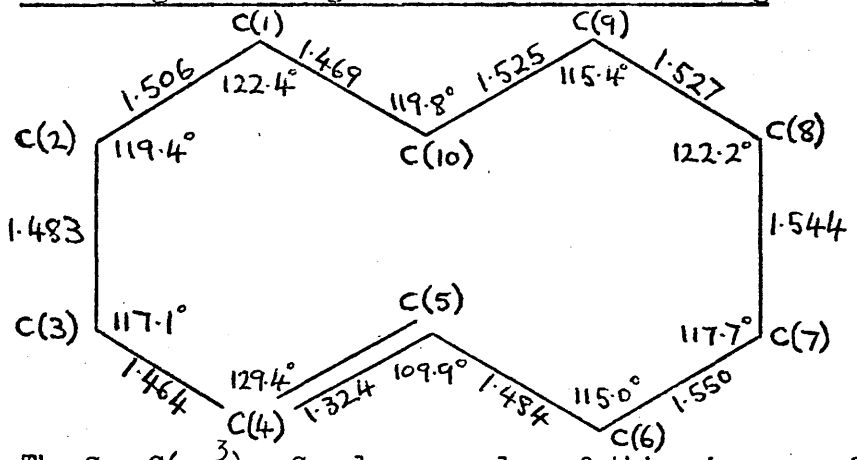
The configuration and stereochemistry of berlandin is that shown above.

The conformation of the 10-membered ring in dihydromikanolide is shown in Figure 1; the unsymmetrical conformation is due to the unsymmetrical substitution of the ring. In this ring there are 2 small torsion angles, i.e. C(1) - C(2) - C(3) - C(4) $\angle -3^{\circ} \rangle$ and C(5) - C(6) - C(7) - C(8) $\angle -2^{\circ} \rangle$. The 2 planes containing these atoms are inclined to each other at 24.4° and the remaining atoms of the ring, C(9) and C(10), both lie below these planes as shown:



As expected the 2 shortest single bonds in this ring are involved with the epoxide linkages.

Bond lengths and angles in the 10-membered ring

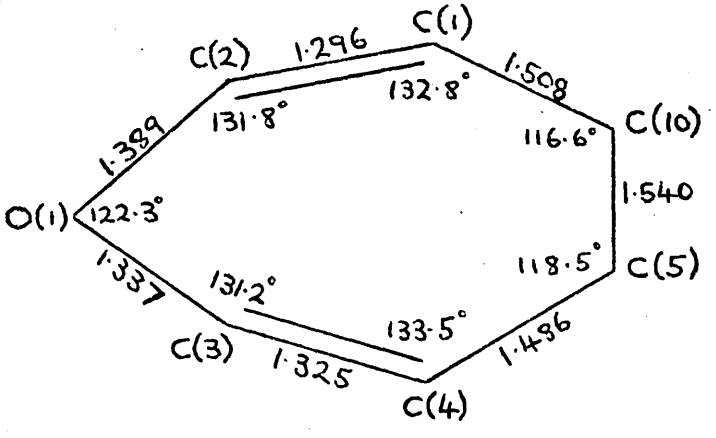


The C - C(sp^3) - C valency angles of this ring vary from 115.4 to 122.4° with a mean of 118.5°; this large deviation from the tetrahedral value indicates a considerable amount of angular strain. There is appreciable angular strain in medium sized saturated carbocycles (including 10-membered rings) and average valency angles of 116 - 117° are common.[11] Eupacunoxin-m-bromobenzoate[12] and eupacunin-o-bromobenzoate[13] contain ring systems of 10 carbon atoms, 4 of which are sp^2 hybridised. In these compounds the average C - C(sp^3) - C valency angles are 113.7° and 113.2° respectively. A similar reduction of angular strain is obtained in the presence of five sp^2 carbon atoms in the cyclodecadiene ring of germacratriene[14]; here the average C - C(sp^3) - C valency angle is 109.2°. The trans double bond, C(4) - C(5), in dihydromikanolide is subject to significant steric strain, the C(3) - C(4) - C(5) - C(6) torsion angle is |163°| which compares well to other trans ethylenic systems

of 10-membered rings: elephantol-p-bromobenzoate[3] ⟨163°⟩, shiromodiol acetate-p-bromobenzoate[15] ⟨167°⟩ and pregeijerene[16] ⟨165°⟩. Since the C(3) - C(4) - C(5) - C(6) torsion angle is 163° and the C(14) - C(4) - C(5) - C(6) torsion angle is 6°, this gives the departure from planar trigonal bonding at C(4) to be 11°. In-plane distortion is also present here with the C(3) - C(4) - C(5) valency angle at 129.4° while at C(4) - C(5) - C(6) the valency angle is 109.9°. The shortest intramolecular contact across the ring is 3.03 Å between C(5) and C(1), also C(5) is separated from O(1) by 2.94 Å, while the remaining transannular contacts are significantly larger than the sum of Van der Waals radii. In the two epoxide rings the valency angles vary from 58.4 to 61.9° and the C - O distances from 1.432 - 1.453 Å, in good agreement with the average values quoted by Sutton et al.[17]

The conformation of the 7-membered cyclic enol ether group in miscandenin is shown in Figure 2.

Bond length and angles in the 7-membered ring of miscandenin



The conformation of the ring may be described as a highly distorted boat form with one apex formed by C(10) [displacement 0.51Å] and the other by O(1) and C(3) [displacements 0.17 and 0.15 Å respectively]. However, the atoms C(1), C(2), C(4) and C(5) lie between -0.04 and 0.06 Å off the plane they describe. The ring is highly strained and the angular strain is shown by the high valency angles at O(1) - C(2) - C(1) [131.8°], C(2) - C(1) - C(10) [132.8°], O(1) - C(3) - C(4) [131.2°] and C(3) - C(4) - C(5) [133.5°]. This gives an average deviation of 12.3° from the expected value of 120°. The torsion angles of the ring show that there is a flattening effect around the O(1) - C(2) and O(1) - C(3) bonds. The torsion angle C(3) - O(1) - C(2) - C(1) is 22° and that of C(2) - O(1) - C(3) - C(4) is -6° while the anisotropic temperature-factor parameters of O(1) are approximately twice as large as those of the other two endocyclic oxygen atoms of the molecule. In fact, the conformation of this ring lies between the two possible boat conformations; one where the apex is O(1) with C(5) and C(10) at the opposite apex and the second where C(10) forms one apex with O(1) and C(3) at the opposite apex. The latter conformation is better described in terms of a fold across the ring between atoms O(1) and C(10) with the two planes of atoms inclined to each other at an obtuse angle. However, C(10) in miscandenin is displaced 0.69 Å below the plane defined by O(1), C(3), C(4) and C(5). It is difficult to envisage steric repulsion of the oxygen as the smallest non-bonded intramolecular separations here are all greater than the normal van der Waals radii, i.e. O(1) - H(9B) [3.30 Å], O(1) - C(5) [3.23 Å] and O(1) - C(10) [3.24 Å]. However, there

may well be repulsion due to transannular π-π overlap:- C(2) - C(3) 2.39 Å, C(2) - C(4) 2.96 Å, C(1) - C(3) 3.00 Å and C(1) - C(4) 3.01 Å are all shorter than the normal van der Waals radii. Trans annular π-π interaction is present in the 10-membered ring of Pregeijerene, here the shortest distances between the carbons of the two trans double bonds are 2.91 and 3.13 Å. The flattening effect observed around the oxygen is such that the double bonds are separated by a greater distance than that for any of the two extreme boat forms.

The cyclohexene ring in miscandenin adopts a distorted chair conformation where the atoms C(6), C(7), C(9) and C(10) define a plane with C(5) displaced by -0.54 Å and C(8) by 0.72 Å.

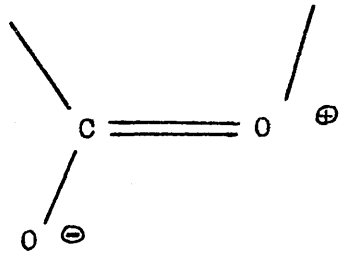
In berlandin the cycloheptene ring contains one double bond and adopts a chair conformation. The out of plane displacements are C(1) /1.11 Å/, C(10) /1.18 Å/ and C(7) /-0.63 Å/. Here the torsion angles of the ring are in good agreement with those calculated for a model of a seven-membered chair.

Torsion angles° for a seven-membered chair

Torsion angle	Theoretical[68]	Berlandin
C(6) -C(7) -C(8) -C(9)	-64	-57
C(5) -C(6) -C(7) -C(8)	+64	64
C(1) -C(5) -C(6) -C(7)	-84	-82
C(10)-C(1) -C(5) -C(6)	66	64
C(5) -C(1) -C(10)-C(9)	0	6
C(1) -C(10)-C(9) -C(8)	-66	-73
C(7) -C(8) -C(9) -C(10)	84	76

Similar atomic displacements for cycloheptene chair conformations have been found for desacetyldihydrogaillardin-p-bromobenzoate[19] and 3 β-methoxy-21-keto-Δ^{13}-serratene.[20] The five membered carbocyclic ring in berlandin adopts a flattened envelope conformation ∠C(1) is displaced by 0.28 Å, with the largest torsion angle at 18° compared to 46° for a theoretical envelope. The flattened conformation of this ring is due to the presence of the epoxide linkage and the exocyclic double bond.

Each of the three sesquiterpenes contain γ-lactone rings which adopt various conformations. The rings all show a small contribution (~10%)[21] from the structure:



the resonance form which is also present in carboxylic acids and esters. The exocyclic carbon-oxygen bond lengths have values ranging from 1.193 - 1.206 Å and the adjacent endocyclic carbon-oxygen bonds range from 1.337 - 1.365 Å. These may be compared with the average values[17] of 1.233 and 1.358 Å found for the shorter and longer bonds in carboxylic acids and esters. The asymmetry of the two endocyclic carbon-oxygen bonds is partly due to the small contribution from the resonance form and partly due to the smaller covalent radius of the sp^2 hybridised carbon compared with the sp^3 carbon atom. The exocyclic valency angles

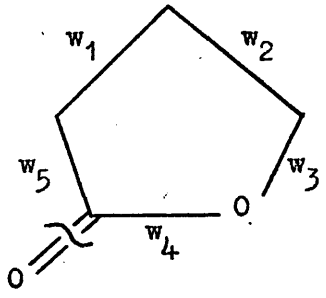
around C(12) [or C(14)] are larger than the internal angle here and these two angles differ by 6.9° - 10.5°. In some acyl groupings these angles have similar values [Table 4], although, generally the difference between the O - C = O and O = C - R' valency angle is not so large. Also the smaller R - C - O angle found in the γ-lactone rings is due to the strain of ring closure.

The above mentioned features of these γ-lactone rings are commonly found in many compounds[22] containing such rings.

The conformations of the γ-lactone rings are varied and are shown by the torsion angles (Table 5).

Table 5

The torsion angles of the γ-lactone rings



Compound	w_1	w_2	w_3	w_4	w_5
Miscandenin α,γ-fused lactone	27	-32	27	-10	-13
Miscandenin γ,β-fused lactone	-36	40	-30	7	19
Dihydromikanolide α,γ-fused lactone	6	-5	2	2	-5
Dihydromikanolide γ,β-fused lactone	-31	31	-20	0	20
Berlandin γ,β-fused lactone	34	-41	35	-14	-14

TABLE 4

The angles around C(12) [or C(14)] in the γ-lactone rings

Compound	Angle° R - C - O	Angle° O - C = O	Angle° O = C - R'
Miscandenin α,γ-lactone	108.8(3)	120.3(4)	130.8(4)
Miscandenin γ,β-lactone	108.3(3)	121.1(4)	130.6(4)
Dihydromikanolide α,γ-lactone	107.5(4)	122.8(4)	129.7(4)
Dihydromikanolide γ,β-lactone	110.0(3)	121.5(3)	128.4(3)
Berlandin γ,β-lactone	108.4(4)	121.8(3)	129.7(5)

Similar angles in some compounds containing acyl groups

Compound	Angle° R - C - O	Angle° O - C = O	Angle° O = C - R'
Bromolythranine hydrobromide[23]	113(2)	122(2)	125(2)
Procaine hydrochloride[24]	112.9(3)	121.0(3)	126.2(3)
Berlandin	111.5(6)	124.9(4)	123.6(4)
Berlandin	108.3(4)	123.2(3)	128.5(5)
Fusidic acid intermediate[25]	111(0.5)	124(0.5)	125(0.5)
Desacetyl dihydrogaillardin[19]	117(1)	119(1)	124(1)
3β-p-bromobenzoyloxy-androst-5-en-17-one[26]	110.5(5)	125.0(5)	124.5(5)
Solaphyllidine[27]	109.9(7)	119.7(7)	130.4(7)

For a theoretical envelope conformation the magnitudes of the torsion angles are such that:

$$w_1 = -w_2 > w_3 = -w_5 > w_4 = 0$$

and for the half-chair conformation:

$$w_2 > w_1 = w_3 > w_4 = w_5$$

The α,γ-cis-fused lactone in miscandenin has a slightly distorted half-chair conformation; a mean plane described by atoms O(3), C(4) and C(14) shows that C(5) is displaced by 0.31 Å and C(6) by -0.23 Å. It can be seen from a Dreiding model that if the seven-membered ring were to adopt the extreme boat conformation with O(1) and C(3) at one apex and C(10) at the other, the γ-lactone ring would adopt the envelope conformation. The flattening effect around the oxygen of this seven-membered ring causes the α,γ-fused lactone to pucker. The γ,β trans-fused lactone in this molecule adopts a highly distorted half-chair conformation with C(7) displaced by -0.47 Å and C(8) by 0.18 Å from the plane defined by O(5), C(11) and C(12). This conformation is closer to the preferred envelope form than that of the α,γ-fused lactone in this compound.

In dihydromikanolide the unsaturated α,γ-cis-fused lactone is almost planar with the largest torsion angle at 6°. A mean plane through this ring gives the atom displacements as O(3) [0.00], C(4) [-0.03], C(5) [0.03], C(6) [-0.02], and C(14) [0.02]. The β,γ-trans-fused lactone in this molecule adopts an almost perfect envelope conformation; here C(7) is displaced by 0.52 Å from the

plane described by O(5), C(8), C(11) and C(12). This is the only fully saturated γ-lactone in the three sesquiterpenes and the only one to adopt the preferred conformation.

In berlandin the γ,β trans-fused lactone has adopted a half-chair conformation with C(7) displaced by -0.35 Å and C(6) by 0.33 Å from the plane described by O(2), C(11) and C(12). Both this lactone group and the γ,β trans-fused lactone in miscandenin have an exocyclic methylene group and the sum of the moduli of the endocyclic torsion angles exceeds, in both cases, the values obtained for the other γ-lactones in these compounds. The presence of an exocyclic double bond on a γ-lactone normally has the effect of flattening the ring by increasing the conjugation of the system. However, this is not the case in these two sesquiterpenes and the conformation of these rings must therefore be affected by the ring system to which they are fused. Also there are no short, non-bonded, intramolecular contacts (which would indicate steric hinderance) around the γ-lactone systems. γ-lactone rings with exocyclic methylene groups are known to adopt various conformations, e.g. in bromomexicanin-E[28], mondoromogaillardin[29] and elephantol-p-bromobenzoate[3] envelope conformations are found; in euparotin bromoacetate[3] the γ-lactone ring has a flat conformation and in vernolepin-p-bromobenzene sulphonate[30] the γ-lactone ring conformation is a half-chair.

The average bond lengths (Å) found in the acetyl side chains of berlandin are compared to the accepted values below:

Table 6

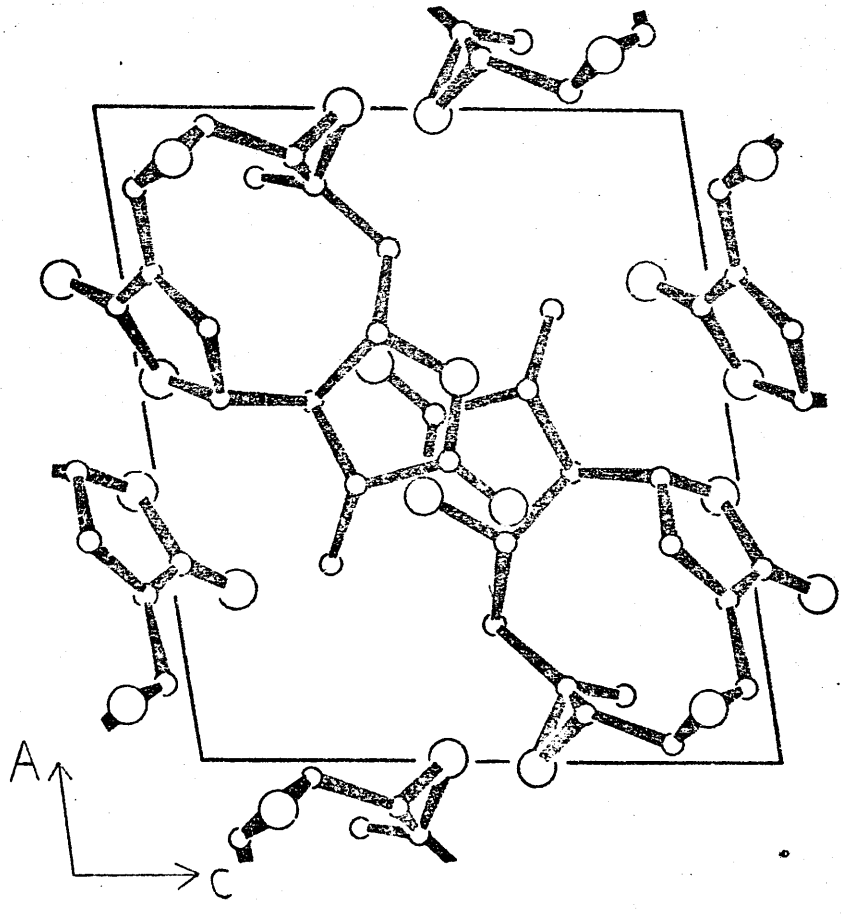
Bond		Berlandin	Accepted value[17]
$C(sp^3)$ - $C(sp^2)$	single bond	1.494	1.510
$C(sp^2)$ - $C(sp^2)$	single bond*	1.528	1.465
$C(sp^2)$ - $C(sp^2)$	double bond*	1.321	1.335
$C(sp^3)$ - O	single bond	1.454	1.426
$C(sp^2)$ - O	single bond	1.344	1.358
$C(sp^2)$ - O	double bond	1.195	1.233

* single values

The C(20) - C(22) bond in the longer acetyl side chain is only 1.454 Å and the methyl hydrogens at C(22) have not been found. This bond length is shorter than the corresponding C(16) - C(17) bond [1.502 Å] in the smaller acetyl side chain, the methyl hydrogens at C(17) have also been clearly located. Either the protons at C(22) are in free rotation or the position of this carbon must be poorly defined.

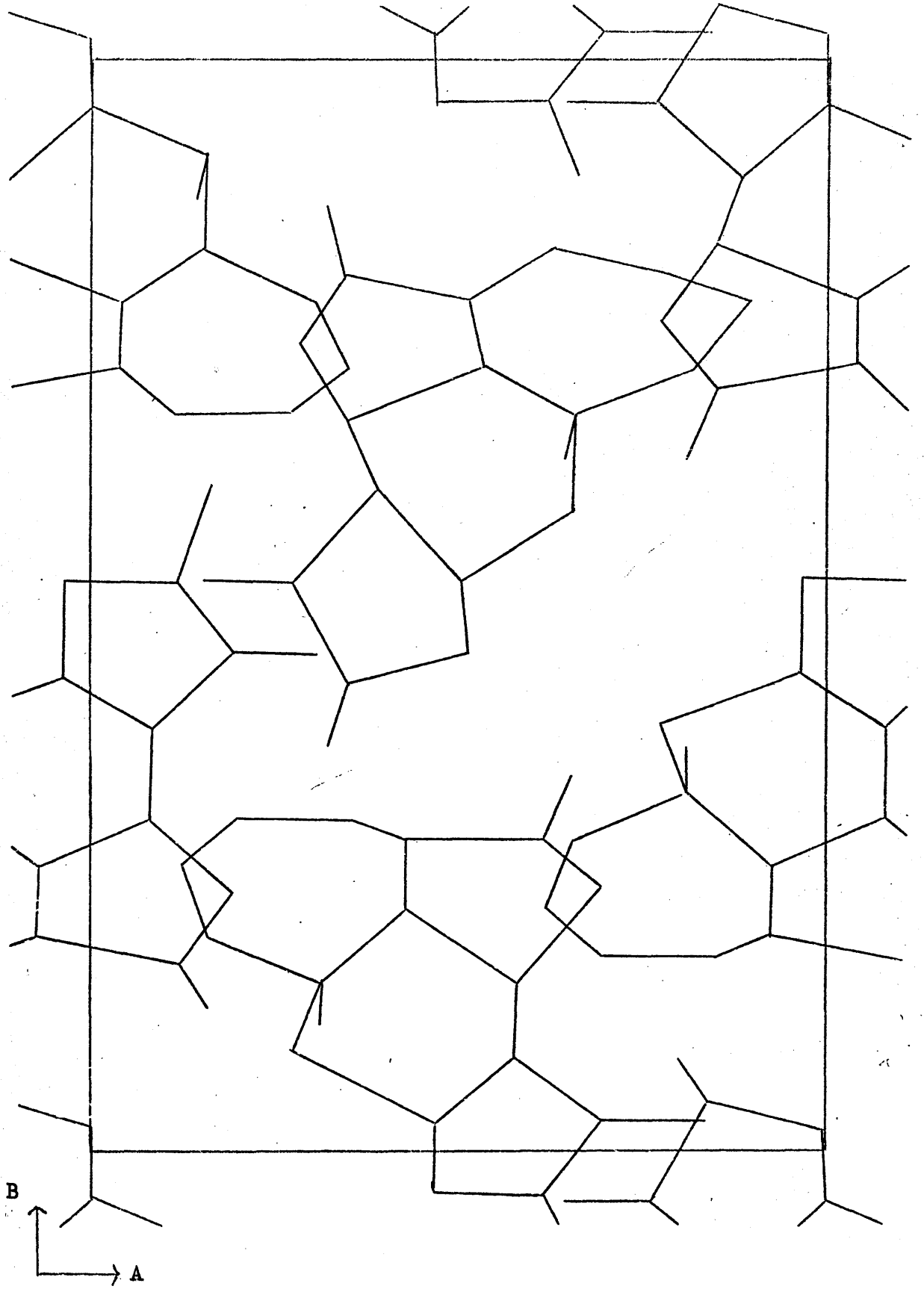
There are no intermolecular contacts in the three sesquiterpenes which are less than the accepted sums of van der Waals radii.

Fig. 4



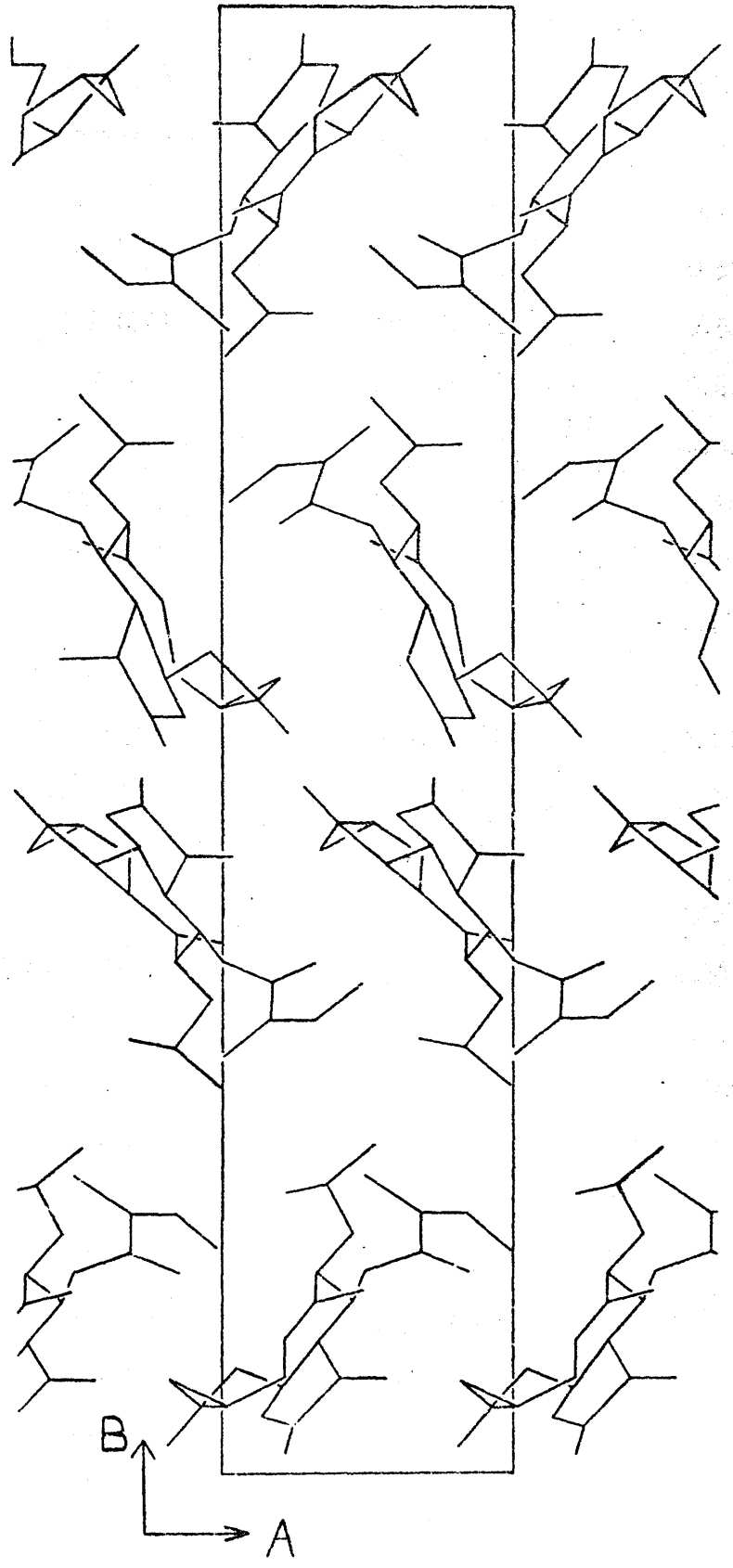
The packing of the molecules of Dihydromikanolide in the crystal, viewed down the b axis.

Fig. 5



The packing of the molecules of Miscandenin in the crystal, viewed down the c axis.

Fig. 6



The packing of the molecules of Berlandin in the crystal, viewed down the c axis.

Table 7

Dihydromikanolide

Fractional Atomic co-ordinates and positional standard deviations.

Atom	x	y	z
O(1)	0.9146(4)	0.7570	0.1139(4)
O(2)	0.7381(4)	0.2414(8)	-0.1061(4)
O(3)	0.5881(3)	0.2932(7)	0.0359(3)
O(4)	0.3918(3)	0.3820(7)	0.5958(3)
O(5)	0.5921(3)	0.3992(7)	0.5465(3)
O(6)	1.0095(3)	0.4180(9)	0.4259(3)
C(1)	0.9263(4)	0.5379(8)	0.3255(4)
C(2)	0.9723(4)	0.5876(9)	0.1844(5)
C(3)	0.8795(4)	0.5805(9)	0.0440(5)
C(4)	0.7475(4)	0.5164(8)	0.0504(4)
C(5)	0.6635(4)	0.5807(7)	0.1308(4)
C(6)	0.5592(4)	0.4402(8)	0.1348(4)
C(7)	0.5538(3)	0.3567(7)	0.2886(4)
C(8)	0.6578(4)	0.4215(7)	0.4182(4)
C(9)	0.7871(4)	0.3192(8)	0.4607(4)
C(10)	0.8842(3)	0.3474(8)	0.3565(4)
C(11)	0.4273(4)	0.4137(8)	0.3413(4)
C(12)	0.4631(4)	0.3944(7)	0.5063(4)
C(13)	0.3048(4)	0.3098(9)	0.2746(5)
C(14)	0.6975(4)	0.3363(9)	-0.0175(4)
C(15)	0.8957(5)	0.1856(8)	0.2557(5)
H(1)	0.8905(52)	0.6311(98)	0.3674(63)
H(2)	1.0637(47)	0.5877(90)	0.1824(58)
H(3)	0.9131(67)	0.5520(118)	-0.0478(74)

Table 7

Fractional Atomic co-ordinates and positional standard deviations (cont.)

Atom	x	y	z
H(5)	0.6807(50)	0.7105(82)	0.1796(59)
H(6)	0.4692(38)	0.4792(65)	0.1017(44)
H(7)	0.5537(35)	0.2270(58)	0.2848(41)
H(8)	0.6750(39)	0.5610(66)	0.4173(45)
H(9A)	0.7724(49)	0.1851(83)	0.4737(56)
H(9B)	0.8387(54)	0.3539(90)	0.5720(63)
H(11)	0.4083(36)	0.5599(59)	0.3193(41)
H(13A)	0.2387(44)	0.3145(83)	0.3232(52)
H(13B)	0.3293(54)	0.1801(89)	0.2759(59)
H(13C)	0.2714(68)	0.3630(149)	0.1524(85)
H(15A)	0.8085(46)	0.1530(86)	0.1970(54)
H(15B)	0.9468(47)	0.2122(78)	0.1912(54)
H(15C)	0.9394(64)	0.0877(116)	0.3170(77)

Table 8

Dihydromikanolide

Anisotropic thermal parameters for the oxygen and carbon atoms ($\times 10^4$).

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
O(1)	162(4)	190(8)	179(5)	-89(10)	101(8)	44(10)
O(2)	156(4)	323(10)	117(4)	5(11)	83(7)	-127(11)
O(3)	105(3)	245(8)	84(3)	-61(8)	25(5)	-75(8)
O(4)	129(3)	180(6)	124(3)	-13(8)	113(6)	-3(8)
O(5)	100(3)	207(6)	87(3)	-14(8)	50(4)	7(8)
O(6)	79(3)	326(10)	136(4)	-43(9)	-24(5)	6(11)
C(1)	81(4)	195(9)	118(5)	-60(9)	8(7)	-43(11)
C(2)	85(4)	206(9)	147(6)	-43(11)	65(7)	-5(13)
C(3)	109(4)	201(10)	126(5)	-26(11)	97(8)	34(12)
C(4)	90(4)	175(8)	86(4)	0(9)	40(6)	29(10)
C(5)	94(3)	141(7)	95(4)	34(9)	46(6)	42(9)
C(6)	73(3)	183(9)	84(4)	30(8)	9(5)	20(9)
C(7)	72(3)	122(6)	82(3)	20(7)	29(5)	12(7)
C(8)	80(3)	138(6)	79(3)	-10(8)	31(5)	17(9)
C(9)	81(3)	171(8)	105(4)	2(9)	2(6)	53(10)
C(10)	69(3)	169(8)	99(4)	23(8)	-14(6)	-11(9)
C(11)	82(3)	171(8)	98(4)	2(9)	57(6)	-10(10)
C(12)	106(4)	109(6)	100(4)	1(8)	66(7)	-19(9)
C(13)	77(3)	241(10)	130(5)	-20(10)	33(7)	7(14)
C(14)	94(4)	231(10)	82(4)	19(10)	18(6)	-30(11)
C(15)	147(6)	160(9)	135(6)	98(12)	35(10)	-20(12)

Anisotropic temperature factors were employed in the form:

$$T = \exp[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)]$$

Table 8 (cont.)

Isotropic thermal parameters for the hydrogen atoms

H(1)	4.37	H(9B)	4.08
H(2)	2.17	H(11)	1.00
H(3)	5.55	H(13A)	2.63
H(5)	3.30	H(13B)	4.10
H(6)	1.34	H(13C)	4.90
H(7)	1.30	H(15A)	1.87
H(8)	1.33	H(15B)	2.21
H(9A)	2.02	H(15C)	7.41

The average standard deviation of the isotropic temperature factors is 0.9$\mathring{A}^2$.

Table 9

Miscandenin

Fractional Atomic co-ordinates and positional standard deviations

Atom	x	y	z
O(1)	0.80691(67)	0.81798(35)	0.12059(62)
O(2)	0.31932(64)	0.86216(26)	0.09616(50)
O(3)	0.28934(35)	0.74523(22)	0.22851(36)
O(4)	0.31964(48)	0.39753(23)	0.03201(36)
O(5)	0.51922(38)	0.46469(20)	0.13114(33)
C(1)	0.84051(65)	0.71345(42)	0.30357(72)
C(2)	0.88477(75)	0.77471(52)	0.22169(97)
C(3)	0.65157(78)	0.82289(40)	0.11549(59)
C(4)	0.54272(59)	0.78606(27)	0.19011(48)
C(5)	0.54743(46)	0.72378(26)	0.30364(40)
C(6)	0.38875(49)	0.67640(29)	0.28538(43)
C(7)	0.40627(45)	0.60114(26)	0.18625(42)
C(8)	0.53643(47)	0.53794(24)	0.22466(42)
C(9)	0.69204(51)	0.58387(31)	0.21985(50)
C(10)	0.69026(54)	0.66231(32)	0.31985(48)
C(11)	0.28132(57)	0.53454(29)	0.15761(44)
C(12)	0.36571(57)	0.45764(31)	0.09867(46)
C(13)	0.12955(57)	0.53387(40)	0.18083(75)
C(14)	0.37886(61)	0.80445(32)	0.16145(53)
C(15)	0.68305(79)	0.62457(41)	0.46239(60)
H(1)	0.9195 (56)	0.6923 (39)	0.3722 (51)
H(2)	0.9747 (86)	0.8037 (44)	0.2186 (58)
H(3)	0.6047 (60)	0.8563 (31)	0.0465 (44)
H(5)	0.5333 (35)	0.7610 (20)	0.3928 (29)

Table 9

Fractional Atomic co-ordinates and positional standard deviations (cont.)

H(6)	0.3433(36)	0.6565(22)	0.3706(31)
H(7)	0.4463(41)	0.6259(24)	0.1002(34)
H(8)	0.5105(44)	0.5076(22)	0.3132(34)
H(9A)	0.7717(44)	0.5410(26)	0.2366(37)
H(9B)	0.7109(59)	0.6041(29)	0.1306(41)
H(13A)	0.0664(42)	0.4796(24)	0.1559(36)
H(13B)	0.0819(43)	0.5811(29)	0.2257(38)
H(15A)	0.7826(67)	0.5809(39)	0.4618(51)
H(15B)	0.5674(64)	0.6009(32)	0.4737(51)
H(15C)	0.7132(59)	0.6784(32)	0.5090(47)

Table 10

Miscandenin

Anisotropic thermal parameters for the oxygen and carbon atoms ($\times 10^4$)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
O(1)	213(9)	76(3)	249(8)	-75(9)	235(16)	- 6(9)
O(2)	320(10)	45(2)	200(6)	39(8)	-247(14)	- 4(6)
O(3)	109(5)	39(2)	163(4)	37(5)	- 22(8)	-22(5)
O(4)	226(7)	48(2)	124(4)	-25(6)	- 81(10)	-41(5)
O(5)	125(5)	38(1)	118(4)	8(5)	4(7)	-19(4)
C(1)	110(8)	70(4)	185(9)	- 1(8)	- 48(13)	-90(10)
C(2)	140(10)	66(4)	270(14)	-60(10)	107(22)	-115(14)
C(3)	231(13)	53(3)	134(7)	-48(10)	84(15)	- 9(8)
C(4)	151(8)	31(2)	96(5)	-19(6)	21(11)	- 7(5)
C(5)	89(5)	37(2)	73(5)	3(6)	2(9)	-16(5)
C(6)	96(6)	35(2)	89(5)	3(6)	13(9)	2(5)
C(7)	86(6)	31(2)	85(4)	8(5)	9(9)	6(5)
C(8)	93(6)	35(2)	86(5)	14(6)	- 10(9)	- 5(5)
C(9)	92(6)	40(2)	145(7)	31(6)	- 11(12)	-17(7)
C(10)	107(7)	47(2)	107(5)	20(7)	- 53(11)	-16(6)
C(11)	127(7)	36(2)	99(5)	- 3(7)	- 54(10)	6(6)
C(12)	149(8)	36(2)	88(5)	-11(7)	- 38(10)	15(6)
C(13)	87(7)	63(3)	219(9)	-32(8)	13(13)	-26(11)
C(14)	150(8)	30(2)	129(6)	19(8)	- 89(12)	-17(7)
C(15)	245(12)	69(3)	124(7)	45(11)	-185(17)	- 4(8)

Table 10 (cont.)

Isotropic thermal parameters for the hydrogen atoms

H(1)	4.17	H(9A)	1.73
H(2)	6.75	H(9B)	3.01
H(3)	3.20	H(13A)	1.37
H(5)	1.11	H(13B)	1.96
H(6)	1.23	H(15A)	5.02
H(7)	1.13	H(15B)	4.68
H(8)	1.27	H(15C)	4.08

The average standard deviation of the isotropic temperature factors is 0.9 $\mathring{A}^2$.

Table 11

Berlandin

Fractional Atomic co-ordinates and positional standard deviations

Atom	x	y	z
O(1)	-0.1943(10)	0.0682(1)	1.2652(7)
O(2)	0.1091(7)	0.0408(1)	0.8386(5)
O(3)	0.2134(10)	0.0177(1)	0.6182(5)
O(4)	0.4768(8)	0.1493(1)	0.7862(5)
O(5)	0.8292(8)	0.1485(1)	0.8255(6)
O(6)	0.4473(9)	0.1782(1)	1.0524(5)
O(7)	0.1679(11)	0.2051(1)	1.1586(8)
C(1)	0.1864(11)	0.0952(1)	1.1881(7)
C(2)	0.1851(15)	0.0693(2)	1.3193(8)
C(3)	-0.0024(13)	0.0464(2)	1.2926(9)
C(4)	-0.0895(10)	0.0517(2)	1.1385(9)
C(5)	0.0513(10)	0.0804(1)	1.0638(7)
C(6)	0.2038(11)	0.0660(1)	0.9481(7)
C(7)	0.2959(9)	0.0951(1)	0.8428(6)
C(8)	0.4355(10)	0.1242(1)	0.9094(6)
C(9)	0.3291(10)	0.1453(1)	1.0319(7)
C(10)	0.3205(11)	0.1232(2)	1.1763(6)
C(11)	0.3852(11)	0.0716(1)	0.7208(7)
C(12)	0.2345(12)	0.0402(2)	0.7134(8)
C(13)	0.5581(14)	0.0733(2)	0.6406(8)
C(14)	-0.2162(14)	0.0245(2)	1.0527(10)
C(15)	0.4766(16)	0.1335(2)	1.2941(8)
C(16)	0.3478(14)	0.2056(2)	1.1177(9)
C(17)	0.4938(17)	0.2371(2)	1.1409(10)

Table 11

Fractional Atomic co-ordinates and positional standard deviations (cont.)

Atom	x	y	z
C(18)	0.6790(13)	0.1602(2)	0.7595(7)
C(19)	0.6746(15)	0.1883(2)	0.6345(8)
C(20)	0.8212(20)	0.1859(3)	0.5296(10)
C(21)	0.5015(17)	0.2170(2)	0.6426(12)
C(22)	0.9855(18)	0.1586(3)	0.5136(11)
H(2A)	0.1691(100)	0.0836(14)	1.4079(62)
H(2B)	0.3250(92)	0.0538(13)	1.3188(56)
H(3)	-0.0210(88)	0.0213(12)	1.3523(56)
H(5)	-0.0650(107)	0.0973(15)	1.0389(66)
H(6)	0.3119(95)	0.0507(13)	1.0096(54)
H(7)	0.1723(87)	0.1107(12)	0.7893(55)
H(8)	0.5736(101)	0.1131(14)	0.9593(63)
H(9)	0.1698(90)	0.1542(12)	1.0036(52)
H(13A)	0.6297(98)	0.0558(14)	0.5842(60)
H(13B)	0.6745(90)	0.0952(13)	0.6373(56)
H(14A)	-0.3345(105)	0.0392(14)	0.9521(63)
H(14B)	-0.1110(90)	0.0013(13)	0.9702(56)
H(14C)	-0.3421(129)	0.0127(17)	1.1103(79)
H(15A)	0.5690(132)	0.1550(19)	1.3012(81)
H(15B)	0.3585(132)	0.1640(19)	1.3773(83)
H(15C)	0.4960(125)	0.1189(19)	1.3580(80)
H(17A)	0.4028(133)	0.2616(19)	1.1593(85)
H(17B)	0.5991(140)	0.2333(21)	1.1481(91)
H(17C)	0.5228(154)	0.2435(22)	1.0177(103)

Table 11

Fractional Atomic co-ordinates and positional standard deviations (cont.)

Atom	x	y	z
H(20)	0.8095(129)	0.2020(18)	0.4249(82)
H(21A)	0.3606(138)	0.2086(19)	0.6802(94)
H(21B)	0.5348(152)	0.2335(21)	0.6984(99)
H(21C)	0.4301(146)	0.2214(20)	0.5584(97)

Table 12

Berlandin

Anisotropic thermal parameters for the oxygen and carbon atoms ($\times 10^4$)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
O(1)	410(19)	11(0)	268(11)	5(5)	367(26)	2(4)
O(2)	247(12)	8(0)	145(6)	-16(3)	-17(16)	2(2)
O(3)	513(22)	9(0)	160(7)	-24(5)	-60(24)	-14(3)
O(4)	298(14)	7(0)	126(6)	-11(4)	-35(16)	14(2)
O(5)	228(13)	15(1)	206(9)	-6(5)	-17(20)	38(4)
O(6)	401(17)	7(0)	166(7)	-18(4)	69(21)	-9(3)
O(7)	542(24)	9(0)	304(13)	21(6)	222(34)	-19(4)
C(1)	262(18)	6(0)	130(8)	16(5)	57(23)	4(3)
C(2)	495(31)	8(1)	126(9)	6(7)	90(32)	4(4)
C(3)	333(23)	8(1)	186(12)	12(6)	195(30)	15(4)
C(4)	196(16)	8(0)	229(13)	14(5)	131(27)	13(5)
C(5)	220(17)	6(0)	163(9)	12(5)	29(23)	16(4)
C(6)	287(19)	6(0)	120(8)	-12(5)	-13(24)	6(3)
C(7)	197(15)	6(0)	120(8)	-3(4)	-27(20)	7(3)
C(8)	218(16)	6(0)	112(7)	-6(4)	-25(20)	7(3)
C(9)	226(16)	6(0)	135(8)	-7(5)	-22(21)	0(3)
C(10)	305(19)	7(0)	100(7)	15(5)	3(22)	-1(3)
C(11)	304(20)	7(0)	108(8)	-3(5)	-70(23)	3(3)
C(12)	334(23)	7(0)	147(10)	-6(6)	-102(27)	8(4)
C(13)	460(29)	9(1)	169(11)	-6(7)	194(34)	-13(4)
C(14)	367(28)	9(1)	265(15)	-43(7)	27(38)	20(5)
C(15)	570(36)	8(0)	167(11)	1(8)	-232(38)	-1(4)
C(16)	374(25)	7(0)	177(12)	0(6)	8(32)	2(4)

Table 12

Anisotropic thermal parameters for the oxygen and carbon atoms (x 10^4) (cont.)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
C(17)	608(39)	9(1)	275(16)	-37(9)	5(49)	-23(5)
C(18)	382(24)	7(0)	117(9)	-31(6)	38(27)	4(3)
C(19)	498(31)	10(1)	139(10)	-80(8)	-35(34)	2(4)
C(20)	633(43)	15(1)	168(13)	-113(11)	-19(45)	4(6)
C(21)	720(42)	7(1)	348(22)	-33(9)	-456(57)	45(6)
C(22)	508(40)	19(1)	237(17)	-1(12)	226(47)	-20(8)

Anisotropic temperature factors were employed in the form:

$$T = \exp[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)]$$

Table 12 (cont.)

Isotropic thermal parameters for the hydrogen atoms

H(2A)	2.31	H(14C)	5.03
H(2B)	1.43	H(15A)	4.84
H(3)	1.40	H(15B)	8.11
H(5)	3.30	H(15C)	7.62
H(6)	1.38	H(17A)	5.99
H(7)	1.22	H(17B)	6.51
H(8)	2.51	H(17C)	7.35
H(9)	1.06	H(20)	5.36
H(13A)	2.18	H(21A)	5.74
H(13B)	1.41	H(21B)	7.43
H(14A)	2.42	H(21C)	6.30
H(14B)	1.34		

The methyl hydrogens at C(15) were not located.

The average standard deviation of the isotropic temperature factors is 1.8Å^2.

Table 13

Dihydromikanolide

Intramolecular bonded distances and estimated standard deviations (Å).

O(1)	-	C(2)	1.453(6)	C(9)	-	C(10)	1.525(6)
O(1)	-	C(3)	1.432(6)	C(10)	-	C(15)	1.499(7)
O(2)	-	C(14)	1.193(7)	C(11)	-	C(12)	1.512(5)
O(3)	-	C(6)	1.454(6)	C(11)	-	C(13)	1.516(7)
O(3)	-	C(14)	1.355(6)	C(1)	-	H(1)	0.88(9)
O(4)	-	C(12)	1.206(6)	C(2)	-	H(2)	0.96(5)
O(5)	-	C(8)	1.475(5)	C(3)	-	H(3)	0.99(7)
O(5)	-	C(12)	1.337(6)	C(5)	-	H(5)	1.00(6)
O(6)	-	C(1)	1.439(7)	C(6)	-	H(6)	0.97(5)
O(6)	-	C(10)	1.447(6)	C(7)	-	H(7)	0.92(3)
C(1)	-	C(2)	1.506(6)	C(8)	-	H(8)	0.99(4)
C(1)	-	C(10)	1.469(8)	C(9)	-	H(9A)	0.98(5)
C(2)	-	C(3)	1.483(7)	C(9)	-	H(9B)	1.11(6)
C(3)	-	C(4)	1.464(7)	C(11)	-	H(11)	1.07(4)
C(4)	-	C(5)	1.324(6)	C(13)	-	H(13A)	0.90(5)
C(4)	-	C(14)	1.483(8)	C(13)	-	H(13B)	0.97(7)
C(5)	-	C(6)	1.484(7)	C(13)	-	H(13C)	1.15(7)
C(6)	-	C(7)	1.550(5)	C(15)	-	H(15A)	1.00(5)
C(7)	-	C(8)	1.544(5)	C(15)	-	H(15B)	0.91(5)
C(7)	-	C(11)	1.539(6)	C(15)	-	H(15C)	0.98(8)
C(8)	-	C(9)	1.527(6)				

Table 14

Dihydromikanolide

Valency angles (degrees) and estimated standard deviations.

C(3)	-	O(1)	-	C(2)	61.9(3)
C(1)	-	C(2)	-	C(1)	114.4(3)
C(3)	-	C(2)	-	O(1)	58.4(3)
C(2)	-	C(3)	-	O(1)	59.7(3)
C(4)	-	C(3)	-	O(1)	115.3(4)
O(3)	-	C(14)	-	O(2)	122.8(4)
C(4)	-	C(14)	-	O(2)	129.7(4)
C(14)	-	O(3)	-	C(6)	110.1(3)
C(5)	-	C(6)	-	O(3)	103.8(3)
C(7)	-	C(6)	-	O(3)	110.0(3)
C(4)	-	C(14)	-	O(3)	107.5(4)
O(5)	-	C(12)	-	O(4)	121.5(3)
C(11)	-	C(12)	-	O(4)	128.4(3)
C(12)	-	O(5)	-	C(8)	111.4(2)
C(7)	-	C(8)	-	O(5)	103.2(2)
C(9)	-	C(8)	-	O(5)	104.8(3)
C(11)	-	C(12)	-	O(5)	110.0(3)
C(10)	-	O(6)	-	C(1)	61.2(3)
C(2)	-	C(1)	-	O(6)	116.7(3)
C(10)	-	C(1)	-	O(6)	59.7(3)
C(1)	-	C(10)	-	O(6)	59.1(4)
C(9)	-	C(10)	-	O(6)	114.5(3)
C(15)	-	C(10)	-	O(6)	112.4(3)
C(10)	-	C(1)	-	C(2)	122.4(4)
C(3)	-	C(2)	-	C(1)	119.4(3)

Table 14

Valency angles (degrees) and estimated standard deviations (cont.).

C(9)	-	C(10)	-	C(1)	119.8(3)
C(15)	-	C(10)	-	C(1)	122.1(3)
C(4)	-	C(3)	-	C(2)	117.1(3)
C(5)	-	C(4)	-	C(3)	129.4(3)
C(14)	-	C(4)	-	C(3)	121.3(4)
C(14)	-	C(4)	-	C(5)	108.5(4)
C(6)	-	C(5)	-	C(4)	109.9(4)
C(7)	-	C(6)	-	C(5)	115.0(3)
C(8)	-	C(7)	-	C(6)	117.7(3)
C(11)	-	C(7)	-	C(6)	110.8(3)
C(11)	-	C(7)	-	C(8)	101.9(3)
C(9)	-	C(8)	-	C(7)	122.2(3)
C(12)	-	C(11)	-	C(7)	102.4(3)
C(13)	-	C(11)	-	C(7)	117.0(3)
C(10)	-	C(9)	-	C(8)	115.4(3)
C(15)	-	C(10)	-	C(9)	115.0(4)
C(13)	-	C(11)	-	C(12)	114.4(3)

The average O - $C(sp^3)$ - H valency angle is 111°

The average H - $C(sp^3)$ - H valency angle is 108°

The average H - $C(sp^3)$ - $C(sp^3)$ valency angle is 110°

Table 15

Miscandenin

Intramolecular bonded distances and estimated standard deviations (Å)

O(1)	-	C(2)	1.389(11)	C(9)	-	C(10)	1.553(7)
O(1)	-	C(3)	1.337(9)	C(10)	-	C(15)	1.562(8)
O(2)	-	C(14)	1.203(7)	C(11)	-	C(12)	1.484(7)
O(3)	-	C(6)	1.456(5)	C(11)	-	C(13)	1.324(7)
O(3)	-	C(14)	1.356(6)	C(1)	-	H(1)	1.02(5)
O(4)	-	C(12)	1.193(6)	C(2)	-	H(2)	0.89(7)
O(5)	-	C(8)	1.459(5)	C(3)	-	H(3)	0.95(5)
O(5)	-	C(12)	1.363(6)	C(5)	-	H(5)	1.07(3)
C(1)	-	C(2)	1.296(11)	C(6)	-	H(6)	1.00(3)
C(1)	-	C(10)	1.508(7)	C(7)	-	H(7)	1.01(4)
C(3)	-	C(4)	1.325(8)	C(8)	-	H(8)	1.04(4)
C(4)	-	C(5)	1.486(6)	C(9)	-	H(9A)	0.95(4)
C(4)	-	C(14)	1.463(7)	C(9)	-	H(9B)	0.97(4)
C(5)	-	C(6)	1.546(6)	C(13)	-	H(13A)	1.01(4)
C(5)	-	C(10)	1.540(6)	C(13)	-	H(13B)	0.94(4)
C(6)	-	C(7)	1.519(6)	C(15)	-	H(15A)	1.08(6)
C(7)	-	C(8)	1.514(6)	C(15)	-	H(15B)	1.06(6)
C(7)	-	C(11)	1.491(6)	C(15)	-	H(15C)	0.97(5)
C(8)	-	C(9)	1.502(6)				

Table 16

Miscandenin

Valency Angles (degrees) and estimated standard deviations (degrees)

C(3)	-	O(1)	-	C(2)	122.3(5)
C(4)	-	C(3)	-	O(1)	131.2(4)
C(4)	-	C(14)	-	O(2)	130.8(4)
C(5)	-	C(6)	-	O(3)	104.0(3)
O(5)	-	C(12)	-	O(4)	121.1(4)
C(12)	-	O(5)	-	C(8)	108.4(3)
C(7)	-	C(8)	-	O(5)	102.8(3)
C(5)	-	C(10)	-	C(1)	111.6(3)
C(15)	-	C(10)	-	C(1)	108.6(4)
C(14)	-	C(4)	-	C(3)	119.0(4)
C(10)	-	C(5)	-	C(4)	118.5(3)
C(9)	-	C(10)	-	C(5)	112.7(3)
C(8)	-	C(7)	-	C(6)	111.1(3)
C(13)	-	C(11)	-	C(7)	132.7(3)
C(1)	-	C(2)	-	O(1)	131.8(4)
O(3)	-	C(14)	-	O(2)	120.3(4)
C(14)	-	O(3)	-	C(6)	109.2(3)
C(7)	-	C(6)	-	O(3)	108.3(3)
C(4)	-	C(14)	-	O(3)	108.8(3)
C(11)	-	C(12)	-	O(4)	130.6(4)
C(9)	-	C(8)	-	O(5)	114.2(3)
C(11)	-	C(12)	-	O(5)	108.3(3)
C(10)	-	C(1)	-	C(2)	132.8(5)
C(9)	-	C(10)	-	C(1)	107.5(4)
C(5)	-	C(4)	-	C(3)	133.5(4)
C(14)	-	C(4)	-	C(5)	107.4(4)

Table 16

Valency Angles (degrees) and estimated standard deviations (degrees) (cont.)

C(6)	-	C(5)	-	C(4)	99.7(3)
C(10)	-	C(5)	-	C(6)	116.3(3)
C(7)	-	C(6)	-	C(5)	109.3(3)
C(15)	-	C(10)	-	C(5)	106.5(4)
C(11)	-	C(7)	-	C(6)	123.5(3)
C(11)	-	C(7)	-	C(8)	99.6(3)
C(9)	-	C(8)	-	C(7)	111.3(3)
C(12)	-	C(11)	-	C(7)	104.1(3)
C(10)	-	C(9)	-	C(8)	108.3(3)
C(15)	-	C(10)	-	C(9)	110.0(4)
C(13)	-	C(11)	-	C(12)	123.2(3)

The average O - $C(sp^3)$ - H valency angle is 108°

The average H - $C(sp^3)$ - H valency angle is 113°

The average H - $C(sp^3)$ - $C(sp^3)$ valency angle is 110°

The average H - $C(sp^2)$ - $C(sp^2)$ valency angle is 120°

Table 17

Berlandin

Intramolecular bonded distances (Å) and estimated standard deviations

O(1)	- C(3)	1.476(10)	C(18)	- C(19)	1.528(10)
O(1)	- C(4)	1.450(10)	C(19)	- C(20)	1.321(14)
O(2)	- C(6)	1.480(7)	C(19)	- C(21)	1.526(13)
O(2)	- C(12)	1.372(8)	C(20)	- C(22)	1.454(16)
O(3)	- C(12)	1.201(8)	C(2)	- H(2A)	0.96(6)
O(4)	- C(8)	1.468(7)	C(2)	- H(2B)	1.05(6)
O(4)	- C(18)	1.358(9)	C(3)	- H(3)	1.08(5)
O(5)	- C(18)	1.198(9)	C(5)	- H(5)	0.99(6)
O(6)	- C(9)	1.440(7)	C(6)	- H(6)	1.04(5)
O(6)	- C(16)	1.330(9)	C(7)	- H(7)	1.08(5)
O(7)	- C(16)	1.192(11)	C(8)	- H(8)	1.06(6)
C(1)	- C(2)	1.517(9)	C(9)	- H(9)	1.09(6)
C(1)	- C(5)	1.505(9)	C(13)	- H(13A)	0.94(6)
C(1)	- C(10)	1.342(9)	C(13)	- H(13B)	1.10(5)
C(2)	- C(3)	1.473(12)	C(14)	- H(14A)	1.29(6)
C(3)	- C(4)	1.499(11)	C(14)	- H(14B)	1.31(5)
C(4)	- C(5)	1.538(9)	C(14)	- H(14C)	1.04(8)
C(4)	- C(14)	1.497(11)	C(15)	- H(15A)	0.99(8)
C(5)	- C(6)	1.512(9)	C(15)	- H(15B)	1.54(7)
C(6)	- C(7)	1.547(8)	C(15)	- H(15C)	0.80(7)
C(7)	- C(8)	1.513(8)	C(17)	- H(17A)	1.08(8)
C(7)	- C(11)	1.508(8)	C(17)	- H(17B)	0.68(9)
C(8)	- C(9)	1.506(8)	C(17)	- H(17C)	1.14(9)

Table 17

Intramolecular bonded distances (Å) and estimated standard deviations (cont.)

C(9)	-	C(10)	1.533(8)	C(20)	-	H(20)	1.12(7)
C(10)	-	C(15)	1.494(11)	C(21)	-	H(21A)	1.00(9)
C(11)	-	C(12)	1.503(9)	C(21)	-	H(21B)	0.82(8)
C(11)	-	C(13)	1.308(11)	C(21)	-	H(21C)	0.89(9)
C(16)	-	C(17)	1.502(12)				

Table 18

Berlandin

Valency angles (degrees) and estimated standard deviations

C(4)	-	O(1)	-	C(3)	61.6(5)
C(2)	-	C(3)	-	O(1)	111.8(5)
C(4)	-	C(3)	-	O(1)	58.3(5)
C(3)	-	C(4)	-	O(1)	60.0(4)
C(5)	-	C(4)	-	O(1)	108.2(4)
C(14)	-	C(4)	-	O(1)	116.3(5)
C(12)	-	O(2)	-	C(6)	108.6(4)
C(5)	-	C(6)	-	O(2)	114.9(4)
C(7)	-	C(6)	-	O(2)	100.8(4)
O(3)	-	C(12)	-	O(2)	121.8(3)
C(11)	-	C(12)	-	O(2)	108.4(4)
C(11)	-	C(12)	-	O(3)	129.7(5)
C(18)	-	O(4)	-	C(8)	119.2(4)
C(7)	-	C(8)	-	O(4)	105.0(3)
C(9)	-	C(8)	-	O(4)	107.2(3)
O(5)	-	C(18)	-	O(4)	123.2(3)
C(19)	-	C(18)	-	O(4)	108.3(4)
C(19)	-	C(18)	-	O(5)	128.5(5)
C(16)	-	O(6)	-	C(9)	117.3(5)
C(8)	-	C(9)	-	O(6)	107.6(4)
C(10)	-	C(9)	-	O(6)	111.3(4)
O(7)	-	C(16)	-	O(6)	124.9(4)
C(17)	-	C(16)	-	O(6)	111.5(6)
C(17)	-	C(16)	-	O(7)	123.6(6)

Table 18

Valency angles (degrees) and estimated standard deviations (cont.)

C(5)	-	C(1)	-	C(2)	109.9(4)
C(10)	-	C(1)	-	C(2)	123.6(4)
C(3)	-	C(2)	-	C(1)	104.0(5)
C(10)	-	C(1)	-	C(5)	125.4(4)
C(4)	-	C(5)	-	C(1)	104.8(4)
C(6)	-	C(5)	-	C(1)	106.0(4)
C(9)	-	C(10)	-	C(1)	120.1(5)
C(15)	-	C(10)	-	C(1)	123.9(5)
C(4)	-	C(3)	-	C(2)	111.6(5)
C(5)	-	C(4)	-	C(3)	106.2(4)
C(14)	-	C(4)	-	C(3)	125.5(5)
C(14)	-	C(4)	-	C(5)	123.3(5)
C(6)	-	C(5)	-	C(4)	114.9(4)
C(7)	-	C(6)	-	C(5)	114.2(4)
C(8)	-	C(7)	-	C(6)	118.3(4)
C(11)	-	C(7)	-	C(6)	100.2(4)
C(11)	-	C(7)	-	C(8)	118.7(4)
C(9)	-	C(8)	-	C(7)	113.4(4)
C(12)	-	C(11)	-	C(7)	104.1(4)
C(13)	-	C(11)	-	C(7)	133.0(4)
C(10)	-	C(9)	-	C(8)	110.7(4)
C(15)	-	C(10)	-	C(9)	115.9(5)
C(13)	-	C(11)	-	C(12)	122.8(4)
C(20)	-	C(19)	-	C(18)	117.6(6)

Table 18

Valency angles (degrees) and estimated standard deviations (cont.)

C(21)	-	C(19)	-	C(18)		116.9(6)
C(21)	-	C(19)	-	C(20)		125.5(6)
C(22)	-	C(20)	-	C(19)		127.9(7)

The average O - $C(sp^3)$ - H valency angle is 111°

The average H - $C(sp^3)$ - H valency angle is 102°

The average H - $C(sp^3)$ - $C(sp^3)$ valency angle is 112°

The average H - $C(sp^3)$ - $C(sp^2)$ valency angle is 112°

Table 19

Dihydromikanolide

Torsion Angles (degrees)

C(3)	-	O(1)	-	C(2)	-	C(1)		-111
C(2)	-	O(1)	-	C(3)	-	C(4)		108
C(14)	-	O(3)	-	C(6)	-	C(5)		2
C(14)	-	O(3)	-	C(6)	-	C(7)		-122
C(6)	-	O(3)	-	C(14)	-	O(2)		-177
C(6)	-	O(3)	-	C(14)	-	C(4)		2
C(12)	-	O(5)	-	C(8)	-	C(7)		-20
C(12)	-	O(5)	-	C(8)	-	C(9)		-149
C(8)	-	O(5)	-	C(12)	-	O(4)		-178
C(8)	-	O(5)	-	C(12)	-	C(11)		0
C(10)	-	O(6)	-	C(1)	-	C(2)		-114
C(1)	-	O(6)	-	C(10)	-	C(9)		-111
C(1)	-	O(6)	-	C(10)	-	C(15)		115
O(6)	-	C(1)	-	C(2)	-	O(1)		-158
O(6)	-	C(1)	-	C(2)	-	C(3)		136
C(10)	-	C(1)	-	C(2)	-	O(1)		132
C(10)	-	C(1)	-	C(2)	-	C(3)		66
O(6)	-	C(1)	-	C(10)	-	C(9)		102
O(6)	-	C(1)	-	C(10)	-	C(15)		-99
C(2)	-	C(1)	-	C(10)	-	O(6)		104
C(2)	-	C(1)	-	C(10)	-	C(9)		-153
C(2)	-	C(1)	-	C(10)	-	C(15)		6
O(1)	-	C(2)	-	C(3)	-	C(4)		-105
C(1)	-	C(2)	-	C(3)	-	O(1)		102
C(1)	-	C(2)	-	C(3)	-	C(4)		-3

Table 19

Torsion Angles (degrees) (cont.)

O(1)	-	C(3)	-	C(4)	-	C(5)		-12
O(1)	-	C(3)	-	C(4)	-	C(14)		180
C(2)	-	C(3)	-	C(4)	-	C(5)		55
C(2)	-	C(3)	-	C(4)	-	C(14)		-113
C(3)	-	C(4)	-	C(5)	-	C(6)		-163
C(14)	-	C(4)	-	C(5)	-	C(6)		6
C(3)	-	C(4)	-	C(14)	-	O(2)		-17
C(3)	-	C(4)	-	C(14)	-	O(3)		165
C(5)	-	C(4)	-	C(14)	-	O(2)		173
C(5)	-	C(4)	-	C(14)	-	O(3)		-5
C(4)	-	C(5)	-	C(6)	-	O(3)		-5
C(4)	-	C(5)	-	C(6)	-	C(7)		116
O(3)	-	C(6)	-	C(7)	-	C(8)		115
O(3)	-	C(6)	-	C(7)	-	C(11)		-129
C(5)	-	C(6)	-	C(7)	-	C(8)		-2
C(5)	-	C(6)	-	C(7)	-	C(11)		115
C(6)	-	C(7)	-	C(8)	-	O(5)		153
C(6)	-	C(7)	-	C(8)	-	C(9)		-90
C(11)	-	C(7)	-	C(8)	-	O(5)		31
C(11)	-	C(7)	-	C(8)	-	C(9)		148
C(6)	-	C(7)	-	C(11)	-	C(12)		-157
C(6)	-	C(7)	-	C(11)	-	C(13)		77
C(8)	-	C(7)	-	C(11)	-	C(12)		-31
C(8)	-	C(7)	-	C(11)	-	C(13)		-157
O(5)	-	C(8)	-	C(9)	-	C(10)		-171

Table 19

Torsion Angles (degrees) (cont.)

C(7)	-	C(8)	-	C(9)	-	C(10)	73
C(8)	-	C(9)	-	C(10)	-	O(6)	124
C(8)	-	C(9)	-	C(10)	-	C(1)	57
C(8)	-	C(9)	-	C(10)	-	C(15)	-103
C(7)	-	C(11)	-	C(12)	-	O(4)	-162
C(7)	-	C(11)	-	C(12)	-	O(5)	20
C(13)	-	C(11)	-	C(12)	-	O(4)	-34
C(13)	-	C(11)	-	C(12)	-	O(5)	148

The sign convention used for the torsion angles is such that the sign is negative if an anticlockwise rotation is required of atom (1) to eclipse atom (4) whilst looking down the (2) - (3) bond.

The average standard deviation of the torsion angle is 0.74°.

Table 20

Dihydromikanolide

Mean Plane Calculations

	Atoms in plane	Atoms out of plane	Deviation (Å)
(1)	C(1)		0.01
	C(2)		-0.01
	C(3)		0.01
	C(4)		-0.01
		C(5)	0.81
		C(6)	0.18
		C(7)	-0.13
		C(8)	0.18
		C(9)	-0.84
		C(10)	-1.11
(2)	C(5)		0.01
	C(6)		-0.01
	C(7)		0.01
	C(8)		-0.01
		C(1)	-1.48
		C(2)	-1.92
		C(3)	-1.70
		C(4)	-1.12
		C(9)	-1.31
		C(10)	-2.10

Table 20

Mean Plane Calculations (cont.)

	Atoms in plane	Atoms out of plane	Deviation (Å)
(3)	O(3)		0.00
	C(4)		0.03
	C(5)		-0.03
	C(6)		0.02
	C(14)		-0.02
(4)	O(5)		0.00
	C(8)		0.00
	C(11)		0.00
	C(12)		0.00
		C(7)	-0.52

The angles between planes (1) and (2) is 24.4°.

Table 21

Miscandenin

Torsion Angles (degrees)

C(3)	-	O(1)	-	C(2)	-	C(1)		22
C(2)	-	O(1)	-	C(3)	-	C(4)		-6
C(14)	-	O(3)	-	C(6)	-	C(5)		27
C(14)	-	O(3)	-	C(6)	-	C(7)		-89
C(6)	-	O(3)	-	C(14)	-	O(2)		173
C(6)	-	O(3)	-	C(14)	-	C(4)		-10
C(12)	-	O(5)	-	C(8)	-	C(7)		-30
C(12)	-	O(5)	-	C(8)	-	C(9)		-151
C(8)	-	O(5)	-	C(12)	-	O(4)		-173
C(8)	-	O(5)	-	C(12)	-	C(11)		7
C(10)	-	C(1)	-	C(2)	-	O(1)		2
C(2)	-	C(1)	-	C(10)	-	C(5)		-42
C(2)	-	C(1)	-	C(10)	-	C(9)		82
C(2)	-	C(1)	-	C(10)	-	C(15)		-159
O(1)	-	C(3)	-	C(4)	-	C(5)		-2
O(1)	-	C(3)	-	C(4)	-	C(14)		179
C(3)	-	C(4)	-	C(5)	-	C(6)		-151
C(3)	-	C(4)	-	C(5)	-	C(10)		-24
C(14)	-	C(4)	-	C(5)	-	C(6)		27
C(14)	-	C(4)	-	C(5)	-	C(10)		154
C(3)	-	C(4)	-	C(14)	-	O(2)		-17
C(3)	-	C(4)	-	C(14)	-	O(3)		166
C(5)	-	C(4)	-	C(14)	-	O(2)		164
C(5)	-	C(4)	-	C(14)	-	O(3)		-13
C(4)	-	C(5)	-	C(6)	-	O(3)		-32
C(4)	-	C(5)	-	C(6)	-	C(7)		83

Table 21

Torsion Angles (degrees)

C(10)	-	C(5)	-	C(6)	-	O(3)		-161
C(10)	-	C(5)	-	C(6)	-	C(7)		-45
C(4)	-	C(5)	-	C(10)	-	C(1)		47
C(4)	-	C(5)	-	C(10)	-	C(9)		-74
C(4)	-	C(5)	-	C(10)	-	C(15)		166
C(6)	-	C(5)	-	C(10)	-	C(1)		166
C(6)	-	C(5)	-	C(10)	-	C(9)		45
C(6)	-	C(5)	-	C(10)	-	C(15)		-76
O(3)	-	C(6)	-	C(7)	-	C(8)		167
O(3)	-	C(6)	-	C(7)	-	C(11)		-75
C(5)	-	C(6)	-	C(7)	-	C(8)		54
C(5)	-	C(6)	-	C(7)	-	C(11)		172
C(6)	-	C(7)	-	C(8)	-	O(5)		172
C(6)	-	C(7)	-	C(8)	-	C(9)		-66
C(11)	-	C(7)	-	C(8)	-	O(5)		40
C(11)	-	C(7)	-	C(8)	-	C(9)		163
C(6)	-	C(7)	-	C(11)	-	C(12)		-159
C(6)	-	C(7)	-	C(11)	-	C(13)		17
C(8)	-	C(7)	-	C(11)	-	C(12)		-36
C(8)	-	C(7)	-	C(11)	-	C(13)		141
O(5)	-	C(8)	-	C(9)	-	C(10)		178
C(7)	-	C(8)	-	C(9)	-	C(10)		62
C(8)	-	C(9)	-	C(10)	-	C(1)		-174
C(8)	-	C(9)	-	C(10)	-	C(5)		-51
C(8)	-	C(9)	-	C(10)	-	C(15)		68
C(7)	-	C(11)	-	C(12)	-	O(4)		-160
C(7)	-	C(11)	-	C(12)	-	O(5)		19
C(13)	-	C(11)	-	C(12)	-	O(4)		23
C(13)	-	C(11)	-	C(12)	-	O(5)		-158

Table 21

Torsion Angles (degrees)

The sign convention used for the torsion angles is such that the sign is negative if an anticlockwise rotation is required of atom (1) to eclipse atom (4) whilst looking down the (2) - (3) bond.

The average standard deviation of the torsion angle is 0.62°.

Table 22

Miscandenin

Mean Plane Calculations

	Atoms in plane	Atoms out of plane	Deviation (Å)
(1)	C(1)		-0.06
	C(2)		0.05
	C(4)		-0.04
	C(5)		0.05
		O(1)	-0.17
		C(3)	-0.15
		C(10)	0.51
(2)	C(1)		-0.05
	C(2)		0.07
	C(3)		-0.07
	C(4)		0.05
		O(1)	-0.12
		C(10)	-0.48
		C(5)	0.12
(3)	O(1)		0.00
	C(3)		-0.01
	C(4)		0.01
	C(5)		0.00
		C(1)	-0.06
		C(2)	0.15
		C(10)	-0.59

Table 22

Mean Plane Calculations (cont.)

	Atoms in plane	Atoms out of plane	Deviation (Å)
(4)	O(1)		0.00
	C(2)		-0.01
	C(1)		0.01
	C(10)		0.00
		C(3)	0.45
		C(4)	0.86
		C(5)	0.93
(5)	C(6)		0.01
	C(7)		-0.01
	C(9)		0.01
	C(10)		-0.01
		C(5)	-0.54
		C(8)	0.72
(6)	O(3)		0.00
	C(4)		0.00
	C(14)		0.00
		C(5)	0.31
		C(6)	-0.23
(7)	O(5)		0.00
	C(11)		0.00
	C(12)		0.00
		C(7)	-0.47
		C(8)	0.18

Table 23

Berlandin

Torsion angles (degrees)

C(4)	-	O(1)	-	C(3)	-	C(2)		103
C(3)	-	O(1)	-	C(4)	-	C(5)		-99
C(3)	-	O(1)	-	C(4)	-	C(14)		118
C(12)	-	O(2)	-	C(6)	-	C(5)		158
C(12)	-	O(2)	-	C(6)	-	C(7)		35
C(6)	-	O(2)	-	C(12)	-	O(3)		167
C(6)	-	O(2)	-	C(12)	-	C(11)		-14
C(18)	-	O(4)	-	C(8)	-	C(7)		-132
C(18)	-	O(4)	-	C(8)	-	C(9)		107
C(8)	-	O(4)	-	C(18)	-	O(5)		5
C(8)	-	O(4)	-	C(18)	-	C(19)		-176
C(16)	-	O(6)	-	C(9)	-	C(8)		159
C(16)	-	O(6)	-	C(9)	-	C(10)		-80
C(9)	-	O(6)	-	C(16)	-	O(7)		-1
C(9)	-	O(6)	-	C(16)	-	C(17)		176
C(5)	-	C(1)	-	C(2)	-	C(3)		-19
C(10)	-	C(1)	-	C(2)	-	C(3)		173
C(2)	-	C(1)	-	C(5)	-	C(4)		18
C(2)	-	C(1)	-	C(5)	-	C(6)		-104
C(10)	-	C(1)	-	C(5)	-	C(4)		-174
C(10)	-	C(1)	-	C(5)	-	C(6)		64
C(2)	-	C(1)	-	C(10)	-	C(9)		173
C(2)	-	C(1)	-	C(10)	-	C(15)		-3
C(5)	-	C(1)	-	C(10)	-	C(9)		6

Table 23

Torsion angles (degrees) (cont.)

C(5)	-	C(1)	-	C(10)	-	C(15)		-170
C(1)	-	C(2)	-	C(3)	-	O(1)		-52
C(1)	-	C(2)	-	C(3)	-	C(4)		12
O(1)	-	C(3)	-	C(4)	-	C(5)		102
O(1)	-	C(3)	-	C(4)	-	C(14)		-102
C(2)	-	C(3)	-	C(4)	-	O(1)		-103
C(2)	-	C(3)	-	C(4)	-	C(5)		-1
C(2)	-	C(3)	-	C(4)	-	C(14)		155
O(1)	-	C(4)	-	C(5)	-	C(1)		53
O(1)	-	C(4)	-	C(5)	-	C(6)		169
C(3)	-	C(4)	-	C(5)	-	C(1)		-10
C(3)	-	C(4)	-	C(5)	-	C(6)		106
C(14)	-	C(4)	-	C(5)	-	C(1)		-166
C(14)	-	C(4)	-	C(5)	-	C(6)		-51
C(1)	-	C(5)	-	C(6)	-	O(2)		163
C(1)	-	C(5)	-	C(6)	-	C(7)		-82
C(4)	-	C(5)	-	C(6)	-	O(2)		47
C(4)	-	C(5)	-	C(6)	-	C(7)		163
O(2)	-	C(6)	-	C(7)	-	C(8)		-172
O(2)	-	C(6)	-	C(7)	-	C(11)		-41
C(5)	-	C(6)	-	C(7)	-	C(8)		64
C(5)	-	C(6)	-	C(7)	-	C(11)		-165
C(6)	-	C(7)	-	C(8)	-	O(4)		-174
C(6)	-	C(7)	-	C(8)	-	C(9)		-57
C(11)	-	C(7)	-	C(8)	-	O(4)		64

Table 23

Torsion angles (degrees) (cont.)

C(11)	-	C(7)	-	C(8)	-	C(9)	-179
C(6)	-	C(7)	-	C(11)	-	C(12)	34
C(6)	-	C(7)	-	C(11)	-	C(13)	-141
C(8)	-	C(7)	-	C(11)	-	C(12)	164
C(8)	-	C(7)	-	C(11)	-	C(13)	-11
O(4)	-	C(8)	-	C(9)	-	O(6)	-47
O(4)	-	C(8)	-	C(9)	-	C(10)	-169
C(7)	-	C(8)	-	C(9)	-	O(6)	-162
C(7)	-	C(8)	-	C(9)	-	C(10)	76
O(6)	-	C(9)	-	C(10)	-	C(1)	168
O(6)	-	C(9)	-	C(10)	-	C(15)	-16
C(8)	-	C(9)	-	C(10)	-	C(1)	-73
C(8)	-	C(9)	-	C(10)	-	C(15)	104
C(7)	-	C(11)	-	C(12)	-	O(2)	-14
C(7)	-	C(11)	-	C(12)	-	O(3)	165
C(13)	-	C(11)	-	C(12)	-	O(2)	162
C(13)	-	C(11)	-	C(12)	-	O(3)	-19
O(4)	-	C(18)	-	C(19)	-	C(20)	-137
O(4)	-	C(18)	-	C(19)	-	C(21)	43
O(5)	-	C(18)	-	C(19)	-	C(20)	42
O(5)	-	C(18)	-	C(19)	-	C(21)	-137
C(18)	-	C(19)	-	C(20)	-	C(22)	3
C(21)	-	C(19)	-	C(20)	-	C(22)	-178

Table 23

Torsion angles (degrees) (cont.)

The sign convention of the torsion angles is such that the sign is negative if an anticlockwise rotation is required of atom (1) to eclipse atom (4) whilst looking down the (2) - (3) bond.

The average standard deviation of the torsion angles is 0.8°.

Table 24

Berlandin

Mean Plane Calculations

	Atoms in plane	Atoms out of plane	Deviation
(1)	C(5)		-0.03
	C(6)		0.04
	C(7)		-0.04
	C(8)		0.03
		C(1)	1.09
		C(10)	1.18
		C(7)	-0.63
(2)	C(2)		0.00
	C(3)		0.01
	C(4)		-0.01
	C(5)		0.00
		C(1)	0.28
(3)	O(2)		0.00
	C(12)		0.00
	C(11)		0.00
		C(6)	0.33
		C(7)	-0.35

Table 25

Dihydromikanolide

Intermolecular contacts (Å) of less than 3.85 Å.

O(2)	$O(5)_{I}$	3.495	O(5)	$O(4)_{V}$	3.695
O(1)	$C(15)_{II}$	3.340	O(5)	$C(11)_{V}$	3.823
O(6)	$C(13)_{III}$	3.680	O(5)	$C(12)_{V}$	3.594
C(3)	$C(13)_{IV}$	3.620	O(5)	$C(13)_{V}$	3.440
C(4)	$C(13)_{IV}$	3.621	C(5)	$O(4)_{V}$	3.435
C(5)	$O(3)_{IV}$	3.194	C(8)	$O(4)_{V}$	3.319
C(6)	$O(2)_{IV}$	3.748	C(8)	$C(12)_{V}$	3.705
C(6)	$O(3)_{IV}$	3.217	C(11)	$O(4)_{V}$	3.829
C(6)	$C(14)_{IV}$	3.917	C(11)	$O(5)_{V}$	3.625
C(11)	$O(2)_{IV}$	3.446	C(11)	$C(12)_{V}$	3.803
C(13)	$O(2)_{IV}$	3.440	C(12)	$O(5)_{V}$	3.661
O(4)	$C(7)_{V}$	3.562	C(12)	$C(7)_{V}$	3.817
O(4)	$C(9)_{V}$	3.624	C(12)	$C(12)_{V}$	3.650

The subscripts refer to the following transformations of the atomic co-ordinates:

(I) x, y, z-1

(II) x, 1+y, z

(III) 1+x, y, z

(IV) 1-x, $\frac{1}{2}$+y, -z

(V) 1-x, $\frac{1}{2}$+y, 1-z

Table 26

Miscandenin

Intermolecular contacts (Å) of less than 3.85 Å

O(3)	$C(2)_{I}$	3.502	O(2)	$O(5)_{VI}$	3.466
C(6)	$O(4)_{II}$	3.280	O(2)	$C(8)_{VI}$	3.429
C(13)	$O(4)_{II}$	3.754	O(2)	$C(9)_{VI}$	3.805
O(5)	$C(15)_{III}$	3.358	C(1)	$O(4)_{VI}$	3.500
O(1)	$O(2)_{IV}$	3.483	C(2)	$O(4)_{VI}$	3.572
O(1)	$O(3)_{IV}$	3.690	C(3)	$O(4)_{VI}$	3.776
O(1)	$C(7)_{IV}$	3.464	C(3)	$O(5)_{VI}$	3.649
O(1)	$C(11)_{IV}$	3.600	C(3)	$C(12)_{VI}$	3.547
O(1)	$C(14)_{IV}$	3.466	C(4)	$O(4)_{VI}$	3.495
C(3)	$O(2)_{IV}$	3.790	C(4)	$O(5)_{VI}$	3.273
C(3)	$O(3)_{IV}$	3.843	C(4)	$C(12)_{VI}$	3.438
C(3)	$C(11)_{IV}$	3.680	C(5)	$O(4)_{VI}$	3.292
C(3)	$C(13)_{IV}$	3.709	C(5)	$O(5)_{VI}$	3.700
C(9)	$O(2)_{IV}$	3.501	C(5)	$C(12)_{VI}$	3.704
O(3)	$C(15)_{V}$	3.817	C(10)	$O(4)_{VI}$	3.822
O(1)	$C(12)_{VI}$	3.841	C(14)	$O(5)_{VI}$	3.311
O(1)	$C(13)_{VI}$	3.845	C(14)	$C(8)_{VI}$	3.743

The subscripts refer to the following transformations of the atomic co-ordinates:

(I)	$x - 1, y, z$	(IV)	$x + \frac{1}{2}, -y + \frac{3}{2}, -z$
(II)	$-x + \frac{1}{2}, -y + 1, z + \frac{1}{2}$	(V)	$x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$
(III)	$-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}$	(VI)	$-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$

Table 27

Berlandin

Intermolecular contacts (Å) of less than 3.85 Å

O(3)	$C(2)_{I}$	3.295	O(7)	$C(22)_{III}$	3.796
O(3)	$C(3)_{I}$	3.390	C(15)	$C(22)_{III}$	3.784
C(11)	$C(2)_{I}$	3.813	O(2)	$O(3)_{IV}$	3.494
C(12)	$C(2)_{I}$	3.704	C(2)	$O(3)_{IV}$	3.745
C(13)	$O(2)_{I}$	3.720	C(3)	$O(3)_{IV}$	3.376
C(20)	$C(15)_{I}$	3.597	C(3)	$C(12)_{IV}$	3.695
O(1)	$C(10)_{II}$	3.760	C(4)	$O(3)_{IV}$	3.501
O(1)	$C(15)_{II}$	3.197	C(6)	$O(3)_{IV}$	3.491
C(5)	$O(5)_{II}$	3.588	C(14)	$O(3)_{IV}$	3.583
C(7)	$O(5)_{II}$	3.548	C(14)	$C(13)_{IV}$	3.839
C(9)	$O(5)_{II}$	3.656	O(3)	$C(14)_{V}$	3.552
O(1)	$C(13)_{III}$	3.713			

The subscripts refer to the following transformations of the atomic co-ordinates:

(I)	x, y, 1 + z	(IV)	$\frac{1}{2}$ - x, - y, $\frac{1}{2}$ + z
(II)	x - 1, y, z	(V)	$-\frac{1}{2}$ - x, - y, $-\frac{1}{2}$ + z
(III)	x - 1, y, 1 + z		

Table 28 Structure factor listings ($|F_o|$ and $|F_c|$ x 10)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
10	7	2	57	42	9	6	3	41	45	8	9	6	27	28	8	4	3	26	21	7	12	5	63	56
10	7	0	25	4	9	6	1	29	24	8	9	5	42	38	8	4	2	60	61	7	12	4	55	54
10	6	3	25	40	9	6	0	32	11	8	9	4	50	43	8	4	1	36	34	7	12	3	29	8
10	6	1	29	46	9	5	5	27	29	8	9	3	35	27	8	4	0	79	83	7	12	2	38	42
10	5	3	41	29	9	5	3	40	31	8	9	2	73	63	8	3	6	54	46	7	12	0	49	42
10	5	2	37	17	9	5	1	50	44	8	9	0	49	42	8	3	5	37	34	7	11	6	32	21
10	4	4	28	11	9	4	6	55	51	8	8	7	26	24	8	3	4	32	7	7	11	3	43	39
10	4	2	33	44	9	4	5	26	2	8	8	5	31	22	8	3	3	61	61	7	11	2	34	36
10	4	0	67	66	9	4	4	34	39	8	8	3	63	65	8	3	2	27	26	7	11	1	68	61
10	3	2	29	30	9	4	3	29	40	8	8	1	36	48	8	3	1	75	80	7	11	0	96	88
10	2	2	30	14	9	4	2	59	51	8	8	0	60	55	8	2	7	34	22	7	10	6	25	11
10	2	1	49	47	9	4	1	41	16	8	7	6	36	35	8	2	6	33	41	7	10	4	44	38
10	2	0	26	1	9	4	0	61	57	8	7	5	45	38	8	2	4	66	65	7	10	3	36	36
10	1	5	30	18	9	3	3	38	32	8	7	4	28	23	8	2	3	52	45	7	10	2	51	38
10	1	4	27	28	9	3	1	57	53	8	7	3	37	32	8	2	2	32	16	7	10	0	53	58
10	1	3	32	31	9	3	0	25	25	8	7	1	34	33	8	2	1	61	52	7	9	6	39	32
10	1	1	35	26	9	2	5	37	33	8	6	7	34	37	8	2	0	75	81	7	9	5	32	33
10	1	0	41	39	9	2	3	36	45	8	6	5	36	46	8	1	6	51	40	7	9	4	36	31
10	0	2	29	27	9	2	2	30	19	8	6	4	59	60	8	1	5	45	50	7	9	3	33	26
10	0	0	48	51	9	2	0	42	32	8	6	2	49	52	8	1	4	25	33	7	9	2	97	96
9	10	1	36	24	9	1	4	34	6	8	6	1	43	37	8	1	3	34	40	7	9	1	91	97
9	9	4	27	14	9	1	3	39	38	8	6	0	72	72	8	1	2	109	109	7	8	7	38	39
9	9	3	50	45	9	1	1	37	33	8	5	8	34	19	8	1	1	105	105	7	8	6	25	14
9	9	1	36	21	9	0	5	35	37	8	5	6	25	23	8	1	0	133	147	7	8	4	83	83
9	9	0	39	34	9	0	2	38	35	8	5	5	37	24	8	0	8	27	19	7	8	2	85	88
9	8	5	33	37	9	0	1	48	39	8	5	4	61	58	8	0	7	30	5	7	8	1	86	80
9	8	4	30	16	8	13	0	57	50	8	5	3	39	24	8	0	4	31	44	7	8	0	65	57
9	8	2	43	35	8	12	3	27	38	8	5	2	85	90	8	0	3	146	148	7	7	7	40	22
9	8	0	41	45	8	12	2	39	31	8	5	1	29	27	8	0	1	62	68	7	7	6	48	46
9	7	5	65	56	8	12	1	38	29	8	5	0	76	82	8	0	0	43	57	7	7	5	33	21
9	7	4	27	27	8	12	0	27	55	8	4	8	28	22	7	14	2	52	53	7	7	4	55	57
9	7	2	32	35	8	11	4	30	29	8	4	7	74	77	7	14	0	33	18	7	7	3	88	84
9	7	1	48	46	8	11	2	60	59	8	4	6	28	24	7	13	4	26	39	7	7	2	82	83
9	7	0	32	17	8	10	4	29	12	8	4	5	60	51	7	13	3	41	32	7	7	1	79	80
9	6	5	43	44	8	10	2	42	40	8	4	4	46	50	7	13	0	32	21	7	6	7	35	29

Table 28 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
7	6	6	47	52	7	2	0	155	196	6	11	2	32	47	6	6	0	63	70	6	2	2	60	69
7	6	5	33	36	7	1	10	32	33	6	11	1	66	61	6	5	7	47	48	6	2	1	118	116
7	6	4	84	88	7	1	9	30	35	6	11	0	48	48	6	5	6	32	36	6	2	0	37	33
7	6	3	104	99	7	1	7	105	106	6	10	5	82	74	6	5	5	78	74	6	1	10	58	52
7	6	1	146	147	7	1	5	80	81	6	10	4	63	51	6	5	4	46	43	6	1	9	36	39
7	6	0	140	146	7	1	4	43	41	6	10	3	109	106	6	5	3	83	85	6	1	8	125	121
7	5	8	26	9	7	1	3	76	78	6	10	2	116	114	6	5	2	32	22	6	1	7	82	85
7	5	7	37	35	7	1	2	146	151	6	9	8	25	25	6	5	1	67	65	6	1	6	98	100
7	5	6	27	22	7	1	1	212	224	6	9	7	34	42	6	5	0	112	111	6	1	5	93	90
7	5	5	63	64	7	1	0	215	236	6	9	6	51	57	6	4	8	39	31	6	1	4	110	106
7	5	4	72	74	7	0	9	38	34	6	9	5	36	33	6	4	7	43	49	6	1	2	155	153
7	5	3	48	54	7	0	7	107	99	6	9	4	48	48	6	4	6	199	203	6	1	1	152	151
7	5	2	148	146	7	0	6	88	92	6	9	3	55	41	6	4	5	94	98	6	1	0	161	169
7	5	1	29	10	7	0	4	64	71	6	9	2	106	111	6	4	4	185	195	6	0	8	54	52
7	4	8	42	31	7	0	3	188	195	6	9	1	106	106	6	4	3	44	43	6	0	4	77	77
7	4	7	31	42	6	15	2	43	40	6	9	0	203	222	6	4	2	83	78	6	0	3	25	35
7	4	5	164	169	6	15	1	53	55	6	8	8	37	42	6	4	1	75	74	6	0	2	75	80
7	4	4	72	74	6	15	0	67	70	6	8	7	53	54	6	4	0	44	30	6	0	1	93	94
7	4	3	193	193	6	14	5	43	37	6	8	6	34	39	6	3	10	31	34	6	0	0	214	250
7	4	2	57	63	6	14	2	34	47	6	8	4	53	41	6	3	9	44	30	5	16	2	38	33
7	4	1	115	114	6	14	1	31	20	6	8	2	89	87	6	3	8	27	20	5	16	1	45	44
7	4	0	55	48	6	13	5	38	49	6	8	1	41	37	6	3	7	63	58	5	15	3	40	28
7	3	9	45	45	6	13	4	31	19	6	8	0	35	29	6	3	6	100	101	5	15	1	47	39
7	3	8	61	52	6	13	2	30	27	6	7	5	73	74	6	3	4	142	148	5	15	0	88	90
7	3	4	97	99	6	13	0	45	40	6	7	4	146	152	6	3	2	163	160	5	14	5	44	31
7	3	3	86	87	6	12	7	40	33	6	7	2	91	100	6	3	1	127	132	5	14	2	40	32
7	3	2	115	114	6	12	6	47	52	6	7	1	65	57	6	3	0	66	71	5	14	0	28	11
7	3	1	33	45	6	12	5	37	22	6	7	0	95	98	6	2	10	30	32	5	13	7	34	37
7	2	9	33	19	6	12	3	45	51	6	6	9	28	35	6	2	9	106	106	5	13	6	49	52
7	2	8	80	75	6	12	1	77	75	6	6	6	28	27	6	2	8	46	47	5	13	4	28	13
7	2	7	54	46	6	12	0	36	41	6	6	5	45	54	6	2	7	96	99	5	13	3	72	73
7	2	6	94	94	6	11	6	36	41	6	6	4	169	176	6	2	6	59	63	5	13	2	42	48
7	2	4	120	125	6	11	5	28	23	6	6	3	88	89	6	2	5	30	25	5	13	1	61	61
7	2	3	89	86	6	11	4	29	39	6	6	2	223	231	6	2	4	105	109	5	13	0	67	70
7	2	1	77	80	6	11	3	54	59	6	6	1	53	52	6	2	3	91	89	5	12	8	43	43

Table 28 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	12	7	30	30	5	7	8	35	18	5	4	1	223	215	5	0	9	74	69	4	11	3	150	147
5	12	6	33	27	5	7	7	47	39	5	4	0	38	33	5	0	6	48	48	4	11	2	78	80
5	12	5	29	41	5	7	6	90	96	5	3	11	34	30	5	0	5	71	73	4	11	1	147	155
5	12	4	48	50	5	7	5	113	119	5	3	10	28	16	5	0	4	38	32	4	10	9	29	20
5	12	3	52	61	5	7	3	163	158	5	3	9	44	36	5	0	3	74	76	4	10	7	33	32
5	12	2	94	96	5	7	2	88	83	5	3	8	38	39	5	0	2	132	129	4	10	6	65	70
5	11	7	39	41	5	7	1	77	81	5	3	7	79	76	5	0	1	339	339	4	10	5	97	97
5	11	3	74	71	5	6	10	38	21	5	3	6	104	100	4	17	2	25	26	4	10	4	69	64
5	11	2	52	54	5	6	9	49	41	5	3	5	65	68	4	17	1	35	21	4	10	3	164	172
5	11	1	56	62	5	6	7	70	72	5	3	3	133	129	4	16	4	33	33	4	10	2	122	126
5	10	8	36	40	5	6	6	30	38	5	3	2	70	69	4	16	2	39	25	4	10	1	70	69
5	10	7	39	21	5	6	5	122	130	5	3	1	79	71	4	15	5	26	33	4	10	0	135	136
5	10	5	82	81	5	6	4	65	62	5	3	0	199	185	4	15	2	30	23	4	9	9	26	12
5	10	4	64	63	5	6	3	119	114	5	2	10	69	68	4	15	1	49	47	4	9	7	37	33
5	10	3	77	73	5	6	1	147	140	5	2	9	45	45	4	15	0	30	16	4	9	6	52	51
5	10	2	39	32	5	6	0	120	115	5	2	8	64	73	4	14	6	41	40	4	9	5	40	35
5	10	1	170	176	5	5	11	36	20	5	2	7	39	43	4	14	5	58	45	4	9	4	118	116
5	10	0	53	59	5	5	8	35	32	5	2	6	26	19	4	14	3	48	50	4	9	3	48	47
5	9	9	29	18	5	5	7	76	72	5	2	5	127	123	4	14	2	31	10	4	9	2	116	111
5	9	6	40	33	5	5	6	114	114	5	2	4	38	26	4	14	1	32	39	4	9	1	43	32
5	9	5	59	53	5	5	4	105	102	5	2	3	120	122	4	13	8	61	55	4	9	0	159	156
5	9	4	36	33	5	5	3	186	182	5	2	2	146	145	4	13	6	55	47	4	8	9	25	37
5	9	2	87	87	5	5	2	119	116	5	2	1	138	135	4	13	5	42	31	4	8	6	193	199
5	9	0	109	108	5	5	1	73	74	5	2	0	48	46	4	13	4	55	51	4	8	5	43	32
5	8	10	26	23	5	5	0	76	74	5	1	11	54	58	4	13	2	67	62	4	8	4	207	219
5	8	8	66	64	5	4	11	27	6	5	1	10	35	43	4	13	1	54	55	4	8	3	74	79
5	8	7	47	48	5	4	10	31	18	5	1	9	77	77	4	13	0	128	131	4	8	2	165	162
5	8	6	74	78	5	4	9	26	9	5	1	8	124	125	4	12	8	43	38	4	8	1	59	66
5	8	5	152	152	5	4	8	40	41	5	1	7	63	57	4	12	5	45	50	4	8	0	119	118
5	8	4	66	62	5	4	7	93	89	5	1	6	76	76	4	12	3	43	44	4	7	11	24	19
5	8	3	45	52	5	4	6	78	82	5	1	4	100	97	4	12	2	37	35	4	7	8	35	22
5	8	2	25	16	5	4	5	122	126	5	1	3	109	110	4	12	1	60	68	4	7	7	107	111
5	8	1	140	130	5	4	4	140	138	5	1	2	84	85	4	11	9	32	26	4	7	6	29	28
5	8	0	118	122	5	4	3	185	171	5	1	1	122	122	4	11	8	30	34	4	7	5	34	29
5	7	10	26	17	5	4	2	148	146	5	1	0	188	195	4	11	6	37	42	4	7	4	72	74

Table 28 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	7	3	52	53	4	3	6	74	79	4	0	6	38	39	3	12	5	25	20	3	8	4	75	77
4	7	2	96	99	4	3	5	85	83	4	0	5	26	29	3	12	4	60	54	3	8	3	199	193
4	7	1	90	89	4	3	4	142	143	4	0	3	40	40	3	12	3	150	159	3	8	2	91	96
4	7	0	51	63	4	3	3	126	126	4	0	1	466	448	3	12	1	191	190	3	8	1	142	135
4	6	11	31	25	4	3	2	201	199	4	0	0	207	234	3	11	10	32	37	3	8	0	38	44
4	6	10	27	22	4	3	1	371	345	3	18	1	40	37	3	11	7	26	34	3	7	11	38	26
4	6	9	28	4	4	3	0	589	560	3	17	4	27	6	3	11	6	79	76	3	7	9	36	31
4	6	7	45	40	4	2	12	41	30	3	17	2	27	40	3	11	4	88	92	3	7	8	152	154
4	6	5	35	37	4	2	11	36	32	3	16	3	28	35	3	11	3	47	51	3	7	7	90	92
4	6	4	79	80	4	2	10	48	49	3	16	2	26	24	3	11	2	132	134	3	7	6	98	97
4	6	3	208	210	4	2	8	54	58	3	16	1	72	70	3	11	1	83	81	3	7	5	96	101
4	6	2	77	77	4	2	7	64	61	3	15	7	38	31	3	11	0	63	63	3	7	4	185	178
4	6	1	114	113	4	2	6	45	48	3	15	6	37	31	3	10	9	49	55	3	7	3	199	184
4	6	0	82	83	4	2	5	53	53	3	15	3	44	44	3	10	8	43	48	3	7	2	39	43
4	5	8	72	75	4	2	4	65	66	3	15	2	30	24	3	10	7	43	41	3	7	1	287	275
4	5	7	58	58	4	2	3	101	97	3	15	1	43	43	3	10	6	38	45	3	7	0	55	51
4	5	6	59	60	4	2	2	286	274	3	14	7	52	50	3	10	5	75	75	3	6	11	29	5
4	5	5	38	41	4	2	1	76	66	3	14	6	38	26	3	10	4	135	135	3	6	9	45	49
4	5	4	217	228	4	2	0	219	199	3	14	5	34	26	3	10	3	108	106	3	6	8	68	64
4	5	3	102	102	4	1	12	47	44	3	14	4	26	34	3	10	2	149	154	3	6	7	34	25
4	5	2	294	290	4	1	10	72	69	3	14	3	45	43	3	10	1	66	70	3	6	6	50	52
4	5	1	182	180	4	1	9	94	91	3	14	2	58	58	3	10	0	113	113	3	6	5	105	107
4	5	0	261	241	4	1	8	25	25	3	14	1	57	60	3	9	10	30	20	3	6	4	169	170
4	4	10	25	20	4	1	7	53	56	3	14	0	72	69	3	9	7	40	51	3	6	3	68	61
4	4	9	45	47	4	1	6	61	66	3	13	7	55	49	3	9	6	65	73	3	6	2	174	163
4	4	7	47	44	4	1	5	58	59	3	13	6	32	27	3	9	5	165	168	3	6	1	91	89
4	4	6	39	37	4	1	4	68	68	3	13	5	65	72	3	9	4	58	69	3	5	11	42	31
4	4	5	116	124	4	1	3	71	68	3	13	4	41	28	3	9	3	177	173	3	5	9	50	48
4	4	4	48	49	4	1	2	267	248	3	13	3	67	61	3	9	2	61	67	3	5	8	71	72
4	4	3	174	179	4	1	1	69	63	3	13	2	25	21	3	9	1	261	256	3	5	7	33	28
4	4	2	59	54	4	1	0	204	190	3	13	1	104	99	3	8	10	37	28	3	5	6	65	69
4	4	1	150	157	4	0	11	35	37	3	13	0	50	53	3	8	9	39	31	3	5	5	92	95
4	4	0	229	211	4	0	10	46	49	3	12	8	26	20	3	8	7	100	104	3	5	4	202	198
4	3	10	45	41	4	0	8	48	49	3	12	7	32	17	3	8	6	140	149	3	5	3	187	182
4	3	8	72	85	4	0	7	31	27	3	12	6	36	25	3	8	5	189	193	3	5	2	154	147

Table 28 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	5	1	432	398	3	1	11	41	34	2	15	2	80	82	2	10	5	101	103	2	7	3	129	127
3	5	0	208	194	3	1	10	61	59	2	15	1	46	48	2	10	4	68	70	2	7	2	274	255
3	4	11	51	52	3	1	8	89	95	2	14	8	35	36	2	10	3	89	89	2	7	1	266	247
3	4	10	41	28	3	1	7	46	56	2	14	7	30	34	2	10	2	102	105	2	6	12	35	11
3	4	8	27	24	3	1	6	62	60	2	14	6	42	40	2	10	1	73	69	2	6	10	29	30
3	4	7	106	104	3	1	5	94	89	2	14	4	51	41	2	10	0	54	47	2	6	9	50	53
3	4	6	42	40	3	1	4	94	95	2	14	2	87	88	2	9	11	25	16	2	6	8	50	56
3	4	5	69	70	3	1	3	254	245	2	14	1	47	52	2	9	10	32	16	2	6	7	47	52
3	4	4	209	206	3	1	2	152	144	2	14	0	31	33	2	9	8	51	58	2	6	6	100	101
3	4	3	125	125	3	1	1	172	149	2	13	9	34	33	2	9	7	108	108	2	6	5	179	172
3	4	2	56	53	3	1	0	209	202	2	13	8	54	47	2	9	6	93	98	2	6	4	288	294
3	4	1	490	472	3	0	12	53	45	2	13	5	45	34	2	9	4	94	98	2	6	3	125	120
3	4	0	87	85	3	0	11	28	3	2	13	4	54	50	2	9	3	120	123	2	6	2	195	200
3	3	11	41	40	3	0	10	63	62	2	13	3	54	59	2	9	2	177	171	2	6	1	249	235
3	3	10	27	27	3	0	9	27	39	2	13	2	88	88	2	9	1	121	124	2	5	10	84	84
3	3	9	53	50	3	0	7	25	20	2	13	1	33	36	2	9	0	61	58	2	5	9	54	50
3	3	7	71	74	3	0	6	83	84	2	12	9	34	23	2	8	10	30	33	2	5	7	129	127
3	3	6	164	171	3	0	5	234	220	2	12	8	44	29	2	8	9	53	52	2	5	6	98	96
3	3	5	147	144	3	0	4	28	26	2	12	6	44	37	2	8	8	78	77	2	5	5	141	148
3	3	4	79	73	3	0	3	260	249	2	12	5	88	93	2	8	7	126	134	2	5	4	173	164
3	3	3	270	266	3	0	1	68	67	2	12	4	57	56	2	8	6	49	46	2	5	3	196	181
3	3	2	185	176	2	18	2	37	37	2	12	3	46	34	2	8	5	150	154	2	5	2	56	62
3	3	1	504	488	2	18	0	28	43	2	12	2	130	132	2	8	4	88	89	2	5	1	168	166
3	3	0	275	242	2	17	4	42	23	2	12	1	71	73	2	8	3	131	132	2	5	0	174	163
3	2	12	25	20	2	17	1	46	43	2	11	7	79	84	2	8	1	125	121	2	4	12	56	49
3	2	11	36	32	2	17	0	80	77	2	11	6	54	61	2	8	0	95	93	2	4	10	33	23
3	2	9	55	59	2	16	6	29	19	2	11	5	77	76	2	7	11	37	11	2	4	9	64	68
3	2	8	78	83	2	16	5	33	20	2	11	4	122	123	2	8	2	47	41	2	4	8	57	52
3	2	7	67	65	2	16	4	36	37	2	11	3	41	41	2	7	10	59	52	2	4	7	94	93
3	2	6	147	147	2	16	2	44	51	2	11	2	52	55	2	7	9	47	62	2	4	6	31	34
3	2	5	56	59	2	16	1	37	18	2	11	1	80	80	2	7	8	38	29	2	4	5	167	177
3	2	4	77	80	2	16	0	69	64	2	10	9	45	55	2	7	7	130	138	2	4	4	184	189
3	2	3	91	92	2	15	6	35	33	2	10	8	47	45	2	7	6	119	124	2	4	3	268	260
3	2	2	277	263	2	15	4	45	43	2	10	7	50	52	2	7	5	142	138	2	4	2	165	165
3	2	1	89	90	2	15	3	66	60	2	10	6	40	47	2	7	4	77	76	2	4	0	533	519

Table 28 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	3	12	46	16	2	1	0	387	397	1	14	0	100	100	1	9	8	47	51	1	6	4	301	290
2	3	11	30	38	2	0	12	26	22	1	13	9	26	31	1	9	7	34	31	1	6	3	230	217
2	3	10	48	50	2	0	11	63	63	1	13	6	27	17	1	9	6	73	77	1	6	2	102	107
2	3	8	64	67	2	0	10	53	58	1	13	4	46	52	1	9	4	149	151	1	6	1	247	241
2	3	7	112	110	2	0	9	87	83	1	13	3	138	138	1	9	3	48	47	1	6	0	231	239
2	3	6	100	99	2	0	7	58	61	1	13	1	92	90	1	9	2	175	171	1	5	12	29	32
2	3	5	147	140	2	0	6	66	64	1	13	0	117	115	1	9	1	259	257	1	5	11	47	59
2	3	4	286	286	2	0	5	33	47	1	12	7	42	33	1	9	0	36	41	1	5	10	32	18
2	3	3	332	325	2	0	4	38	41	1	12	5	92	101	1	8	10	68	67	1	5	9	70	70
2	3	2	241	246	2	0	3	87	88	1	12	4	27	35	1	8	9	55	59	1	5	8	75	75
2	3	1	124	115	2	0	2	281	260	1	12	3	75	81	1	8	8	63	62	1	5	7	121	122
2	3	0	624	676	2	0	1	591	618	1	12	2	133	136	1	8	7	107	110	1	5	6	241	237
2	2	12	33	32	2	0	0	484	546	1	12	1	69	76	1	8	6	84	80	1	5	5	286	268
2	2	11	36	36	1	18	0	44	38	1	11	10	32	34	1	8	5	55	57	1	5	4	190	183
2	2	10	48	54	1	17	5	31	21	1	11	9	58	52	1	8	4	167	172	1	5	3	236	222
2	2	9	26	24	1	17	2	56	53	1	11	8	29	5	1	8	3	77	74	1	5	2	315	305
2	2	8	124	137	1	17	1	47	59	1	11	7	31	22	1	8	2	215	221	1	5	1	187	174
2	2	7	72	69	1	17	0	45	47	1	11	6	44	46	1	8	1	117	117	1	5	0	267	280
2	2	6	134	125	1	16	6	33	21	1	11	5	137	140	1	8	0	141	142	1	4	12	46	30
2	2	5	151	148	1	16	5	31	24	1	11	4	107	108	1	7	11	26	21	1	4	9	68	74
2	2	4	78	70	1	16	4	47	41	1	11	3	40	46	1	7	9	62	66	1	4	8	92	93
2	2	3	297	301	1	16	3	52	55	1	11	2	107	107	1	7	8	32	38	1	4	7	94	91
2	2	2	275	282	1	16	2	90	82	1	11	0	86	84	1	7	7	151	154	1	4	6	56	62
2	2	1	75	66	1	16	1	70	67	1	10	9	32	19	1	7	6	68	72	1	4	5	117	112
2	2	0	282	289	1	16	0	61	59	1	10	8	77	73	1	7	5	64	68	1	4	4	346	327
2	1	11	38	30	1	15	5	25	9	1	10	7	110	113	1	7	4	111	106	1	4	3	87	86
2	1	10	35	37	1	15	3	125	127	1	10	6	34	38	1	7	3	48	54	1	4	2	83	80
2	1	9	97	92	1	15	1	100	102	1	10	5	179	187	1	7	2	267	246	1	4	1	315	328
2	1	8	48	51	1	15	0	173	165	1	10	4	89	86	1	7	1	133	135	1	4	0	117	114
2	1	6	125	127	1	14	8	48	42	1	10	3	85	87	1	7	0	168	160	1	3	12	31	40
2	1	5	172	170	1	14	6	51	48	1	10	2	106	108	1	6	11	29	11	1	3	11	33	21
2	1	4	65	64	1	14	4	38	40	1	10	1	42	43	1	6	10	56	60	1	3	9	103	99
2	1	3	275	276	1	14	3	81	74	1	10	0	98	96	1	6	8	26	30	1	3	8	136	127
2	1	2	547	577	1	14	2	68	73	1	9	10	42	30	1	6	7	83	79	1	3	7	42	33
2	1	1	201	199	1	14	1	89	90	1	9	9	30	18	1	6	6	125	128	1	3	6	173	172

Table 28 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	3	5	355	350	1	0	5	48	38	0	12	4	135	137	0	8	0	111	108	0	4	0	209	218
1	3	4	176	171	1	0	4	59	59	0	12	3	73	72	0	7	11	33	36	0	3	8	74	66
1	3	3	295	292	1	0	3	173	174	0	12	2	27	31	0	7	10	28	32	0	3	7	129	125
1	3	2	132	127	1	0	2	614	678	0	12	0	166	162	0	7	9	55	62	0	3	6	27	30
1	3	1	411	417	0	19	1	33	14	0	11	9	46	44	0	7	8	25	11	0	3	5	149	141
1	3	0	288	285	0	18	4	30	30	0	11	6	159	163	0	7	7	94	94	0	3	4	444	459
1	2	12	30	19	0	18	0	33	35	0	11	5	83	93	0	7	6	49	48	0	3	3	413	409
1	2	11	36	33	0	17	5	42	31	0	11	4	28	15	0	7	4	251	258	0	3	1	356	373
1	2	9	107	112	0	17	4	33	32	0	11	3	159	164	0	7	3	205	188	0	2	10	63	68
1	2	8	64	72	0	17	2	38	53	0	11	2	116	118	0	7	1	171	169	0	2	9	63	72
1	2	7	165	164	0	17	1	66	63	0	11	1	49	44	0	6	8	31	37	0	2	8	106	104
1	2	6	142	144	0	16	7	50	39	0	10	11	29	11	0	6	7	46	40	0	2	7	177	185
1	2	5	93	92	0	16	6	63	57	0	10	8	89	86	0	6	6	57	46	0	2	5	84	80
1	2	4	313	304	0	16	5	25	17	0	10	7	43	38	0	6	5	208	200	0	2	4	211	207
1	2	3	317	307	0	16	3	74	72	0	10	6	141	154	0	6	4	490	494	0	2	3	788	894
1	2	2	458	474	0	16	2	73	74	0	10	5	36	27	0	6	3	295	277	0	2	2	528	563
1	2	1	112	111	0	16	1	65	75	0	10	4	58	58	0	6	2	159	150	0	2	1	353	371
1	1	11	51	49	0	16	0	141	134	0	10	2	68	70	0	6	0	37	35	0	2	0	482	547
1	1	10	46	42	0	15	8	50	37	0	10	0	56	48	0	5	12	58	52	0	1	13	30	24
1	1	9	60	63	0	15	7	35	31	0	9	11	36	18	0	5	11	55	48	0	1	12	34	15
1	1	7	99	98	0	15	6	29	9	0	9	7	71	71	0	5	9	46	45	0	1	10	47	46
1	1	6	103	100	0	15	2	160	162	0	9	6	30	37	0	5	7	128	128	0	1	9	34	35
1	1	5	78	74	0	15	1	30	15	0	9	5	100	98	0	5	6	259	253	0	1	5	207	193
1	1	4	184	174	0	14	8	55	54	0	9	4	100	100	0	5	5	549	558	0	1	4	234	236
1	1	3	297	296	0	14	5	45	44	0	9	3	126	129	0	5	4	470	458	0	1	3	549	575
1	1	2	102	99	0	14	2	34	42	0	9	1	62	61	0	5	3	87	85	0	1	2	385	400
1	1	1	335	338	0	14	1	145	151	0	8	11	32	37	0	5	2	573	585	0	1	1	181	166
1	1	0	308	299	0	14	0	219	226	0	8	10	34	18	0	5	1	256	248	0	0	12	44	50
1	0	12	55	45	0	13	4	54	59	0	8	8	32	20	0	4	11	37	41	0	0	10	92	92
1	0	11	76	75	0	13	3	55	48	0	8	7	143	149	0	4	8	41	40	0	0	8	70	66
1	0	10	73	74	0	13	2	144	146	0	8	6	94	84	0	4	5	97	97	0	0	6	129	126
1	0	9	45	50	0	13	1	38	30	0	8	5	46	49	0	4	4	36	23	0	0	4	135	140
1	0	8	140	140	0	12	10	24	2	0	8	4	195	205	0	4	3	60	68					
1	0	7	53	59	0	12	9	57	47	0	8	3	198	203	0	4	2	799	926					
1	0	6	232	227	0	12	6	38	50	0	8	2	158	144	0	4	1	481	519					

Table 29 Structure factor listings ($|F_o|$ and $|F_c| \times 10$)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
14	1	0	20	17	12	3	-1	39	40	11	4	3	32	29	11	1	-5	27	25	10	3	0	43	41
14	1	-1	29	27	12	2	5	22	15	11	4	2	20	19	11	1	-6	30	27	10	3	-1	57	59
14	1	-2	42	37	12	2	3	25	26	11	4	0	26	30	11	1	-7	47	42	10	3	-2	22	31
14	0	-3	27	21	12	2	2	28	25	11	4	-1	21	22	11	1	-8	28	23	10	3	-3	36	38
14	0	-6	31	29	12	2	1	34	29	11	4	-2	23	15	11	1	-10	24	23	10	3	-5	43	44
13	4	-1	19	17	12	2	0	28	30	11	4	-3	20	21	11	0	5	35	30	10	3	-6	21	23
13	4	-2	39	34	12	2	-1	23	20	11	4	-4	28	29	11	0	4	28	26	10	3	-9	22	13
13	4	-4	23	21	12	2	-2	30	31	11	3	5	38	29	11	0	3	25	21	10	2	6	19	8
13	4	-5	21	17	12	2	-4	33	23	11	3	3	21	17	11	0	2	38	36	10	2	3	20	17
13	3	0	20	23	12	2	-5	22	24	11	3	2	40	36	11	0	1	23	18	10	2	2	41	34
13	3	-1	24	24	12	2	-8	34	30	11	3	1	19	17	11	0	-6	49	49	10	2	1	39	40
13	3	-2	34	34	12	1	5	19	21	11	3	0	29	31	11	0	-8	62	54	10	2	0	66	67
13	3	-4	19	10	12	1	3	32	27	11	3	-1	34	38	11	0	-10	50	44	10	2	-2	69	73
13	2	3	23	21	12	1	2	29	31	11	3	-2	22	19	10	7	0	22	20	10	2	-4	28	26
13	2	-1	37	33	12	1	1	19	11	11	3	-6	22	16	10	7	-1	26	23	10	2	-5	37	39
13	2	-6	31	33	12	1	-1	37	35	11	3	-7	24	25	10	7	-2	22	19	10	2	-8	34	29
13	2	-7	27	22	12	1	-2	31	31	11	3	-8	21	23	10	7	-3	31	30	10	2	-9	23	19
13	1	3	23	21	12	1	-6	27	20	11	3	-9	26	24	10	6	3	22	17	10	1	3	19	20
13	1	-2	21	19	12	1	-7	25	23	11	2	5	35	33	10	6	2	28	24	10	1	2	50	50
13	1	-3	28	25	12	1	-8	36	29	11	2	3	21	20	10	6	-2	30	29	10	1	1	61	56
13	1	-6	27	26	12	1	-9	34	29	11	2	2	35	34	10	6	-5	27	22	10	1	0	47	51
13	1	-7	22	20	12	0	2	33	31	11	2	1	19	19	10	5	1	19	16	10	1	-2	39	45
13	0	4	36	32	12	0	1	38	33	11	2	0	23	17	10	5	-3	30	34	10	1	-3	77	83
13	0	-2	20	21	12	0	-3	21	23	11	2	-2	23	18	10	5	-4	26	28	10	1	-4	25	23
13	0	-6	46	41	12	0	-4	36	36	11	2	-3	52	55	10	5	-6	19	15	10	1	-7	20	16
12	5	-2	23	19	12	0	-8	36	33	11	2	-4	21	18	10	4	6	21	19	10	1	-9	24	23
12	5	-3	20	17	12	0	-9	25	17	11	2	-5	33	30	10	4	3	26	27	10	0	5	32	28
12	5	-4	19	16	11	6	0	21	17	11	2	-8	44	42	10	4	2	30	26	10	0	4	25	20
12	4	3	21	15	11	6	-4	39	36	11	2	-9	30	30	10	4	1	24	24	10	0	3	39	40
12	4	1	33	32	11	5	-1	34	35	11	1	6	44	40	10	4	0	29	29	10	0	2	82	82
12	4	0	35	32	11	5	-2	34	34	11	1	4	24	21	10	4	-1	23	23	10	0	1	22	23
12	4	-1	28	28	11	5	-3	28	30	11	1	0	37	41	10	4	-3	28	26	10	0	0	34	33
12	4	-4	28	26	11	5	-5	23	19	11	1	-2	24	26	10	4	-4	25	26	10	0	-1	50	50
12	4	-7	19	10	11	4	5	20	16	11	1	-3	27	29	10	4	-5	30	29	10	0	-2	25	33
12	3	2	40	39	11	4	4	42	38	11	1	-4	29	26	10	4	-7	23	23	10	0	-3	20	14

Table 29 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
10	0	-4	46	45	9	3	4	37	36	9	1	-6	73	68	8	5	-3	63	65	8	2	8	23	26
10	0	-5	41	40	9	3	3	26	24	9	1	-7	24	24	8	5	-4	39	45	8	2	7	38	37
10	0	-6	35	33	9	3	2	44	39	9	1	-8	23	22	8	5	-6	37	36	8	2	6	37	38
10	0	-8	31	28	9	3	1	65	66	9	0	7	38	36	8	5	-8	22	19	8	2	4	46	44
9	7	3	20	21	9	3	0	53	51	9	0	4	22	22	8	5	-9	19	22	8	2	3	42	46
9	7	2	28	26	9	3	-1	25	25	9	0	3	28	26	8	4	8	26	18	8	2	2	82	85
9	7	1	31	30	9	3	-2	141	161	9	0	0	118	121	8	4	7	31	33	8	2	1	100	105
9	7	-3	21	21	9	3	-3	98	106	9	0	-1	54	58	8	4	6	36	36	8	2	0	50	53
9	7	-4	30	29	9	3	-4	39	43	9	0	-2	25	18	8	4	4	60	59	8	2	-1	26	29
9	6	4	38	36	9	3	-5	29	30	9	0	-5	63	63	8	4	1	44	44	8	2	-2	41	47
9	6	3	36	33	9	3	-7	29	24	9	0	-7	31	26	8	4	-1	27	31	8	2	-3	38	46
9	6	-1	20	14	9	2	7	27	25	8	7	4	28	28	8	4	-2	35	43	8	2	-4	142	154
9	6	-2	42	41	9	2	5	31	34	8	7	3	32	30	8	4	-3	28	28	8	2	-5	84	88
9	6	-4	25	24	9	2	4	24	23	8	7	-2	38	42	8	4	-4	24	28	8	2	-6	59	61
9	6	-5	20	19	9	2	3	30	22	8	7	-3	29	29	8	4	-5	64	65	8	2	-7	61	58
9	6	-7	22	26	9	2	2	81	79	8	7	-5	30	31	8	4	-6	24	22	8	2	-8	30	26
9	5	4	21	22	9	2	1	52	56	8	6	5	20	14	8	4	-7	53	54	8	2	-9	32	33
9	5	-1	66	70	9	2	0	52	56	8	6	4	40	37	8	4	-9	28	26	8	1	8	24	20
9	5	-2	27	27	9	2	-1	59	68	8	6	3	29	26	8	4	-10	26	22	8	1	7	29	29
9	5	-3	55	55	9	2	-2	38	45	8	6	-1	27	32	8	3	8	29	29	8	1	6	27	29
9	5	-4	34	29	9	2	-3	81	87	8	6	-3	52	52	8	3	6	28	26	8	1	5	50	46
9	5	-5	40	39	9	2	-4	49	51	8	6	-4	24	24	8	3	5	74	77	8	1	4	74	75
9	4	7	29	26	9	2	-5	37	36	8	6	-5	29	26	8	3	4	60	58	8	1	3	82	81
9	4	5	22	24	9	2	-6	57	57	8	6	-6	31	32	8	3	3	22	23	8	1	2	80	78
9	4	3	32	33	9	2	-8	25	22	8	6	-7	24	19	8	3	2	37	36	8	1	1	136	148
9	4	2	35	34	9	2	-11	23	23	8	6	-8	21	14	8	3	1	52	57	8	1	0	39	44
9	4	1	36	35	9	1	5	42	39	8	5	6	26	29	8	3	0	33	37	8	1	-1	58	58
9	4	0	45	49	9	1	4	34	31	8	5	5	53	49	8	3	-1	41	46	8	1	-2	71	76
9	4	-1	27	32	9	1	3	56	56	8	5	4	32	33	8	3	-3	37	43	8	1	-4	85	85
9	4	-2	30	29	9	1	1	75	80	8	5	3	36	34	8	3	-4	45	41	8	1	-5	92	95
9	4	-5	31	31	9	1	-1	124	133	8	5	2	19	20	8	3	-5	70	71	8	1	-6	116	112
9	4	-6	35	35	9	1	-2	151	168	8	5	1	31	30	8	3	-6	33	33	8	1	-9	34	32
9	4	-7	26	18	9	1	-3	108	120	8	5	0	37	43	8	3	-7	24	22	8	1	-11	27	28
9	4	-8	33	31	9	1	-4	107	106	8	5	-1	39	36	8	3	-8	24	26	8	0	7	31	36
9	3	7	20	18	9	1	-5	45	45	8	5	-2	33	38	8	3	-10	22	25	8	0	6	27	25

Table 29 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
8	0	5	35	36	7	5	7	21	26	7	3	2	28	34	7	1	0	76	80	6	7	6	25	24
8	0	3	66	68	7	5	5	36	36	7	3	0	32	30	7	1	-1	93	104	6	7	5	28	25
8	0	2	126	130	7	5	4	31	30	7	3	-1	118	132	7	1	-2	76	85	6	7	4	35	36
8	0	1	114	115	7	5	3	28	25	7	3	-2	36	36	7	1	-3	41	44	6	7	1	41	37
8	0	0	27	34	7	5	1	37	34	7	3	-3	80	87	7	1	-4	56	58	6	7	0	40	39
8	0	-1	92	95	7	5	-1	42	41	7	3	-4	66	70	7	1	-5	29	23	6	7	-3	42	43
8	0	-2	26	23	7	5	-2	50	52	7	3	-5	41	46	7	1	-6	21	19	6	7	-4	27	24
8	0	-3	69	70	7	5	-3	39	42	7	3	-6	96	94	7	1	-7	66	65	6	7	-6	23	17
8	0	-4	55	56	7	5	-4	35	33	7	3	-8	32	30	7	1	-8	45	42	6	7	-7	27	33
8	0	-5	99	100	7	5	-5	32	32	7	3	-9	36	30	7	1	-10	41	41	6	7	-8	21	20
8	0	-6	216	210	7	5	-7	40	41	7	3	-11	29	27	7	0	9	26	29	6	6	3	26	24
8	0	-7	61	55	7	5	-8	35	33	7	2	9	19	21	7	0	7	21	15	6	6	2	38	39
8	0	-8	75	70	7	5	-9	26	22	7	2	7	27	33	7	0	6	79	81	6	6	1	24	25
7	8	3	23	23	7	4	8	19	4	7	2	6	25	24	7	0	5	28	30	6	6	0	39	41
7	8	2	22	13	7	4	7	29	31	7	2	5	25	28	7	0	4	61	59	6	6	-1	61	61
7	8	1	28	22	7	4	6	29	27	7	2	4	31	34	7	0	3	39	37	6	6	-3	51	52
7	8	-1	25	23	7	4	5	28	23	7	2	3	82	82	7	0	2	86	80	6	6	-5	68	66
7	8	-2	30	26	7	4	2	29	26	7	2	2	21	16	7	0	0	140	149	6	6	-6	25	20
7	8	-3	25	28	7	4	1	46	46	7	2	1	37	41	7	0	-1	47	51	6	6	-7	37	39
7	7	4	37	32	7	4	0	66	71	7	2	0	130	142	7	0	-2	32	30	6	6	-8	21	15
7	7	3	30	23	7	4	-1	60	69	7	2	-1	72	79	7	0	-3	119	122	6	6	-9	20	10
7	7	2	34	29	7	4	-2	54	57	7	2	-2	36	36	7	0	-4	160	162	6	5	7	40	39
7	7	-2	25	25	7	4	-3	100	110	7	2	-3	94	103	7	0	-5	105	100	6	5	6	22	22
7	7	-3	42	40	7	4	-4	88	90	7	2	-4	29	35	7	0	-6	157	156	6	5	5	32	27
7	7	-4	32	28	7	4	-5	87	88	7	2	-5	89	94	7	0	-8	54	57	6	5	4	33	35
7	7	-6	37	35	7	4	-6	40	41	7	2	-6	94	93	7	0	-10	20	11	6	5	3	111	114
7	6	6	24	22	7	4	-7	50	49	7	2	-8	35	35	6	9	0	27	28	6	5	1	38	39
7	6	5	22	18	7	4	-9	22	20	7	2	-10	25	22	6	9	-1	36	30	6	5	0	43	49
7	6	3	22	15	7	4	-10	31	25	7	1	8	28	29	6	8	4	19	26	6	5	-1	29	31
7	6	2	30	26	7	3	8	24	18	7	1	6	26	17	6	8	2	26	25	6	5	-2	22	18
7	6	1	27	27	7	3	7	25	23	7	1	5	57	54	6	8	0	32	29	6	5	-3	117	123
7	6	-1	62	64	7	3	6	27	29	7	1	4	92	91	6	8	-1	22	25	6	5	-4	53	52
7	6	-3	27	28	7	3	5	54	53	7	1	3	51	47	6	8	-2	25	27	6	5	-5	72	69
7	6	-6	30	32	7	3	4	33	34	7	1	2	86	91	6	8	-4	20	19	6	5	-6	63	64
7	6	-7	24	25	7	3	3	78	82	7	1	1	56	54	6	8	-6	25	22	6	5	-8	30	32

Table 29 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
6	5	-9	28	25	6	3	-11	27	26	6	1	-8	54	53	5	7	0	43	45	5	4	5	56	54
6	5	-10	34	25	6	2	10	25	25	6	1	-9	58	57	5	7	-1	45	43	5	4	4	63	63
6	4	8	33	35	6	2	6	33	33	6	1	-10	22	25	5	7	-2	25	19	5	4	3	104	100
6	4	6	28	24	6	2	5	82	84	6	1	-12	24	22	5	7	-4	22	24	5	4	2	89	86
6	4	4	70	69	6	2	4	46	47	6	0	10	35	36	5	7	-6	32	33	5	4	1	107	107
6	4	3	58	60	6	2	3	109	107	6	0	7	63	62	5	7	-7	26	26	5	4	0	109	120
6	4	2	46	47	6	2	1	63	64	6	0	6	27	28	5	6	7	23	23	5	4	-1	37	41
6	4	1	83	83	6	2	0	102	114	6	0	5	100	97	5	6	3	38	38	5	4	-2	79	84
6	4	0	62	65	6	2	-1	48	57	6	0	4	31	30	5	6	2	25	25	5	4	-3	57	55
6	4	-1	124	133	6	2	-2	96	105	6	0	3	74	75	5	6	1	62	59	5	4	-4	71	69
6	4	-2	77	81	6	2	-3	22	27	6	0	2	23	26	5	6	0	41	39	5	4	-5	49	50
6	4	-3	36	41	6	2	-4	64	61	6	0	1	89	85	5	6	-1	33	33	5	4	-6	32	30
6	4	-4	34	37	6	2	-5	77	77	6	0	0	253	258	5	6	-2	52	51	5	4	-7	70	66
6	4	-5	56	55	6	2	-6	138	128	6	0	-1	112	122	5	6	-3	82	83	5	4	-9	45	44
6	4	-6	72	73	6	2	-7	45	45	6	0	-2	48	44	5	6	-4	57	56	5	4	-10	31	36
6	4	-8	37	33	6	2	-8	69	67	6	0	-3	141	141	5	6	-5	61	61	5	3	10	19	18
6	4	-11	20	23	6	2	-9	43	46	6	0	-4	98	100	5	6	-6	20	15	5	3	9	22	18
6	3	7	57	58	6	2	-10	32	33	6	0	-5	115	118	5	5	9	20	24	5	3	8	20	19
6	3	6	19	23	6	2	-12	25	28	6	0	-6	38	43	5	5	8	40	38	5	3	7	38	41
6	3	5	127	127	6	1	9	35	39	6	0	-7	62	58	5	5	7	23	19	5	3	6	26	27
6	3	4	93	91	6	1	7	28	29	6	0	-10	26	27	5	5	5	59	58	5	3	5	46	47
6	3	3	82	85	6	1	6	73	71	5	9	1	27	28	5	5	4	53	59	5	3	4	55	57
6	3	2	184	188	6	1	5	87	88	5	9	-1	23	17	5	5	3	84	82	5	3	3	42	42
6	3	1	39	46	6	1	4	226	228	5	8	4	23	19	5	5	2	48	48	5	3	2	82	76
6	3	0	28	32	6	1	3	189	185	5	8	3	39	36	5	5	1	38	38	5	3	1	87	87
6	3	-1	41	44	6	1	2	82	81	5	8	2	40	39	5	5	0	80	79	5	3	0	77	77
6	3	-2	90	98	6	1	1	87	92	5	8	0	24	21	5	5	-1	108	110	5	3	-1	82	86
6	3	-3	107	106	6	1	0	44	55	5	8	-1	21	21	5	5	-2	66	65	5	3	-2	69	66
6	3	-4	38	44	6	1	-1	63	69	5	8	-4	27	22	5	5	-3	89	88	5	3	-3	113	114
6	3	-5	111	108	6	1	-2	91	102	5	8	-5	23	17	5	5	-5	50	53	5	3	-4	86	86
6	3	-6	70	72	6	1	-3	49	48	5	7	7	23	23	5	5	-7	37	33	5	3	-5	72	68
6	3	-7	20	16	6	1	-4	158	163	5	7	5	23	22	5	5	-8	45	45	5	3	-7	114	115
6	3	-8	46	47	6	1	-5	35	33	5	7	4	34	35	5	5	-9	20	22	5	3	-8	36	37
6	3	-9	23	21	6	1	-6	74	73	5	7	3	55	57	5	4	9	40	39	5	3	-9	32	30
6	3	-10	20	20	6	1	-7	147	143	5	7	2	36	34	5	4	6	56	57	5	3	-10	40	39

Table 29 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	3	-11	31	33	5	1	-4	111	99	4	8	-1	21	28	4	5	1	73	76	4	3	1	98	100
5	3	-12	35	40	5	1	-5	55	59	4	8	-2	48	47	4	5	0	116	120	4	3	0	113	119
5	2	11	22	16	5	1	-6	34	37	4	8	-4	21	22	4	5	-1	63	60	4	3	-1	91	98
5	2	10	24	25	5	1	-7	119	115	4	8	-7	21	26	4	5	-2	64	66	4	3	-2	43	44
5	2	9	41	43	5	1	-8	34	34	4	7	5	31	29	4	5	-4	95	97	4	3	-3	249	236
5	2	7	40	40	5	1	-9	32	31	4	7	3	21	18	4	5	-5	32	30	4	3	-4	144	134
5	2	6	100	104	5	1	-10	44	48	4	7	1	61	59	4	5	-6	22	20	4	3	-5	143	131
5	2	5	50	50	5	1	-11	30	32	4	7	0	26	27	4	5	-8	41	40	4	3	-6	58	57
5	2	4	35	36	5	1	-12	30	30	4	7	-1	33	38	4	5	-9	36	36	4	3	-7	94	91
5	2	3	69	66	5	0	10	28	31	4	7	-2	29	25	4	4	8	23	26	4	3	-8	44	47
5	2	2	227	226	5	0	8	40	42	4	7	-3	36	35	4	4	7	21	18	4	3	-10	37	37
5	2	1	129	135	5	0	7	80	86	4	7	-4	30	30	4	4	6	50	51	4	3	-12	22	28
5	2	0	211	223	5	0	6	41	39	4	7	-5	36	37	4	4	5	88	90	4	2	11	35	41
5	2	-1	113	125	5	0	5	124	117	4	7	-6	30	28	4	4	3	35	31	4	2	9	36	36
5	2	-2	154	159	5	0	4	63	58	4	7	-7	25	21	4	4	2	39	37	4	2	8	41	44
5	2	-3	61	63	5	0	3	222	208	4	7	-8	41	41	4	4	1	63	66	4	2	7	41	42
5	2	-4	150	145	5	0	2	257	248	4	6	8	27	27	4	4	0	87	89	4	2	6	28	27
5	2	-6	57	56	5	0	1	235	225	4	6	5	28	22	4	4	-1	59	58	4	2	5	123	126
5	2	-7	55	60	5	0	-1	277	307	4	6	4	28	30	4	4	-2	153	152	4	2	4	102	98
5	2	-8	90	92	5	0	-2	92	93	4	6	2	61	62	4	4	-3	76	73	4	2	3	52	50
5	2	-9	28	30	5	0	-3	50	49	4	6	1	84	84	4	4	-4	120	118	4	2	2	141	132
5	2	-10	29	30	5	0	-4	87	81	4	6	0	33	37	4	4	-5	142	135	4	2	1	173	173
5	2	-11	52	56	5	0	-5	112	118	4	6	-1	90	87	4	4	-6	35	33	4	2	0	36	33
5	1	10	35	34	5	0	-6	21	16	4	6	-2	45	45	4	4	-7	55	56	4	2	-1	214	233
5	1	8	27	32	5	0	-7	57	56	4	6	-3	51	49	4	4	-8	26	25	4	2	-2	161	160
5	1	6	33	28	5	0	-8	128	131	4	6	-5	35	34	4	4	-10	20	14	4	2	-3	57	58
5	1	5	76	76	5	0	-11	21	22	4	6	-6	42	41	4	3	10	20	16	4	2	-4	170	170
5	1	4	63	60	4	9	3	32	33	4	6	-7	45	49	4	3	9	33	32	4	2	-5	80	74
5	1	3	153	146	4	9	2	22	20	4	6	-9	31	34	4	3	8	36	37	4	2	-7	104	107
5	1	2	173	172	4	9	-1	21	17	4	5	9	28	30	4	3	7	36	35	4	2	-8	111	110
5	1	1	173	166	4	9	-3	31	32	4	5	7	20	10	4	3	6	97	93	4	2	-9	41	42
5	1	0	68	69	4	9	-5	22	16	4	5	6	21	27	4	3	5	55	51	4	2	-10	31	33
5	1	-1	113	119	4	8	3	23	19	4	5	5	27	23	4	3	4	26	27	4	2	-11	33	29
5	1	-2	167	186	4	8	2	29	29	4	5	4	67	65	4	3	3	49	44	4	1	11	21	13
5	1	-3	164	168	4	8	1	23	22	4	5	2	47	45	4	3	2	108	114	4	1	10	33	31

Table 29 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	1	9	36	41	4	0	-8	87	90	3	6	-3	103	107	3	4	-2	113	107	3	2	5	84	80
4	1	8	23	23	4	0	-9	20	17	3	6	-4	59	58	3	4	-3	53	54	3	2	4	211	199
4	1	7	79	78	4	0	-11	69	72	3	6	-5	31	27	3	4	-4	70	72	3	2	3	221	204
4	1	6	111	111	3	9	3	20	13	3	6	-6	30	30	3	4	-5	68	61	3	2	2	200	185
4	1	5	78	74	3	9	2	22	21	3	6	-7	46	49	3	4	-6	120	116	3	2	1	318	326
4	1	4	102	94	3	9	0	19	21	3	6	-8	19	20	3	4	-7	84	85	3	2	0	75	86
4	1	3	19	13	3	9	-2	30	25	3	6	-9	36	38	3	4	-8	88	91	3	2	-1	81	92
4	1	2	133	121	3	8	6	21	23	3	5	10	27	27	3	4	-9	32	33	3	2	-2	219	211
4	1	1	102	105	3	8	3	20	25	3	5	8	20	23	3	4	-10	26	24	3	2	-3	166	137
4	1	0	246	258	3	8	1	46	44	3	5	7	19	16	3	3	11	32	34	3	2	-4	107	93
4	1	-1	84	95	3	8	-3	33	35	3	5	6	27	29	3	3	9	59	62	3	2	-5	255	235
4	1	-2	91	87	3	8	-5	21	25	3	5	4	107	102	3	3	8	33	33	3	2	-6	187	179
4	1	-3	250	223	3	7	8	28	24	3	5	3	128	124	3	3	7	43	49	3	2	-7	130	131
4	1	-4	284	265	3	7	4	29	24	3	5	2	141	140	3	3	6	54	55	3	2	-8	130	136
4	1	-5	218	202	3	7	3	35	33	3	5	1	35	34	3	3	5	170	165	3	2	-9	37	35
4	1	-6	61	59	3	7	2	69	70	3	5	0	78	78	3	3	4	54	49	3	2	-11	40	40
4	1	-7	85	87	3	7	1	25	29	3	5	-1	33	39	3	3	3	283	270	3	2	-12	32	34
4	1	-8	59	55	3	7	0	62	64	3	5	-3	26	29	3	3	2	140	144	3	1	12	26	19
4	1	-9	24	24	3	7	-1	97	95	3	5	-4	51	52	3	3	1	170	168	3	1	11	26	27
4	1	-11	32	33	3	7	-2	42	44	3	5	-5	122	120	3	3	0	20	21	3	1	10	38	41
4	1	-12	40	41	3	7	-4	24	27	3	5	-6	46	43	3	3	-1	85	86	3	1	9	52	55
4	0	11	38	35	3	7	-5	34	35	3	5	-7	43	43	3	3	-2	151	129	3	1	8	41	45
4	0	10	34	39	3	7	-6	31	31	3	5	-8	28	25	3	3	-3	119	104	3	1	7	73	75
4	0	9	37	35	3	7	-7	19	20	3	5	-9	28	25	3	3	-4	141	129	3	1	6	70	64
4	0	8	98	100	3	7	-8	32	32	3	5	-11	21	22	3	3	-5	28	26	3	1	5	61	61
4	0	5	168	160	3	7	-9	27	31	3	4	10	24	21	3	3	-6	48	48	3	1	4	212	200
4	0	3	109	110	3	6	6	36	35	3	4	8	62	59	3	3	-7	83	80	3	1	3	175	171
4	0	2	37	37	3	6	5	26	26	3	4	7	64	68	3	3	-8	48	45	3	1	2	118	97
4	0	1	115	97	3	6	4	56	55	3	4	6	95	93	3	3	-9	44	44	3	1	1	82	75
4	0	0	119	114	3	6	3	36	40	3	4	5	94	91	3	3	-10	24	24	3	1	0	117	120
4	0	-2	82	78	3	6	2	103	96	3	4	4	94	95	3	3	-12	35	37	3	1	-1	197	226
4	0	-3	266	255	3	6	1	66	65	3	4	3	68	68	3	2	11	23	20	3	1	-2	258	255
4	0	-4	157	137	3	6	0	64	69	3	4	2	163	152	3	2	8	56	58	3	1	-3	150	142
4	0	-5	63	60	3	6	-1	38	39	3	4	1	170	178	3	2	7	36	31	3	1	-4	301	270
4	0	-6	41	42	3	6	-2	145	144	3	4	-1	66	66	3	2	6	79	77	3	1	-5	127	124

Table 29 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	1	-6	28	25	2	8	-1	36	38	2	5	9	22	19	2	3	7	58	57	2	2	-7	108	105
3	1	-7	28	30	2	8	-2	38	36	2	5	8	22	22	2	3	6	109	107	2	2	-8	113	121
3	1	-9	73	74	2	8	-3	39	39	2	5	7	51	51	2	3	4	241	219	2	2	-9	83	84
3	1	-10	50	53	2	8	-4	24	24	2	5	6	38	36	2	3	3	73	70	2	2	-11	23	27
3	1	-12	39	39	2	8	-6	54	56	2	5	4	83	79	2	3	2	84	78	2	2	-12	27	29
3	0	12	32	26	2	7	8	27	23	2	5	3	98	95	2	3	1	136	125	2	1	10	43	45
3	0	11	25	20	2	7	7	24	23	2	5	2	49	47	2	3	0	49	53	2	1	8	30	27
3	0	10	43	48	2	7	6	55	51	2	5	0	144	147	2	3	-1	237	225	2	1	7	123	124
3	0	9	35	32	2	7	5	22	23	2	5	-1	138	135	2	3	-2	85	79	2	1	6	71	69
3	0	8	53	50	2	7	4	54	51	2	5	-2	26	22	2	3	-3	66	65	2	1	5	101	95
3	0	7	33	34	2	7	3	37	31	2	5	-3	85	85	2	3	-4	124	115	2	1	4	182	163
3	0	6	66	65	2	7	2	48	50	2	5	-4	47	50	2	3	-5	73	67	2	1	3	283	250
3	0	5	72	72	2	7	0	40	41	2	5	-5	52	48	2	3	-6	60	61	2	1	2	356	346
3	0	4	125	112	2	7	-2	20	19	2	5	-6	19	20	2	3	-7	60	60	2	1	1	374	483
3	0	2	238	232	2	7	-3	46	48	2	5	-7	32	34	2	3	-8	106	107	2	1	0	81	85
3	0	1	405	477	2	7	-4	35	38	2	5	-9	39	40	2	3	-10	32	36	2	1	-1	267	336
3	0	0	245	285	2	7	-5	30	26	2	5	-11	22	25	2	3	-11	30	29	2	1	-2	200	193
3	0	-2	218	206	2	7	-6	39	43	2	4	10	23	24	2	2	11	27	30	2	1	-3	211	197
3	0	-3	127	107	2	7	-8	24	20	2	4	9	36	34	2	2	10	19	23	2	1	-4	150	134
3	0	-4	364	342	2	6	9	23	24	2	4	8	39	42	2	2	9	53	56	2	1	-5	116	99
3	0	-5	281	244	2	6	8	30	26	2	4	4	38	39	2	2	8	74	78	2	1	-6	62	62
3	0	-6	103	105	2	6	7	39	39	2	4	3	101	100	2	2	7	132	132	2	1	-7	139	134
3	0	-7	253	245	2	6	6	29	33	2	4	2	122	113	2	2	6	131	124	2	1	-8	77	77
3	0	-8	134	137	2	6	4	78	76	2	4	1	153	141	2	2	5	140	131	2	1	-9	43	43
3	0	-9	21	17	2	6	3	29	26	2	4	0	191	192	2	2	4	93	84	2	1	-10	48	45
3	0	-11	52	58	2	6	2	78	75	2	4	-1	51	50	2	2	3	145	122	2	1	-11	21	22
2	9	2	36	29	2	6	1	87	84	2	4	-2	61	56	2	2	2	188	168	2	1	-12	47	51
2	9	-2	27	25	2	6	0	107	102	2	4	-5	92	87	2	2	1	334	349	2	0	12	31	33
2	9	-5	48	49	2	6	-1	85	89	2	4	-6	66	62	2	2	0	276	296	2	0	11	31	32
2	8	6	23	17	2	6	-2	45	41	2	4	-7	99	101	2	2	-1	52	58	2	0	10	23	26
2	8	5	42	38	2	6	-5	28	25	2	4	-8	45	49	2	2	-2	146	154	2	0	9	35	36
2	8	3	29	32	2	6	-6	27	27	2	4	-9	55	59	2	2	-3	46	46	2	0	8	137	145
2	8	2	52	52	2	6	-7	51	53	2	4	-10	23	25	2	2	-4	178	158	2	0	7	81	79
2	8	1	42	45	2	6	-8	19	17	2	3	9	20	20	2	2	-5	106	96	2	0	6	24	25
2	8	0	23	22	2	6	-9	23	27	2	3	8	45	47	2	2	-6	92	89	2	0	4	100	81

Table 29 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	Fc	H	K	L	FO	FC
2	0	3	167	166	1	7	-1	22	22	1	5	-3	114	118	1	3	1	116	113	1	1	5	92	90
2	0	2	219	175	1	7	-2	42	48	1	5	-4	80	83	1	3	0	176	159	1	1	4	353	332
2	0	1	57	55	1	7	-3	69	73	1	5	-5	76	78	1	3	-1	215	198	1	1	3	156	144
2	0	0	235	291	1	7	-4	27	30	1	5	-6	62	64	1	3	-2	143	148	1	1	1	206	191
2	0	-2	55	60	1	7	-5	44	46	1	5	-7	48	51	1	3	-3	231	221	1	1	-2	67	72
2	0	-3	100	80	1	7	-6	34	38	1	5	-8	30	32	1	3	-4	87	88	1	1	-3	217	196
2	0	-4	220	193	1	7	-7	37	38	1	5	-9	25	27	1	3	-5	139	128	1	1	-4	255	236
2	0	-5	19	19	1	6	10	43	44	1	4	10	26	29	1	3	-6	108	101	1	1	-5	139	128
2	0	-6	128	122	1	6	9	23	23	1	4	9	41	43	1	3	-8	26	26	1	1	-6	76	69
2	0	-7	86	82	1	6	6	23	23	1	4	8	53	55	1	3	-9	44	43	1	1	-7	112	108
2	0	-8	115	118	1	6	4	20	18	1	4	7	84	83	1	3	-11	31	36	1	1	-8	64	66
2	0	-9	64	65	1	6	3	21	24	1	4	6	70	68	1	2	10	36	32	1	1	-9	58	53
2	0	-10	37	36	1	6	2	62	64	1	4	5	33	32	1	2	9	34	39	1	1	-10	55	56
1	9	4	24	23	1	6	1	139	131	1	4	4	49	53	1	2	8	26	28	1	1	-11	20	23
1	9	0	21	20	1	6	0	35	32	1	4	3	75	63	1	2	7	68	66	1	1	-12	24	25
1	9	-2	21	26	1	6	-1	90	94	1	4	2	76	71	1	2	6	32	29	1	0	11	20	13
1	9	-5	21	20	1	6	-2	49	48	1	4	1	174	167	1	2	5	64	62	1	0	9	40	42
1	8	7	25	23	1	6	-3	62	67	1	4	0	201	189	1	2	4	291	273	1	0	8	22	18
1	8	6	23	22	1	6	-4	41	43	1	4	-1	109	105	1	2	3	288	271	1	0	7	41	38
1	8	3	32	26	1	6	-5	27	32	1	4	-2	21	20	1	2	2	244	221	1	0	6	41	37
1	8	2	30	29	1	6	-7	38	38	1	4	-3	162	156	1	2	1	174	164	1	0	5	116	105
1	8	1	34	36	1	6	-8	58	61	1	4	-4	136	133	1	2	-1	159	127	1	0	4	136	117
1	8	0	33	35	1	6	-9	20	18	1	4	-5	117	116	1	2	-2	157	150	1	0	3	234	199
1	8	-1	46	51	1	5	10	30	31	1	4	-6	66	64	1	2	-3	179	160	1	0	2	285	260
1	8	-2	37	38	1	5	8	24	22	1	4	-7	97	101	1	2	-4	85	74	1	0	1	316	387
1	8	-4	51	53	1	5	7	22	24	1	4	-8	30	33	1	2	-5	101	97	1	0	0	181	200
1	8	-5	32	33	1	5	6	55	54	1	3	11	21	24	1	2	-6	68	67	1	0	-1	154	119
1	8	-6	22	28	1	5	5	131	123	1	3	9	22	23	1	2	-7	37	35	1	0	-2	233	210
1	8	-7	26	32	1	5	4	50	44	1	3	8	41	43	1	2	-8	94	95	1	0	-3	302	300
1	7	8	27	23	1	5	3	100	100	1	3	7	59	62	1	2	-9	63	66	1	0	-4	56	55
1	7	7	22	17	1	5	2	77	75	1	3	6	66	65	1	1	12	25	25	1	0	-5	20	18
1	7	4	23	19	1	5	1	66	71	1	3	5	120	113	1	1	11	36	37	1	0	-6	119	110
1	7	2	23	24	1	5	0	76	75	1	3	4	192	183	1	1	9	41	45	1	0	-7	100	99
1	7	1	25	18	1	5	-1	114	118	1	3	3	282	254	1	1	8	49	45	1	0	-8	101	106
1	7	0	30	33	1	5	-2	69	67	1	3	2	167	146	1	1	6	27	29	1	0	-10	26	28

Table 29 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	0	-11	34	36	0	4	4	79	79	0	0	12	25	23										
1	0	-12	45	49	0	4	3	137	123	0	0	10	34	32										
0	9	4	20	18	0	4	2	38	35	0	0	9	21	21										
0	9	3	27	27	0	4	1	406	387	0	0	7	134	128										
0	9	2	25	26	0	4	0	225	206	0	0	6	40	41										
0	9	1	20	21	0	3	10	46	44	0	0	5	84	84										
0	8	7	21	22	0	3	9	40	37	0	0	4	119	90										
0	8	2	37	36	0	3	8	38	36	0	0	3	60	61										
0	8	1	45	46	0	3	7	113	119	0	0	2	348	395										
0	8	0	31	29	0	3	6	75	79	0	0	1	104	90										
0	7	9	24	21	0	3	5	145	135															
0	7	6	40	43	0	3	4	62	60															
0	7	5	24	23	0	3	3	96	100															
0	7	4	50	51	0	3	2	65	54															
0	7	3	68	68	0	3	1	20	23															
0	7	2	33	31	0	2	11	42	45															
0	7	1	63	67	0	2	10	24	22															
0	6	9	25	21	0	2	9	21	20															
0	6	7	30	28	0	2	8	64	69															
0	6	4	97	101	0	2	7	92	88															
0	6	3	106	107	0	2	6	51	51															
0	6	2	53	51	0	2	5	106	102															
0	6	1	84	87	0	2	4	90	81															
0	6	0	148	139	0	2	3	92	81															
0	5	11	19	17	0	2	2	366	366															
0	5	10	32	30	0	1	11	33	31															
0	5	8	35	35	0	1	10	44	47															
0	5	7	38	37	0	1	9	26	24															
0	5	6	45	42	0	1	8	67	65															
0	5	5	90	91	0	1	7	79	83															
0	5	3	60	61	0	1	6	38	39															
0	5	2	76	78	0	1	5	156	134															
0	4	7	30	31	0	1	4	205	175															
0	4	6	89	89	0	1	3	377	365															
0	4	5	85	81	0	1	2	387	434															

Table 30 Structure factor listings ($|F_o|$ and $|F_c|$ x 10)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
8	5	0	25	45	7	12	3	42	43	7	4	2	18	24	6	25	3	82	71	6	18	1	55	35
8	4	0	23	76	7	12	2	21	26	7	4	1	25	39	6	25	2	29	22	6	18	0	44	47
8	3	1	39	44	7	12	1	20	15	7	4	0	28	39	6	24	2	27	27	6	17	6	22	23
8	3	0	23	13	7	12	0	22	42	7	3	4	28	20	6	24	0	61	65	6	17	4	42	25
8	2	1	28	24	7	11	5	23	20	7	3	2	48	53	6	23	4	41	40	6	17	1	78	76
8	1	1	51	47	7	11	4	35	19	7	3	1	61	64	6	23	3	53	47	6	17	0	28	47
8	0	1	22	0	7	11	2	55	47	7	3	0	21	44	6	23	2	23	22	6	16	5	24	11
8	0	0	36	79	7	11	1	17	16	7	2	5	29	24	6	23	1	27	34	6	16	3	23	37
7	23	1	34	20	7	10	4	23	11	7	2	4	43	35	6	23	0	31	25	6	16	2	23	14
7	23	0	29	11	7	10	2	30	38	7	2	1	97	76	6	22	5	41	38	6	16	1	22	24
7	22	0	20	27	7	10	1	33	37	7	1	5	25	18	6	22	4	42	45	6	16	0	50	64
7	21	2	27	12	7	9	5	17	19	7	1	4	17	18	6	22	3	21	17	6	15	6	20	23
7	21	1	32	21	7	9	4	23	15	7	1	3	28	23	6	22	2	24	18	6	15	5	32	36
7	21	0	17	11	7	9	3	29	27	7	1	2	64	66	6	22	1	66	64	6	15	4	41	45
7	20	2	27	24	7	9	2	75	63	7	1	1	80	66	6	22	0	36	32	6	15	3	70	66
7	20	0	27	20	7	9	1	48	43	7	0	5	37	26	6	21	4	32	22	6	15	2	29	17
7	19	3	30	28	7	9	0	25	46	7	0	3	40	44	6	21	1	94	94	6	15	1	109	114
7	19	2	35	29	7	8	5	44	31	7	0	2	51	63	6	21	0	25	15	6	15	0	36	47
7	19	1	18	27	7	8	4	28	21	7	0	1	30	43	6	20	5	31	22	6	14	5	35	25
7	18	3	28	16	7	8	3	71	69	6	31	1	31	32	6	20	4	28	27	6	14	4	40	30
7	18	1	18	14	7	7	5	26	25	6	31	0	54	41	6	20	3	40	31	6	14	3	40	23
7	17	3	27	34	7	7	4	35	40	6	30	1	50	36	6	20	2	52	44	6	14	2	38	37
7	17	1	20	16	7	7	3	21	30	6	30	0	19	3	6	20	1	27	30	6	14	1	96	97
7	17	0	24	6	7	7	2	27	15	6	29	3	24	24	6	20	0	68	74	6	14	0	74	106
7	16	4	26	18	7	7	1	37	49	6	29	1	25	17	6	19	6	37	38	6	13	6	25	16
7	16	3	29	16	7	6	5	28	23	6	29	0	23	26	6	19	5	48	46	6	13	4	69	50
7	16	2	34	34	7	6	4	32	34	6	28	2	47	41	6	19	4	21	33	6	13	3	51	54
7	16	1	23	22	7	6	2	21	14	6	28	1	26	23	6	19	2	22	24	6	13	2	97	80
7	16	0	31	44	7	6	1	36	36	6	27	2	32	30	6	19	1	67	63	6	13	1	30	25
7	15	4	29	19	7	6	0	25	67	6	27	1	25	30	6	19	0	55	52	6	12	7	29	22
7	15	0	23	22	7	5	5	35	27	6	26	4	62	46	6	18	6	50	34	6	12	6	21	24
7	13	4	17	12	7	5	4	40	32	6	26	3	61	46	6	18	5	22	12	6	12	5	29	29
7	13	2	28	26	7	5	0	20	58	6	26	2	32	31	6	18	4	50	48	6	12	3	43	26
7	13	1	40	40	7	4	4	20	20	6	26	1	41	48	6	18	3	32	17	6	12	1	36	36
7	12	4	35	27	7	4	3	32	32	6	26	0	20	3	6	18	2	54	59	6	11	7	29	14

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
6	11	6	35	17	6	6	7	49	43	6	1	7	23	31	5	30	4	38	38	5	23	4	27	29
6	11	4	80	75	6	6	6	26	24	6	1	6	47	45	5	30	2	84	75	5	23	2	65	63
6	11	3	34	34	6	6	5	21	23	6	1	5	88	94	5	29	5	22	7	5	23	1	27	26
6	11	2	48	41	6	6	4	49	35	6	1	4	68	66	5	29	4	40	39	5	23	0	40	40
6	11	1	23	16	6	6	3	97	88	6	1	3	57	58	5	29	3	51	51	5	22	7	36	41
6	11	0	38	65	6	6	2	23	2	6	1	2	49	41	5	29	1	34	38	5	22	5	92	86
6	10	7	29	21	6	6	1	76	83	6	1	1	29	17	5	29	0	77	70	5	22	3	75	64
6	10	6	24	23	6	6	0	23	80	6	1	0	20	48	5	28	5	47	47	5	22	2	72	62
6	10	5	49	43	6	5	7	27	10	6	0	7	29	22	5	28	3	42	40	5	22	1	81	80
6	10	4	87	89	6	5	6	24	20	6	0	6	50	47	5	28	2	25	26	5	22	0	22	17
6	10	3	44	59	6	5	5	61	60	6	0	5	22	12	5	28	1	49	43	5	21	7	27	21
6	10	2	17	23	6	5	4	31	16	6	0	4	58	52	5	28	0	56	61	5	21	6	47	27
6	10	1	46	47	6	5	3	119	110	6	0	3	128	113	5	27	6	37	30	5	21	4	30	26
6	10	0	22	18	6	5	2	40	39	6	0	2	97	77	5	27	5	71	61	5	21	3	50	47
6	9	7	31	18	6	5	1	59	68	6	0	1	68	61	5	27	4	45	31	5	21	2	56	58
6	9	5	80	63	6	5	0	44	97	5	37	0	18	12	5	27	3	28	21	5	21	1	128	116
6	9	4	78	75	6	4	7	24	27	5	36	2	46	36	5	27	2	23	35	5	21	0	42	38
6	9	3	25	13	6	4	6	33	47	5	35	1	43	40	5	27	1	55	45	5	20	6	41	44
6	9	2	112	113	6	4	5	31	6	5	35	0	26	35	5	27	0	43	39	5	20	5	51	42
6	9	1	53	50	6	4	4	56	48	5	34	3	19	15	5	26	5	22	24	5	20	4	38	38
6	9	0	55	110	6	4	3	85	86	5	34	2	31	45	5	26	3	74	71	5	20	3	69	61
6	8	6	35	38	6	4	2	93	85	5	34	0	20	5	5	26	2	35	33	5	20	2	30	43
6	8	5	40	43	6	4	1	103	98	5	33	4	39	39	5	26	0	82	73	5	20	1	89	92
6	8	4	49	35	6	4	0	39	117	5	33	3	28	26	5	25	6	27	26	5	20	0	111	121
6	8	3	48	35	6	3	7	21	23	5	33	1	32	27	5	25	5	58	50	5	19	7	28	26
6	8	2	39	30	6	3	6	27	27	5	32	4	41	35	5	25	4	28	18	5	19	6	34	29
6	8	1	94	76	6	3	5	45	49	5	32	3	28	36	5	25	3	41	41	5	19	4	79	71
6	7	7	46	47	6	3	4	47	35	5	32	2	33	30	5	25	2	24	13	5	19	2	128	121
6	7	6	21	39	6	3	2	85	74	5	32	1	46	45	5	25	1	31	45	5	19	1	87	87
6	7	5	54	56	6	3	1	45	47	5	32	0	54	54	5	24	6	69	59	5	19	0	57	60
6	7	4	63	57	6	2	7	32	34	5	31	4	43	38	5	24	4	23	24	5	18	7	21	8
6	7	3	51	72	6	2	6	19	18	5	31	2	21	31	5	24	3	54	39	5	18	6	37	37
6	7	2	35	21	6	2	4	100	76	5	31	1	60	51	5	24	0	90	83	5	18	5	63	50
6	7	1	50	37	6	2	3	62	64	5	31	0	20	14	5	23	7	20	27	5	18	4	20	15
6	7	0	21	20	6	2	2	99	95	5	30	5	33	36	5	23	6	27	24	5	18	3	42	36

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	18	1	92	83	5	13	6	36	20	5	9	3	77	81	5	4	8	29	18	5	0	3	152	142
5	18	0	142	157	5	13	5	18	16	5	9	2	37	30	5	4	7	57	59	5	0	2	150	135
5	17	6	25	15	5	13	4	20	12	5	9	1	108	109	5	4	6	105	101	5	0	1	110	103
5	17	5	45	40	5	13	3	78	71	5	9	0	34	74	5	4	5	83	81	4	39	2	55	38
5	17	4	34	34	5	13	2	163	151	5	8	6	70	61	5	4	4	153	157	4	38	3	26	26
5	17	3	92	71	5	13	1	55	64	5	8	5	67	49	5	4	3	61	63	4	38	2	22	7
5	17	2	129	124	5	13	0	35	38	5	8	4	90	82	5	4	2	173	156	4	37	4	24	20
5	17	1	59	63	5	12	8	30	17	5	8	3	67	80	5	4	0	38	117	4	37	0	37	33
5	17	0	31	64	5	12	6	25	17	5	8	2	110	93	5	3	8	23	16	4	36	4	17	11
5	16	8	35	28	5	12	5	24	21	5	8	1	105	97	5	3	7	33	28	4	36	3	65	59
5	16	7	45	42	5	12	4	108	111	5	8	0	30	51	5	3	6	33	27	4	36	1	66	61
5	16	6	29	42	5	12	3	104	90	5	7	8	35	19	5	3	5	27	20	4	35	4	28	23
5	16	5	20	40	5	12	2	104	104	5	7	7	18	13	5	3	4	87	86	4	35	3	30	31
5	16	4	79	86	5	12	1	68	49	5	7	6	25	17	5	3	3	171	162	4	35	2	65	61
5	16	3	47	37	5	11	8	40	43	5	7	4	72	73	5	3	2	79	68	4	35	0	29	31
5	16	2	23	20	5	11	7	20	28	5	7	3	104	101	5	3	1	25	43	4	34	5	19	11
5	16	1	143	144	5	11	5	57	55	5	7	2	179	148	5	3	0	40	107	4	34	4	19	13
5	16	0	114	146	5	11	4	43	27	5	7	1	79	62	5	2	8	27	37	4	34	3	31	31
5	15	8	37	35	5	11	3	141	124	5	7	0	72	141	5	2	7	67	62	4	33	5	18	18
5	15	7	29	34	5	11	2	165	152	5	6	8	31	19	5	2	6	39	34	4	33	4	36	33
5	15	5	33	30	5	11	1	64	63	5	6	7	43	30	5	2	5	47	53	4	33	2	26	29
5	15	4	51	46	5	11	0	27	45	5	6	6	54	50	5	2	4	74	73	4	33	1	19	10
5	15	3	20	25	5	10	8	28	27	5	6	5	72	63	5	2	3	31	25	4	33	0	71	72
5	15	2	105	95	5	10	7	43	43	5	6	4	128	134	5	2	2	55	49	4	32	4	31	12
5	15	1	52	54	5	10	6	70	62	5	6	3	118	119	5	2	1	65	52	4	32	3	79	68
5	15	0	31	48	5	10	5	56	49	5	6	2	52	52	5	1	8	41	35	4	32	2	21	21
5	14	7	56	60	5	10	4	60	61	5	6	1	75	79	5	1	7	35	27	4	32	1	89	93
5	14	6	78	66	5	10	3	96	92	5	6	0	45	103	5	1	6	78	70	4	32	0	28	26
5	14	5	56	46	5	10	2	79	77	5	5	8	29	33	5	1	5	81	82	4	31	6	40	36
5	14	4	102	89	5	10	1	129	109	5	5	7	28	30	5	1	4	43	49	4	31	5	29	29
5	14	3	109	106	5	10	0	67	105	5	5	6	47	40	5	1	3	176	177	4	31	4	35	39
5	14	2	139	127	5	9	8	33	38	5	5	4	45	53	5	1	2	33	38	4	31	3	33	22
5	14	1	63	70	5	9	7	20	43	5	5	3	75	53	5	1	1	168	178	4	31	1	32	26
5	13	8	48	41	5	9	5	137	125	5	5	2	53	55	5	0	5	40	46	4	31	0	27	24
5	13	7	29	34	5	9	4	53	53	5	5	1	111	103	5	0	4	129	120	4	30	6	19	27

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	30	4	30	19	4	25	2	30	27	4	20	5	95	88	4	16	4	112	98	4	12	4	159	162
4	30	2	39	51	4	25	1	113	106	4	20	4	133	129	4	16	3	112	103	4	12	3	52	53
4	30	1	53	55	4	25	0	80	64	4	20	3	128	126	4	16	2	134	136	4	12	2	208	174
4	30	0	37	34	4	24	8	44	37	4	20	2	129	128	4	16	1	211	208	4	12	1	22	43
4	29	7	20	28	4	24	7	50	37	4	20	1	85	83	4	16	0	90	90	4	12	0	93	102
4	29	5	35	37	4	24	5	69	68	4	20	0	62	52	4	15	7	66	67	4	11	9	17	26
4	29	4	37	38	4	24	4	42	54	4	19	8	26	23	4	15	6	63	58	4	11	8	50	56
4	29	3	50	52	4	24	3	53	41	4	19	7	34	33	4	15	5	92	102	4	11	7	90	88
4	29	2	32	35	4	24	2	163	159	4	19	5	100	98	4	15	4	77	74	4	11	6	43	42
4	29	1	91	93	4	24	1	47	56	4	19	4	57	67	4	15	3	124	124	4	11	5	85	89
4	29	0	65	68	4	24	0	79	79	4	19	3	104	101	4	15	2	214	208	4	11	4	104	100
4	28	7	28	22	4	23	7	18	26	4	19	2	190	174	4	15	1	60	81	4	11	3	160	150
4	28	6	42	40	4	23	6	27	10	4	19	1	101	111	4	15	0	143	159	4	11	2	47	55
4	28	5	37	49	4	23	5	67	61	4	19	0	113	121	4	14	9	28	25	4	11	1	97	109
4	28	3	41	41	4	23	4	68	67	4	18	8	60	58	4	14	7	34	28	4	11	0	19	41
4	28	2	21	27	4	23	3	24	27	4	18	7	23	31	4	14	6	22	17	4	10	9	21	13
4	28	1	28	27	4	23	2	39	38	4	18	6	36	41	4	14	5	42	42	4	10	8	25	23
4	27	7	32	39	4	23	1	85	83	4	18	5	63	65	4	14	4	39	39	4	10	7	49	43
4	27	6	56	52	4	23	0	34	31	4	18	4	111	116	4	14	3	109	103	4	10	6	56	57
4	27	5	41	37	4	22	7	25	9	4	18	3	54	39	4	14	2	92	84	4	10	5	120	112
4	27	4	48	44	4	22	6	72	61	4	18	2	181	185	4	14	1	84	87	4	10	4	98	101
4	27	3	53	55	4	22	5	57	62	4	18	1	170	171	4	13	9	37	35	4	10	3	64	56
4	27	2	89	89	4	22	4	68	63	4	17	9	26	30	4	13	8	31	30	4	10	2	85	82
4	27	1	75	75	4	22	3	66	60	4	17	8	20	20	4	13	7	32	31	4	10	1	60	44
4	26	7	19	20	4	22	2	197	204	4	17	7	26	25	4	13	6	79	79	4	10	0	72	71
4	26	5	25	19	4	22	1	60	63	4	17	6	35	41	4	13	5	206	184	4	9	9	31	13
4	26	4	47	38	4	22	0	32	15	4	17	5	134	135	4	13	4	64	55	4	9	8	73	75
4	26	3	23	28	4	21	7	50	47	4	17	4	153	151	4	13	3	79	75	4	9	7	38	30
4	26	1	33	33	4	21	5	80	79	4	17	3	113	106	4	13	2	40	48	4	9	6	109	120
4	26	0	38	32	4	21	4	19	17	4	17	2	68	57	4	13	1	115	115	4	9	5	140	141
4	25	7	38	41	4	21	3	72	84	4	17	1	114	121	4	13	0	73	79	4	9	3	201	196
4	25	6	34	30	4	21	2	69	67	4	17	0	57	49	4	12	8	41	37	4	9	2	53	30
4	25	5	49	42	4	21	1	184	182	4	16	8	32	41	4	12	7	44	34	4	9	1	108	114
4	25	4	20	7	4	21	0	38	38	4	16	6	48	41	4	12	6	64	55	4	8	9	40	46
4	25	3	98	102	4	20	7	18	28	4	16	5	94	83	4	12	5	104	106	4	8	8	34	34

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	8	7	36	34	4	5	0	17	28	4	0	9	35	31	3	37	0	29	19	3	31	3	94	97
4	8	6	95	95	4	4	9	50	58	4	0	8	33	15	3	36	5	28	13	3	31	2	35	28
4	8	5	133	136	4	4	8	32	36	4	0	7	80	86	3	36	4	38	37	3	31	1	65	64
4	8	4	106	103	4	4	7	58	63	4	0	6	66	78	3	36	3	32	26	3	31	0	24	32
4	8	3	78	76	4	4	6	21	5	4	0	5	35	26	3	36	2	89	82	3	30	7	48	45
4	8	2	116	115	4	4	5	90	87	4	0	4	104	125	3	36	0	53	39	3	30	6	60	39
4	8	1	185	167	4	4	4	159	150	4	0	3	110	105	3	35	5	17	15	3	30	5	35	38
4	8	0	91	145	4	4	3	77	77	4	0	1	42	51	3	35	4	28	15	3	30	4	28	35
4	7	9	25	18	4	4	2	85	53	4	0	0	29	87	3	35	3	42	39	3	30	3	110	109
4	7	8	27	29	4	4	1	147	139	3	43	2	20	9	3	35	2	50	47	3	30	2	110	102
4	7	7	42	43	4	3	8	24	14	3	43	1	23	26	3	34	6	25	20	3	30	1	218	227
4	7	6	51	55	4	3	7	72	73	3	43	0	39	38	3	34	5	38	40	3	30	0	87	76
4	7	5	93	93	4	3	6	55	62	3	42	3	39	26	3	34	4	27	26	3	29	6	27	36
4	7	4	57	45	4	3	5	32	29	3	42	2	32	33	3	34	3	62	61	3	29	5	44	53
4	7	3	179	178	4	3	4	82	65	3	42	1	40	32	3	34	2	63	64	3	29	4	62	67
4	7	2	89	78	4	3	3	100	91	3	42	0	28	23	3	34	1	50	50	3	29	3	47	43
4	7	1	169	165	4	3	2	149	128	3	41	2	30	26	3	34	0	81	82	3	29	2	76	75
4	7	0	93	148	4	3	0	29	77	3	41	1	29	22	3	33	7	29	23	3	29	1	39	37
4	6	8	17	23	4	2	8	20	32	3	40	3	48	44	3	33	6	47	36	3	28	8	31	38
4	6	7	63	74	4	2	7	38	30	3	40	1	57	50	3	33	5	35	34	3	28	7	39	30
4	6	6	27	29	4	2	6	93	81	3	40	0	37	32	3	33	4	38	28	3	28	6	21	19
4	6	5	45	28	4	2	5	34	30	3	39	4	24	19	3	33	3	52	48	3	28	5	46	50
4	6	4	89	86	4	2	4	172	187	3	39	2	22	22	3	33	2	50	45	3	28	4	61	58
4	6	3	114	109	4	2	3	69	73	3	39	1	19	23	3	33	1	43	34	3	28	3	73	74
4	6	2	188	168	4	2	2	38	31	3	39	0	70	62	3	33	0	58	47	3	28	2	89	81
4	6	1	70	65	4	2	1	104	96	3	38	5	33	30	3	32	7	47	53	3	28	1	72	71
4	5	9	24	20	4	1	8	18	23	3	38	3	18	9	3	32	6	37	42	3	28	0	85	82
4	5	8	36	36	4	1	7	90	92	3	38	2	21	19	3	32	4	27	25	3	27	8	30	28
4	5	7	25	14	4	1	6	61	62	3	38	1	61	54	3	32	3	76	81	3	27	6	61	61
4	5	6	112	106	4	1	5	223	233	3	38	0	49	52	3	32	2	21	33	3	27	5	37	31
4	5	5	165	161	4	1	4	42	44	3	37	5	21	25	3	32	1	56	70	3	27	4	42	33
4	5	4	70	63	4	1	3	59	54	3	37	4	19	27	3	32	0	23	21	3	27	3	123	124
4	5	3	174	179	4	1	2	71	61	3	37	3	26	19	3	31	6	29	30	3	27	2	71	74
4	5	2	77	71	4	1	1	65	79	3	37	2	24	35	3	31	5	70	65	3	27	1	95	86
4	5	1	55	52	4	1	0	28	80	3	37	1	37	39	3	31	4	30	25	3	27	0	125	121

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	26	8	34	42	3	22	5	101	110	3	18	7	50	46	3	15	2	143	126	3	11	2	255	241
3	26	7	82	80	3	22	4	85	83	3	18	6	77	79	3	15	1	162	171	3	11	1	69	72
3	26	5	30	37	3	22	3	174	172	3	18	5	154	148	3	15	0	52	60	3	11	0	18	17
3	26	4	82	81	3	22	2	133	130	3	18	4	80	69	3	14	10	24	31	3	10	9	58	54
3	26	2	112	109	3	22	1	184	186	3	18	3	61	63	3	14	9	31	25	3	10	8	72	76
3	26	1	125	121	3	22	0	59	61	3	18	2	231	223	3	14	8	38	37	3	10	7	147	147
3	26	0	210	207	3	21	7	39	48	3	18	1	123	112	3	14	6	85	91	3	10	6	49	45
3	25	8	26	11	3	21	6	82	86	3	18	0	151	159	3	14	5	21	8	3	10	5	108	114
3	25	7	59	64	3	21	5	98	98	3	17	9	24	33	3	14	4	169	170	3	10	4	144	139
3	25	6	85	90	3	21	4	68	66	3	17	8	44	43	3	14	3	254	257	3	10	3	109	114
3	25	5	19	15	3	21	3	338	331	3	17	7	36	31	3	14	2	91	95	3	10	2	256	243
3	25	4	156	150	3	21	2	43	48	3	17	6	109	113	3	14	1	121	115	3	10	1	352	345
3	25	3	67	69	3	21	1	39	45	3	17	5	192	200	3	14	0	86	104	3	10	0	86	100
3	25	2	160	168	3	21	0	99	85	3	17	4	135	141	3	13	10	18	19	3	9	10	26	28
3	25	1	39	38	3	20	9	32	25	3	17	3	220	215	3	13	6	154	163	3	9	9	27	33
3	25	0	82	96	3	20	7	54	49	3	17	2	172	162	3	13	5	84	79	3	9	8	63	63
3	24	7	52	47	3	20	6	117	118	3	17	1	182	189	3	13	4	177	182	3	9	7	23	12
3	24	6	60	59	3	20	5	115	123	3	17	0	29	35	3	13	3	184	166	3	9	6	111	111
3	24	5	88	77	3	20	4	82	89	3	16	9	19	0	3	13	2	406	391	3	9	5	16	12
3	24	4	63	65	3	20	3	134	136	3	16	8	21	16	3	13	1	174	162	3	9	4	200	193
3	24	3	133	153	3	20	2	113	109	3	16	7	65	72	3	13	0	40	59	3	9	3	201	195
3	24	2	93	99	3	20	1	106	101	3	16	6	113	107	3	12	8	28	5	3	9	2	169	158
3	24	1	50	59	3	20	0	25	15	3	16	5	121	116	3	12	7	43	35	3	9	1	232	230
3	24	0	40	31	3	19	9	38	38	3	16	4	60	64	3	12	6	82	73	3	9	0	116	130
3	23	9	18	13	3	19	8	36	31	3	16	3	98	95	3	12	5	66	67	3	8	8	51	55
3	23	8	41	42	3	19	7	44	38	3	16	2	261	256	3	12	4	125	133	3	8	7	50	37
3	23	5	43	36	3	19	6	59	64	3	16	1	165	162	3	12	3	131	129	3	8	6	105	105
3	23	4	113	124	3	19	5	128	132	3	16	0	182	184	3	12	2	457	458	3	8	5	145	165
3	23	3	60	54	3	19	4	88	94	3	15	9	23	16	3	12	1	398	360	3	8	4	197	195
3	23	2	167	160	3	19	3	90	78	3	15	8	30	33	3	12	0	184	183	3	8	3	182	189
3	23	1	55	59	3	19	2	105	109	3	15	7	41	44	3	11	7	17	23	3	8	2	173	155
3	23	0	61	59	3	19	1	78	80	3	15	6	190	189	3	11	6	179	183	3	8	1	389	363
3	22	9	32	30	3	19	0	228	239	3	15	5	153	144	3	11	5	40	43	3	8	0	49	45
3	22	8	31	35	3	18	9	41	37	3	15	4	105	104	3	11	4	122	122	3	7	9	51	44
3	22	6	63	50	3	18	8	43	36	3	15	3	226	230	3	11	3	127	131	3	7	8	63	64

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
3	7	6	96	107	3	4	2	32	53	3	0	2	223	219	2	37	4	37	46	2	31	8	36	36
3	7	5	174	181	3	4	0	26	41	3	0	1	21	26	2	37	3	57	51	2	31	6	66	74
3	7	4	179	166	3	3	10	28	19	2	45	1	45	37	2	37	2	44	44	2	31	5	39	39
3	7	3	103	108	3	3	9	28	29	2	44	3	36	29	2	37	1	69	66	2	31	4	77	74
3	7	2	35	33	3	3	7	24	19	2	44	2	17	17	2	37	0	26	44	2	31	3	77	73
3	7	1	93	86	3	3	6	173	173	2	44	1	38	37	2	36	6	34	38	2	31	0	136	134
3	7	0	71	95	3	3	5	96	96	2	44	0	76	78	2	36	5	39	34	2	30	8	50	43
3	6	10	46	54	3	3	4	88	73	2	43	2	18	22	2	36	4	55	59	2	30	6	35	24
3	6	9	28	36	3	3	3	197	181	2	43	0	81	66	2	36	3	48	48	2	30	5	78	71
3	6	8	39	43	3	3	2	282	248	2	42	4	34	31	2	36	2	60	63	2	30	4	45	41
3	6	7	65	69	3	3	1	102	81	2	42	3	36	21	2	36	1	77	78	2	30	3	69	73
3	6	6	90	91	3	2	10	39	39	2	42	2	35	31	2	36	0	75	74	2	30	2	123	126
3	6	5	159	155	3	2	9	27	25	2	42	1	80	84	2	35	7	36	37	2	30	1	91	97
3	6	4	89	94	3	2	8	82	77	2	42	0	40	42	2	35	5	37	45	2	30	0	151	157
3	6	3	236	219	3	2	7	38	43	2	41	4	54	50	2	35	3	27	21	2	29	8	18	8
3	6	2	206	203	3	2	6	101	97	2	41	3	42	44	2	35	2	17	20	2	29	7	52	54
3	6	1	393	381	3	2	5	88	85	2	41	2	25	17	2	35	1	43	36	2	29	6	17	19
3	6	0	147	222	3	2	4	96	95	2	41	1	60	56	2	35	0	70	80	2	29	5	85	88
3	5	10	47	47	3	2	3	133	108	2	41	0	81	79	2	34	7	29	36	2	29	4	108	115
3	5	9	60	58	3	2	2	363	360	2	40	5	20	14	2	34	6	57	54	2	29	3	84	73
3	5	8	19	28	3	2	1	231	220	2	40	4	20	20	2	34	5	48	51	2	29	2	121	116
3	5	7	62	66	3	1	8	44	45	2	40	3	27	28	2	34	3	22	18	2	29	1	103	98
3	5	6	128	128	3	1	7	53	52	2	40	2	21	12	2	34	1	79	83	2	29	0	37	48
3	5	5	155	159	3	1	6	126	124	2	40	1	81	80	2	33	6	34	30	2	28	8	33	36
3	5	4	211	208	3	1	5	84	80	2	40	0	74	64	2	33	5	50	52	2	28	5	33	40
3	5	3	159	143	3	1	4	145	145	2	39	5	35	25	2	33	3	39	37	2	28	4	70	77
3	5	2	359	335	3	1	3	152	140	2	39	4	23	32	2	33	1	69	80	2	28	3	79	84
3	5	1	199	169	3	1	2	143	128	2	39	2	28	18	2	33	0	102	108	2	28	2	34	19
3	5	0	54	97	3	1	1	73	74	2	39	1	37	35	2	32	7	20	3	2	28	1	38	48
3	4	8	64	69	3	0	10	17	5	2	39	0	70	65	2	32	5	55	58	2	28	0	35	41
3	4	7	65	74	3	0	8	42	44	2	38	6	40	33	2	32	4	65	59	2	27	7	36	34
3	4	6	63	68	3	0	7	55	60	2	38	3	46	42	2	32	3	83	81	2	27	6	29	25
3	4	5	45	31	3	0	6	105	129	2	38	1	52	48	2	32	2	48	40	2	27	5	64	54
3	4	4	21	38	3	0	4	314	302	2	38	0	123	116	2	32	1	40	39	2	27	4	59	61
3	4	3	141	130	3	0	3	207	192	2	37	5	48	46	2	32	0	130	134	2	27	3	71	66

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	27	2	94	83	2	23	1	120	114	2	19	5	121	124	2	15	9	24	32	2	12	5	55	60
2	27	1	128	126	2	23	0	176	179	2	19	3	51	54	2	15	8	30	18	2	12	4	84	71
2	27	0	111	105	2	22	9	37	34	2	19	2	124	121	2	15	7	94	97	2	12	3	130	133
2	26	6	99	96	2	22	8	29	29	2	19	1	97	83	2	15	6	98	91	2	12	2	303	290
2	26	5	35	38	2	22	7	44	50	2	19	0	102	118	2	15	5	63	75	2	12	1	297	264
2	26	4	153	152	2	22	6	69	72	2	18	9	32	27	2	15	4	52	65	2	12	0	34	20
2	26	3	134	137	2	22	5	208	204	2	18	7	37	37	2	15	3	70	71	2	11	10	18	10
2	26	1	182	178	2	22	4	207	219	2	18	6	186	187	2	15	2	164	155	2	11	9	41	37
2	26	0	101	108	2	22	3	196	203	2	18	5	47	47	2	15	1	363	345	2	11	8	71	71
2	25	9	17	20	2	22	2	115	119	2	18	4	118	120	2	15	0	66	80	2	11	7	97	105
2	25	7	20	19	2	22	1	94	98	2	18	3	258	259	2	14	10	35	38	2	11	6	212	211
2	25	6	47	44	2	22	0	287	296	2	18	2	125	124	2	14	9	28	31	2	11	5	121	117
2	25	5	155	163	2	21	9	32	35	2	18	1	43	42	2	14	8	64	72	2	11	4	31	27
2	25	4	144	148	2	21	8	31	32	2	18	0	193	178	2	14	7	114	117	2	11	3	268	250
2	25	3	221	226	2	21	7	23	29	2	17	10	35	35	2	14	6	39	23	2	11	2	298	274
2	25	2	83	82	2	21	6	167	160	2	17	8	32	28	2	14	5	141	159	2	11	1	239	239
2	25	1	90	81	2	21	5	35	35	2	17	7	96	93	2	14	4	146	141	2	11	0	195	191
2	24	9	27	25	2	21	4	108	103	2	17	6	142	140	2	14	3	201	199	2	10	10	31	41
2	24	8	34	32	2	21	3	139	135	2	17	5	81	85	2	14	2	322	302	2	10	8	71	78
2	24	7	55	45	2	21	2	66	59	2	17	4	193	196	2	14	1	116	113	2	10	7	77	88
2	24	6	42	48	2	21	1	184	189	2	17	3	81	94	2	13	10	42	42	2	10	6	144	147
2	24	5	58	52	2	20	9	31	36	2	17	2	249	237	2	13	9	26	33	2	10	5	196	193
2	24	4	96	98	2	20	8	33	45	2	17	1	327	327	2	13	8	40	35	2	10	4	211	191
2	24	3	89	88	2	20	7	32	40	2	17	0	184	174	2	13	7	64	70	2	10	3	441	413
2	24	2	193	192	2	20	6	38	36	2	16	10	26	26	2	13	6	44	51	2	10	2	260	240
2	24	1	189	203	2	20	5	63	61	2	16	9	31	36	2	13	5	178	180	2	10	1	110	129
2	24	0	220	221	2	20	4	101	103	2	16	8	41	48	2	13	4	79	91	2	10	0	512	498
2	23	9	38	28	2	20	3	55	46	2	16	7	50	43	2	13	3	26	42	2	9	10	40	31
2	23	8	18	15	2	20	2	118	114	2	16	6	33	39	2	13	2	583	577	2	9	9	71	70
2	23	7	79	70	2	20	1	263	267	2	16	5	51	60	2	13	1	513	503	2	9	8	84	88
2	23	6	63	65	2	20	0	94	104	2	16	4	148	157	2	13	0	287	282	2	9	7	34	34
2	23	5	93	98	2	19	10	20	14	2	16	3	176	164	2	12	9	80	82	2	9	6	88	94
2	23	4	142	153	2	19	8	34	23	2	16	2	306	307	2	12	8	32	34	2	9	5	107	101
2	23	3	107	112	2	19	7	76	81	2	16	1	350	336	2	12	7	100	107	2	9	4	205	210
2	23	2	69	68	2	19	6	56	60	2	16	0	92	73	2	12	6	59	63	2	9	3	394	390

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	9	2	263	238	2	5	10	32	26	2	2	8	53	54	1	42	1	74	73	1	36	1	89	90
2	9	1	371	331	2	5	9	17	14	2	2	7	67	63	1	42	0	66	71	1	36	0	32	30
2	9	0	318	305	2	5	8	130	134	2	2	6	107	124	1	41	4	45	44	1	35	7	21	25
2	8	10	30	21	2	5	7	92	107	2	2	5	57	62	1	41	3	19	16	1	35	6	28	34
2	8	9	27	25	2	5	6	196	203	2	2	4	199	191	1	41	2	68	72	1	35	5	41	46
2	8	8	86	96	2	5	5	106	101	2	2	3	165	151	1	41	1	47	45	1	35	4	69	72
2	8	7	107	113	2	5	4	188	176	2	2	2	173	158	1	41	0	21	23	1	35	3	54	44
2	8	6	75	70	2	5	3	239	233	2	2	1	61	47	1	40	5	31	28	1	35	2	71	64
2	8	5	184	191	2	5	2	393	365	2	1	11	31	17	1	40	4	18	17	1	35	0	66	69
2	8	4	131	132	2	5	1	292	282	2	1	10	37	43	1	40	2	32	29	1	34	7	26	22
2	8	3	147	149	2	4	11	36	25	2	1	9	85	91	1	40	1	81	87	1	34	6	35	30
2	8	2	343	328	2	4	10	57	51	2	1	8	124	121	1	39	6	46	48	1	34	5	26	17
2	8	1	530	503	2	4	9	66	67	2	1	7	73	70	1	39	5	28	29	1	34	4	54	59
2	8	0	254	264	2	4	8	25	23	2	1	6	62	68	1	39	4	17	19	1	34	3	81	85
2	7	10	20	16	2	4	7	38	32	2	1	5	146	157	1	39	3	31	25	1	34	2	81	77
2	7	8	25	21	2	4	6	178	197	2	1	4	218	216	1	39	2	21	16	1	34	1	138	139
2	7	7	80	81	2	4	5	73	79	2	1	3	267	256	1	39	1	66	66	1	34	0	129	129
2	7	6	85	81	2	4	4	319	296	2	1	2	239	238	1	39	0	41	41	1	33	8	41	26
2	7	5	121	117	2	4	3	238	231	2	1	1	310	274	1	38	6	45	40	1	33	7	27	35
2	7	4	188	184	2	4	2	345	314	2	0	10	37	38	1	38	3	67	69	1	33	6	18	24
2	7	3	348	326	2	4	1	187	200	2	0	7	108	107	1	38	2	39	32	1	33	5	38	37
2	7	2	699	670	2	4	0	103	144	2	0	6	80	81	1	38	1	28	35	1	33	4	65	60
2	7	1	85	74	2	3	9	45	50	2	0	5	207	208	1	38	0	41	34	1	33	3	40	41
2	7	0	110	116	2	3	8	48	48	2	0	3	143	171	1	37	6	45	38	1	33	2	49	52
2	6	10	22	26	2	3	7	54	51	2	0	2	199	180	1	37	4	48	42	1	33	1	129	130
2	6	9	23	24	2	3	6	56	55	2	0	1	400	387	1	37	3	30	30	1	33	0	25	24
2	6	8	90	87	2	3	5	218	227	1	45	2	18	7	1	37	2	38	42	1	32	8	21	16
2	6	7	117	126	2	3	4	162	161	1	45	1	39	47	1	37	1	91	101	1	32	7	36	38
2	6	6	18	39	2	3	3	32	18	1	44	3	58	59	1	37	0	285	282	1	32	6	31	15
2	6	5	151	161	2	3	2	264	275	1	44	1	33	27	1	36	7	34	25	1	32	5	58	64
2	6	4	282	292	2	3	1	378	357	1	43	4	44	34	1	36	6	19	18	1	32	4	76	83
2	6	3	111	111	2	3	0	36	51	1	43	2	23	16	1	36	5	26	21	1	32	3	22	30
2	6	2	363	359	2	2	11	34	30	1	43	1	20	26	1	36	4	57	50	1	32	2	131	134
2	6	1	319	289	2	2	10	37	31	1	42	5	33	18	1	36	3	90	89	1	32	1	60	60
2	6	0	34	41	2	2	9	38	37	1	42	2	47	49	1	36	2	71	70	1	32	0	63	67

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	31	8	72	74	1	27	6	69	63	1	23	8	19	16	1	20	3	158	158	1	16	5	100	105
1	31	7	38	30	1	27	5	112	124	1	23	7	61	55	1	20	2	113	123	1	16	4	66	64
1	31	6	67	67	1	27	4	225	238	1	23	6	53	52	1	20	1	172	175	1	16	3	131	116
1	31	5	63	68	1	27	3	85	87	1	23	5	155	164	1	20	0	26	25	1	16	2	424	405
1	31	4	40	46	1	27	2	104	98	1	23	4	173	176	1	19	9	52	52	1	16	1	115	115
1	31	3	86	85	1	27	1	81	72	1	23	3	171	166	1	19	7	89	91	1	16	0	120	134
1	31	2	126	129	1	27	0	143	147	1	23	2	171	170	1	19	6	131	141	1	15	10	18	15
1	31	1	87	88	1	26	9	31	25	1	23	1	83	87	1	19	5	168	179	1	15	8	30	23
1	31	0	52	54	1	26	7	36	34	1	23	0	198	203	1	19	4	120	108	1	15	7	17	16
1	30	8	54	56	1	26	6	88	85	1	22	10	38	30	1	19	3	139	148	1	15	6	187	179
1	30	7	32	33	1	26	5	139	135	1	22	8	19	6	1	19	2	101	110	1	15	5	50	62
1	30	5	75	71	1	26	4	47	46	1	22	7	49	60	1	19	1	198	186	1	15	4	44	44
1	30	4	53	55	1	26	3	179	177	1	22	6	150	163	1	19	0	78	69	1	15	3	135	132
1	30	3	79	85	1	26	2	96	82	1	22	5	91	103	1	18	7	75	82	1	15	2	250	230
1	30	2	103	109	1	26	1	81	79	1	22	4	147	154	1	18	6	64	69	1	15	1	238	247
1	30	1	114	113	1	26	0	158	162	1	22	3	146	141	1	18	5	63	63	1	15	0	132	117
1	29	7	52	52	1	25	9	58	49	1	22	2	208	205	1	18	4	136	147	1	14	10	53	47
1	29	6	36	32	1	25	8	35	33	1	22	1	192	194	1	18	3	237	246	1	14	8	59	54
1	29	5	87	83	1	25	7	30	27	1	22	0	67	72	1	18	2	104	97	1	14	7	34	28
1	29	4	44	39	1	25	6	44	45	1	21	10	25	21	1	18	1	146	136	1	14	6	84	88
1	29	3	191	199	1	25	5	101	109	1	21	9	21	21	1	18	0	481	464	1	14	5	118	124
1	29	2	141	143	1	25	4	64	63	1	21	8	37	43	1	17	9	55	58	1	14	4	57	59
1	29	1	61	64	1	25	3	105	111	1	21	7	24	31	1	17	8	74	69	1	14	3	122	116
1	29	0	173	173	1	25	2	157	159	1	21	5	80	82	1	17	7	123	135	1	14	2	486	473
1	28	9	19	9	1	25	1	79	79	1	21	4	203	207	1	17	6	44	45	1	14	1	648	648
1	28	6	48	47	1	25	0	53	53	1	21	3	111	124	1	17	5	199	211	1	14	0	50	50
1	28	5	58	61	1	24	8	49	48	1	21	2	128	131	1	17	4	99	87	1	13	8	33	36
1	28	4	62	60	1	24	7	37	35	1	21	1	121	131	1	17	3	63	67	1	13	7	80	89
1	28	3	166	174	1	24	6	50	49	1	21	0	51	64	1	17	2	116	111	1	13	6	31	34
1	28	2	54	45	1	24	5	102	110	1	20	9	22	16	1	17	1	282	275	1	13	5	284	284
1	28	1	23	23	1	24	4	52	53	1	20	8	20	19	1	17	0	296	284	1	13	4	114	106
1	28	0	72	67	1	24	3	170	174	1	20	7	91	94	1	16	10	32	33	1	13	3	299	275
1	27	9	24	24	1	24	2	193	193	1	20	6	59	71	1	16	8	53	55	1	13	2	594	587
1	27	8	19	23	1	24	1	56	55	1	20	5	34	22	1	16	7	53	56	1	13	1	185	184
1	27	7	59	60	1	24	0	20	5	1	20	4	57	53	1	16	6	67	66	1	13	0	235	242

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
1	12	10	32	26	1	9	8	149	153	1	6	5	100	110	1	3	5	97	111	1	0	2	142	156
1	12	9	36	29	1	9	7	120	127	1	6	4	54	68	1	3	4	284	269	1	0	1	701	733
1	12	8	45	45	1	9	6	53	54	1	6	3	337	330	1	3	3	396	383	0	45	3	20	18
1	12	7	64	61	1	9	5	299	303	1	6	2	615	598	1	3	2	512	495	0	45	2	44	45
1	12	5	196	192	1	9	4	241	218	1	6	1	511	491	1	3	1	860	871	0	44	4	31	34
1	12	4	143	139	1	9	3	527	513	1	6	0	714	742	1	3	0	119	145	0	44	2	38	39
1	12	3	614	590	1	9	2	474	452	1	5	11	37	33	1	2	10	59	60	0	44	1	44	40
1	12	2	350	338	1	9	1	396	367	1	5	10	44	44	1	2	9	75	74	0	44	0	56	47
1	12	1	165	179	1	9	0	552	558	1	5	9	67	72	1	2	8	118	118	0	43	3	20	25
1	12	0	310	282	1	8	8	165	168	1	5	8	145	146	1	2	7	77	81	0	42	5	24	30
1	11	9	61	56	1	8	7	28	23	1	5	7	90	93	1	2	6	154	151	0	42	3	35	36
1	11	8	25	22	1	8	6	183	198	1	5	6	149	154	1	2	5	153	137	0	42	2	44	46
1	11	7	77	80	1	8	5	215	221	1	5	5	164	162	1	2	4	20	17	0	42	0	99	103
1	11	6	22	23	1	8	4	389	350	1	5	4	490	489	1	2	3	150	160	0	41	3	40	40
1	11	5	45	52	1	8	3	677	655	1	5	3	219	204	1	2	2	534	502	0	41	1	69	66
1	11	4	106	117	1	8	2	445	415	1	5	2	601	588	1	2	1	828	883	0	40	5	45	30
1	11	3	184	186	1	8	1	904	904	1	5	1	1038	1133	1	1	11	20	22	0	40	3	82	81
1	11	2	249	227	1	8	0	474	409	1	5	0	485	482	1	1	10	21	25	0	40	1	107	100
1	11	1	97	78	1	7	11	33	33	1	4	11	17	14	1	1	9	63	60	0	40	0	84	88
1	11	0	141	158	1	7	10	34	37	1	4	10	20	36	1	1	8	144	151	0	39	6	20	10
1	10	11	48	45	1	7	9	73	72	1	4	9	75	81	1	1	7	139	140	0	39	5	26	32
1	10	10	51	59	1	7	8	83	90	1	4	8	101	100	1	1	6	179	187	0	39	4	45	50
1	10	9	22	23	1	7	7	33	36	1	4	7	116	113	1	1	5	126	144	0	39	3	20	1
1	10	8	46	50	1	7	6	107	114	1	4	6	205	209	1	1	4	246	233	0	39	2	77	70
1	10	7	93	98	1	7	5	52	59	1	4	5	53	44	1	1	3	377	366	0	39	1	66	69
1	10	6	94	93	1	7	4	93	82	1	4	4	105	102	1	1	2	450	457	0	38	6	36	43
1	10	5	197	200	1	7	3	104	127	1	4	3	101	105	1	1	1	635	666	0	38	5	17	4
1	10	4	22	28	1	7	2	377	359	1	4	2	282	257	1	0	10	44	45	0	38	4	41	33
1	10	3	370	370	1	7	1	755	713	1	4	1	551	531	1	0	9	44	47	0	38	2	74	70
1	10	2	233	234	1	7	0	511	503	1	3	11	16	11	1	0	8	129	122	0	38	1	20	25
1	10	1	480	458	1	6	11	32	26	1	3	10	24	15	1	0	7	140	153	0	38	0	70	67
1	10	0	374	343	1	6	10	34	24	1	3	9	69	77	1	0	6	126	137	0	37	7	31	20
1	9	11	30	27	1	6	8	101	100	1	3	8	65	75	1	0	5	18	9	0	37	6	35	35
1	9	10	58	61	1	6	7	145	145	1	3	7	123	131	1	0	4	310	301	0	37	5	33	25
1	9	9	30	31	1	6	6	69	65	1	3	6	74	61	1	0	3	267	273	0	37	4	25	35

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	37	2	67	69	0	32	0	18	1	0	26	6	16	8	0	22	0	158	170	0	18	0	352	343
0	36	6	41	50	0	31	8	31	36	0	26	5	153	149	0	21	9	63	68	0	17	9	23	30
0	36	5	20	19	0	31	7	110	100	0	26	4	121	141	0	21	8	17	16	0	17	8	42	45
0	36	4	42	43	0	31	6	29	27	0	26	2	148	150	0	21	7	26	13	0	17	7	110	118
0	36	3	40	44	0	31	5	112	123	0	26	1	218	225	0	21	6	17	22	0	17	6	24	14
0	36	2	130	130	0	31	4	184	190	0	26	0	65	78	0	21	5	142	149	0	17	5	73	72
0	36	1	29	23	0	31	3	65	76	0	25	8	19	18	0	21	4	191	199	0	17	4	267	283
0	36	0	375	384	0	31	2	219	226	0	25	7	78	71	0	21	3	187	192	0	17	3	571	569
0	35	6	22	30	0	30	8	28	24	0	25	5	62	64	0	21	2	175	175	0	17	2	33	48
0	35	5	23	37	0	30	7	35	38	0	25	4	110	133	0	21	1	28	30	0	17	1	126	127
0	35	4	31	34	0	30	5	75	66	0	25	3	175	180	0	20	8	36	45	0	16	8	40	30
0	35	3	168	174	0	30	4	44	49	0	25	2	76	74	0	20	7	41	36	0	16	7	64	56
0	35	2	30	25	0	30	3	171	173	0	25	1	92	89	0	20	6	163	167	0	16	6	100	89
0	35	1	209	217	0	30	2	128	143	0	24	9	25	15	0	20	5	186	200	0	16	5	61	62
0	34	5	26	24	0	30	1	20	26	0	24	8	21	2	0	20	4	20	14	0	16	3	23	27
0	34	4	22	27	0	30	0	56	62	0	24	7	26	24	0	20	3	136	149	0	16	2	192	204
0	34	3	96	106	0	29	9	19	6	0	24	6	34	30	0	20	2	292	281	0	16	0	93	101
0	34	2	136	143	0	29	8	65	65	0	24	5	142	143	0	20	1	47	50	0	15	10	31	36
0	34	1	132	130	0	29	7	29	20	0	24	4	130	134	0	20	0	43	18	0	15	9	23	18
0	34	0	20	24	0	29	3	160	166	0	24	3	107	105	0	19	10	22	21	0	15	8	94	90
0	33	8	33	34	0	29	2	19	18	0	24	2	97	98	0	19	8	36	32	0	15	7	117	109
0	33	6	24	24	0	29	1	18	12	0	24	1	133	143	0	19	7	117	111	0	15	6	209	224
0	33	5	52	55	0	28	8	16	33	0	24	0	51	51	0	19	6	102	111	0	15	5	279	275
0	33	4	18	15	0	28	5	106	103	0	23	10	21	26	0	19	5	167	159	0	15	4	177	171
0	33	3	60	63	0	28	4	147	156	0	23	6	127	131	0	19	4	54	60	0	15	3	59	56
0	33	2	23	6	0	28	3	73	75	0	23	5	153	167	0	19	3	527	541	0	15	2	99	95
0	33	1	161	165	0	28	1	349	369	0	23	4	25	28	0	19	2	220	215	0	15	1	76	74
0	32	8	32	36	0	28	0	124	115	0	23	2	16	30	0	19	1	276	280	0	14	9	21	31
0	32	7	41	34	0	27	7	23	12	0	23	1	37	49	0	18	9	25	17	0	14	7	37	24
0	32	6	30	31	0	27	6	67	60	0	22	8	54	62	0	18	8	22	24	0	14	6	28	36
0	32	5	26	24	0	27	4	143	148	0	22	7	48	39	0	18	7	132	144	0	14	5	226	226
0	32	4	29	27	0	27	3	212	210	0	22	6	103	108	0	18	4	40	47	0	14	4	128	121
0	32	3	139	150	0	27	2	171	162	0	22	5	53	46	0	18	3	386	382	0	14	3	401	385
0	32	2	38	29	0	27	1	51	47	0	22	2	36	40	0	18	2	49	39	0	14	2	392	388
0	32	1	74	79	0	26	7	34	30	0	22	1	69	62	0	18	1	389	383	0	14	1	635	635

Table 30 (contd.)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	14	0	635	629	0	10	3	152	138	0	6	5	77	82	0	2	8	78	71					
0	13	9	27	35	0	10	2	585	583	0	6	4	255	262	0	2	7	159	152					
0	13	8	20	13	0	10	0	805	844	0	6	3	27	32	0	2	5	80	84					
0	13	7	132	137	0	9	10	45	42	0	6	2	628	607	0	2	4	40	30					
0	13	6	148	141	0	9	8	19	8	0	6	1	178	181	0	2	3	51	64					
0	13	5	237	234	0	9	7	52	64	0	5	10	42	39	0	2	2	474	455					
0	13	4	225	220	0	9	5	161	163	0	5	9	94	98	0	2	1	213	202					
0	13	3	60	58	0	9	4	578	578	0	5	8	39	36	0	2	0	490	597					
0	13	2	111	108	0	9	3	206	205	0	5	7	244	245	0	1	11	17	11					
0	13	1	120	124	0	9	2	559	567	0	5	6	115	103	0	1	10	75	66					
0	12	11	19	18	0	9	1	315	338	0	5	5	342	327	0	1	9	77	83					
0	12	10	56	57	0	8	11	20	5	0	5	4	201	175	0	1	7	69	65					
0	12	9	54	63	0	8	10	80	78	0	5	3	576	566	0	1	6	126	125					
0	12	8	19	26	0	8	9	39	50	0	5	2	1028	1142	0	1	5	17	18					
0	12	7	50	61	0	8	8	23	4	0	5	1	66	44	0	1	4	493	470					
0	12	6	92	92	0	8	7	32	28	0	4	11	21	9	0	1	3	389	364					
0	12	5	222	227	0	8	5	128	127	0	4	10	19	20	0	1	2	391	363					
0	12	4	326	330	0	8	4	106	107	0	4	9	42	36	0	0	10	35	36					
0	12	3	143	114	0	8	3	305	289	0	4	8	134	130	0	0	8	86	95					
0	12	2	309	315	0	8	2	60	63	0	4	7	19	4	0	0	6	249	261					
0	12	0	188	184	0	7	11	33	33	0	4	6	22	22	0	0	4	260	239					
0	11	11	55	57	0	7	10	44	54	0	4	5	111	122										
0	11	8	58	61	0	7	9	48	52	0	4	4	503	509										
0	11	7	54	38	0	7	8	127	138	0	4	3	521	531										
0	11	6	207	197	0	7	6	46	31	0	4	2	315	329										
0	11	5	104	103	0	7	5	65	63	0	4	1	327	294										
0	11	4	44	44	0	7	4	441	431	0	3	9	152	149										
0	11	3	259	245	0	7	3	290	283	0	3	8	235	251										
0	11	2	480	475	0	7	2	833	866	0	3	7	51	34										
0	10	10	18	8	0	7	1	263	274	0	3	5	54	53										
0	10	9	85	87	0	6	11	21	9	0	3	4	263	260										
0	10	8	33	44	0	6	9	36	31	0	3	3	336	333										
0	10	7	43	50	0	6	8	85	88	0	3	2	231	218										
0	10	5	59	74	0	6	7	103	112	0	3	1	564	595										
0	10	4	552	545	0	6	6	45	50	0	2	9	81	73										

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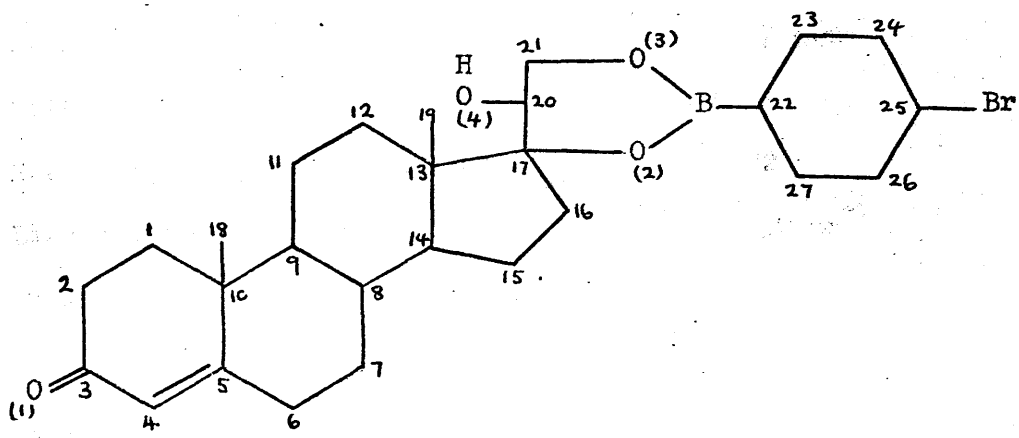
Appendix I

The crystal structure of 17, 20β,21-Trihydroxypregn-4-en-3-one 17,21-p-bromophenylboronate.



The crystals of this compound were very small and the limited data which were collected led to high standard deviations for the parameters involved. Dr. P. D. Cradwick was responsible for solving the structure by Patterson techniques and by applying tangent formula calculations to the phases of partial structure factors. The author completed the refinement of the atom parameters.

Crystal data

Molecular formula	$C_{27}H_{34}O_4BrB$
Molecular weight	513.3 a.m.u.
Crystal system	orthorhombic
Space group	$P2_12_12_1$

Cell dimensions	$\underline{a}$ = 16.847(28) Å
	$\underline{b}$ = 13.294(18) Å
	$\underline{c}$ = 11.082(10) Å
Cell volume (u)	2482.0 $Å^3$
Density (obs.)	1.42 $g.cm^{-3}$
Density (calc.)	1.37 $g.cm^{-3}$
Molecules per unit cell (z)	4
No. electrons per unit cell ($F_{(000)}$)	1072
Linear absorption coefficient, μ(MoKα)	17.90 cm^{-1}

The space group $P2_12_12_1$ was deduced from Weissenberg and precession photographs, and after collecting data on the diffractometer 3053 independent structure amplitudes were obtained. Many of the structure amplitudes were unobserved or not very intense, so only 1382 amplitudes were used in the calculation of a sharpened Patterson. The bromine co-ordinates were located and partial structure factors were calculated on the basis of this position. The phases of these structure factors were used in tangent formula calculations for 274 E values > 1.0 and much of the structure was found from the resulting E map. When all the atoms were located only those reflections with $I \geq 2.5\sigma I$ were accepted as significantly above background, this left 776 reflections. The structure refined to R = 0.136 and at this stage those reflections where $\sin\theta/\lambda$ was > 0.52 were removed as the agreement between the observed and calculated structure factors in this region was low. The remaining 699 reflections refined to a final R value of 0.096; unit weights were used in the least

squares calculations. Determining the absolute configuration of the molecule was not experimentally achieved [R = 0.0960 or 0.0961] so the absolute configuration of the steroid molecule was assumed.

Discussion

The stereochemistry of the molecule has been determined and is shown in Figure 1, also the atom positions, bond lengths and valency angles are listed in tables 1, 2 and 3.

C(20) and C(22) are displaced from the plane defined by atoms C(17), C(21), O(2), O(3) and B by -0.69 Å and 0.26 Å respectively (table 4). Although it is possible for an interaction involving the unfilled p orbital of the boron and the lone pair on the oxygen the distance O(4) - B is 3.05 Å (van der Waals contact 3.07 Å) which is larger than that required for such a case.

There is a short intermolecular contact of 2.77 Å between O(1) and the atom O(4) through x, y-1, z, which indicates hydrogen bonding. The remaining intermolecular separations are all of the normal van der Waals type.

Fig. 1

A general view of the 17,20β,21-Trihydroxypregn-4-en-3-one 17,21-p-bromophenylboronate.

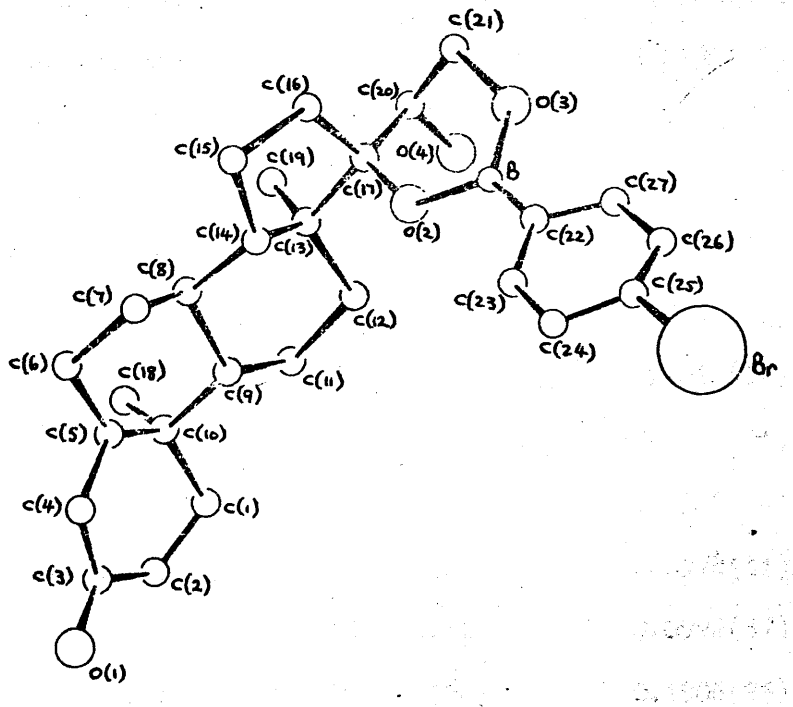


TABLE 1

Fractional Atomic co-ordinates, positional standard deviations and temperature factors ($Å^2$)

Atom	x	y	z	B
Br	-0.1469(3)	0.3054(4)	0.4776(5)	≠
O(1)	0.4029(16)	-0.3465(20)	0.1703(35)	≠
O(2)	0.1921(17)	0.3373(22)	0.1116(28)	4.65
O(3)	0.1632(20)	0.5152(25)	0.1409(32)	≠
O(4)	0.3236(13)	0.4718(18)	0.1844(21)	≠
C(1)	0.4193(23)	-0.0721(32)	0.2239(39)	3.46
C(2)	0.4484(17)	-0.1840(24)	0.2339(28)	3.08
C(3)	0.4044(16)	-0.2571(22)	0.1423(29)	4.51
C(4)	0.3760(24)	-0.2081(28)	0.0391(33)	3.51
C(5)	0.3801(20)	-0.1077(28)	0.0045(33)	3.02
C(6)	0.3545(17)	-0.0770(19)	-0.1224(27)	4.74
C(7)	0.3006(17)	0.0224(26)	-0.1089(31)	4.22
C(8)	0.3424(23)	0.0997(28)	-0.0362(34)	2.03
C(9)	0.3546(20)	0.0585(29)	0.0978(31)	3.80
C(10)	0.4141(22)	-0.0348(32)	0.0992(37)	2.16
C(11)	0.3900(16)	0.1418(20)	0.1906(25)	3.14
C(12)	0.3311(21)	0.2361(26)	0.1860(31)	3.89
C(13)	0.3199(19)	0.2739(25)	0.0540(31)	1.62
C(14)	0.2874(23)	0.1951(25)	-0.0250(29)	4.06
C(15)	0.2635(19)	0.2491(22)	-0.1443(27)	4.83
C(16)	0.2393(20)	0.3557(26)	-0.0997(31)	3.71
C(17)	0.2595(18)	0.3616(27)	0.0337(27)	5.31
C(18)	0.4989(18)	-0.0070(23)	0.0539(27)	2.86

TABLE 1

Fractional Atomic co-ordinates, positional standard deviations and temperature factors ($Å^2$) (cont.)

Atom	x	y	z	B
C(19)	0.4062(18)	0.3181(24)	0.0075(31)	4.12
C(20)	0.2891(26)	0.4710(34)	0.0625(42)	6.24
C(21)	0.2289(23)	0.5479(29)	0.0458(36)	5.38
C(22)	0.0742(17)	0.3847(24)	0.2348(26)	2.03
C(23)	0.0420(23)	0.2809(28)	0.2457(32)	4.54
C(24)	-0.0237(21)	0.2565(27)	0.3104(33)	3.94
C(25)	-0.0575(21)	0.3362(30)	0.3729(35)	4.92
C(26)	-0.0266(20)	0.4325(28)	0.3829(32)	3.79
C(27)	0.0356(22)	0.4564(27)	0.3110(33)	4.04
B	0.1493(33)	0.4121(38)	0.0549(43)	5.22

The average standard deviation of the isotropic temperature factors is $0.8Å^2$.

/ For these atoms anisotropic temperature factors were employed.

TABLE 1 (cont.)

The anisotropic thermal parameters ($\times 10^4$)

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Br	75(3)	134(5)	155(6)	-92(6)	83(8)	-67(11)
O(1)	50(14)	36(19)	338(65)	-11(31)	6(50)	7(57)
O(3)	42(15)	100(26)	197(39)	1(32)	50(42)	-92(55)
O(4)	85(22)	119(33)	202(45)	-7(41)	102(53)	18(69)

TABLE 2

Intramolecular bonded distances and estimated standard deviations (Å)

Br	-	C(25)	1.95(4)	C(9)	-	C(11)	1.62(5)
O(1)	-	C(3)	1.23(5)	C(10)	-	C(18)	1.56(4)
O(2)	-	C(17)	1.46(5)	C(11)	-	C(12)	1.60(5)
O(2)	-	B	1.38(6)	C(12)	-	C(13)	1.56(4)
O(3)	-	C(21)	1.59(5)	C(13)	-	C(14)	1.47(4)
O(3)	-	B	1.42(6)	C(13)	-	C(17)	1.56(5)
O(4)	-	C(20)	1.47(6)	C(13)	-	C(19)	1.65(4)
C(1)	-	C(2)	1.57(5)	C(14)	-	C(15)	1.56(5)
C(1)	-	C(10)	1.47(5)	C(15)	-	C(16)	1.56(5)
C(2)	-	C(3)	1.59(5)	C(16)	-	C(17)	1.52(5)
C(3)	-	C(4)	1.40(5)	C(17)	-	C(20)	1.57(6)
C(4)	-	C(5)	1.39(4)	C(20)	-	C(21)	1.45(6)
C(5)	-	C(6)	1.53(5)	C(22)	-	C(23)	1.49(5)
C(5)	-	C(10)	1.54(4)	C(22)	-	C(27)	1.43(5)
C(6)	-	C(7)	1.61(5)	C(22)	-	B	1.51(6)
C(7)	-	C(8)	1.48(5)	C(23)	-	C(24)	1.36(5)
C(8)	-	C(9)	1.60(4)	C(24)	-	C(25)	1.39(5)
C(8)	-	C(14)	1.58(4)	C(25)	-	C(26)	1.39(5)
C(9)	-	C(10)	1.60(5)	C(26)	-	C(27)	1.36(5)

TABLE 3

Valency angles (degrees) and estimated standard deviations

C(24)	-	C(24)	-	Br	117(2)
C(26)	-	C(25)	-	Br	116(2)
C(2)	-	C(3)	-	O(1)	116(3)
C(4)	-	C(3)	-	O(1)	130(3)
B	-	O(2)	-	C(17)	121(3)
C(13)	-	C(17)	-	O(2)	105(2)
C(16)	-	C(17)	-	O(2)	113(2)
C(20)	-	C(17)	-	O(2)	109(3)
O(3)	-	B	-	O(2)	121(2)
C(22)	-	B	-	O(2)	119(2)
B	-	O(3)	-	C(21)	121(3)
C(20)	-	C(21)	-	O(3)	102(2)
C(22)	-	B	-	O(3)	118(3)
C(17)	-	C(20)	-	O(4)	109(3)
C(21)	-	C(20)	-	O(4)	113(3)
C(10)	-	C(1)	-	C(2)	114(2)
C(3)	-	C(2)	-	C(1)	113(2)
C(5)	-	C(10)	-	C(1)	117(2)
C(9)	-	C(10)	-	C(1)	108(2)
C(18)	-	C(10)	-	C(1)	109(2)
C(4)	-	C(3)	-	C(2)	113(2)
C(5)	-	C(4)	-	C(3)	130(2)
C(6)	-	C(5)	-	C(4)	120(2)
C(10)	-	C(5)	-	C(4)	116(2)
C(10)	-	C(5)	-	C(6)	124(2)
C(7)	-	C(6)	-	C(5)	107(2)

TABLE 3

Valency angles (degrees) and estimated standard deviations (cont.)

C(9)	-	C(10)	-	C(5)	104(2)
C(18)	-	C(10)	-	C(5)	106(2)
C(8)	-	C(7)	-	C(6)	111(2)
C(9)	-	C(8)	-	C(7)	109(2)
C(14)	-	C(8)	-	C(7)	109(2)
C(14)	-	C(8)	-	C(9)	106(2)
C(10)	-	C(9)	-	C(8)	111(2)
C(11)	-	C(9)	-	C(8)	114(2)
C(13)	-	C(14)	-	C(8)	114(2)
C(15)	-	C(14)	-	C(8)	117(2)
C(11)	-	C(9)	-	C(10)	107(2)
C(18)	-	C(10)	-	C(9)	113(2)
C(12)	-	C(11)	-	C(9)	107(2)
C(13)	-	C(12)	-	C(11)	111(2)
C(14)	-	C(13)	-	C(12)	112(2)
C(17)	-	C(13)	-	C(12)	117(2)
C(19)	-	C(13)	-	C(12)	107(2)
C(17)	-	C(13)	-	C(14)	102(2)
C(19)	-	C(13)	-	C(14)	113(2)
C(15)	-	C(14)	-	C(13)	106(2)
C(19)	-	C(13)	-	C(17)	105(2)
C(16)	-	C(17)	-	C(13)	104(3)
C(20)	-	C(17)	-	C(13)	117(2)
C(16)	-	C(15)	-	C(14)	103(2)
C(17)	-	C(16)	-	C(15)	107(3)
C(20)	-	C(17)	-	C(16)	108(3)

TABLE 3

Valency angles (degrees) and estimated standard deviations (cont.)

C(21)	-	C(20)	-	C(17)	114(3)
C(27)	-	C(22)	-	C(23)	114(2)
B	-	C(22)	-	C(23)	125(3)
C(24)	-	C(23)	-	C(22)	124(2)
B	-	C(22)	-	C(27)	121(3)
C(26)	-	C(27)	-	C(22)	123(2)
C(25)	-	C(24)	-	C(23)	115(3)
C(26)	-	C(25)	-	C(24)	126(2)
C(27)	-	C(26)	-	C(25)	117(2)

TABLE 4

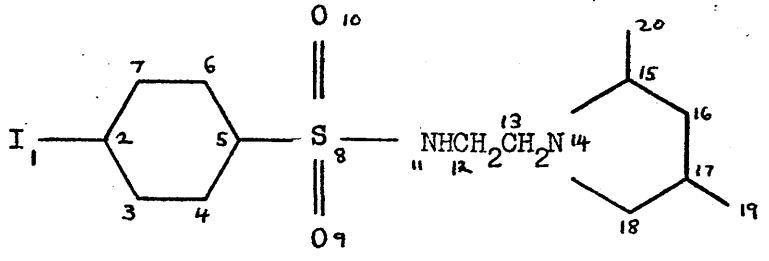
Mean Plane calculations

	Atoms in plane	Atoms out of plane	Deviation (Å)
(1)	O(2)		0.04
	O(3)		-0.04
	C(21)		0.04
	C(17)		-0.04
		C(20)	-0.69
		B	-0.03
(2)	O(2)		0.05
	O(3)		-0.03
	C(21)		0.03
	C(17)		-0.04
	B		-0.01
		C(20)	-0.70
		C(22)	0.26

Appendix II

The crystal structure of N-2-(2,4-dimethyl-1-pyrrolidinyl)-ethyl-p-iodobenzene-sulphonamide

The structural study of this compound was undertaken to verify the results obtained from the Weissenberg X-ray data of the bromo derivative (unpublished).



The iodo compound crystallises in space group $P\bar{1}$ whereas the space group for the bromo derivative is $P2_1/c$. Although the structure of the compound was solved by this study, very high isotropic temperature factors (B(max.) = 18.6) were found to be associated with a number of atoms. The high temperature factors were also a feature of the bromo derivative (B(max.) = 15.0) and both sets of data produced high standard deviations for all the required parameters.

Crystal data

Molecular formula	$C_{14}H_{21}N_2O_2SI$
Molecular weight	408.3 a.m.u.
Crystal system	triclinic
Space group	$P\bar{1}$ (C_i^1)
Cell dimensions	$\underline{a}$ = 12.575(9) Å
	$\underline{b}$ = 13.280(8) Å
	$\underline{c}$ = 10.535(6) Å
	$\underline{\alpha}$ = 95.65(5)°
	$\underline{\beta}$ = 95.58(5)°
	$\underline{\gamma}$ = 85.55(5°)
Cell volume (u)	1738.4 $Å^3$
Density (obs.)	1.56 $g.cm^{-3}$
Density (calc.)	1.56 $g.cm^{-3}$
Molecules per unit cell (z)	4
No. electrons per unit cell ($F_{(000)}$)	816
Linear absorption coefficient, μ (MoKα)	19.83 cm^{-1}

The crystal used in the analysis was colourless and rectangular in shape. Weissenberg and precession photographs showed the crystal system to be triclinic and the unit cell dimensions were obtained.

The crystal was transferred to the diffractometer and data for the octants hkl, $hk\bar{l}$, $h\bar{k}l$ and $h\bar{k}\bar{l}$ were collected out to $\theta \leq 27°$. The data were corrected for Lorentz and polarisation effects and only those

reflections with $I \geq 2.5\sigma I$ were accepted as significantly above background, 3104 independent structure amplitudes being obtained.

Structure analysis

With the assumption that the space group was $P\bar{1}$ the co-ordinates of the iodine atoms in the 2 molecules of the assymetric unit were deduced from a sharpened Patterson synthesis. Structure-factor calculations based on these co-ordinates gave R = 0.391. The remaining atoms were located after a number of difference Fourier syntheses; the atoms of the pyrrolidine ring were clearly located but the peak heights were very small. Unit weights were applied in all least-squares calculations, with the iodine and sulphur atoms assigned anisotropic thermal parameters and the oxygen, nitrogen and carbon atoms isotropic parameters. The least-squares calculations converged to R = 0.130.

Discussion

The methyl groups are in a cis-configuration on the pyrrolidine ring as shown in Figure 1; this configuration is in agreement with that found in the bromo derivative. The packing of the molecules in the crystal is shown in Figure 2 and tables 1, 2 and 3 list the atomic positions, the bond lengths and the valency angles respectively. For both the iodo and bromo derivatives the atoms of the pyrrolidine ring have not been accurately determined and it is here that the highest temperature factors are found.

It is possible the molecules of the crystal are disordered but the mode of disorder, if present, is not clear.

Figure 1

A general view of the N-2-(2,4-dimethyl-1-pyrrolidinyl)-ethyl-p-iodobenzene-sulphonamide molecule.

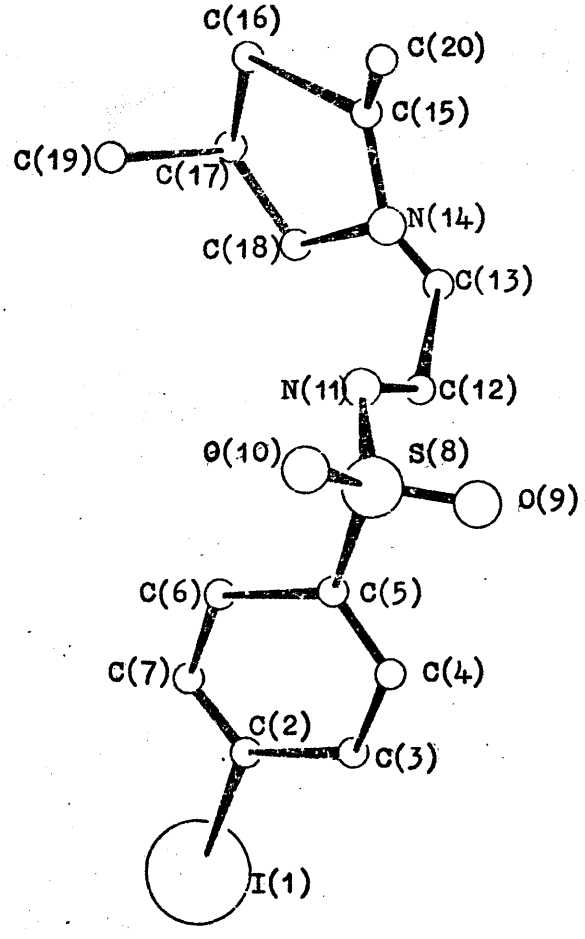


Figure 2

The packing of the molecules in N-2-(2,4-dimethyl-1-pyrrolidinyl)-ethyl-p-iodobenzene-sulphonamide viewed on the ba plane.

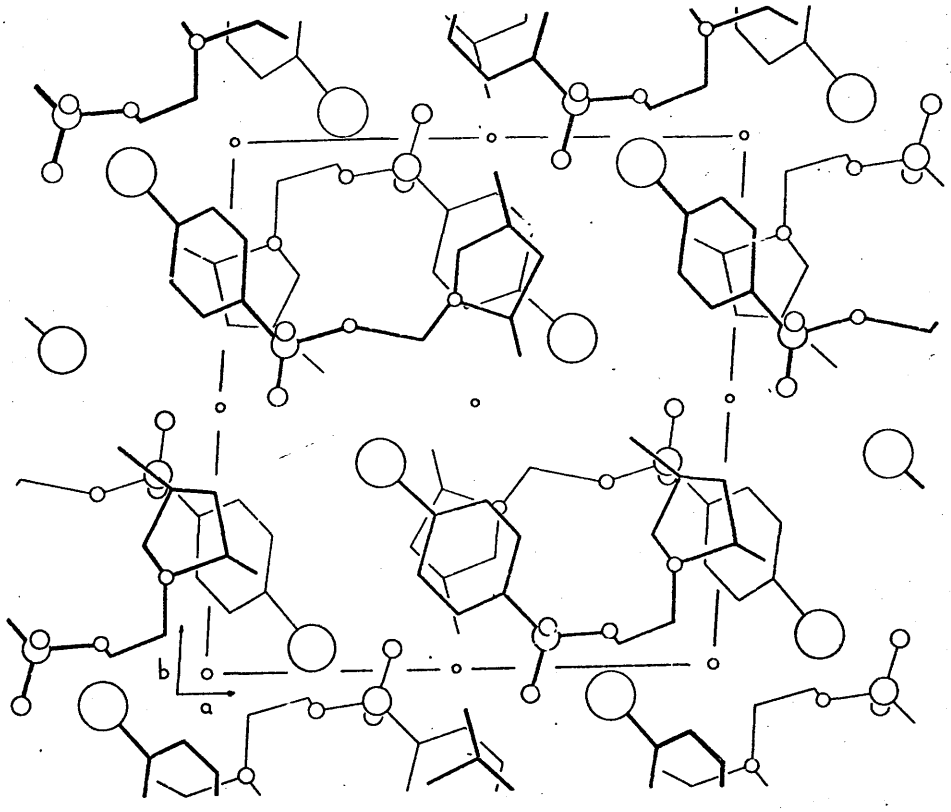


TABLE 1

Molecule 1

Fractional atomic co-ordinates, positional standard deviations and temperature factors

Atom	X	Y	Z	B
I(1)	-0.2157(2)	0.9370(2)	-0.1092(3)	✓
C(2)	-0.1085(41)	0.8425(39)	0.0002(40)	5.65
C(3)	-0.1208(42)	0.7351(41)	-0.0297(42)	5.83
C(4)	-0.0426(42)	0.6728(40)	0.0377(41)	5.82
C(5)	0.0370(41)	0.7090(38)	0.1222(40)	5.35
C(6)	0.0393(52)	0.8242(50)	0.1444(50)	6.90
C(7)	-0.0366(36)	0.8853(32)	0.0817(35)	4.66
S(8)	0.1352(7)	0.6361(5)	0.2022(7)	✓
O(9)	0.1179(20)	0.5308(18)	0.1520(23)	8.64
O(10)	0.1388(16)	0.6658(14)	0.3379(19)	6.55
N(11)	0.2543(20)	0.6611(18)	0.1656(24)	6.14
C(12)	0.2746(35)	0.6440(30)	0.0252(39)	9.34
C(13)	0.3916(45)	0.6247(39)	0.0241(51)	12.80
N(14)	0.4525(27)	0.7032(25)	0.0970(31)	9.34
C(15)	0.5661(46)	0.6680(41)	0.1305(52)	13.36
C(16)	0.6293(53)	0.7808(49)	0.1818(63)	16.32
C(17)	0.5472(58)	0.8349(53)	0.0824(69)	16.46
C(18)	0.4456(51)	0.7892(46)	0.0083(58)	17.13
C(19)	0.5261(58)	0.9405(55)	0.1859(70)	18.53
C(20)	0.6017(57)	0.6063(52)	0.2619(70)	18.60

TABLE 1 (cont.)

Molecule 2

Fractional atomic co-ordinates, positional standard deviations and temperature factors

Atom	X	Y	Z	B
I(1)	0.3385(2)	0.4124(2)	0.2996(2)	✓
C(2)	0.4600(37)	0.3214(37)	0.3832(40)	5.30
C(3)	0.4375(47)	0.2069(44)	0.3818(45)	7.53
C(4)	0.5167(41)	0.1396(40)	0.4399(41)	6.94
C(5)	0.6133(35)	0.1773(32)	0.4882(33)	4.55
C(6)	0.6363(48)	0.2857(45)	0.4854(47)	5.70
C(7)	0.5600(38)	0.3475(34)	0.4258(36)	5.27
S(8)	0.7081(7)	0.0091(5)	0.5623(8)	✓
O(9)	0.6780(17)	-0.0048(15)	0.5260(20)	7.22
O(10)	0.7238(16)	0.1344(14)	0.6942(19)	6.33
N(11)	0.8241(18)	0.1081(16)	0.5075(22)	5.62
C(12)	0.8315(27)	0.0720(24)	0.3680(31)	6.93
C(13)	0.9448(40)	0.1052(37)	0.3382(46)	11.97
N(14)	0.9447(22)	0.2182(20)	0.3699(25)	7.24
C(15)	1.0628(32)	0.2572(29)	0.3883(38)	8.96
C(16)	1.0248(31)	0.3724(28)	0.3927(36)	8.71
C(17)	0.9309(38)	0.3753(34)	0.2969(42)	10.41
C(18)	0.8822(33)	0.2729(31)	0.2777(39)	9.40
C(19)	0.8356(44)	0.4526(40)	0.3257(51)	13.51
C(20)	1.1280(35)	0.2359(32)	0.5203(42)	10.52

TABLE 1

Molecule 1 (cont.)

/ For the iodine and sulphur atoms anisotropic temperature factors were employed, having the form:-

$$T = \exp.\left[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)\right]$$

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
I(1)	0.0134	0.0078	0.0227	-0.0004	-0.0010	0.0063
S(8)	0.0147	0.0043	0.0141	-0.0034	-0.0021	0.0019

TABLE 1

Molecule 2 (cont.)

For the iodine and sulphur atoms anisotropic temperature factors were employed, having the form:-

$$T = \exp.[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{13}hl + b_{23}kl)]$$

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
I (1)	0.0142	0.0066	0.0216	-0.0022	-0.0028	0.0060
S (8)	0.0129	0.0035	0.0157	-0.0051	-0.0009	0.0036

TABLE 2

Intermolecular bonded distances and estimated standard deviations (Å)

			Molecule 1	Molecule 2
I(1)	-	C(2)	2.11(5)	2.06(5)
C(2)	-	C(3)	1.45(8)	1.57(9)
C(3)	-	C(4)	1.42(8)	1.42(9)
C(4)	-	C(5)	1.36(7)	1.38(8)
C(5)	-	C(6)	1.53(8)	1.49(7)
C(6)	-	C(7)	1.37(8)	1.36(7)
C(5)	-	S(8)	1.72(5)	1.70(5)
S(8)	-	O(9)	1.47(3)	1.46(3)
S(8)	-	O(10)	1.44(2)	1.42(2)
S(8)	-	N(11)	1.65(3)	1.64(3)
N(11)	-	C(12)	1.52(5)	1.51(4)
C(12)	-	C(13)	1.48(8)	1.59(6)
C(13)	-	N(14)	1.45(7)	1.51(6)
N(14)	-	C(15)	1.49(7)	1.60(5)
C(15)	-	C(20)	1.68(10)	1.58(6)
C(15)	-	C(16)	1.76(10)	1.57(6)
C(16)	-	C(17)	1.58(10)	1.48(6)
C(17)	-	C(19)	1.71(10)	1.55(8)
C(17)	-	C(18)	1.56(10)	1.52(7)
N(14)	-	C(18)	1.54(8)	1.41(5)

TABLE 3

Valency angles (degrees) and estimated standard deviations (degrees)

	Molecule 1	Molecule 2
C(3) - C(2) - I(1)	115(2)	116(2)
O(10) - S(8) - O(9)	121(1)	119(1)
C(5) - S(8) - O(9)	105(2)	107(2)
C(5) - S(8) - O(10)	110(2)	109(2)
C(12) - N(11) - S(8)	117(2)	116(1)
C(6) - C(9) - S(8)	118(3)	118(2)
C(15) - N(14) - C(13)	113(4)	112(3)
C(12) - C(13) - N(14)	114(4)	107(3)
C(16) - C(15) - N(14)	104(5)	95(3)
C(17) - C(18) - N(14)	91(4)	102(3)
C(4) - C(3) - C(2)	114(3)	119(4)
C(5) - C(4) - C(3)	124(4)	118(4)
C(7) - C(6) - C(5)	120(3)	117(3)
C(17) - C(16) - C(15)	87(4)	104(3)
C(19) - C(17) - C(16)	93(5)	118(3)
C(7) - C(2) - I(1)	118(2)	127(3)
N(11) - S(8) - O(9)	107(1)	107(1)
N(11) - S(8) - O(10)	103(1)	104(1)
C(5) - S(8) - N(11)	110(2)	110(2)
C(4) - C(5) - S(8)	125(3)	119(3)
C(13) - C(12) - N(11)	105(3)	104(3)
C(18) - N(14) - C(13)	104(4)	113(3)

TABLE 3

Valency angles (degrees) and estimated standard deviations (degrees) (cont.)

	Molecule 1	Molecule 2
C(18) - N(14) - C(15)	111(4)	109(2)
C(20) - C(15) - N(14)	121(4)	115(3)
C(7) - C(2) - C(3)	127(3)	117(3)
C(6) - C(7) - C(2)	118(4)	125(4)
C(6) - C(5) - C(4)	116(5)	123(4)
C(20) - C(15) - C(16)	98(4)	109(3)
C(18) - C(17) - C(16)	126(5)	110(4)
C(19) - C(17) - C(18)	117(5)	104(4)