CRYSTAL STRUCTURE ANALYSES OF ORGANIC AND ORGANOMETALLIC COMPOUNDS

by

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Summary

The thesis is divided into three parts: the first part is a brief review of the theory and methods of x-ray crystallography, the second part describes a number of computer programmes devised either wholly or partly by the author, and in the third part accounts of three structure analyses are presented.

The computer programmes described in Part II are written in ALGOL for the English Electric KDF9 Computer. The molecular functions system is a group of six programmes for interpreting the results of a structure analysis: bond lengths and interbond angles with their standard deviations, intermolecular contacts, and mean plane equations may be calculated and rigid-body vibrational analysis can be carried out. The automatic structure solution (ASS) system allows semi-automatic Fourier refinement to be performed. The minimum residual programme permits crystal structures to be refined in projection by direct calculation of the minimum R-factor.

The structure analyses presented in Part III are applications of the x-ray method to organic and organo-metallic structural problems.

It has been known for more than twenty years that indene can form a 1:2 adduct with dimethylacetylene-dicarboxylate. Earlier chemical and spectroscopic studies

on the adduct did not lead to a successful structure determination. The molecular structure of the adduct has now been definitely established by x-ray analysis of its dibromo-derivative.

The structure analyses of phenanthrenechromium tricarbonyl, $C_{14}H_{10}Cr(CO)_3$, and of 9,10-dihydrophenanthrenechromium tricarbonyl, $C_{14}H_{12}Cr(CO)_3$, were undertaken to obtain accurate dimensions for aromatic rings bonded to chromium. In both analyses the standard deviations of the C-C bonds range from 0.006 to 0.010 Å. The results suggest that the chromium atom causes a slight increase in the mean bond length of the bonded ring without alteration of the ring symmetry. Structural studies on related arenechromium complexes are discussed.

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PART I

SOME METHODS OF X-RAY ANALYSIS

1.1 INTRODUCTION

X-radiation is produced when high energy electrons collide with matter. It was shown by von Laue in 1912 that x-ray wavelengths are of the same order of magnitude as the distances between adjacent atoms in solids and that, consequently, diffraction patterns are produced when an x-ray beam strikes a crystal.

The science of x-ray crystallography is mainly concerned with the interpretation of such diffraction patterns. The angles at which diffracted beams occur are determined solely by the translations of the crystal lattice. Because x-rays are scattered by electrons the intensities of the diffracted beams are related to the distribution of electrons in the crystal. From a study of the x-ray diffraction pattern it is therefore possible to determine not only the geometry of the unit cell of the crystal and its space group, but also the electron density distribution and the positions of the constituent atoms.

The last fifty years have seen the methods of x-ray structure analysis being applied to more and more complex structures. Initially, greatest progress was made in the field of ionic crystals. Molecular crystals constituted more of a problem, due both to the greater difficulty of determining the electron density distribution from the x-ray intensities and to the scale of the calculations involved. The discovery that the interpretation of a diffraction pattern is greatly simplified when the structure contains a small number of atoms of much greater scattering power than the rest and, more recently, the advent of the electronic computer have removed these problems to a large extent. Today many complex organic molecules - steroids, carbohydrates, terpenoids, alkaloids, and even proteins - have yielded to the x-ray analyst.

1.2 THE GEOMETRY OF X-RAY DIFFRACTION

Consider monochromatic x-radiation of wavelength λ to be incident upon a crystal in a direction defined by the unit vector $\lambda\,\underline{s}_0$ (Fig. 1.1). The path difference, dp, between a wave scattered at a point A in a direction defined by the unit vector $\lambda\,\underline{s}$ is, relative to a wave scattered at the origin O in the same direction,

$$dp = \underline{OB}-\underline{AC} = \lambda\underline{r}.(\underline{s}-\underline{s}_0) = \lambda\underline{r}.\underline{S} \qquad (1)$$

where $\underline{OA} = \underline{r}$ and $\underline{S} = \underline{s}-\underline{s}_0$. The vector $\underline{S}$ defines the spatial relationship of the incident and diffracted beams. From Fig. 1.1 it is easily seen that if 2θ is the angle between incident and diffracted beams, then

$$|\underline{S}| = 2\sin\theta/\lambda \qquad (2)$$

The path difference $\lambda\,\underline{r}.\underline{S}$ corresponds to a phase difference $2\pi\underline{r}.\underline{S}$. If the electron density at A in electrons per unit volume is $p(\underline{r})$, then the wave scattered by the electron density in the volume element dV about A is defined in amplitude and phase, relative to the wave scattered by a single electron at the origin, by the expression

$$G_A(\underline{S}) = p(\underline{r})dV\exp 2\pi i\underline{r}.\underline{S} \qquad (3)$$

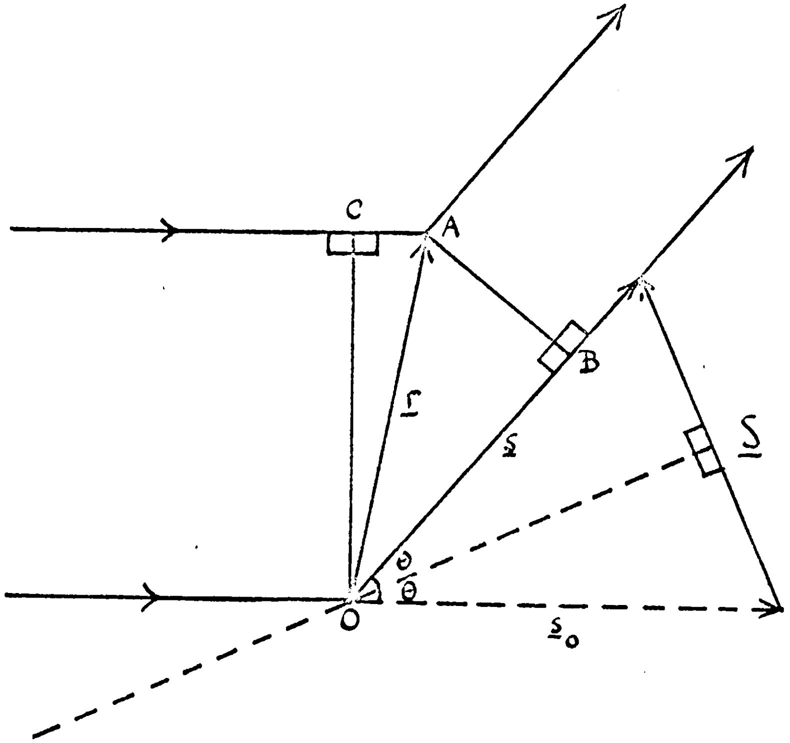


FIG. 1.1

The electron density $p(\underline{r})$ is a periodic function. If $\underline{a}$, $\underline{b}$, and $\underline{c}$ are the translations of the crystal lattice and u,v,w any three integers, then the points which lie on the lattice defined by the vector equation

$$\underline{R} = \underline{r} + u\underline{a} + v\underline{b} + w\underline{c} \qquad (4)$$

have identical electron density. The wave scattered from anyone of these points, B, in the direction $\lambda\ \underline{s}$ is therefore

$$\begin{aligned} G_B(\underline{S}) &= p(\underline{r})dV\exp 2\pi i\underline{R}.\underline{S} \\ &= G_A(\underline{S})\exp 2\pi i(u\underline{a} + v\underline{b} + w\underline{c}).\underline{S} \qquad (5) \end{aligned}$$

The wave scattered by the crystal will have an appreciable amplitude only if all unit cells scatter in phase, that is if the path difference between $G_A(\underline{S})$ and $G_B(\underline{S})$ is always an integral number of wavelengths. If n is an integer this condition may be written as

$$\lambda(u\underline{a} + v\underline{b} + w\underline{c})\underline{S} = n\lambda \text{ for all values of u,v, and w,} \qquad (6)$$

so that

$$\left.\begin{aligned} \underline{a}.\underline{S} &= h \\ \underline{b}.\underline{S} &= k \\ \underline{c}.\underline{S} &= \ell \end{aligned}\right\} \quad \text{where h, k, and } \ell \text{ are integers.} \qquad (7)$$

Equations (7) are called the Laue equations. $\underline{a}.\underline{S} = h$ defines, in the space of $\underline{S}$, a family of planes normal to $\underline{a}$. The spacing between any two adjacent planes is $1/|\underline{a}|$. Since $\underline{a}$, $\underline{b}$, and $\underline{c}$ are never parallel, the Laue equations define three sets of equally spaced planes whose intersections form a lattice in the space of $\underline{S}$. The equation which defines such a lattice is

$$\underline{S} = h\underline{a}^* + k\underline{b}^* + \ell \underline{c}^* \qquad (8)$$

From (7) and (8) it immediately follows that $\underline{a}^*$ is normal to $\underline{b}$ and $\underline{c}$ and that the projection of $\underline{a}^*$ upon $\underline{a}$ is $1/|\underline{a}|$. Similar results follow for $\underline{b}^*$ and $\underline{c}^*$. The primitive translations of the lattice defined by (8), which is termed the reciprocal lattice of the crystal, are related to the primitive translations of the real space lattice of the crystal by

$$\begin{aligned} \underline{a}^* &= \underline{b} \times \underline{c}/V \\ \underline{b}^* &= \underline{c} \times \underline{a}/V \qquad (9) \\ \underline{c}^* &= \underline{a} \times \underline{b}/V \end{aligned}$$

where V is the volume of the unit cell in real space.

The physical significance of the Laue equations may now be stated. They define the values of the vector $\underline{S}$, and hence the relationship between incident and diffracted beams, which result in the beam diffracted by a crystal having an appreciable amplitude. The values of $\underline{S}$ which fulfill this condition are functions only of the lattice translations of the crystal. Each such value of $\underline{S}$ is associated with a point on the reciprocal lattice of the crystal and is uniquely defined by the lattice coordinates h,k, and ℓ.

The Laue equations may be rewritten as

$$(\underline{a}/h).\underline{S} = (\underline{b}/k).\underline{S} = (\underline{c}/\ell).\underline{S} = 1 \qquad (10)$$

By definition $\underline{a}/h$, $\underline{b}/k$, and $\underline{c}/\ell$ are the intercepts which the plane with Miller indices hkℓ makes on the crystal axes. From (10) the projections of three points on this plane on to $\underline{S}$ are equal. $\underline{S}$ is therefore normal to the plane and $|\underline{S}| = 1/d$ where d is the origin to plane distance. Substituting for $|\underline{S}|$ from equation (2) gives

$$2d\sin\theta = \lambda \qquad (11)$$

From Fig. 1.1 it can be seen that $\underline{s}$ and $\underline{s}_0$ make equal angles θ with the plane which is normal to $\underline{S}$. When the diffraction conditions (7) hold, therefore, the incident and diffracted beams stand in the same relationship to the plane with Miller indices hkℓ as incident and reflected beams do to a mirror. This treatment, which is due to W.L. Bragg (1913), allows diffraction by a crystal to be considered in terms of the simpler concept of reflection by a crystal plane.

1.3 THE STRUCTURE FACTOR

The wave scattered by the entire contents of one unit cell, $G(\underline{S})$, is completely defined by

$$G(\underline{S}) = \int p(\underline{r})\exp(2\pi i\underline{r}.\underline{S})dV \qquad (12)$$

where the integration is over the volume of the unit cell. $G(\underline{S})$ is thus the Fourier transform of the electron density distribution. The electron density function, $p(\underline{r})$, may be regarded as a sum of N independent atomic electron densities and (12) may then be rewritten as

$$G(\underline{S}) = \sum_{n=1}^{N}\int_{-\infty}^{+\infty} p_n(\underline{r})\exp\{2\pi i(\underline{r}+\underline{r}_n).\underline{S}\}dV \qquad (13)$$

In (13) $p_n(\underline{r})$ is the electron density distribution of the n^{th} atom referred to an origin in the atom. This origin is connected to the origin of the unit cell by the vector $\underline{r}_n$.

The function

$$f_n(\underline{S}) = \int_{-\infty}^{+\infty} p_n(\underline{r})\exp 2\pi i\underline{r}.\underline{S}\ dV \qquad (14)$$

is the Fourier transform of the atomic electron density and is termed the atomic scattering factor. If the atom is centrosymmetric and if the origin of $\underline{r}$ has been taken at the centre of symmetry, $f_n(\underline{S})$ is a real function; if $p_n(\underline{r})$ is spherically symmetric and hence a function of $|\underline{r}|$ only, $f_n(\underline{S})$ is a function of $|\underline{S}| = 2\sin\theta/\lambda$ only. Since $p_n(\underline{r})$ is known exactly only for the isolated hydrogen atom the atomic scattering factor can in general only be calculated approximately. Tabulated results of such calculations are given for spherically symmetrical atoms in International Tables Vol. III (1962). The physical interpretation of the scattering factor is that it describes the total wave scattered by an atom. There are phase differences between the waves scattered at different parts of the same atom and such phase differences increase with scattering angle. Accordingly the amplitude of the total wave scattered by the atom, and hence $f_n(\underline{S})$, decreases as $\sin\theta/\lambda$ increases.

Substitution of (14) into (13) yields

$$G(\underline{S}) = \sum_1^N f_n(\underline{S})\exp 2\pi i \underline{r}_n\cdot\underline{S} \qquad (15)$$

The total wave scattered by the crystal has an appreciable amplitude only if

$$\underline{S} = h\underline{a}^* + k\underline{b}^* + \ell\,\underline{c}^* \qquad (8)$$

If the fractional coordinates of the n^{th} atom are x_n, y_n, and z_n then

$$\underline{r}_n = x_n\underline{a} + y_n\underline{b} + z_n\underline{c} \qquad (16)$$

Making use of the relations $\underline{a}.\underline{a}^* = 1$, $\underline{a}.\underline{b}^* = \underline{a}.\underline{c}^* = 0$ and similar ones involving $\underline{b}$ and $\underline{c}$, it is found that

$$\underline{r}_n.\underline{S} = hx_n + ky_n + \ell z_n \tag{17}$$

Substitution of (17) into (15) gives the structure factor expression

$$G(\underline{S}) = F(hk\ell) = \sum_1^N f_n(hk\ell)\exp 2\pi i(hx_n+ky_n+\ell z_n) \tag{18}$$

The structure factor, $F(hk\ell)$, is defined only when the vector $\underline{S}$ takes values which result in the total wave scattered by the crystal having a non-zero amplitude. It then describes the amplitude and phase of the wave scattered by one unit cell, and, since all unit cells are scattering in phase, also describes the amplitude and phase of the total wave scattered by the crystal. $F(hk\ell)$ is generally complex and may be written as

$$F(hk\ell) = A + iB \tag{19}$$

where

$$A = \sum_1^N f_n(hk\ell)\cos 2\pi(hx_n+ky_n+\ell z_n) \tag{20}$$

$$B = \sum_1^N f_n(hk\ell)\sin 2\pi(hx_n+ky_n+\ell z_n) \tag{21}$$

The The modulus, $|F(hk\ell)|$, and phase, $\alpha\ (hk\ell)$, are defined by

$$|F(hk\ell)| = (A^2 + B^2)^{\frac{1}{2}} \tag{22}$$

$$\alpha\ (hk\ell) = \tan^{-1} B/A \tag{23}$$

If the space group is centrosymmetric, provided the origin of coordinates has been taken at a centre of symmetry, then $B=0$ and $\alpha(hk\ell)$ is restricted to the values of 0° or 180°.

The atomic scattering factor is normally calculated from the electron density of an atom at rest. Atoms in crystals have an appreciable motion at room temperature due to thermal vibration. The effect of such motion is to make the atomic electron density more diffuse and so to increase the rate at which the amplitude of the wave scattered by the atom falls off with scattering angle. To allow for the effect it is necessary to replace the atomic scattering factor in the structure factor expression by the transform of the electron density of the vibrating atom. If the smearing function, $t(\underline{x})$, gives the probability that the atomic centre is at $\underline{x}$, the origin of $\underline{x}$ being taken at the maximum of the electron density of the vibrating atom, then the electron density of the vibrating atom $p_v(\underline{r})$ is given by

$$p_v(\underline{r}) = \int_{-\infty}^{+\infty} p(\underline{u})t(\underline{r}-\underline{u})d\underline{u} \qquad (24)$$

where $p(\underline{u})$ is the electron density of the atom at rest. $p_v(\underline{r})$ is thus the convolution of $p(\underline{u})$ and $t(\underline{x})$, and its transform is the product of the transform of $t(\underline{x})$ and the atomic scattering factor (which has already been shown to be the transform of $p(\underline{u})$). Bloch (1932) showed that for an atom vibrating in an isotropic harmonic potential the smearing function, $t(\underline{x})$, is a Gaussian and that its transform is given by

$$q(\underline{S}) = \exp-2\pi^2 U\underline{S}^2 = \exp-8\pi^2 U\sin^2\theta/\lambda^2 \qquad (25)$$

where $U = u^2$ and u is the root mean square amplitude of vibration.

If the atomic vibrations are anisotropic U must be replaced by the symmetrical third order tensor $\underline{U}$ and the mean square amplitude of vibration in the direction of the unit vector $\underline{\ell}$ is then

$$u^2 = \sum_{i=1}^{3}\sum_{j=1}^{3} U_{ij}\,\ell_i\,\ell_j \qquad (26)$$

where both $\underline{\ell}$ and $\underline{U}$ are referred to the reciprocal lattice axes. In the anisotropic case the transform of the smearing function becomes

$$q(\underline{S}) = q(hk\ell) = \exp-2\pi^2 \quad (U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{23}k\ell b^*c^* + 2U_{31}\ell hc^*a^* + 2U_{12}hka^*b^*) \qquad (27)$$

The structure factor expression may therefore be written as

$$F(hk\ell) = \sum_{1}^{N} f_n(hk\ell)q_n(hk\ell)\exp2\pi i(hx_n+ky_n+\ell z_n) \qquad (28)$$

1.4 THE FOURIER SERIES REPRESENTATION OF ELECTRON DENSITY

The electron density function, $p(\underline{r})$, is a finite single-valued function which is periodic in three dimensions. It may therefore be represented by a Fourier series. If u,v, and w are integers and x,y, and z fractional coordinates then

$$p(\underline{r}) = p(xyz) = \sum_{u} \sum_{v=-\infty}^{+\infty} \sum_{w} A(uvw)\exp-2\pi i(ux+vy+wz) \qquad (29)$$

The structure factor is the Fourier transform of p(xyz), so that

$$F(hk\ell) = V\int_{0}^{1}\int_{0}^{1}\int_{0}^{1} p(xyz)\exp 2\pi i(hx+ky+\ell z)dxdydz \qquad (30)$$

Replacing p(xyz) in the above expression by the Fourier series (29) gives, with some rearrangement,

$$F(hk\ell) = V \sum_{u} \sum_{v=-\infty}^{+\infty} \sum_{w} \left[\int_{0}^{1}\int_{0}^{1}\int_{0}^{1} A(uvw)\exp 2\pi i(h-u)x.\exp 2\pi i(k-v)y \times \exp 2\pi i(l-w)z.dxdydz \right] \qquad (31)$$

The integral in (31) enclosed in square brackets is zero, unless h = u, k = v, and ℓ= w. Therefore

$$F(hk\ell) = VA(uvw) \qquad (32)$$

which on substitution in (29) yields

$$p(xyz) = \frac{1}{V} \sum_{h} \sum_{k=-\infty}^{+\infty} \sum_{\ell} F(hk\ell)\exp-2\pi i(hx+ky+\ell z) \qquad (33)$$

The hkℓ coefficient of the Fourier series which represents the electron density function is thus the structure factor F(hkℓ), scaled by the reciprocal of the cell volume.

1.5 THE MEASUREMENT OF STRUCTURE AMPLITUDES

The total energy, $E(hk\ell)$, of the x-ray beam reflected from the set of planes with Miller indices $hk\ell$ of a small rotating crystal may be shown to be

$$E(hk\ell) = K.L(hk\ell).p(hk\ell).\ |F(hk\ell)|^2 \qquad (34)$$

where K is constant for the experiment and is given by

$$K = \frac{I_o \lambda^3 N^2 dV}{w} \quad \frac{e^4}{m^2 c^4} \qquad (35)$$

The symbols in (35) have the following meanings:-

I_o is the intensity of the incident beam,

λ is the wavelength of the x-radiation,

N is the number of unit cells per unit volume,

dV is the volume of crystal irradiated,

w is the angular velocity of the crystal,

e is the electronic charge,

m is the mass of an electron, and

c is the speed of light.

The polarisation factor, $p(hk\ell)$, takes into account the unpolarised nature of the radiation used. For all experimental conditions it is given by

$$p(hk\ell) = (1+\cos^2 2\theta)/2 \qquad (36)$$

The Lorentz factor, $L(hk\ell)$, allows for the different times during which the reflecting condition is obeyed by different crystal planes. It depends on the experimental method used. For equi-inclination Weissenberg photographs it takes the form (Tunell, 1939)

$$L(hk\ell) = \sin\theta\,(\cos^2\mu - \cos^2\theta)^{-\frac{1}{2}}\,(\sin 2\theta)^{-1} \qquad (37)$$

where μ is the angle between the incident beam and the plane normal to the rotation axis.

The energy of the diffracted beam is proportional to its intensity, $I(hk\ell)$, which may be measured by either the blackening produced by the beam on a photographic film or by the number of quanta detected by a radiation counter held in the beam.

Therefore

$$I(hk\ell) \propto L(hk\ell).p(hk\ell).\,|F(hk\ell)|^2 \qquad (38)$$

Using (38) the structure amplitude, $|F_o|$, of a Bragg reflection may be determined from measurable quantities, albeit on an arbitrary scale. The absolute scale may be determined by experimental comparison with a standard (Robertson, 1934). Alternatively, it may be deduced from the decrease in average structure amplitude with scattering angle (Wilson, 1942) or at a somewhat later stage in the analysis by comparison with structure factors calculated from a reliable model of the structure.

Equations (34) and (38) are strictly applicable only to microscopic crystals but they are also found to apply to the larger crystals used in diffraction experiments

Such crystals have a mosaic structure, that is, their lattice contains regions of disregistry, and they behave like an aggregation of approximately alligned microscopic crystals rather than as a single block of ideal crystal. However even with small mosaic crystals some effects which are negligible in the case of diffraction by a microscopic crystal become important, and, if neglected, they may lead to systematic errors in the structure amplitudes calculated by equation (38).

Chief amongst these is absorption. As an x-ray beam passes through a crystal its intensity decreases due to absorption and the beam incident on the lower layers of the crystal is weaker than that incident on the surface layers. The diffracted beam is also partly absorbed. The resultant weakening of the intensity of the diffracted beam is different for different reflections and is greatest for the low order spectra. Adequate correction for the effect is possible only for crystals of spherical or cylindrical shape.

It is a consequence of the geometry of x-ray diffraction that the beam reflected from a set of crystal planes obeys the Bragg reflection condition for these planes and may therefore be reflected again. Such a doubly reflected beam is parallel to the incident beam and exactly out of phase with it. Primary extinction, as the effect is called, thus results in the beam incident on the lower layers of the crystal being weaker than the beam incident on the upper layers. Correction for the effect is difficult.

When the Bragg reflection condition is satisfied part of the incident beam is reflected by the upper layers of the crystal and the beam incident on the lower layers is consequently weakened. This effect is called secondary extinction. Methods of correcting for the effect are available.

1.6 THE PHASE PROBLEM

To calculate, using the Fourier series expression, the electron density distribution in a crystal it is necessary to know the amplitude and phase of each structure factor. The structure amplitude is an experimentally accessible quantity but there is no experimental method which allows phases to be determined; this constitutes the phase problem of crystal structure analysis.

Many ingenious methods of surmounting this problem have been devised and some of the more commonly used of these are described below. It is, however, still true that a proportion of structures cannot be solved by currently known methods.

1.6.1 THE PATTERSON FUNCTION

The function defined by Patterson (1934) is the self-convolution of the electron density. Itis defined by

$$P(uvw) = V\int_{0}^{1}\int_{0}^{1}\int_{0}^{1} p(xyz).p(x+u,y+v,z+w).dxdydz \qquad (39)$$

where u, v, and w are fractional coordinates. If Fourier series are substituted for the electron density functions in equation (39), P(uvw) is found to be a sum of integrals of the form

$$T = \int_{0}^{1}\int_{0}^{1}\int_{0}^{1} F(hk\ell)F(h'k'\ell')\exp-2\pi i(h+h')x.\exp-2\pi i(k+k')y \times\exp-2\pi i(\ell+\ell')z.\exp-2\pi i(hu+kv+\ell w).dxdydz \qquad (40)$$

The integral T is zero unless $h = -h'$, $k = -k'$, and $\ell = -\ell'$ when

$$T = F(hk\ell)F(\overline{hk\ell})\exp-2\pi i(hu+kv+\ell w) \qquad (41)$$

Since $F(hk\ell)$ and $F(\overline{hk\ell})$ are complex conjugates

$$F(hk\ell)F(\overline{hk\ell}) = |F(hk\ell)|^2 = |F(\overline{hk\ell})|^2 \qquad (42)$$

and the Patterson function may be written as

$$P(uvw) = \frac{1}{V}\sum_{h}\sum_{k=-\infty}^{+\infty}\sum_{\ell}|F(hk\ell)|^2\exp-2\pi i(hu+kv+\ell w) \qquad (43)$$

To compute the Patterson function from equation (43) only a knowledge of the structure amplitudes is required. From equation (39) it can be seen that the Patterson function will attain large values only if the vector defined by (uvw) corresponds to a vector between two peaks in the electron density distribution; the value of P(uvw) will then be approximately the product of the electron density values at the two peaks. Harker (1936) pointed out that the presence of certain elements of symmetry results in peaks being concentrated on special lines and sections through the three-dimensional Patterson function.

In a unit cell containing N atoms the number of distinct interatomic vectors which can occur is N(N-1). This also is the number of peaks which should appear in the corresponding Patterson function. It is therefore difficult to obtain the positions of all the atoms in even a moderately complicated structure by inspection of the Patterson synthesis.

1.6.2 THE HEAVY ATOM METHOD

If a structure contains a small number of heavy atoms whose scattering power is approximately equal to the combined scattering power of the other atoms then the dominant peaks in the Patterson function will correspond to vectors between the heavy atoms and it will be possible to determine their positions. The phases of structure factors in which only the heavy atom contributions have been included are, under such circumstances, a good first approximation to the true phases and may be used to calculate an electron density distribution.

The heavy atom method, as this technique is called, is the most frequently used way of surmounting the phase problem and is often the only way if the structure is at all complicated. Its main disadvantage is that the major part of each structure amplitude comes from the scattering of the heavy atoms and the accuracy with which the positions of the lighter atoms can be fixed is correspondingly lessened.

This difficulty is minimised in the method of isomorphous substitution. A heavy atom derivative is used to determine the phases but the final refinement is carried out on an isomorphous derivative in which the heavy atom has been replaced by a much lighter one.

The structural studies of the phthalocyanines by Robertson (1935), (1936), and Robertson and Woodward (1937), (1940) are classical examples of the successful application of both heavy atom and isomorphous replacement methods.

1.6.3 TRIAL AND ERROR METHODS

Models of a crystal structure which stand a reasonable chance of being close to the true structure can sometimes be developed from a consideration of such factors as the limitations imposed by space group symmetry, the chemical and physical properties of the crystal, the dominant features of the diffraction pattern, and from possible similarities to known structures. The calculated diffraction patterns of the models may then be compared with the observed diffraction pattern of the crystal and those which show violent disagreement discarded. The method is usually only applicable when the molecular structure is known. The solutions of the structures of pyrene (Robertson and White, 1947) and of violanthrone (Stadler, 1953) are examples of this approach.

1.6.4 DIRECT METHODS

A number of authors, notably Harker and Kasper (1948) and Sayre (1952), have derived relationships between structure factors which arise, for example, if the electron density is constrained to be greater than zero. Such relationships allow phases for the larger structure factors to be calculated directly. The method has been mainly applied to centrosymmetric structures. A recent example of its use is the determination of the structure of the alkaloid jamine by Karle and Karle (1964).

1.7 METHODS OF STRUCTURE REFINEMENT

From the approximate electron density synthesis obtained by one of the methods outlined in the preceding section the positions of most atoms in the structure can usually be determined. The process of structure refinement may then be started.

The general aim is to minimise some function of the difference between the observed structure amplitudes and those calculated for the model which is being refined. In the early stages of refinement the usual function minimised is the discrepancy index or R-factor which is defined by

$$R = \Sigma \big| |F_o| - |F_c| \big| / \Sigma |F_o| \qquad (44)$$

where $|F_o|$ is the observed structure amplitude, $|F_c|$ that calculated for the model, and the summation is over the structure amplitudes used in the refinement.

1.7.1 FOURIER REFINEMENT METHODS

The atomic positions obtained from an approximate electron density synthesis may be used to compute phases which are closer to the true values than those on which the original synthesis was based. It is therefore possible, by preparing successive electron density syntheses, to calculate continually better approximations to the true phases. Such a process of refinement is complete when the phases derived from a synthesis are the same as those used to calculate it.

The chief advantage of this method of refinement is that it can be started before all atoms in the structure have been located. Under such circumstances Woolfson (1956) and Sim (1960) have suggested that the Fourier coefficient should be multiplied by a weight proportional to the probability that the phase being applied to it is correct. The main disadvantage of the Fourier method is that the atomic positions derived from it are affected by termination of series errors. Due to experimental limitations it is necessary to truncate the Fourier series used to calculate the electron density distribution after a finite number of terms. In a typical organic structure this may lead to errors in derived positions of the order of 0.02 Å. Booth (1946) has suggested a method of allowing for this effect by computing an electron density map with the calculated structure factors as coefficients. The corrections for termination of series errors to the coordinates derived from this map can be estimated. These corrections may then be applied to the coordinates derived from the electron density map calculated with the observed structure amplitudes since series termination errors should be the same in the two maps.

The properties of the difference synthesis, which is derived from a Fourier series whose coefficients are

$(F_o - F_c)$, have been described by Booth (1948a) and Cochran (1951). The difference synthesis of a completely refined structure has a flat topography in which only random fluctuations in density are apparent. A small error in an atomic position results in the atom lying on a steep gradient of density in the difference map. Temperature factor errors have also a characteristic appearance. The main applications of the difference synthesis in modern structure analysis have been in checking the results of a least-squares refinement (see below) and in determining the positions of hydrogen atoms.

1.7.2 LEAST-SQUARES REFINEMENT

The application of the method of least-squares to structure refinement was first suggested by Hughes (1941). The object is to minimise some function of the differences between the observed and calculated intensities with respect to the structure parameters. The function most commonly minimised is

$$M = \sum_m w(|F_o| - |F_c|)^2 \qquad (45)$$

where the summation is over all m independent reflections and w is a weight for each term. If the standard deviation of $|F_o(hk\ell)|$ is $\sigma(hk\ell)$ it can be shown that the choice of weights which gives the lowest standard deviations in the derived parameters is

$$w(hk\ell) = 1/\sigma^2(hk\ell) \qquad (46)$$

If $p_1, p_2, \ldots, p_n$ are the n parameters whose values are to be determined the condition that M is a minimum is that

$$\partial M/\partial p_j = 0 \qquad (j = 1,2,\ldots,n) \qquad (47)$$

i.e. $\Sigma w\Delta\partial|F_c|/\partial p_j = 0$

where $\Delta = |F_o| - |F_c|$. The parameters have to be varied until these n conditions are satisfied. For a trial set of p_j close to the correct values Δ may be expanded as a function of the parameters by a Taylor series of the first order

$$\Delta(\underline{p}+\underline{e}) = \Delta(\underline{p}) - \sum_{i=1}^{n} e_i \partial|F_c|/\partial p_i \qquad (48)$$

where e_i is a small change in the parameter p_i and $\underline{p}$ and $\underline{e}$ stand for the parameters and changes as a whole. Substitution of (48) into (47) yields the normal equations

$$\sum_{i=1}^{n} \left(\sum_m w \frac{\partial|F_c|}{\partial p_i} \frac{\partial|F_c|}{\partial p_j}\right) e_i = \sum_m w\Delta \frac{\partial|F_c|}{\partial p_j} \qquad (j = 1,2,\ldots,n) \qquad (49)$$

The normal equations may be written in matrix notation as

$$\sum_{i=1}^{n} a_{ij} e_i = b_j \qquad (j=1,2,\ldots\ldots,n), \tag{50}$$

where

$$a_{ij} = \sum_{m} w \frac{\partial |F_c|}{\partial p_i} \frac{\partial |F_c|}{\partial p_j} \tag{51}$$

and

$$b_j = \sum_{m} w\Delta \frac{\partial |F_c|}{\partial p_j} \tag{52}$$

The solution of (50) is

$$e_j = \sum_{i=1}^{n} (a^{-1})_{ij} b_i \tag{53}$$

where $(\underline{a}^{-1})$ is the matrix inverse to $\underline{a}$

The number of independent elements of the matrix $\underline{a}$ is proportional to the square of n, the number of parameters being refined. Since the capacity of a computer for storing numbers is limited, it is often necessary to make some approximation to $\underline{a}$. The DEUCE least-squares programme (Rollett, 1961) used in the work described in Chapter I of Part III of this thesis calculated a chain of 3 x 3 and 6 x 6 matrices down the diagonal of $\underline{a}$ for the refinement of the fractional coordinates and anisotropic temperature factors for each atom plus a 2 x 2 matrix for scale and overall temperature factor refinement. The programme written by Cruickshank and Smith which was used for the rest of the work described in Part III calculates a 9 x 9 matrix for the parameters of each atom instead; if an isotropic temperature factor is being refined a 4 x 4 matrix is calculated.

Due to the omission of higher terms in the Taylor series for Δ (48) it is usually necessary to calculate several cycles of refinement before the minimum of M is obtained. The criterion generally used to decide when a refinement should be terminated is that the ratio of the shift, e_i, of each parameter to its standard deviation should be less than unity and preferably less than a half. The course of the refinement may be followed from the change in M or from the function

$$R' = \Sigma w\Delta^2/\Sigma wF_o^2 \qquad (54)$$

The discrepancy index defined by equation (44) may also be used and has the advantage that it is unaffected by changes in the weighting scheme.

1.8 THE ANALYSIS OF RESULTS

At the conclusion of a structure analysis it is often important to decide whether some function of the refined parameters, a bond length say, differs from its theoretical or standard value. Such a problem can be solved by a statistical significance test, the application of which requires a knowledge of the standard deviation of the function in question.

The method of least-squares allows the standard deviations of the refined parameters to be estimated without much additional calculation. The variance of the parameter p_i is given by

$$\sigma(p_i) = (\underline{a}^{-1})_{ii}(\Sigma w\Delta^2/m-n) \tag{55}$$

and the covariance of the parameters p_i and p_j is given by

$$\begin{aligned} \mathrm{cov}(p_i p_j) &= (\underline{a}^{-1})_{ij}(\Sigma w\Delta^2/m-n) \\ &= \sigma(p_i)\,\sigma(p_j) r_{ij} \end{aligned} \tag{56}$$

where r_{ij} is the correlation coefficient of the parameters. These equations are valid only if the weighting scheme is appropriate to the data; the usual test applied is that the average $w\Delta^2$ should be approximately constant if the data are examined in a systematic manner.

The standard deviations of functions of the refined parameters may be calculated from the parameter variances and covariances obtained from equations (55) and (56), by established statistical methods. A set of programmes which allows such calculations to be performed is described in Part II Chapter I. Alternatively, if the experiment has resulted in several independent measurements of a quantity the root mean square deviation of these measurements from their mean value gives an estimate of the standard deviation of an individual measurement.

If x is the value of an experimentally derived quantity whose standard deviation is σ (x), the probability, P, that x differs from its theoretical or expected value, m, due to random experimental errors may be determined from the value of t, where t is a random variable distributed in Student's distribution, and defined by

$$t = |x-m| \;/\; \sigma(x) \qquad (57)$$

when $t = 2.6$, $P = 1\%$ and when $t = 3.3$, $P = 0.1\%$.

If the goodness of fit of a set of experimental results to their expected values is under consideration the χ^2 test may be used. If, for instance, d_i is the deviation of the i^{th} of a set of n points from the least-squares plane through the points, then

$$\chi^2 = \sum_{i=1}^{n} d_i^{\,2}/\sigma^2 \qquad (58)$$

where σ is the average positional standard deviation of a point. The probability that the deviations from the plane are due to random experimental errors can then be found by looking up tables of χ^2 for n-3 degrees of freedom (Fisher and Yates, 1953).

PART II

CHAPTER I

THE MOLECULAR FUNCTIONS SYSTEM

1.1 INTRODUCTION

The molecular functions system consists of a group of six programmes for interpreting the results of a crystal structure analysis. With these programmes it is possible, in a single run on the computer, to calculate all bond lengths and interbond angles in the asymmetric unit, with our without their standard deviations, to determine the best plane through a specified group of atoms, and to find all intermolecular contacts less than a given value. It is also possible to perform an analysis of the molecular vibrations and to prepare tables of such quantities as fractional atomic coordinates in a form suitable for presentation in a thesis or paper. All the programmes are written in ALGOL for the English Electric KDF9 computer. As an illustration of the programming methods the ALGOL texts of two of the programmes are given in Appendix II.

The basic input data consists of the cell dimensions, the fractional coordinates and temperature factors punched in the same form as the output from the Glasgow least-squares programme, and, optionally, the coordinate standard deviations and correlation coefficients. This information is written on magnetic tape at the start of a run and is then available to any of the programmes described in sections 1.3 to 1.7. The rest of the input data consists of instructions to the computer as to which of the programmes are required and the small amounts of information needed to control the calculations. Output formats have been designed to be intelligible without any external key. Atoms are identified by a chemical type symbol and bracketed integer and care has been taken that all the programmes use the same system of atomic identifiers.

Most of the programmes have been in general use in this laboratory for over a year and they have in addition been used by crystallographers in the University of Newcastle. Working copies of the programmes have also been sent to five other crystallographic laboratories which use KDF9 computers.

In the case of two of the programmes the role of the present author has been to adapt existing programmes so that they could fit into the system; the bond length and angle standard deviation programme was originally written by Dr. W.S. Macdonald and the mean plane programme by Dr. W. Oberhansli. Dr. W.S. Macdonald is also a co-author of the molecular vibrations analysis programme. The donation of subroutines by Dr. J.G. Sime, Mr. D. Macgregor and Mr. J.G.F. Smith is also acknowledged.

1.2 ORTHOGONALISATION FORMULAE

In all of the programmes the first step is to transform the imput data so that it refers to equal orthogonal axes. In this section the equations required to orthogonalise fractional coordinates, their standard deviations, and anisotropic vibration tensors are stated.

We take as a standard set of orthogonal axes unit $\underline{Z}$ parallel to $\underline{c}$, unit $\underline{X}$ parallel to $\underline{a}^*$, and unit $\underline{Y}$ normal to $\underline{X}$ and $\underline{Z}$. Such a set of axes should always be understood where orthogonal axes are referred to in other parts of this thesis.

Let $\underline{x}$ be the vector defining the position of an atom with fractional coordinates (x_1, x_2, x_3) and let $\underline{X}$ be the same vector referred to unit orthogonal axes. If $\underline{N}$ is a square matrix of order three then

$$\underline{X} = \underline{Nx} \qquad (1)$$

$\underline{N}$ is a lower triangular matrix and is given by

$$\underline{N} = \begin{bmatrix} a\sin\beta\,\sin\gamma^* & 0 & 0 \\ -a\sin\beta\,\cos\gamma^* & b\sin\alpha & 0 \\ a\cos\beta & b\cos\alpha & c \end{bmatrix} \qquad (2)$$

The variance of the ith component of $\underline{X}$ is then

$$\sigma^2(X_i) = \sum_{j=1}^{3}\sum_{k=1}^{3} N_{ij}N_{ik}r_{jk}\sigma(x_j)\sigma(x_k) \qquad (3)$$

where r_{jk} is the correlation coefficient between the j and kth components of $\underline{x}$.

The anisotropic vibration tensor referred to orthogonal axes, $\underline{V}$, is given by the matrix equation

$$\underline{V} = (\underline{N}\ \underline{E})\ \underline{U}\ (\underline{N}\ \underline{E})^T \tag{4}$$

Here $\underline{U}$ is the anisotropic vibration tensor referred to reciprocal crystal axes, $\underline{E}$ is a square diagonal matrix of order three such that $E_{ii} = a_i^*$, and superscript T indicates the transposed matrix. If $\underline{H}$ is a unit vector expressed in terms of the orthogonal axes then u^2, the mean square amplitude of vibration in the direction of $\underline{H}$, is given by

$$u^2 = \sum_{i=1}^{3} \sum_{j=1}^{3} V_{ij} H_i H_j \tag{5}$$

1.3 THE BOND ANGLE E.S.D. PROGRAMME

In an orthogonal coordinate system the distance, M, between atoms 1 and 2 is given by

$$M^2 = (X_2-X_1)^2 + (Y_2-Y_1)^2 + (Z_2-Z_1)^2 \tag{6}$$

The direction cosines of the vector between atoms 1 and 2 are

$$\begin{aligned} m_1 &= (X_2-X_1)/M \\ m_2 &= (Y_2-Y_1)/M \\ m_3 &= (Z_2-Z_1)/M \end{aligned} \tag{7}$$

and the variance of M is

$$\sigma^2(M) = m_1{}^2\left(\sigma^2(X_1)+\sigma^2(X_2)\right)+m_2{}^2\left(\sigma^2(Y_1)+\sigma^2(Y_2)\right) + m_3{}^2\left(\sigma^2(Z_1)+\sigma^2(Z_2)\right) \tag{8}$$

This formula neglects all covariances between the orthogonal coordinates and is therefore inapplicable if these covariances are large, say because atoms 1 and 2 are related by symmetry.

If N is the distance between atoms 2 and 3 and n_1, n_2, n_3 the direction cosines of the vector joining 2 and 3 then θ, the angle 1-2-3, and its variance (Darlow, 1960) can be obtained from

$$\cos\theta = m_1n_1 + m_2n_2 + m_3n_3 \tag{9}$$

$$\sigma^2(\theta) = (MN\sin\theta)^{-2}\left\{A_3{}^2\sigma^2(X_1)+(A_1+A_3)^2\sigma^2(X_2)+A_1{}^2\sigma^2(X_3) + \text{similar terms in } Y \text{ and } Z\right\} \tag{10}$$

where

$A_1 = M(m_1 - \cos\theta\, n_1)$

$A_3 = N(n_1 - \cos\theta\, m_1)$ etc.

For each atom in the asymmetric unit the programme first finds those distances to other atoms in the asymmetric unit which are less than a value specified on the input tape. The interatomic distances are then taken in pairs and the angle they define at the atom under consideration calculated. For each such angle the identifiers of the three atoms involved, the two distances and their standard deviations, and the angle and its standard deviation are printed.

1.4 THE DISTANCE AND ANGLE PROGRAMME

The object of this programme is to find, for each atom in the asymmetric unit, the distances of its nearest neighbours and the angles between the points of contact. The data consists of the symmetry operations which define the space group, the maximum interatomic distance required (DMAX), and the maximum interatomic distance to be used in the angle calculation (AMAX). This information is read from paper tape; the unit cell dimensions and fractional coordinates are read from magnetic tape.

Each atom in the asymmetric unit is taken in turn and the following calculations are performed.

(1) From the list of atoms in the asymmetric unit (list A) a second list of atoms (list B) is compiled by applying in turn each of the symmetry operations specified on the input tape. List B thus normally covers all the atoms in a single unit cell.

(2) A third atom list (list C) is prepared from list B by applying each of the twenty seven possible combinations

of unit or zero lattice translations. List C thus covers all the atoms in a block of 3 x 3 x 3 unit cells. This step is optional.

(3) The distance of the atom in the asymmetric unit from each of the atoms in list C is calculated and stored if it is less than DMAX.

(4) When all the required nearest neighbour distances have been found they are sorted in ascending order and printed.

(5) All the angles defined by pairs of nearest neighbours distances, both of which are less than AMAX, are calculated and printed.

For a large structure list C may contain entries for more than five thousand atoms. It is therefore not usually possible to hold in the store of the computer all the orthogonal coordinates required for stage (3). The programme generates them in the following way. The vector of orthogonal coordinates of the q^{th} atom in the asymmetric unit, transformed by the r^{th} symmetry operation of the space group, and translated by the s^{th} of the twenty seven combinations of zero or unit lattice translations is defined by

$$\underline{X}_{qrs} = \underline{N}(\underline{R}_r\underline{x}_q+\underline{t}_r) + \underline{NC}_s \qquad (11)$$

where $\underline{R}_r$ and $\underline{t}_r$ are the rotation matrix and translation vector (Cruickshank, 1961) defining the r^{th} symmetry operation and $\underline{C}_s$ is a vector of order three with components ± 1 or 0. The programme calculates and stores the orthogonal coordinates required for list B by evaluating the first term in (11) for all values of r and q. $\underline{NC}_s$ is also calculated for all values of S and stored. The orthogonal coordinates required for list C may then be obtained without any further matrix multiplications.

Redundancy in the output in stages (4) and (5) is kept to a minimum by arranging that, if required, atoms of different chemical types may have different DMAXs and by excluding the atoms in list A from list C if intermolecular contacts only are wanted.

For a structure containing twenty atoms with four equivalent positions a complete contacts search takes about eight minutes.

1.5 THE MOLECULAR VIBRATIONS ANALYSIS PROGRAMME

This programme was written with the aims of providing sufficient information to decide whether a molecule behaves as a rigid body, of determining the tensors of molecular translational and librational motion, and of correcting atomic coordinates for the effects of libration.

The programme uses the treatment of Cruickshank (1956) to determine the rigid body motions. In the following discussion it is assumed that the atomic coordinates, $\underline{X}$, and vibration tensors, $\underline{V}$, are referred to orthogonal axes and that the mass centre of the molecule has been taken as origin.

The molecular translational and librational motions may be described by the symmetrical third order tensors, $\underline{T}$ and $\underline{W}$, which have respectively the dimensions $\mathring{A}^2$s and radians^2. The mean square amplitude of vibration, u^2, of the rth atom in the molecule in the direction defined by the unit vector $\underline{l}$ may then be written as

$$u^2 = \sum_{i=1}^{3}\sum_{j=1}^{3} V^r_{ij} l_i l_j = \sum_{i=1}^{3}\sum_{j=1}^{3} T_{ij} l_i l_j + \sum_{i=1}^{3}\sum_{j=1}^{3} W_{ij} \times (\underline{l} \times \underline{X}_r)_i (\underline{l} \times \underline{X}_r)_j \qquad (12)$$

By equating coefficients of $l_i l_j$ in (12) a set of linear observational equations can be obtained from which it is possible to derive the twelve independent elements of $\underline{T}$ and $\underline{W}$ by a least-squares treatment.

The effect of a librational motion of the molecule is to make all atoms appear closer to the axis about which the libration occurs. The corrections (E) which should then be added to the coordinates to allow for the effect of librations have been shown by Cruickshank (1961a) to be

$$\begin{aligned} E_X &= \tfrac{1}{2}(X(B_{22}-B_{33}) - YB_{12}-ZB_{13}) \\ E_Y &= \tfrac{1}{2}(Y(B_{33}-B_{11}) - ZB_{23}-XB_{12}) \\ E_Z &= \tfrac{1}{2}(Z(B_{11}-B_{22}) - XB_{13}-YB_{23}) \end{aligned} \qquad (13)$$

where $\underline{B} = \underline{A}^{-1}$ and $\underline{A}$ is a symmetric matrix of order three whose typical elements are

$$A_{11} = (Y^2-Z^2)/q^2 + W^{-1}{}_{11}; \quad A_{12} = -XY/q^2-W^{-1}_{12}.$$

(q^2 is the Gaussian peak width parameter for the atom involved).

The programme is similar to the Pegasus programme described by Cruickshank (1961). The calculation proceeds in the following stages.

(1) The atomic coordinates and vibration tensors, U_{obs}, obtained from a least-squares refinement are referred to orthogonal axes.

(2) The latent roots and vectors of the vibration tensors (see Appendix) are found w.r.t. orthogonal and crystal axes.

(3) The mass centre and principal moments of inertia of the molecule are found.

(4) The coordinates and vibration tensors are referred to inertial axes and the mass centre is taken as origin.

(5) The normal equations for $\underline{T}$ and $\underline{W}$ are set up and solved. The standard deviations of the elements of $\underline{T}$ and $\underline{W}$ are also found.

(6) The latent roots and vectors of $\underline{T}$ and $\underline{W}$ are found w.r.t. the inertial axes.

(7) $\underline{U}_{calc}$ is computed from $\underline{T}$ and $\underline{W}$ w.r.t. inertial, orthogonal and crystal axes.

(8) $\Delta U = U_{obs} - U_{calc}$ and the root mean square ΔU are found.

(9) The amplitude of vibration of each atom along the line joining it to the centre of mass of the molecule is calculated from $\underline{U}_{obs}$ and $\underline{U}_{calc}$.

(10) The librational corrections to coordinates are found.

(11) The revised coordinates w.r.t. inertial, orthogonal, and crystal axes are calculated.

Apart from the normal equations all other results are printed. A discussion of some of the mathematics used is given in the Appendix to this chapter.

1.6 THE MEAN PLANE PROGRAMME

Using the method of Schomaker et al. (1959) the programme finds the plane through a set of atoms which obeys the condition that the sum of weighted squared deviations of the atoms from the plane is a minimum. The atoms which define the plane are specified on the input paper tape. Any number of plane calculations can be performed during a single run. For each plane the output includes the plane equation, the sum of weighted squared deviations, the root mean square deviation and the deviations of individual atoms from the plane.

1.7 THE TABLES PROGRAMME

This programme prepares paginated tables of fractional and orthogonal coordinates, anisotropic temperature factors, and principal values and directions of atomic thermal motion, in a form suitable for direct inclusion in a thesis or paper. The tables of such quantities presented in Part III of this thesis are almost untouched examples of the output. The chief advantages of preparing tables in this way are that typing and transcribing errors are avoided and that the same data tape is used to prepare the tables and for the final structure factor and distance and angle calculations.

APPENDIX

Let $\underline{V}$ be a square matrix and $\underline{p}$ a vector, both of order n. There are n values of the scalar λ which yield a non-trivial ($\underline{p} \neq 0$) solution of the system of homogeneous equations

$$\underline{V}.\underline{p} = \lambda \underline{p}. \tag{14}$$

These values are termed the latent roots of $\underline{V}$ and the corresponding vectors, $\underline{p}$, are the latent vectors of $\underline{V}$. If $\underline{I}$ is a unit matrix the condition that (14) has a solution may be written as

$$\det(\lambda \underline{I}-\underline{V}) = 0 \tag{15}$$

If n = 3, expansion of (15) yields a cubic in λ which may be solved by the methods of International Tables Vol. II (1959) p. 26. Substitution of λ into (14) with the additional requirement that $\underline{p}$ be a unit vector yields the latent vectors. It can be shown (e.g. Rollett, 1965) that the latent vectors are orthogonal, provided two latent roots do not coincide.

If the magnitude of a quantity U^2 in the direction defined by the unit vector $\underline{\ell}$ is given by the quadratic form

$$U^2 = \sum_i \sum_j V_{ij} \ell_i \ell_j \tag{16}$$

then transformation to the system of orthogonal axes defined by the latent vectors of $\underline{V}$ gives U^2 as

$$U^2 = \sum_{i=1}^{3} \lambda_i m_i^2 \tag{17}$$

where $\underline{m}$ is the unit vector $\underline{\ell}$ referred to the new axes and λ_i is the i^{th} latent root of $\underline{V}$. It can be shown that the maximum and minimum values of U^2 are the maximum and minimum latent roots of $\underline{V}$.

The mean square amplitude of atomic vibration in a given direction is defined by an equation of the form of (16). The latent roots and vectors of the anisotropic vibration tensor thus define the amplitudes and directions of greatest and least thermal motion.

If the vector between the centre of mass and the r^{th} atom in the molecule is $\underline{X}_r$, the moment of inertia, I, of the molecule about an axis passing through the mass centre and defined by the unit vector $\underline{p}$ is

$$I = \sum_{1}^{N} w_r \underline{X}_r^T \underline{X}_r - \sum_{i=1}^{3}\sum_{j=1}^{3} A_{ij} p_i p_j \tag{18}$$

where, for example, $A_{12} = \Sigma \; w_r X_r Y_r$; the summations are over the N atoms in the molecule and w_r is the mass of the r^{th} atom. The latent vectors of $\underline{A}$ thus define the axes of greatest and least inertia and are termed the inertial axes of the molecule. For a planar molecule the axis of greatest inertia is parallel to the normal of the molecular plane.

CHAPTER II

THE ASS SYSTEM

2.1 INTRODUCTION

The automatic structure solution (ASS) system is a group of programmes which allow all the calculations necessary for a cycle of Fourier refinement to be performed during a single run on the computer. It also contains programmes which attempt to interpret the results of such a cycle of refinement.

Given a list of fractional coordinates derived either from study of a Patterson function or from a previous electron density synthesis the programmes will produce the fractional coordinates of the peaks in the electron density synthesis based on phases calculated from the input coordinates. At the option of the user the coordinates of certain atoms on the input list are used in the phasing calculation only if they are likely to improve structure factor agreement.

The system has proved reasonably efficient in meeting the computational requirements of the early stages of a structure analysis. It has been used in nearly all current work in this laboratory and in the last ten months at least fifteen structures have been solved using its programmes. In most of these structures the interpretative programmes have at least accelerated the process of finding a solution.

The overall planning of the system was the joint work of Mr. D. MacGregor and the present author. Dr. J.G. Sime kindly made available his Fourier programme. The present writer devised the modified structure factor programme used in the system. Mr. D. MacGregor wrote the Fourier map scanning programme and the programmes required for writing primary data on to magnetic tape. Mr. R. Pollard contributed the Fourier coefficient weighting programme which is based, in part, on an earlier programme of the present writer.

2.2. GENERAL DESCRIPTION OF THE SYSTEM

When work is started on a new structure, a magnetic file tape is prepared which contains for each Bragg reflection the indices, the observed structure amplitude $|F_o|$ on an arbitrary scale, $\sin\theta/\lambda$, and interpolated form factors for each chemical species present in the structure. This information is then available to any other programme in the system and is, for example, invariably part of the input data for a structure factor calculation.

The isotropic structure factor programme reads coordinates, temperature factors and equivalent positions from paper tape and the rest of the information required from the magnetic file tape. The output consists of structure factors with the structure amplitudes scaled so that $\sum |F_o| = \sum |F_c|$ either for the data as a whole or for each reciprocal net separately. The scaled structure factors are stored on magnetic tape and may optionally be printed. A summary of the scale and R-factors for each reciprocal net is also printed. The programme contains one novel feature. Atoms admitted to the structure factor calculation may be classed either as reliable or tentative. Structure factors are first calculated over part of the data, usually about four hundred reflections, with only the reliable atoms included and a value of R is obtained. The tentative atoms are then admitted to the structure factor calculation one at a time. If they reduce R by more than a specified amount they are accepted as genuine atoms and included in all further calculations. Otherwise they are ignored. The structure factors finally output are thus calculated over all the reliable atoms and those tentative atoms which have reduced R over the selected part of the data.

A separate programme calculates the weight which should be assigned to the Fourier coefficient to allow for the errors in phasing which result from omission of as yet unlocated atoms from the structure factor calculation. The formulae of Sim (1960) or Woolfson (1956) are used to compute the weights. The weighted structure factors are scaled so that $\Sigma w |F_o| = \Sigma |F_o|$ and stored on magnetic tape.

The Fourier programme reads structure factors or weighted structure factors from magnetic tape and the rest of the required information from paper tape. The output consists of printed number fields. The sections are also stored on magnetic tape as they are computed.

The map scanning programme requires as its main input data the three-dimensional Fourier synthesis stored on magnetic tape by the Fourier programme. The interpolated grid and fractional coordinates of all peaks greater than a specified threshold value are computed by least-squares fitting of the function

$$\rho = a+bx^2+cy^2+dz^2+ex+fy+gz+hxy+iyz+jzx \qquad (1)$$

to the electron density values at the twenty seven grid points nearest the peak and printed. The interpolated peak height and integrated peak density are also printed. The fractional coordinates are finally output on paper tape in order of decreasing integrated peak density. This paper tape is accepted as a list of atomic coordinates by the structure factor programme.

2.3 EXPERIENCE WITH THE PROGRAMMES

Many cycles of Fourier refinement have now been completed using the system. It has generally been found that most atoms which can be located from a contoured Fourier map are included in the output from the map scanning programme. Diffraction ripples and peaks due to incorrect phasing are also picked up by the programme but quite often such peaks are few in number and may be easily recognised from their low integrated peak density or from their position. The facility for including atoms in the structure factor calculation only after they have lowered R over part of the data has mainly been used to check atoms which are being introduced into the refinement for the first time. Under such circumstances an electron density peak which does not correspond to an atomic position is generallyrejected by the programme. Less frequently all the peaks produced by the map scanning programme, with the exceptions of obvious diffraction ripples and heavy atom peaks, have been tested in this manner. If the structure is centrosymmetric and if most peaks in the electron density synthesis correspond to atoms, then the results are reliable. The system may then be used for semi-automatic Fourier refinement and the contouring of most of the electron density maps calculated in successive cycles can be avoided.

CHAPTER III

THE MINIMUM RESIDUAL PROGRAMME

3.1 INTRODUCTION

Crystal structure refinement by direct calculation of the minimum residual was first described by Bhuiya and Stanley (1963). The method works as follows. Structure factors are calculated from starting values of the atomic coordinates and temperature factors and a value of R, the usual discrepancy index is obtained. The x coordinate of the first atom is then varied from -nDx to +nDx in 2n+1 steps of Dx, and for each value of the coordinate structure factors and the corresponding R-factor are calculated. The refined value of the coordinate is that which yields the lowest R-factor and it is used in all subsequent calculations. In one cycle each atomic coordinate or temperature factor is in turn varied in this manner.

3.2 DESCRIPTION OF THE PROGRAMME

The minimum residual programme uses the above technique to refine crystal structures in projection. Triclinic, monoclinic, and orthorhombic space groups can be handled. For each atom two coordinate parameters and one temperature parameter may be refined. An overall temperature factor can also be refined and provision has been made to keep the parameters of one or more atoms fixed to allow for atoms in special positions. The R-factor is always calculated from

$$R = \Sigma \big| k|F_o| - |F_c| \big| / \Sigma k|F_o| ; \quad k\Sigma|F_o| = \Sigma|F_c| \qquad (1)$$

3.3 EXPERIENCE WITH THE PROGRAMME

The programme has proved useful in a number of analyses carried out in this laboratory. The maximum drop in R achieved in one cycle is 0.1 and drops of 0.05 have not been uncommon. For projections in which the atoms overlap the method has advantages over full matrix least-squares or difference map refinement. Its main disadvantage is that it requires more extensive calculations than either of these methods and, even with careful programming, uses more machine time. For a problem involving thirty atoms and two hundred reflections, with n=5 for both coordinate and temperature parameters one cycle takes about twenty minutes.

PART III

CHAPTER I

THE DIMETHYLACETYLENE DICARBOXYLATE INDENE ADDUCT

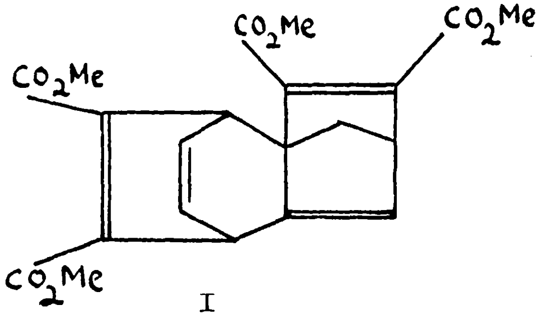
1.1 INTRODUCTION

The preparation of the 1:2 adduct of indene and dimethyl acetylenedicarboxylate was first described by Alder, Pascher, and Vagt (1942). On the basis of known Diels - Alder chemistry Pascher (1944) favoured I as the most likely of a number of possible structures for the adduct.

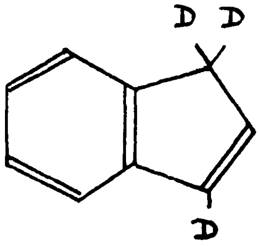
The reaction was reinvestigated by Strachan and Huebner (Muir, Sim, Strachan, and Huebner, 1964) who showed that the adduct is formed under mild conditions even at room temperature. Their nuclear magnetic resonance studies indicated that the adduct contains four vinyl protons thus precluding I from further consideration. They also prepared a trideutero adduct by reacting dimethyl acetylenedicarboxylate with indene-1,1,3-d_3(II) and showed that its n.m.r. spectrum contains peaks corresponding to four vinyl protons. These results suggested that both acetylene moieties are attached to the five membered ring of the indene system.

Further chemical and spectroscopic investigations by Strachan and Huebner did not lead to a definitive solution of the structural problem.

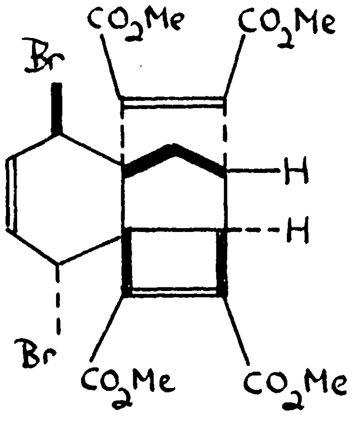
The adduct forms a crystalline dibromo-derivative (Alder, Pascher, and Vagt, 1942) from which it may be


CO$_2$Me
CO$_2$Me
CO$_2$Me
CO$_2$Me

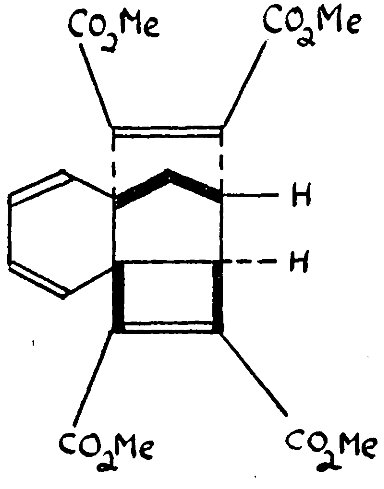
I


D D
D

II


CO$_2$Me
CO$_2$Me
Br
H
H
Br
CO$_2$Me
CO$_2$Me

III


CO$_2$Me
CO$_2$Me
H
H
CO$_2$Me
CO$_2$Me

IV

regenerated by treatment with zinc in ether/tetrahydrofuran. The x-ray analysis of the crystal structure of the dibromo-adduct is described in the other sections of this chapter. The results establish the molecular structure as III from which it may be inferred that the adduct has structure IV. Structure IV has been shown by Strachan and Huebner to be in conformity with the n.m.r. spectrum of the adduct.

1.2 EXPERIMENTAL

Crystal Data

Dibromo-adduct

$C_{21}H_{20}Br_2O_8$

F.W. 560.2 M.P. 182-183 °C

Monoclinic, $a = 8.48 \pm 2$, $b = 7.48 \pm 2$, $c = 34.63 \pm 1$ Å

$\beta = 98°2' \pm 20'$.

$U = 2175$ Å^3

$D_m = 1.67$ gmcm^{-3} (by flotation in aqueous $ZnBr_2$)

$Z = 4$

$D_x = 1.711$ gmcm^{-3}

Linear absorption coefficient μ(Cu Kα, λ = 1.5418 Å)

= 56.9cm^{-1}

F(000) = 1120

Systematic absences

0k0 when k is odd

h0ℓ when ℓ is odd

Space group $P2_1/c$ (No. 14).

The crystals used in the analysis were supplied by Dr. C.F. Huebner. They consisted of pale yellow needles elongated about the b axis. The cell dimensions were measured from rotation and equatorial layer Weissenberg photographs taken about the b axis with copper Kα radiation (wavelength 1.5418 Å) and from precession photographs of the hk0 and 0kℓ zones taken with molybdenum K α radiation (wavelength 0.7107 Å).

The intensity data were measured from equatorial and equi-inclination Weissenberg photographs of the reciprocal nets $h0\ell$ to $h5\ell$, taken with copper K α radiation, by visual comparison with a calibrated intensity strip. The multiple film technique of Robertson (1943) with four films per pack was used; the interfilm scale factors were those of Rossman (1956). An empirical spot shape correction was applied to the data but no absorption corrections were made. The intensities were reduced to structure amplitudes using a DEUCE computer programme written by Dr. J.G. Sime (Sime, 1961); the Lorentz, polarisation and rotation factors (Tunell, 1939) appropriate to a small mosaic crystal being applied. In all 1982 independent structure amplitudes (Table 1.4) were obtained, being approximately 40% of the data accessible with copper K α radiation. No unobserved reflections were used in the analysis.

The data were put on a rough absolute scale by comparison with the first set of calculated structure factors. The final scale factors were determined by least-squares refinement.

1.3 STRUCTURE SOLUTION AND REFINEMENT

The x and z coordinates of both bromine atoms were obtained from the Patterson projection on to (010) and the y coordinates were thereafter derived from line sections through the three-dimensional Patterson function.

The plane group of the (010) projection is p2, with equivalent positions x,z; $\bar{x},\bar{z}$. The c axis is halved and accordingly there are four bromine atoms in the projected unit cell. Twelve non-zero vector peaks should therefore appear in the corresponding Patterson function, six peaks being related to other six by the inversion centre at the origin. Using subscripts to denote bromines 1 and 2 the analytical expressions for the six independent vectors are:-

$$(x_1 + x_2),\ (z_1 + z_2);\quad \text{(twice)}$$
$$(x_1 - x_2),\ (z_1 - z_2);\quad \text{(twice)}$$
$$2x_1,\ 2z_1;$$
$$2x_2,\ 2z_2;$$

The asymmetric unit of the projected Patterson function should thus show two doubleweight and two singleweight peaks. The projected Patterson is shown in Fig. 1.1. The peaks marked A and B were taken as doubleweight peaks and those marked C and D were taken as singleweight peaks. The coordinates of these peaks were worked out using Booth's (1948) interpolation formula and the fractional coordinates of the bromine atoms were then derived from the analytical expressions given above.

Line sections parallel with the b axis were next computed through the three-dimensional Patterson function to obtain the y coordinates of the bromine atoms. In all seventeen such sections were calculated, one through each heavy atom vector found within the area bounded by the three-dimensional unit cell projected down b.

The coordinates of the bromine atoms so obtained were:-

	X/a	Y/b	Z/c
Br(1)	0.8094	0.4166	0.4636
Br(2)	0.2494	0.3210	0.3393

A three-dimensional electron density distribution based on phases calculated from these positions revealed almost the entire structure. In addition to the two bromines twenty carbon atoms and eight oxygen atoms could be located; oxygens were distinguished from carbons partly by peak height and partly by chemical considerations. There was a peak in the position subsequently assigned to C(19); there was, however, also a peak opposite O(5) which could have been a methyl carbon although its position suggested that it was more probably a diffraction ripple from Br(2). C(19) was accordingly omitted from the second structure factor calculation for which the R-factor was 0.193. The R-factor with the heavy atoms alone was 0.39. A second electron density distribution allowed the position of C(19) to be determined unambiguously. A third set of structure factors calculated from positions derived from the second electron density map, with all atoms included gave an R-factor of 0.187.

Six cycles of minimisation of the function $\Sigma w(|F_o| - |F_c|)^2$ were now calculated using the least-squares programme by Dr. J.S. Rollett for the DEUCE computer (Rollett, 1961). Three coordinates and six anisotropic temperature parameters for each atom were refined. A block diagonal approximation to the normal matrix was generally employed. In cycles 1 and 2 a diagonal approximation was used for the parameters of both bromine atoms and in cycles 4,5, and 6 the bromine parameters were left unchanged, while in cycle 3 only bromine parameters were refined. This course was rendered necessary by limitations on the size of elements of the normal equations which the programme could handle. During this stage of refinement a number of indexing and card-punching errors were corrected. At the end of the sixth cycle R stood at 0.118. Throughout this course of refinement scale factors were chosen so as to equalise $\Sigma|F_o|$ and $\Sigma|F_c|$ for each layer of data.

A difference synthesis using all the data was now computed to check the refinement and to find if it would be worthwhile including hydrogen atoms in the calculations. In this map peaks corresponding to all twenty hydrogen atoms could be made out. Hydrogen peak heights ranged from 0.32 to 0.64e/$\mathring{A}^3$ with a mean of 0.5e/$\mathring{A}^3$. The other most obvious feature of the map was that nearly all the heavier atoms lay in negative troughs. This suggested that either the scale factors or the overall temperature factor had been underestimated and that further refinement was desirable.

Inclusion of the hydrogen atoms into the structure factor computations in positions calculated from the coordinates of the heavier atoms and using an assumed isotropic temperature facture U of 0.075 $\mathring{A}^2$ led to a drop in R of 0.004, most of the improvement being in the lower order reflections. This drop was regarded as satisfactory and hydrogen atoms were included in all subsequent calculations.

The refinement was now completed using the least-squares programme written for the KDF9 computer by Cruickshank and Smith. In the first cycle of refinement with the new programme the only parameters refined were separate scale factors for each layer of photographic data and an overall temperature factor. R fell to 0.109.

Two further cycles of block diagonal refinement produced convergence with a final value of R of 0.087 and of R' ($\Sigma w\Delta^2/\Sigma wF_o^2$) of 0.016. In the final cycle the ratios of average shift to average standard deviation were 0.4, 0.4 and 0.3 for the coordinates of bromine, carbon and oxygen respectively.

The weighting scheme used in the last three cycles of refinement was one of the form recommended by Cruickshank (1961) as suitable for photographic data, namely

$$\sqrt{w} = (10 + F + 0.009F^2)^{-\frac{1}{2}}$$

The atomic form factors used were for carbon Hoerni and Ibers (1954), for oxygen Berghuis et al. (1955), for bromine Thomas and Umeda (1957), and for hydrogen Stewart, Davidson, and Simpson (1965).

The last set of structure factors was used to phase electron density and difference syntheses. A composite view of the final electron density synthesis is shown in Fig. 1.2. The mean peak heights were 40.9, 5.5, and 7.8e/$\mathring{A}^3$ for bromine, carbon, and oxygen respectively. The standard deviation of $\rho(xyz)$, estimated by the approximate formula of Cruickshank (1949), was 0.22e/Å^3. In the final difference synthesis there were regions of positive and negative density greater than three times this standard deviation; the highest function value was 1.2 and the lowest -1.6e/Å^3. These regions were associated with each heavy atom position and are probably due to uncorrected absorption.

Tables 1.1 and 1.2 contain the final values of the fractional coordinates and anisotropic temperature factors of the heavier atoms, together with their standard deviations derived from the inverse of the normal least-squares matrix. In Table 1.3 the assumed fractional coordinates and isotropic temperature factors of the hydrogen atoms are presented. The final list of calculated and observed structure factors is given in Table 1.4. Tables 1.5 and 1.6 show the coordinates of all the atoms referred to a set of orthogonal axes parallel to a*,b and c, while Table 1.7 contains the principal values and directions of the anisotropic vibration tensors. Tables 1.8 and 1.9 contain all the covalent bond lengths and interbond angles in the structure together with their estimated standard deviations. Table 1.10 lists all intermolecular contacts between the heavier atoms which are less than 4Å and in Table 1.11 the equations of some molecular planes are given, together with some deviations of atoms from these planes. The results listed in Tables

1.5 to 1.11 were all calculated with the programmes described in Part II of this thesis and the equations given there apply. Standard deviations, if quoted, are in units of the last decimal place of the quantity to which they refer.

A molecular drawing illustrating the numbering of the heavier atoms is shown in Fig. 1.3. The numbering of the hydrogen atoms is explained in Fig. 1.4. A view of the molecular packing down b is shown in Fig. 1.5.

Course of the Analysis

1. Fourier Refinement

S.F. Cycle No.	Atoms Included	R
1	2 Br	0.39
2	2 Br + 20 C + 8O	0.193
3	2 Br + 21 C + 8O	0.187

2. Least-Squares Refinement

S.F.L.S. Cycle No.	Comments	R
1	Block diagonal for C and O; diagonal for Br	0.187
2	Block diagonal for C and O; diagonal for Br	0.152
3	Block diagonal for Br; C and O not refined	0.133
4	Block diagonal for C and O; Br not refined	0.130
5	Block diagonal for C and O; Br not refined	0.122
6	Structure factors only	0.118
7	Structure factors only: hydrogens included	0.114
8	Layer scales and overall temperature factor refined	0.114
9	Block diagonal on all atoms	0.109
10	Block diagonal on all atoms	0.091
11	Structure factors only	0.087

FIG. 1.1

The Patterson projection on to (010). Contours are at arbitrary intervals.

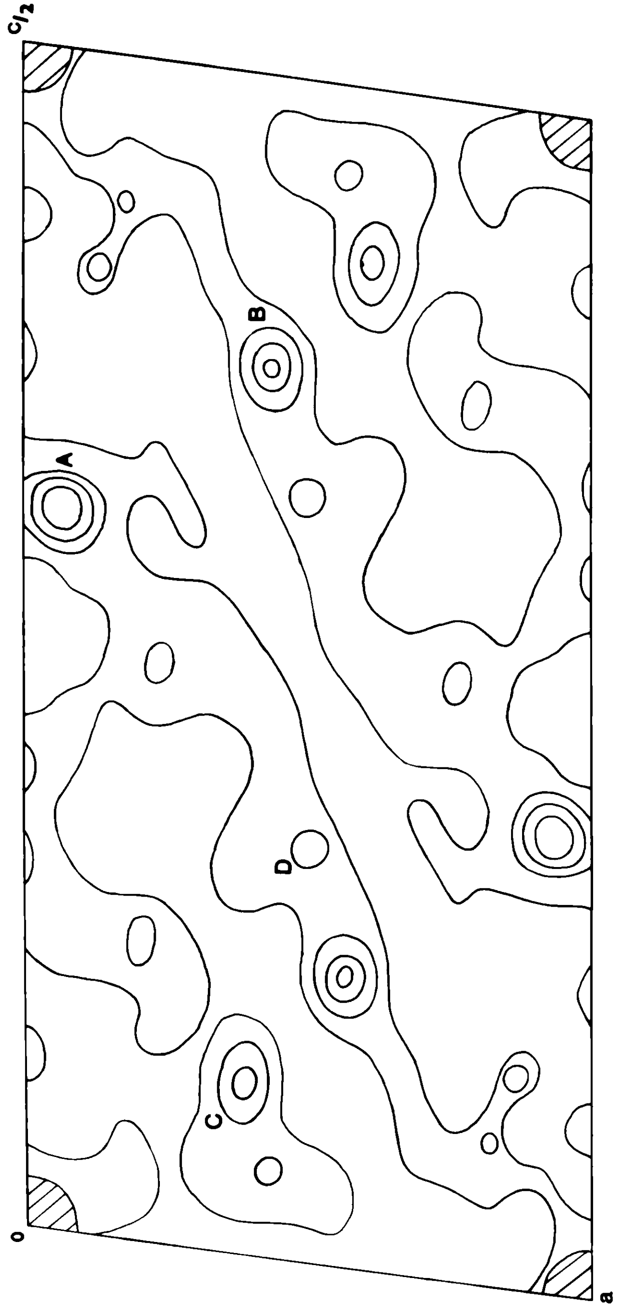

c/2
0
a
A
B
C
D

FIG. 1.2

The composite final electron density synthesis viewed down the b axis. Contours are at 1 e/Å^3 intervals starting at 2 e/Å^3 except round the bromine atoms which are contoured at 5 e/Å^3 intervals starting at 5 e/Å^3.The broken contours are those of O(4).

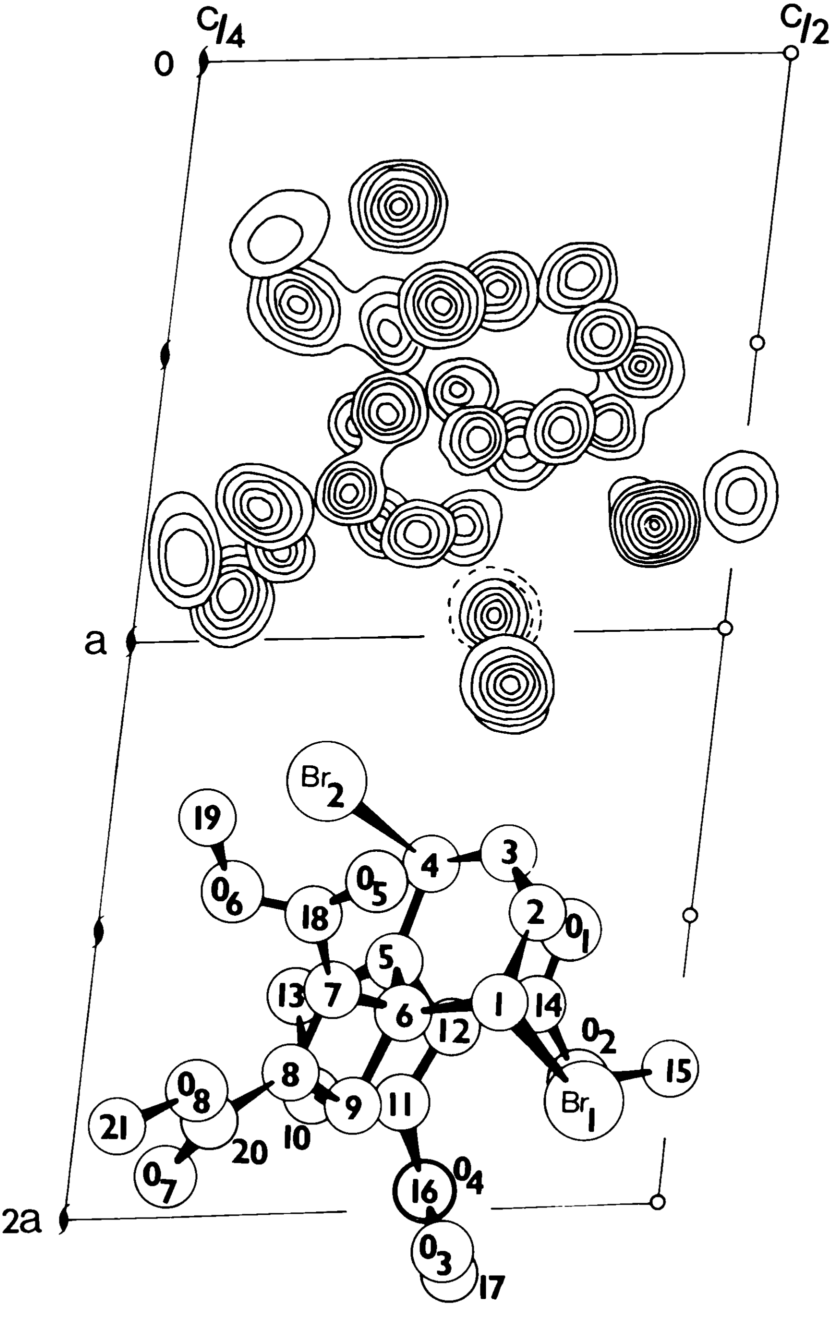
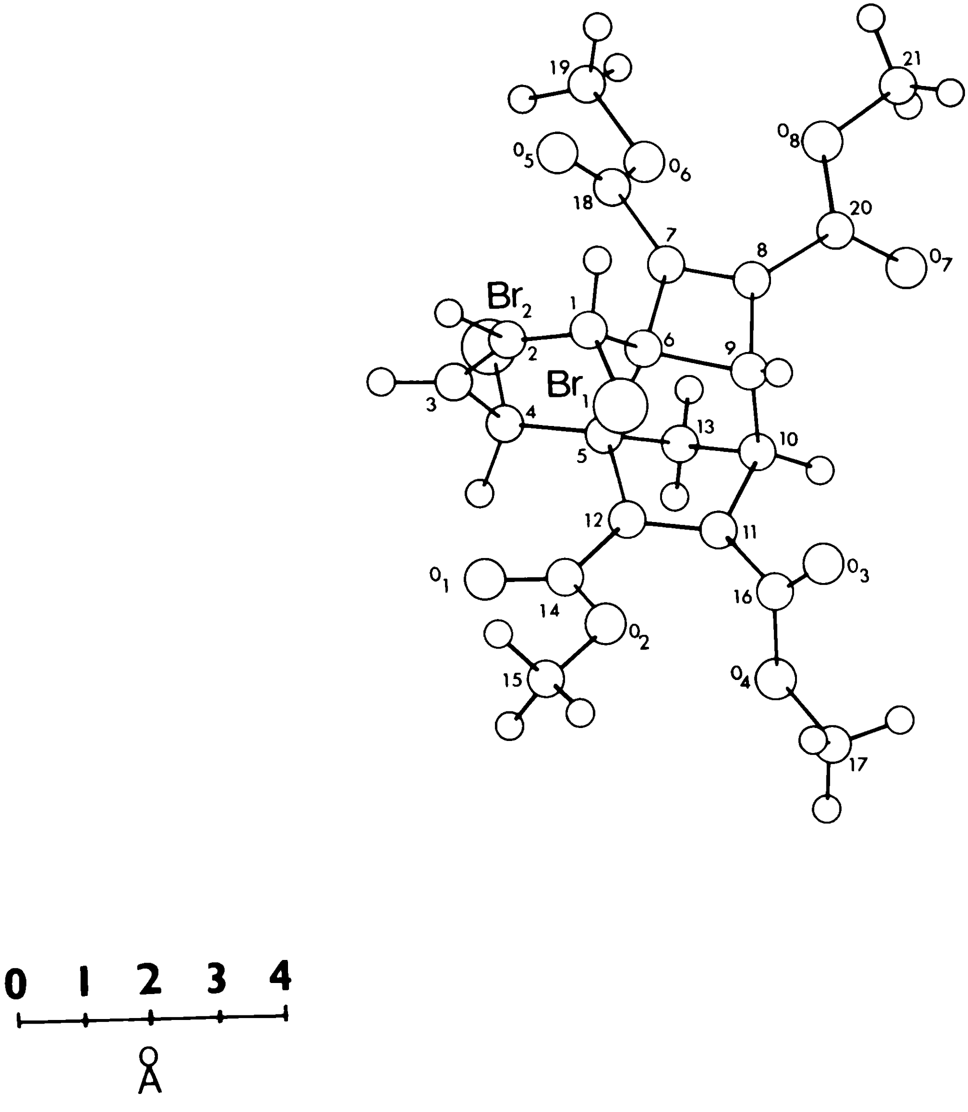

c/4
c/2
0
a
2a
Br2
19
4
3
O6
18
O5
2
O1
5
13
7
6
1
14
12
O2
15
8
O8
9
11
Br1
21
10
20
O7
16
O4
O3
17

FIG. 1.3

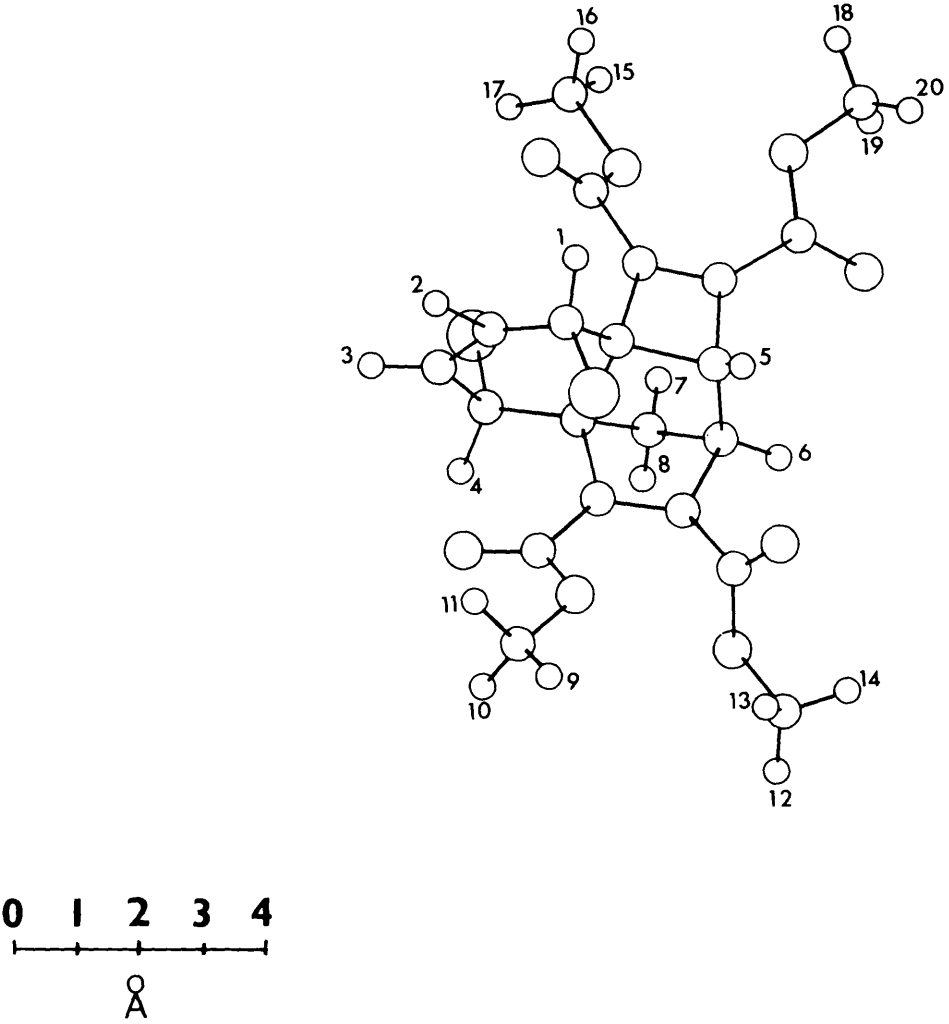
Molecular drawing showing the numbering of the heavier atoms.



19
21
O_5
O_6
O_8
18
20
7
8
O_7
Br_2
1
2
6
9
Br_1
3
4
13
10
5
12
11
O_1
14
O_3
16
O_2
15
O_4
17
0
1
2
3
4
Å

FIG. 1.4

The numbering of the hydrogen atoms.


1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
0 1 2 3 4
Å

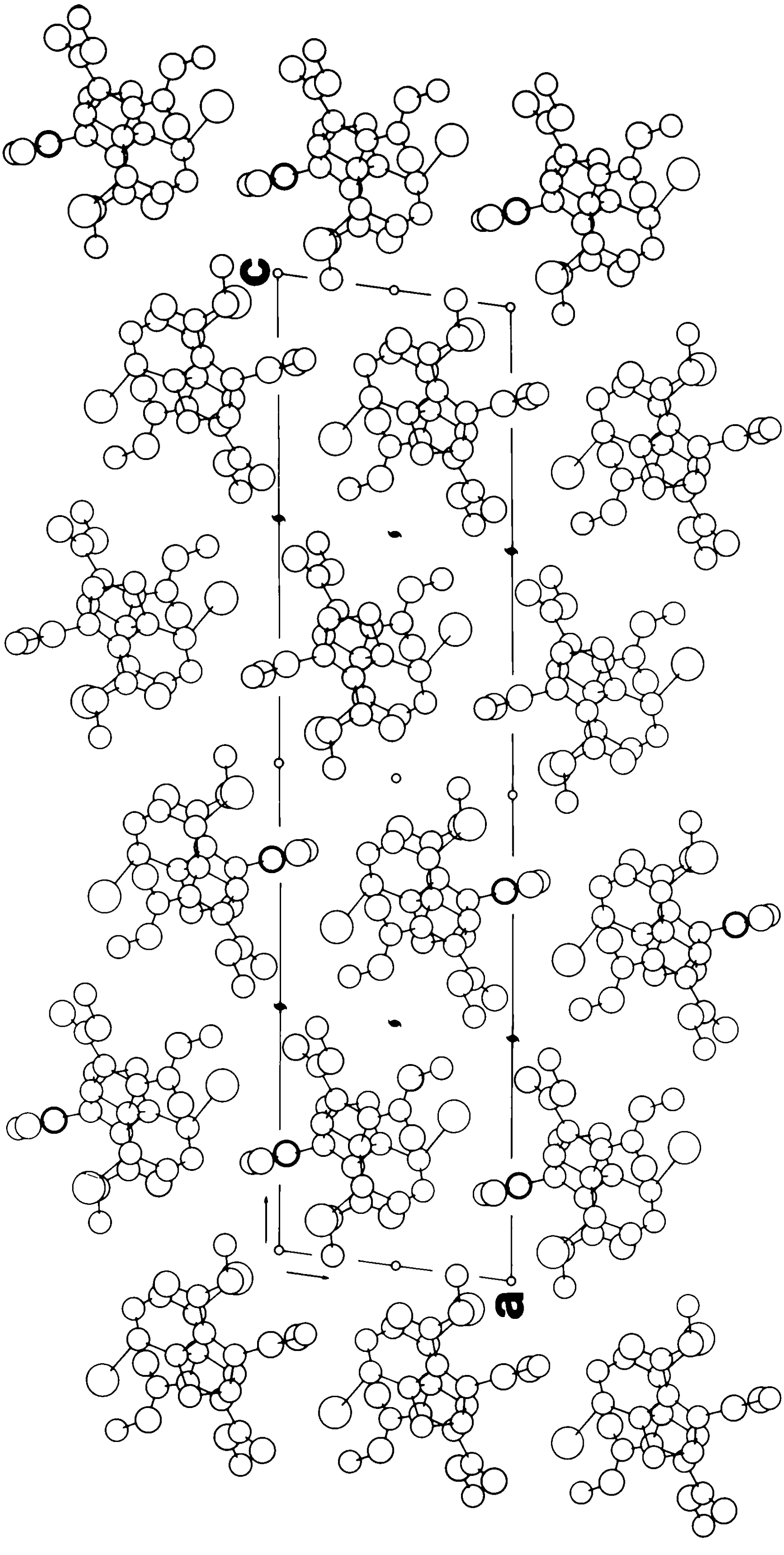

c
a

TABLE 1.1

FRACTIONAL COORDINATES AND E.S.D.S.

ATOM	X/a	Y/b	Z/c
Br(1)	0.8146 ± 2	0.4205 ± 3	0.46407 ± 5
Br(2)	0.2498 ± 2	0.3259 ± 3	0.34035 ± 5
C(1)	0.6431 ± 18	0.5047 ± 22	0.4228 ± 4
C(2)	0.4871 ± 18	0.4708 ± 24	0.4359 ± 4
C(3)	0.3792 ± 16	0.3546 ± 23	0.4190 ± 4
C(4)	0.3976 ± 15	0.2378 ± 23	0.3856 ± 4
C(5)	0.5663 ± 17	0.2349 ± 21	0.3764 ± 4
C(6)	0.6556 ± 19	0.4251 ± 23	0.3834 ± 4
C(7)	0.6137 ± 17	0.5606 ± 22	0.3505 ± 4
C(8)	0.7528 ± 18	0.5417 ± 22	0.3369 ± 4
C(9)	0.8144 ± 15	0.3947 ± 20	0.3648 ± 4
C(10)	0.7923 ± 15	0.2035 ± 23	0.3484 ± 4
C(11)	0.8131 ± 18	0.0849 ± 21	0.3846 ± 4
C(12)	0.6813 ± 17	0.1059 ± 22	0.4020 ± 4
C(13)	0.6161 ± 16	0.1837 ± 23	0.3367 ± 4
C(14)	0.6518 ± 17	0.0210 ± 20	0.4390 ± 4
C(15)	0.7655 ± 22	-0.1086 ± 27	0.4982 ± 4
C(16)	0.9659 ± 17	0.0004 ± 24	0.4002 ± 4
C(17)	1.1145 ± 21	-0.2658 ± 26	0.4142 ± 6
C(18)	0.4804 ± 18	0.6863 ± 23	0.3403 ± 5

C(19)	0.3043 ± 26	0.8195 ± 30	0.2898 ± 7
C(20)	0.8320 ± 17	0.6220 ± 22	0.3057 ± 4
C(21)	0.8386 ± 28	0.8799 ± 31	0.2658 ± 6
O(1)	0.5218 ± 12	0.0055 ± 18	0.4488 ± 3
O(2)	0.7835 ± 14	-0.0356 ± 18	0.4598 ± 3
O(3)	1.0815 ± 13	0.0855 ± 17	0.4104 ± 4
O(4)	0.9647 ± 12	-0.1755 ± 15	0.3991 ± 3
O(5)	0.4251 ± 15	0.7705 ± 17	0.3641 ± 4
O(6)	0.4361 ± 13	0.6974 ± 16	0.3021 ± 3
O(7)	0.9288 ± 16	0.5480 ± 20	0.2899 ± 4
O(8)	0.7804 ± 15	0.7864 ± 17	0.2978 ± 3

TABLE 1.2

ANISOTROPIC TEMPERATURE FACTORS AND E.S.D.S.

ATOM	U11	U22	U33	2U23	2U31	2U12
Br(1)	0.0637	0.0603	0.0586	-0.0077	-0.0048	0.0088
	11	15	9	18	15	20
Br(2)	0.0447	0.0657	0.0674	0.0189	0.0029	0.0022
	8	15	9	18	14	18
C(1)	0.0520	0.0296	0.0594	0.0110	0.0010	-0.0013
	89	110	84	141	130	153
C(2)	0.0491	0.0554	0.0595	0.0050	0.0331	-0.0116
	88	128	85	159	133	174
C(3)	0.0302	0.0528	0.0666	0.0128	0.0278	0.0151
	67	123	86	159	116	150
C(4)	0.0248	0.0505	0.0674	0.0257	0.0095	-0.0008
	58	120	84	154	109	143
C(5)	0.0485	0.0300	0.0528	0.0041	-0.0236	-0.0250
	79	106	75	135	121	147
C(6)	0.0600	0.0530	0.0431	-0.0002	0.0216	0.0197
	92	128	69	143	125	170
C(7)	0.0479	0.0387	0.0565	0.0036	0.0386	0.0038
	84	117	79	143	127	154
C(8)	0.0544	0.0344	0.0558	-0.0045	-0.0005	0.0075
	90	117	80	141	130	157
C(9)	0.0297	0.0327	0.0534	0.0006	0.0197	-0.0066
	63	105	70	131	103	134
C(10)	0.0320	0.0612	0.0503	0.0076	0.0226	-0.0032
	67	128	73	147	106	152
C(11)	0.0547	0.0262	0.0514	-0.0041	0.0027	-0.0346
	86	108	72	134	121	152

C(12)	0.0478	0.0279	0.0597	0.0056	0.0237	-0.0098
	81	106	79	139	124	146
C(13)	0.0403	0.0499	0.0506	0.0088	0.0232	-0.0025
	74	123	72	144	112	152
C(14)	0.0478	0.0162	0.0607	0.0005	0.0285	0.0046
	82	103	82	129	123	138
C(15)	0.0760	0.0776	0.0483	0.0058	0.0135	0.0305
	116	149	80	174	148	219
C(16)	0.0427	0.0518	0.0543	0.0051	0.0173	-0.0206
	80	127	79	150	120	160
C(17)	0.0541	0.0336	0.1280	0.0033	0.0226	-0.0029
	102	127	160	215	196	185
C(18)	0.0471	0.0330	0.0760	0.0063	0.0338	0.0053
	85	117	98	158	140	158
C(19)	0.0739	0.0614	0.1370	0.0174	-0.0384	0.0125
	134	167	191	267	246	235
C(20)	0.0452	0.0371	0.0582	0.0071	0.0206	-0.0013
	81	113	80	143	124	151
C(21)	0.1228	0.0670	0.0836	0.0701	0.1010	0.0311
	183	164	126	224	245	264
O(1)	0.0432	0.0886	0.0712	0.0503	0.0371	0.0093
	60	101	69	134	100	128
O(2)	0.0715	0.0687	0.0547	0.0220	0.0255	0.0183
	75	97	59	115	105	134
O(3)	0.0476	0.0456	0.1115	0.0297	-0.0055	-0.0094
	63	89	95	137	120	120
O(4)	0.0406	0.0360	0.0930	-0.0145	-0.0061	0.0067
	55	81	78	117	101	103
O(5)	0.0733	0.0535	0.0940	0.0048	0.0551	0.0410
	82	90	85	137	132	138
O(6)	0.0633	0.0413	0.0799	0.0077	0.0048	0.0203
	71	84	74	120	113	122

O(7)	0.0891	0.0890	0.0924	0.0412	0.0905	0.0180
	97	114	90	162	153	169
O(8)	0.0818	0.0557	0.0690	0.0269	0.0506	0.0117
	84	92	68	124	119	138

TABLE 1.3

ASSUMED FRACTIONAL COORDINATES AND TEMPERATURE FACTORS OF HYDROGEN ATOMS.

ATOM	X/a	Y/b	Z/c	U
H(1)	0.648	0.643	0.419	0.075
H(2)	0.459	0.546	0.460	0.075
H(3)	0.269	0.346	0.430	0.075
H(4)	0.374	0.103	0.394	0.075
H(5)	0.917	0.424	0.384	0.075
H(6)	0.864	0.164	0.328	0.075
H(7)	0.571	0.265	0.314	0.075
H(8)	0.577	0.061	0.325	0.075
H(9)	0.871	-0.144	0.514	0.075
H(10)	0.686	-0.219	0.494	0.075
H(11)	0.708	-0.010	0.515	0.075
H(12)	1.104	-0.404	0.413	0.075
H(13)	1.152	-0.227	0.444	0.075
H(14)	1.205	-0.224	0.398	0.075
H(15)	0.278	0.821	0.258	0.075
H(16)	0.336	0.953	0.298	0.075
H(17)	0.201	0.784	0.300	0.075
H(18)	0.783	1.008	0.263	0.075
H(19)	0.798	0.809	0.239	0.075
H(20)	0.958	0.891	0.270	0.075

TABLE 1.4

Final observed and calculated structure factors.

H	K	L	F OBS	F CALC
0	0	4	172.5	-195.2
0	0	6	74.1	70.0
0	0	8	76.4	-80.7
0	0	10	85.1	-81.6
0	0	12	30.8	-36.1
0	0	14	46.4	-53.4
0	0	16	147.1	-159.2
0	0	18	18.1	14.1
0	0	20	67.2	66.4
0	0	22	56.4	-56.3
0	0	24	76.4	79.9
0	0	26	80.7	77.0
0	0	30	48.5	46.3
0	0	32	37.1	35.4
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2	0	16	118.9	114.6
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2	0	-10	221.7	201.2
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H	K	L	F OBS	F CALC
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1	4	23	17.4	16.7
1	4	25	33.1	36.3
1	4	26	10.6	-10.1
1	4	27	11.3	12.2
1	4	29	14.7	15.3
1	4	31	20.1	29.2
1	4	-1	147.3	145.9
1	4	-2	15.3	-13.1
1	4	-3	11.5	-11.6
1	4	-4	18.4	-15.6
1	4	-5	6.1	5.0
1	4	-7	46.5	44.5
1	4	-8	6.6	7.0
1	4	-9	234.5	-247.0
1	4	-10	27.6	-25.3
1	4	-11	43.3	-41.4
1	4	-13	14.0	14.1
1	4	-14	18.2	18.2
1	4	-15	73.9	-82.6
1	4	-16	14.1	-12.0
1	4	-17	25.6	-31.0
1	4	-18	9.6	-8.6
1	4	-19	38.4	29.9
1	4	-20	39.0	37.5
1	4	-21	15.4	15.0
1	4	-23	14.5	12.6
1	4	-25	47.7	53.3
1	4	-27	19.6	22.0
1	4	-28	9.9	10.2
1	4	-31	17.1	20.2
1	4	-35	16.7	-15.9
1	4	-36	9.8	-11.6
2	4	0	85.5	73.2
2	4	1	210.0	191.3
2	4	2	36.6	35.0
2	4	5	80.2	-69.9
2	4	6	46.9	46.0
2	4	7	18.2	16.6
2	4	8	21.7	21.6
2	4	9	65.4	-65.0
2	4	10	20.3	-22.5
2	4	11	94.0	-100.2
2	4	12	20.5	-21.0
2	4	13	18.1	-11.1
2	4	14	11.7	-11.0
2	4	17	34.7	-39.7
2	4	18	15.4	17.5
2	4	19	20.5	30.9
2	4	21	62.0	74.2
2	4	22	12.4	-12.8
2	4	23	11.3	-14.0
2	4	24	9.9	-9.0
2	4	25	16.0	16.0
2	4	26	9.9	11.0
2	4	27	34.5	40.6
2	4	29	11.9	-12.5
2	4	32	12.0	14.4
2	4	35	15.3	-16.5
2	4	37	9.4	-13.1
2	4	-1	18.7	-15.6
2	4	-2	5.4	-1.0
2	4	-3	94.1	81.4
2	4	-4	30.9	-43.1
2	4	-5	150.7	116.3
2	4	-6	23.1	-17.0
2	4	-7	15.2	-16.5
2	4	-8	6.3	5.0
2	4	-9	7.4	-8.0
2	4	-10	15.3	-14.0
2	4	-11	45.0	44.4
2	4	-13	34.5	-32.6
2	4	-15	54.9	-58.4
2	4	-17	18.0	-16.0
2	4	-18	9.9	-6.7
2	4	-19	51.9	-35.0
2	4	-20	25.5	22.9
2	4	-21	30.4	-40.3
2	4	-22	12.0	11.9
2	4	-23	24.0	25.0
2	4	-24	11.1	13.2
2	4	-29	30.0	40.0
2	4	-31	22.3	21.3
2	4	-35	18.3	13.0
3	4	0	15.2	10.9
3	4	1	60.4	-70.9
3	4	2	22.2	20.5
3	4	4	22.9	-27.6
3	4	5	60.4	-67.7
3	4	7	71.0	-76.2
3	4	8	47.4	26.4
3	4	9	17.0	17.1
3	4	10	13.7	-14.6
3	4	11	9.5	7.3
3	4	12	23.9	-25.5
3	4	13	19.6	-20.3
3	4	15	22.7	24.2
3	4	17	41.3	47.0
3	4	18	21.5	-24.0
3	4	21	24.7	27.9
3	4	22	11.3	10.0
3	4	23	19.6	22.7
3	4	24	9.9	-10.0
3	4	25	9.0	-11.5
3	4	26	11.0	13.1
3	4	28	10.5	13.1
3	4	31	19.9	-22.4
3	4	33	15.6	-17.2
3	4	-1	26.6	-23.0
3	4	-3	85.2	82.1
3	4	-4	57.3	53.6
3	4	-5	7.9	7.1
3	4	-6	26.6	25.6
3	4	-7	28.6	24.0
3	4	-8	16.0	-14.2
3	4	-9	82.5	78.2
3	4	-11	25.3	25.3
3	4	-13	17.0	-17.0
3	4	-14	18.5	-17.7
3	4	-15	40.9	40.1
3	4	-19	71.0	-72.0
3	4	-20	21.0	-24.3
3	4	-21	13.5	-13.2
3	4	-24	12.5	11.0
3	4	-25	31.9	-30.6
3	4	-27	16.5	-18.2
3	4	-30	13.5	14.0
3	4	-33	9.9	12.6
3	4	-35	25.0	23.0
4	4	0	6.0	-6.0
4	4	1	87.6	-88.4
4	4	2	22.7	-23.6
4	4	3	39.6	-38.5
4	4	4	6.3	7.1
4	4	5	40.0	39.2
4	4	6	20.4	-27.3
4	4	7	38.4	-36.3
4	4	8	21.0	-21.1
4	4	9	11.3	8.7
4	4	11	53.7	57.1
4	4	12	16.7	-16.2
4	4	15	21.7	24.0
4	4	17	47.9	54.9
4	4	20	11.3	12.4
4	4	21	22.1	-23.0
4	4	22	11.2	13.5
4	4	-2	28.0	22.5
4	4	-3	42.2	-42.0
4	4	-5	64.0	-55.0
4	4	-7	18.2	13.7
4	4	-9	32.0	33.2
4	4	-10	29.2	22.0
4	4	-11	21.3	25.2
4	4	-12	9.9	-13.5
4	4	-13	42.9	48.6
4	4	-14	12.7	-15.5
4	4	-15	42.3	42.0
4	4	-19	21.6	24.5
4	4	-20	12.3	-12.8
4	4	-21	9.9	7.7
4	4	-23	43.3	-46.9
4	4	-24	9.9	-9.6
4	4	-26	12.5	-15.5
4	4	-29	36.3	-34.5
5	4	0	11.5	-14.0
5	4	1	11.5	11.9
5	4	2	40.0	-42.4
5	4	3	14.4	-16.2
5	4	5	24.0	24.1
5	4	7	59.4	61.9
5	4	11	21.9	24.6
5	4	13	45.9	49.5
5	4	15	9.9	-8.5
5	4	16	9.9	11.4
5	4	17	12.5	-18.2
5	4	18	17.6	22.0
5	4	21	27.5	-29.3
5	4	23	21.9	-21.2
5	4	-1	9.0	-7.7
5	4	-3	43.0	-47.3
5	4	-4	31.9	-32.3
5	4	-5	35.1	-34.3
6	4	0	9.8	-9.2
6	4	1	48.1	54.9
6	4	3	30.0	31.7
6	4	8	30.5	3.2
6	4	10	11.3	9.0
6	4	12	27.6	29.0
6	4	13	24.4	18.0
6	4	-1	17.5	-16.6
6	4	-5	31.4	29.3
6	4	-8	34.6	-33.7
6	4	-9	31.6	-49.6
6	4	-10	48.4	-34.4
6	4	-11	32.9	16.5
6	4	-12	12.5	21.1
6	4	-13	24.7	-19.5
6	4	-14	19.6	27.2
6	4	-15	26.3	-38.6
6	4	-16	35.0	12.4
6	4	-18	22.1	12.0
6	4	-25	33.0	17.4
0	5	3	50.8	-46.9
0	5	4	73.6	63.6
0	5	5	8.5	-9.6
0	5	6	27.0	24.7
0	5	7	6.3	6.0
0	5	8	28.0	-26.3
0	5	10	47.4	46.0
0	5	11	62.3	60.9
0	5	12	48.5	44.1
0	5	13	76.9	76.5
0	5	14	46.5	-45.7
0	5	16	24.2	-26.3
0	5	17	22.3	22.2
0	5	18	22.9	19.4
0	5	19	20.7	21.0
0	5	20	21.2	-24.2
0	5	21	13.6	-16.4
0	5	26	13.9	-16.6
0	5	27	13.7	-15.4
0	5	29	21.1	-20.2
0	5	30	18.1	9.6
1	5	0	77.3	51.3
1	5	1	51.7	39.9
1	5	2	26.5	25.2
1	5	3	33.5	29.6
1	5	4	5.9	-4.9
1	5	5	20.0	-21.9
1	5	6	17.4	15.7
1	5	7	92.0	94.7
1	5	8	17.5	18.6
1	5	9	50.1	43.0
1	5	10	35.4	-31.2
1	5	11	18.9	-18.4
1	5	12	8.7	11.3
1	5	13	29.5	24.1
1	5	15	17.2	17.6
1	5	16	19.6	-21.2
1	5	17	10.1	-6.0
1	5	18	13.1	-14.7
1	5	19	23.9	-27.2
1	5	20	18.0	-19.2
1	5	21	18.9	-6.7
1	5	23	24.9	-24.1
1	5	25	12.5	-11.1
1	5	26	15.3	17.5
1	5	29	22.2	-25.0
1	5	32	15.4	16.9
1	5	33	16.9	19.0
1	5	-1	96.4	-68.6
1	5	-2	17.0	13.6
1	5	-3	36.1	-30.5
1	5	-4	26.0	-21.3
1	5	-6	23.2	21.6
1	5	-7	76.0	-69.2
1	5	-8	16.2	-14.5
1	5	-9	40.2	-34.9
1	5	-10	111.4	-36.9
1	5	-13	9.6	9.1
1	5	-14	30.0	-30.3
1	5	-15	10.6	7.1
1	5	-16	19.1	-19.5
1	5	-17	50.7	54.0
1	5	-19	26.1	27.0
1	5	-20	21.1	21.4
1	5	-22	10.9	-11.6
1	5	-23	35.6	39.6
1	5	-26	24.7	27.6
1	5	-27	13.7	-13.5
1	5	-31	15.5	-15.2
1	5	-33	10.2	-13.2
2	5	0	25.0	20.0
2	5	1	19.9	16.7
2	5	2	51.3	49.2
2	5	3	76.0	67.0
2	5	4	18.2	-17.4
2	5	5	62.1	54.8
2	5	6	19.4	-20.2
2	5	7	17.9	-10.1
2	5	8	18.9	16.5
2	5	9	6.6	7.4
2	5	10	42.1	-38.3
2	5	11	9.1	-10.0
2	5	12	22.7	-22.2
2	5	13	24.3	-24.5
2	5	15	21.0	26.0
2	5	16	23.4	-27.5
2	5	17	38.0	-32.3
2	5	18	17.9	-17.1
2	5	19	55.3	-61.9
2	5	20	29.5	36.0
2	5	21	15.5	-16.9
2	5	26	23.9	27.0
2	5	29	12.2	15.0
2	5	33	12.9	13.2
2	5	-1	6.0	-6.9
2	5	-2	30.0	-26.0
2	5	-4	42.3	38.0
2	5	-6	38.8	35.3
2	5	-7	41.9	-48.8
2	5	-8	24.3	-22.1
2	5	-9	9.1	-6.4
2	5	-10	28.3	23.7
2	5	-11	52.9	-40.4
2	5	-12	17.6	13.9
2	5	-13	54.5	-54.2
2	5	-14	53.7	-54.7
2	5	-16	9.0	-8.9
2	5	-17	25.5	-25.7
2	5	-18	18.3	9.4
2	5	-20	22.9	-23.0
2	5	-21	27.3	31.4
2	5	-27	23.6	22.7
2	5	-30	20.5	19.4
2	5	-31	9.7	-10.7
3	5	0	24.5	-22.6
3	5	2	13.9	13.4
3	5	3	37.5	32.3
3	5	5	36.0	31.4
3	5	6	55.5	-53.5
3	5	7	37.5	-35.7
3	5	8	28.3	-22.0
3	5	9	49.6	-52.9
3	5	10	11.2	12.7
3	5	12	14.4	-19.1
3	5	13	26.3	-27.5
3	5	15	21.4	-23.1
3	5	16	27.3	29.7
3	5	17	13.0	-14.9
3	5	19	18.4	-19.0
3	5	21	18.9	13.7
3	5	22	24.5	28.0
3	5	23	27.1	32.0
3	5	25	11.7	15.0
3	5	26	18.0	-18.9
3	5	29	11.1	12.1
3	5	32	18.7	-13.1
3	5	-1	45.6	38.1
3	5	-2	29.9	25.9
3	5	-3	23.0	22.4
3	5	-4	16.0	10.9
3	5	-7	42.1	36.3
3	5	-8	38.9	29.9
3	5	-9	13.9	15.1
3	5	-10	29.6	31.0
3	5	-11	46.6	-45.0
3	5	-12	16.6	-16.0
3	5	-13	29.1	-28.5
3	5	-16	24.0	23.0
3	5	-17	45.4	-46.7
3	5	-18	26.9	-25.5
3	5	-19	24.3	-21.9
3	5	-20	27.3	-30.3
3	5	-22	11.0	11.3
3	5	-24	12.5	-13.0
3	5	-26	18.8	-13.1
3	5	-27	12.1	15.6
4	5	0	23.3	-24.8
4	5	2	27.9	-27.5
4	5	3	32.3	-31.2
4	5	7	14.5	-14.1
4	5	8	23.5	-26.3
4	5	9	51.5	-58.9
4	5	11	15.2	-16.7
4	5	12	24.4	25.0
4	5	13	21.8	24.6
4	5	15	12.5	-11.2
4	5	16	19.7	23.4
4	5	17	13.9	16.3
4	5	18	19.6	25.6
4	5	19	37.0	42.9
4	5	26	18.3	-16.5
4	5	27	12.1	-3.9
4	5	-1	31.6	31.7
4	5	-5	42.1	35.9
4	5	-7	90.1	84.3
4	5	-8	32.4	27.2
4	5	-9	11.4	-10.3
4	5	-11	14.5	13.1
4	5	-12	18.5	20.0
4	5	-13	14.8	13.7
4	5	-14	18.9	18.5
4	5	-15	10.7	-6.7
4	5	-19	11.0	-8.8
4	5	-20	18.4	21.6
4	5	-21	27.0	-32.2
4	5	-23	21.0	-24.0
4	5	-24	24.4	-27.0
4	5	-30	16.5	-13.3
4	5	-31	17.9	19.7
4	5	-33	7.0	12.3
5	5	1	13.5	-12.0
5	5	2	13.5	-13.7
5	5	4	13.6	-14.2
5	5	5	16.1	-16.9
5	5	6	27.5	29.6
5	5	8	12.5	14.4
5	5	12	27.6	33.2
5	5	13	21.9	24.6
5	5	15	27.2	32.2
5	5	16	15.1	-17.9
5	5	22	9.3	-13.7
5	5	23	18.1	-9.4
5	5	-1	58.2	-62.5
5	5	-2	19.0	-15.8
5	5	-4	34.7	-35.2
5	5	-5	24.0	28.6
5	5	-6	15.1	12.4
5	5	-8	13.5	13.5
5	5	-9	27.2	26.5
5	5	-10	27.3	-26.9
5	5	-11	27.4	28.6
5	5	-14	15.4	13.5
5	5	-17	39.4	44.1
5	5	-21	18.0	-19.6
5	5	-27	12.1	-14.0
5	5	-28	9.2	-9.3
5	5	-31	8.9	-12.6
6	5	2	33.2	39.2
6	5	3	13.9	15.6
6	5	4	23.2	25.3
6	5	9	13.6	33.4
6	5	11	12.1	12.7
6	5	12	18.4	-18.9
6	5	15	14.0	17.4
6	5	20	18.4	6.0
6	5	21	16.1	-4.0
6	5	-1	35.3	-37.6
6	5	-2	24.9	-23.0
6	5	-5	19.7	-19.1
6	5	-6	19.7	-17.7
6	5	-7	12.5	-14.2
6	5	-8	31.3	-35.0
6	5	-14	19.5	-16.9
6	5	-15	18.0	9.0
6	5	-17	19.0	21.0
6	5	-18	15.0	14.6

TABLE 1.5

ORTHOGONAL COORDINATES AND E.S.D.S.

ATOM	X	Y	Z
Br(1)	6.840 ± 2	3.145 ± 2	15.105 ± 2
Br(2)	2.097 ± 2	2.438 ± 2	11.490 ± 2
C(1)	5.400 ± 15	3.775 ± 16	13.879 ± 15
C(2)	4.090 ± 15	3.522 ± 18	14.519 ± 15
C(3)	3.184 ± 13	2.652 ± 17	14.060 ± 15
C(4)	3.339 ± 13	1.778 ± 17	12.883 ± 15
C(5)	4.755 ± 14	1.757 ± 16	12.362 ± 14
C(6)	5.505 ± 16	3.179 ± 17	12.499 ± 13
C(7)	5.153 ± 14	4.193 ± 17	11.411 ± 13
C(8)	6.321 ± 15	4.052 ± 17	10.775 ± 15
C(9)	6.838 ± 12	2.952 ± 15	11.668 ± 13
C(10)	6.653 ± 13	1.522 ± 18	11.125 ± 13
C(11)	6.827 ± 15	0.635 ± 15	12.354 ± 14
C(12)	5.721 ± 14	0.792 ± 16	13.115 ± 14
C(13)	5.173 ± 14	1.374 ± 17	10.929 ± 13
C(14)	5.473 ± 14	0.157 ± 15	14.429 ± 14
C(15)	6.428 ± 19	-0.813 ± 20	16.346 ± 15
C(16)	8.110 ± 14	0.003 ± 18	12.714 ± 14
C(17)	9.358 ± 18	-1.988 ± 19	13.024 ± 22
C(18)	4.033 ± 15	5.134 ± 17	11.216 ± 16

C(19)	2.555 ± 22	6.130 ± 23	9.675 ± 26
C(20)	6.986 ± 14	4.652 ± 17	9.601 ± 14
C(21)	7.042 ± 24	6.581 ± 23	8.209 ± 19
O(1)	4.381 ± 10	0.042 ± 14	14.922 ± 11
O(2)	6.579 ± 12	-0.266 ± 13	14.995 ± 10
O(3)	9.081 ± 11	0.640 ± 12	12.928 ± 13
O(4)	8.100 ± 10	-1.313 ± 12	12.677 ± 12
O(5)	3.569 ± 13	5.764 ± 13	12.104 ± 13
O(6)	3.662 ± 11	5.216 ± 12	9.943 ± 11
O(7)	7.799 ± 14	4.099 ± 15	8.938 ± 13
O(8)	6.553 ± 13	5.882 ± 13	9.386 ± 11

TABLE 1.6

ORTHOGONAL HYDROGEN COORDINATES.

ATOM	X	Y	Z
H(1)	5.44	4.81	13.75
H(2)	3.86	4.08	15.37
H(3)	2.26	2.59	14.58
H(4)	3.14	0.77	13.21
H(5)	7.70	3.17	12.19
H(6)	7.25	1.23	10.33
H(7)	4.79	1.98	10.18
H(8)	4.85	0.46	10.57
H(9)	7.32	-1.08	16.77
H(10)	5.76	-1.64	16.31
H(11)	5.94	-0.07	16.98
H(12)	9.27	-3.02	12.99
H(13)	9.68	-1.70	14.00
H(14)	10.12	-1.68	12.34
H(15)	2.34	6.14	8.60
H(16)	2.82	7.13	9.91
H(17)	1.69	5.87	10.16
H(18)	6.57	7.54	8.17
H(19)	6.70	6.05	7.33
H(20)	8.04	6.66	8.21

TABLE 1.7

PRINCIPAL VALUES OF VIBRATION TENSORS AND THEIR DIRECTION COSINES REFERRED TO ORTHOGONAL AXES.

ATOM	U $\mathring{A}^2$	D1	D2	D3
Br(1)	0.0766	-0.6841	-0.3601	0.6343
	0.0512	0.6656	0.0475	0.7448
	0.0579	-0.2983	0.9317	0.2072
Br(2)	0.0773	-0.0948	0.6208	0.7782
	0.0434	0.9616	-0.1453	0.2330
	0.0590	0.2577	0.7704	-0.5831
C(1)	0.0286	0.0235	-0.9845	0.1740
	0.0658	-0.4438	0.1457	0.8842
	0.0486	-0.8958	-0.0981	-0.4334
C(2)	0.0397	-0.7669	-0.3906	0.5092
	0.0636	0.5789	-0.0785	0.8116
	0.0582	-0.2770	0.9172	0.2863
C(3)	0.0262	-0.9508	0.2275	0.2104
	0.0702	0.2875	0.3948	0.8726
	0.0511	0.1154	0.8902	-0.4408
C(4)	0.0749	0.0190	0.4712	0.8818
	0.0247	-0.9985	-0.0362	0.0409
	0.0436	0.0512	-0.8813	0.4698
C(5)	0.0753	-0.6285	0.2361	0.7411
	0.0227	0.5395	0.8187	0.1967
	0.0387	-0.5603	0.5234	-0.6419
C(6)	0.0670	0.8194	0.5714	0.0457
	0.0407	-0.2865	0.3390	0.8961
	0.0473	0.4965	-0.7473	0.4415
C(7)	0.0637	0.6312	0.0957	0.7697
	0.0373	-0.7369	0.3835	0.5567
	0.0387	-0.2419	-0.9186	0.3125

C(8)	0.0651	-0.6237	-0.1465	0.7678
	0.0336	-0.1540	0.9861	0.0631
	0.0482	-0.7664	-0.0789	-0.6376
C(9)	0.0536	0.2339	-0.0011	0.9723
	0.0265	-0.8541	-0.4780	0.2049
	0.0345	0.4645	-0.8784	-0.1128
C(10)	0.0293	-0.9325	-0.0912	0.3494
	0.0624	0.0158	0.9564	0.2917
	0.0502	-0.3607	0.2776	-0.8904
C(11)	0.0179	0.4339	0.8983	0.0688
	0.0657	-0.8256	0.3659	0.4296
	0.0505	0.3608	-0.2432	0.9004
C(12)	0.0261	-0.2507	-0.9572	0.1444
	0.0607	0.3604	0.0462	0.9317
	0.0474	-0.8985	0.2856	0.3334
C(13)	0.0364	-0.8380	-0.2450	0.4876
	0.0550	0.2535	0.6165	0.7455
	0.0479	-0.4832	0.7483	-0.4545
C(14)	0.0160	-0.0758	0.9970	0.0152
	0.0627	0.4579	0.0213	0.8887
	0.0440	0.8858	0.0744	-0.4582
C(15)	0.0922	-0.6914	-0.7207	0.0496
	0.0479	0.2066	-0.1315	0.9695
	0.0624	-0.6922	0.6806	0.2398
C(16)	0.0349	-0.8046	-0.5465	0.2323
	0.0593	-0.4437	0.8132	0.3766
	0.0541	-0.3947	0.1999	-0.8968
C(17)	0.1286	0.0501	0.0189	0.9986
	0.0334	-0.0741	-0.9970	0.0226
	0.0540	0.9960	-0.0752	-0.0486
C(18)	0.0775	0.3291	0.0789	0.9410
	0.0325	0.1599	-0.9868	0.0268
	0.0437	0.9307	0.1416	-0.3374
C(19)	0.1576	-0.3313	0.0558	0.9419
	0.0536	0.6103	-0.7487	0.2590
	0.0708	0.7196	0.6606	0.2140

C(20)	0.0590	0.2689	0.1514	0.9512
	0.0362	-0.1593	-0.9670	0.1990
	0.0443	0.9499	-0.2050	-0.2359
C(21)	0.1505	0.7966	0.3456	0.4960
	0.0350	-0.1577	-0.6733	0.7224
	0.0776	0.5836	-0.6537	-0.4818
O(1)	0.1071	0.1710	0.8050	0.5681
	0.0371	-0.8692	-0.1483	0.4717
	0.0558	0.4640	-0.5745	0.6743
O(2)	0.0820	0.6693	0.6798	0.2998
	0.0486	0.0799	-0.4671	0.8806
	0.0631	0.7387	-0.5654	-0.3669
O(3)	0.1203	-0.1402	0.2117	0.9672
	0.0410	-0.4420	-0.8875	0.1302
	0.0474	0.8860	-0.4093	0.2180
O(4)	0.0990	-0.1553	-0.1295	0.9793
	0.0341	-0.3909	0.9185	0.0595
	0.0401	-0.9072	-0.3736	-0.1933
O(5)	0.0386	-0.5722	0.7944	0.2039
	0.1033	0.6064	0.2424	0.7574
	0.0744	0.5522	0.5570	-0.6204
O(6)	0.0368	0.3786	-0.9197	0.1045
	0.0841	-0.3067	-0.0181	0.9516
	0.0657	-0.8733	-0.3923	-0.2889
O(7)	0.1293	0.6257	0.4488	0.6381
	0.0507	-0.5989	-0.2478	0.7615
	0.0812	0.4998	-0.8586	0.1137
O(8)	0.0933	0.7950	0.3023	0.5259
	0.0463	-0.1184	-0.7730	0.6233
	0.0627	0.5949	-0.5578	-0.5788

TABLE 1.8

BOND LENGTHS AND E.S.D.S.

Br(1) - C(1)	1.993 ± 15 Å	C(11) - C(12)	1.352 ± 21 Å
Br(2) - C(4)	1.979 ± 15	C(7) - C(18)	1.475 ± 22
C(1) - C(2)	1.480 ± 21	C(8) - C(20)	1.477 ± 21
C(1) - C(6)	1.506 ± 21	C(11) - C(16)	1.475 ± 21
C(2) - C(3)	1.337 ± 23	C(12) - C(14)	1.480 ± 21
C(3) - C(4)	1.474 ± 22	O(1) - C(14)	1.203 ± 18
C(4) - C(5)	1.509 ± 19	O(3) - C(16)	1.181 ± 19
C(5) - C(6)	1.614 ± 23	O(5) - C(18)	1.183 ± 20
C(5) - C(12)	1.559 ± 21	O(7) - C(20)	1.186 ± 20
C(5) - C(13)	1.541 ± 20	O(2) - C(14)	1.313 ± 19
C(6) - C(7)	1.528 ± 22	O(4) - C(16)	1.316 ± 21
C(6) - C(9)	1.588 ± 20	O(6) - C(18)	1.328 ± 19
C(7) - C(8)	1.338 ± 21	O(8) - C(20)	1.321 ± 21
C(8) - C(9)	1.508 ± 21	O(2) - C(15)	1.465 ± 19
C(9) - C(10)	1.541 ± 23	O(4) - C(17)	1.469 ± 21
C(10) - C(11)	1.526 ± 21	O(6) - C(19)	1.460 ± 25
C(10) - C(13)	1.500 ± 19	O(8) - C(21)	1.454 ± 24

TABLE 1.9

INTERBOND ANGLES AND E.S.D.S.

Br(1)- C(1) - C(2)	108.6±10°	C(5) - C(6) - C(7)	114.7±12°
Br(1)- C(1) - C(6)	112.9±11	C(5) - C(6) - C(9)	102.7±12
C(2) - C(1) - C(6)	112.9±13	C(7) - C(6) - C(9)	85.2±10
C(1) - C(2) - C(3)	124.3±14	C(6) - C(7) - C(8)	93.9±13
C(2) - C(3) - C(4)	126.0±13	C(6) - C(7) - C(18)	133.8±13
Br(2)- C(4) - C(3)	107.4±10	C(8) - C(7) - C(18)	131.9±14
Br(2)- C(4) - C(5)	110.5±10	C(7) - C(8) - C(9)	95.5±12
C(3) - C(4) - C(5)	112.5±12	C(7) - C(8) - C(20)	136.8±15
C(4) - C(5) - C(6)	113.2±13	C(9) - C(8) - C(20)	127.8±13
C(4) - C(5) - C(12)	115.0±12	C(6) - C(9) - C(8)	85.3±11
C(4) - C(5) - C(13)	125.4±12	C(6) - C(9) - C(10)	102.5±11
C(6) - C(5) - C(12)	102.5±11	C(8) - C(9) - C(10)	115.3±11
C(6) - C(5) - C(13)	99.9±11	C(9) - C(10)- C(11)	104.0±11
C(12)- C(5) - C(13)	97.3±11	C(9) - C(10)- C(13)	104.9±12
C(1) - C(6) - C(5)	113.2±12	C(11)- C(10)- C(13)	99.3±12
C(1) - C(6) - C(7)	112.0±14	C(10)- C(11)- C(12)	107.0±13
C(1) - C(6) - C(9)	126.5±13	C(10)- C(11)- C(16)	123.0±12

C(12)- C(11)- C(16)	128.6±13
C(5) - C(12)- C(11)	107.9±12
C(5) - C(12)- C(14)	126.2±12
C(11)- C(12)- C(14)	125.9±14
C(5) - C(13)- C(10)	97.0±11
O(1) - C(14)- C(12)	123.9±14
O(3) - C(16)- C(11)	121.9±16
O(5) - C(18)- C(7)	122.5±15
O(7) - C(20)- C(8)	124.3±16
O(2) - C(14)- C(12)	112.3±12
O(4) - C(16)- C(11)	114.5±13
O(6) - C(18)- C(7)	112.3±13
O(8) - C(20)- C(8)	111.1±13
O(1) - C(14)- O(2)	123.8±14
O(3) - C(16)- O(4)	123.4±14
O(5) - C(18)- O(6)	125.2±15
O(7) - C(20)- O(8)	124.6±15
C(14)- O(2) - C(15)	115.5±13
C(16)- O(4) - C(17)	116.5±12
C(18)- O(6) - C(19)	115.3±15
C(20)- O(8) - C(21)	118.0±14

TABLE 1.10

INTERMOLECULAR CONTACTS BELOW 4 Å.

C(4).....O(3)	ii	3.14 Å	O(4).....O(8)	iv	3.65 Å
C(21)....O(7)	viii	3.20	Br(2)....C(21)	vi	3.67
C(3).....O(3)	ii	3.21	C(13)....O(5)	iv	3.67
C(15)....O(3)	xi	3.25	C(5).....O(5)	iv	3.68
C(15)....O(1)	x	3.34	C(2).....C(17)	iii	3.71
C(8).....O(4)	i	3.36	C(11)....O(8)	iv	3.72
C(17)....O(5)	v	3.36	C(3).....C(15)	x	3.75
O(1).....O(5)	iv	3.42	Br(1)....C(15)	i	3.76
Br(2)....O(7)	ii	3.45	C(7).....O(4)	i	3.77
C(12)....O(5)	iv	3.46	C(19)....O(7)	ii	3.78
Br(2)....O(3)	ii	3.48	C(1).....O(4)	i	3.80
C(14)....O(5)	iv	3.54	C(1).....O(2)	i	3.80
C(10)....O(8)	iv	3.57	C(10)....C(21)	iv	3.81
C(4).....O(5)	iv	3.59	C(9).....C(17)	i	3.83
C(19)....O(7)	vii	3.59	O(1).....O(3)	ii	3.83
C(9).....O(4)	i	3.60	C(21)....O(6)	vii	3.88
C(20)....O(4)	i	3.61	C(1).....C(14)	i	3.90
C(3).....C(17)	iii	3.61	C(13)....C(18)	iv	3.90
O(1).....O(1)	x	3.62	Br(1)....Br(1)	ix	3.91
C(13)....O(8)	iv	3.62	C(19)....C(21)	vi	3.92

Br(2)....C(9)	ii	3.94	C(6).....O(4)	i	3.96
C(1).....C(15)	i	3.94	C(13)....C(19)	iv	3.98
C(19)....C(21)	ii	3.95	C(15)....C(16)	xi	4.00

Roman numerals refer to the following transformations of the fractional coordinates given in TABLE 1.1.

i	x, 1 + y, z;	vi	1 - x,-1/2 + y,1/2 - z;
ii	-1 + x, y, z;	vii	1 - x, 1/2 + y,1/2 - z;
iii	-1 + x, 1 + y, z;	viii	2 - x, 1/2 + y,1/2 - z;
iv	x,-1 + y, z;	ix	2 - x, 1 - y, 1 - z;
v	1 + x,-1 + y, z;	x	1 - x, - y, 1 - z;
xi	2 - x, - y,1 - z;		

TABLE 1.11

PART I - DEVIATIONS FROM MEAN PLANES (Å).

Plane 1 defined by C(1),C(2),C(3) and C(4).

C(1)	0.003	C(4)	-0.003
C(2)	-0.007	C(5)	-0.299
C(3)	0.007	C(6)	0.327

Plane 2 defined by C(6),C(7),C(8),C(9),C(18) and C(20).

C(6)	-0.040	C(20)	-0.020
C(7)	0.043	O(5)	-0.756
C(8)	0.003	O(6)	0.833
C(9)	0.021	O(7)	0.394
C(18)	-0.008	O(8)	-0.557

Plane 3 defined by C(5),C(6),C(9) and C(10).

C(5)	-0.012	C(11)	-1.374
C(6)	0.017	C(12)	-1.414
C(9)	-0.017	C(13)	0.819
C(10)	0.013		

Plane 4 defined by C(5),C(10),C(11) and C(12).

C(5)	0.008	C(6)	-1.469
C(10)	-0.008	C(9)	-1.449
C(11)	0.013	C(13)	0.818
C(12)	-0.013		

Plane 5 defined by C(6),C(9),C(11) and C(12).

C(6)	0.012	C(5)	0.885
C(9)	-0.012	C(10)	0.872
C(11)	0.014	C(13)	1.886
C(12)	-0.014		

Plane 6 defined by C(4),C(5),C(10) and C(13).

C(4)	-0.010	C(6)	1.293
C(5)	0.014	C(9)	1.207
C(10)	-0.008	C(11)	-1.202
C(13)	0.003	C(12)	-1.181

Plane 7 defined by C(5),C(10),C(11),C(12),C(14) and C(16).

C(5)	-0.047	C(6)	-1.533
C(10)	0.006	C(9)	-1.463
C(11)	0.080	C(13)	0.770
C(12)	0.015	O(1)	0.278
C(14)	0.006	O(2)	-0.332
C(16)	-0.060	O(3)	-1.034
		O(4)	1.016

Plane 8 defined by C(12),C(14),C(15),O(1) and O(2).

C(12)	-0.025	O(1)	0.008
C(14)	0.009	O(2)	0.040
C(15)	-0.031		

Plane 9 defined by C(11),C(16),C(17),O(3) **and** O(4).

C(11)	0.003	O(3)	0.011
C(16)	-0.023	O(4)	0.014
C(17)	-0.005		

Plane 10 defined by C(7),C(18),C(19),O(5) **and** O(6).

C(7)	0.001	O(5)	0.006
C(18)	-0.012	O(6)	0.009
C(19)	-0.004		

Plane 11 defined by C(8),C(20),C(21),O(7) **and** O(8).

C(8)	0.021	O(7)	-0.005
C(20)	-0.008	O(8)	-0.035
C(21)	0.027		

PART II - PLANE EQUATIONS.

In the following table P,Q and R are the direction cosines of the plane normal, S is the plane to origin distance and RMS D is the root mean square deviation in Å s. The plane equation is then

$$PX + QY + RZ = S$$

where X,Y and Z are in Å s and are referred to standard orthogonal axes.

PLANE	P	Q	R	S	RMS D	χ^2
1	-0.4088	0.7108	-0.5724	-7.4717	0.006	0.5
2	-0.4333	-0.6905	-0.5792	-11.7809	0.027	16.8
3	-0.4720	0.3477	-0.8101	-11.6361	0.015	3.6
4	-0.4167	0.7715	-0.4807	-9.2870	0.010	1.7
5	-0.5553	-0.2444	-0.7949	-13.7817	0.013	2.7
6	-0.0679	0.9607	-0.2690	-1.9741	0.009	1.4
7	-0.3743	-0.8022	-0.4652	-8.8919	0.046	49.1
8	-0.0970	-0.8989	-0.4273	-6.8460	0.026	15.7
9	0.2499	-0.0029	-0.9683	-10.2615	0.013	4.2
10	0.6573	0.7365	-0.1597	4.6517	0.007	1.2
11	-0.7239	-0.3774	-0.5776	-12.3496	0.022	11.8

1.4 DISCUSSION

Although the analysis was undertaken to determine only the gross molecular structure the results allow something to be said about the details of the structure of the molecule.

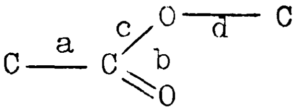
The mean dimensions of the methyl ester groups are given in Table A. The figures in parentheses are the respective root mean square deviations from these means and they are in every case less than the estimated standard deviations of an individual measurement calculated from the least-squares totals. The latter may thus be taken as reliable estimates of the random errors. Table A also contains values for comparable bond lengths and interbond angles obtained in some other recent analyses. They are in reasonable agreement with the results of this analysis.

The ester groups are planar to within the accuracy of the results, the deviations from the mean plane of the five atoms forming the group being significant at the 0.1% level in one instance only.

In table B the means of the other types of covalent bond in the structure are given. With the exception of the C-Br bond which is about three standard deviations longer, they are in good agreement with accepted values.

TABLE A

BOND LENGTHS (Å) AND INTERBOND ANGLES (°) IN SOME ESTER GROUPS



a	b	c	d	Reference
1.477(2)	1.188(9)	1.320(6)	1.462(6)	This analysis
-	1.223	1.351	1.459	1
-	1.196	1.360	1.476	2
	1.188	1.343	1.463	3
1.470	1.189	-	-	4

∠ab	∠ac	∠bc	∠cd	Reference
123.2(10)	112.6(13)	124.3(7)	116.3(11)	This analysis
124.6	111.2	124.2	120.3	1
126.3	110.6	123.1	120.7	2
126.0	108.0	125.8	120.2	3

References

1. d.l-Alphaprodine hydrochloride, Kartha, Ahmed & Barnes (1960).
2. d.l-Betaprodine hydrochloride, Ahmed & Barnes (1963).
3. d.l-Betaprodine hydrobromide, Ahmed, Barnes & Masironi (1963).
4. Maleic anhydride, Marsh, Ubell, & Wilcox (1962).

TABLE B

AVERAGED BOND LENGTHS (Å)

BOND	TYPE	MEAN	NUMBER	LITERATURE VALUE*
C-C	sp^3-sp^3	1.543	7	1.537
	sp^3-sp^2	1.513	6	1.510
	sp^2-sp^2	1.342	3	1.335
C-Br		1.986	2	1.938

* Sutton (1965)

The unusual carbon skeleton of this molecule results in a good deal of steric strain. This is shown by considerable departures from normal valence angles, by significant departures from expected planarity, and in at least one instance by a departure from usual covalent bond lengths.

The C(5)-C(6) bond is 1.614 Å which is more than three standard deviations greater than the mean for this type of bond. Both carbon atoms are fully substituted and lengthening due to steric repulsion is understandable. Such lengthening in bonds involving highly substituted carbon atoms has been observed in other analyses. The central bond in hexamethylethane was found by Bauer and Beach (1942) to be 1.58 Å; 1.59 Å was found for a similar bond in longifolene hydrochloride by Cesur and Grant (1965) and values up to 1.66 Å were claimed in methyl melaleucate iodoacetate by Hall and Maslen (1965).

Angles at sp^3 and sp^2 carbon atoms show highly significant differences from their usual values of 109° and 120°. These differences are most marked at the ring junctions and in the cyclobutene ring. Angles at the sp^3 carbons C(5) and C(6) range from 97° to 125° and 85° to 127° respectively. The average internal angle at sp^2 carbon is 94° in the cyclobutene ring and 107° in the bicycloheptene system. The angle at the bridging C(13) is 97°. These results are comparable with those found in the electron diffraction studies of methylcyclobutene (Shand, Schomaker, and Fischer, 1944), cyclobutene (Goldish, Hedberg, and Schomaker, 1956), and norbornadiene (Schomaker, 1960), and with the x-ray studies of norbornadiene palladium dichloride (Baenziger, Richards, and Doyle, 1965), and anti-8-tricyclo $[3,2,1,0^{2,4}]$ octyl-p-bromo-benzene sulphonate (Macdonald and Trotter, 1965).

The deviations from the planes defined by the carbons in carbon-carbon double bonds and the atoms adjacent to them (Table 1.11, planes 1,2 and 7) are significant at the 0.1% level in the case of the C(7)-C(8) and the C(11)-C(12) double bonds but not in that of the C(2)-C(3) double bond. This may reasonably be attributed to the greater steric strain in the cyclobutene and bicycloheptene ring systems.

Although their standard deviations are large the anisotropic vibration tensors give a physically reasonable description of the atomic vibrations. The atoms in the methyl ester groups, and in particular the methyl carbons, undergo vibrations which are both larger and more anisotropic than the atoms in the main part of the molecular skeleton. In each case the direction of maximum vibration of a methyl carbon is approximately normal to the direction of the Me-O bond. The peak heights and shapes of the final three-dimensional Fourier (Fig. 1.2.) also support this picture.

There are three intermolecular contacts which are smaller than the sum of the van der Waals radii (Pauling, 1960) of the participating atoms, namely two methylcarbon - carbonyl oxygen contacts of 3.20 and 3.25 Å and a contact between C(4) and O(3) of 3.14 Å. All other contacts are normal. Since hydrogen atoms were included in the calculations in assumed positions it has not been considered worthwhile to list intermolecular contacts involving hydrogen.

CHAPTER II

PHENANTHRENECHROMIUM TRICARBONYL

2.1 INTRODUCTION

The structural study of phenanthrenechromium tricarbonyl was prompted by a controversy over the molecular symmetry of dibenzenechromium. In one x-ray analysis of dibenzenechromium (Jellinek, 1963) adjacent bond lengths in the benzene rings were found to differ by 0.07 Å, whereas in a second analysis (Cotton, Dollase, and Wood, 1963) the bond lengths in the aromatic rings were found to be equal. Structure analyses of arenechromium tricarbonyls might be expected to yield information relevant to this problem. When the present work was started x-ray analyses of benzenechromium tricarbonyl and biphenyl bis(chromium tricarbonyl) (Corradini and Allegra, 1959 & 1960), and of a monoclinic modification of phenanthrenechromium tricarbonyl (Deuschl and Hoppe, 1964) had been reported. However, each of these three analyses was based only on projection data and no worthwhile conclusions could be drawn about the effect of the chromium tricarbonyl fragment on the bond lengths of the aromatic ring.

From Deuschl and Hoppe's work on the monoclinic polymorph it was known that the chromium tricarbonyl moiety is bonded to one of the side rings of phenanthrene.

An accurate x-ray analysis of phenanthrenechromium tricarbonyl thus allows direct comparisons to be made between the two side rings, which are different only in the respect that one is bonded to a chromium tricarbonyl fragment while the other is not.

2.2 EXPERIMENTAL

Crystal Data

Phenanthrenechromium Tricarbonyl

$C_{14}H_{10}Cr(CO)_3$

F.W. 314.3

Orthorhombic, a = 12.14, b = 18.08, c = 12.34 Å,

U = 2709 $Å^3$ F(000) = 1280

D_m = 1.52 $gmcm^{-3}$ Z = 8 D_x = 1.540 $gmcm^{-3}$

Linear absorption coefficient (Mo $K\alpha$, wavelength 0.7107 Å) = 8.8 cm^{-1}

Systematic Absences

$0k\ell$ when k is odd

$h0\ell$ when ℓ is odd

hk0 when h is odd

h00 when h is odd

0k0 when k is odd

00ℓ when ℓ is odd

Space Group Pbca (No. 61)

The systematic absences and cell dimensions were determined from equatorial layer and equi-inclination upper layer Weissenberg photographs taken normal to the c axis with copper Kα radiation (wavelength 1.5418 Å) and from h0ℓ and 0kℓ precession photographs taken with molybdenum Kα radiation (wavelength 0.7107 Å). The determination of the space group and density was carried out by Mr. D.R. Pollard who also supplied preliminary values of the cell dimensions (Pollard, 1964).

The intensities of 714 independent reflections were measured by visual comparison with a calibrated intensity strip. Timed series of 30° precession photographs of the reciprocal lattice nets 0kℓ to 4kℓ and h0ℓ to h2ℓ were taken with molybdenum Kα radiation. The charts of Grenville-Wells and Abrahams (1952) were used to correct for Lorentz and polarisation factors. The various reciprocal lattice nets were set on an approximately equal scale by comparison of common reflections. The final scale factors were obtained by making $\Sigma |F_o| = \Sigma |F_c|$ for each reciprocal lattice net.

2.3 STRUCTURE SOLUTION AND REFINEMENT OF PHOTOGRAPHIC DATA

The space group implies that the chromium atom is in a general position in the unit cell. Its fractional coordinates were determined from the Harker sections at $U = \frac{1}{2}$, $V = \frac{1}{2}$, and $W = \frac{1}{2}$.

The space group Pbca is centrosymmetric; there are three sets of non-intersecting two-fold screw axes parallel respectively to each of the crystal axes and three sets of axial glide planes normal to each of the crystal axes. If the origin is taken at a centre of symmetry then the coordinates of the eight general equivalent positions are: $\pm(x,y,z)$, $\pm(x,\frac{1}{2}-y,\frac{1}{2}+z)$, $\pm(\frac{1}{2}+x,y,\frac{1}{2}-z)$, and $\pm(\frac{1}{2}-x,\frac{1}{2}+y,z)$.

If the 2_1 axis parallel to the a axis is considered it is apparent that four equivalent positions are connected to other four by vectors having a component of $\frac{1}{2}$ along a. The analytical expressions for these four vectors and their inverses are found to be:

$$\pm(\tfrac{1}{2},\tfrac{1}{2}+2y,2z),\pm(\tfrac{1}{2},\tfrac{1}{2}-2y,2z),\pm(\tfrac{1}{2},\tfrac{1}{2}+2y,-2z),\pm(\tfrac{1}{2},\tfrac{1}{2}-2y,-2z).$$

Eight vectors between chromium atoms should therefore give rise to four double-weight peaks on the Harker section at $U=\frac{1}{2}$. These four peaks are related to each other by the pmm plane group symmetry of the section.

The a glide plane normal to the c axis connects four equivalent positions to the other four by vectors having components $\frac{1}{2}$ along a and 0 along b. The expressions for these four vectors and their inverses are found to be

$$\pm(\tfrac{1}{2},0,\tfrac{1}{2}+2z),\pm(\tfrac{1}{2},0,\tfrac{1}{2}-2z),$$

each position occuring twice. Another eight vectors between chromium atoms should therefore give rise to two peaks of quadruple weight at V=0 on the Harker section at $U=\frac{1}{2}$. These two peaks are also related by the plane group symmetry of the Harker section. The Harker section at $U=\frac{1}{2}$ therefore contains two independent peaks corresponding to vectors between chromium atoms from which two estimates of the z coordinate and one of the y coordinate of the chromium atom may be derived.

Analogous results may be obtained for the other two Harker sections, and the positions of the independent Harker peaks can then be summarised as:-

Section	Two-fold Peak	Four-fold Peak
$U=\frac{1}{2}$	$\frac{1}{2},\frac{1}{2}+2y,2z$	$\frac{1}{2},0,\frac{1}{2}+2z$
$V=\frac{1}{2}$	$2x,\frac{1}{2},\frac{1}{2}+2z$	$\frac{1}{2}+2x,\frac{1}{2},0$
$W=\frac{1}{2}$	$\frac{1}{2}+2x,2y,\frac{1}{2}$	$0,\frac{1}{2}+2y,\frac{1}{2}$

The asymmetric units of the three Harker sections of the unsharpened three-dimensional Patterson function are shown in Fig. 2.1; the peaks which were taken as vectors between chromium atoms are indicated by crosses. The coordinates of these peaks were determined using Booth's interpolation formula (1948). The chromium atom coordinates were then worked out from the analytical expressions given above and averaged.

The mean values obtained for the chromium coordinates were:-

	X/a	Y/b	Z/c
Cr(1)	0.4304	0.6771	0.1609

An electron density synthesis based on phases calculated from the chromium positions revealed the entire structure except for one carbonyl group. Due to the small number of terms used in the Fourier series the peaks in this synthesis were rather poorly resolved, and there was a good deal of spurious electron density round the chromium. Inclusion of the atoms of the phenanthrene nucleus and of the two located carbonyl groups reduced R by 0.13 to 0.33. A second electron density synthesis allowed the atoms of the missing carbonyl group to be located. Structure factors calculated from the positions derived from this synthesis gave an R-factor of 0.28.

At this stage of the analysis it was apparent that further data collection was necessary, to achieve accurate results. It was therefore decided to collect a more complete set of data and in the meantime to refine the available photographic data in order to start the refinement of the second set with a reasonably good model of the structure.

With the photographic data the structure was refined in eight cycles of least-squares minimisation of the function $M = \Sigma w(|F_o| - |F_c|)^2$. The programme devised by Dr. J.S. Rollett for the DEUCE computer was used (Rollett, 1961). Since this programme did not allow isotropic temperature factors to be refined the temperature factors of the carbon and oxygen atoms were held constant during the first four cycles. Thereafter anisotropic temperature factors were refined for these atoms. At the conclusion of this refinement R stood at 0.106 and the average standard deviation of a C-C bond was 0.03 Å. The bond lengths at this stage of the analysis are presented in Table 2.7. It can be seen that none differ significantly from the final values.

2.4 COLLECTION OF DIFFRACTOMETER DATA

A second set of data was collected on a Hilger-Watts linear diffractometer (see Appendix I) with a crystal mounted about the c axis. Molybdenum radiation was used, with balanced $SrO-ZrO_2$ Ross filters. A half-minute oscillation cycle was employed and each reflection was measured at least four times with each filter. A 3° oscillation angle was used for all reflections. About sixty reflections had to be set by hand. The maximum recording angle was $\theta = 30^\circ$.

The intensities of 4716 independent reflections on the reciprocal lattice nets hk0 to hk17 were measured; of these 505 had intensities of zero and a further 42, including the 00ℓ reflections, were known to be subject to serious systematic error. None of these reflections were used in the analysis. Of the remaining 4169 reflections 1033 had intensities of less than 20 counts per minute and these were introduced into the refinement only in its later stages.

The intensities were reduced to structure amplitudes, using the Lorentz and polarisation corrections appropriate to equi-inclination Weissenberg geometry, by means of DEUCE computer programmes devised by Dr. J.G. Sime. No absorption corrections were applied since the crystal was effectively transparent to molybdenum $K\alpha$ radiation.

The data were placed on approximately absolute scale by comparison with the refined photographic data. The final scale factor was determined by least-squares refinement.

2.5 REFINEMENT OF DIFFRACTOMETER DATA

The structure was now refined in fourteen cycles of least-squares minimisation of the function $M = \Sigma w(|F_o| - |F_c|)^2$, using the programme written by Cruickshank and Smith for the KDF9 computer. A block-diagonal approximation to the normal least-squares matrix was employed. The 1033 weak reflections were first introduced into the refinement in cycle 11 and were then used in all subsequent cycles.

Isotropic temperature factors were refined for carbon and oxygen atoms in the first nine cycles; in the first two cycles an isotropic temperature factor was also refined for the chromium atom but thereafter an anisotropic temperature factor was used.

The first six cycles reduced R from 0.231 to 0.138. After cycle 6 a difference synthesis was computed using the 437 reflections for which $\sin\theta/\lambda$ was less than 0.35 $\mathring{A}^{-1}$. The purpose of this synthesis was to decide whether inclusion of the hydrogen atoms in the calculations was worthwhile. Peaks corresponding to the expected positions of all ten hydrogen atoms were found. The peak heights ranged from 0.2 to 0.4e/$\mathring{A}^3$. The hydrogen atoms were accordingly included in the structure factor calculations in positions consistent with those of the carbon atoms adjacent to them. The isotropic temperature parameter of each hydrogen atom was assumed to be 1.5 times that of the carbon atom to which it was bonded. Inclusion of the hydrogen atoms reduced R from 0.138 in cycle 6 to 0.133 in cycle 7.

In cycle 9 least-squares totals were accumulated to determine the anisotropic temperature factors of the carbon and oxygen atoms. As a result of allowing for the anisotropic vibrations of these atoms R fell from 0.130 in cycle 9 to 0.105 in cycle 10. In cycle 11 all 4169 reflections were used for the first time. R rose to 0.128 but the parameter standard deviations fell by 10% on average.

Unit weights were used in cycles 1 to 8 and in cycles 9 to 12 a weighting scheme of the form $w = 1-\exp(-6\sin^2\theta/\lambda^2)$ was applied. After cycle 12 the unweighted differences between the observed and calculated structure factors were analysed as functions of $|F_o|$, $\sin\theta/\lambda$, and of the layer line index. From this analysis it was apparent that equal weights were appropriate to about three-quarters of the data but that low order reflections and particularly strong reflections required some down-weighting. Similar conclusions have been reached about linear diffractometer data in a number of analyses carried out in this laboratory and elsewhere (e.g. Wheatley 1964). In the present case it was also found that for weak reflections in which $|F_o|$ was greater than $|F_c|$ the mean Δ^2 was about three times the average for the data as a whole. Only a quarter of the 2400 reflections with $|F_o|$ less than 10 showed this effect and the average Δ^2 for the remaining three-quarters was about the same as the average Δ^2 for the data as a whole. The following weighting scheme was devised to allow for these factors:-

$w = 0$ if $|F_c| < \frac{1}{2}|F_o|$ otherwise $w = w_1 \times w_2$ where
$w_1 = 1$ if $|F_o| < 75$ otherwise $w_1 = 75/|F_o|$ and
$w_2 = 1$ if $\sin\theta/\lambda > 0.4$ otherwise $w_2 = (\sin\theta/\lambda)^2/0.16$

This weighting scheme was used in the last two cycles. In all, 671 reflections were given zero weight. The change in weighting scheme had little effect on R or on the atomic coordinates. R', however, fell from 0.0184 to 0.0080 and significant shifts in the scale factor and temperature parameters occurred. The parameter standard deviations fell on average by 15% after allowance had been made for the smaller number of degrees of freedom on which they were based.

In the last cycle of refinement the average shift in coordinates was less than 0.001 Å and the maximum shift was less than one third of the corresponding standard deviation. The shifts in scale and temperature factors were also insignificant.

The atomic form factors used throughout the refinement were those of Freeman and Watson (1961) for chromium, of Hoerni and Ibers (1954) for carbon, of Berghuis et al. (1955) for oxygen, and of Stewart, Davidson and Simpson (1965) for hydrogen.

The structure factors from the final cycle of least-squares were used to calculate electron density and difference syntheses. A composite view of the final electron density synthesis is shown in Fig. 2.2. The standard deviation of the electron density, calculated from the approximate formula of Cruickshank (1949), was $0.1e/\text{Å}^3$. A number of regions in the difference synthesis showed function values greater or less than three times this standard deviation. In particular there were two regions of positive density with maximum function values of 0.8 and $1.1e/\text{Å}^3$ associated with the chromium atom. These were tentatively ascribed to errors in the low order data down-weighted in the least-squares refinement.

Course of the Analysis

(1) Refinement of Photographic Data

S.F. Cycle No.	Atoms Included	R
1	Cr	0.46
2	Cr+16C+2O	0.33
3	Cr+17C+3O	0.28

S.F.L.S. Cycle No.	R	S.F.L.S. Cycle No.	R
1	0.28	5	0.155
2	0.25	6	0.129
3	0.24	7	0.118
4	0.18	8	0.106

(2) Refinement of Partial Diffractometer Data

S.F.L.S. Cycle No.	Remarks	R
1	All atoms isotropic	0.231
2	All atoms isotropic	0.174
3	Chromium set anisotropic	0.155
4	-	0.141
5	-	0.139
6	Structure factors only	0.138
7	Hydrogens included	0.133
8	-	0.131
9	-	0.130
10	All atoms set anisotropic	0.105

(3) Refinement of Complete Diffractometer Data

S.F.L.S. Cycle No.	R	R'	$\Sigma w\Delta^2$
11	0.128	0.0190	19976
12	0.123	0.0184	19087
13	0.123	0.0084	10476
14	0.123	0.0080	9892

The final values of the coordinates of the heavier atoms are presented, with their standard deviations, in Table 2.1. The assumed fractional coordinates of the hydrogen atoms are given in Table 2.2. Table 2.3 contains the anisotropic vibration parameters of the heavier atoms. The final values of the observed and calculated structure factors are given in Table 2.4 and an analysis of the structure factor agreement is presented in Table 2.5. Table 2.6 contains the principal magnitudes and directions of atomic thermal motion. The bond lengths, interbond angles, and intermolecular contacts below 4Å are presented in Tables 2.7, 2.8, and 2.9 respectively. The deviations from least-squares planes through various sets of atoms are given in Table 2.10. Standard deviations, if quoted, are in units of the last decimal place of the quantity to which they refer. The quantities given in Tables 2.6 to 2.10 were calculated with the programmes described in Part II of this thesis and the equations given there apply.

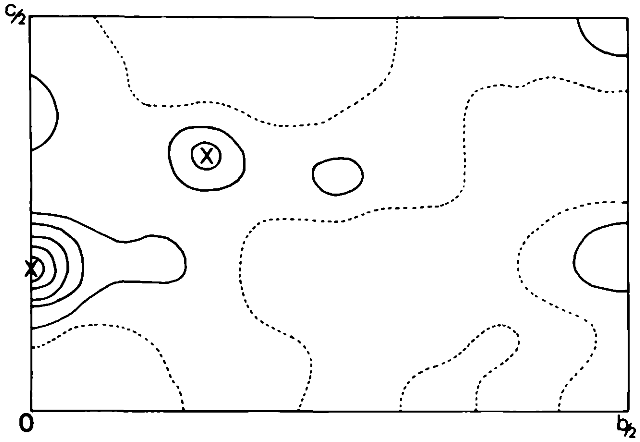
A view of the molecular packing down the c axis is given in Fig. 2.3.

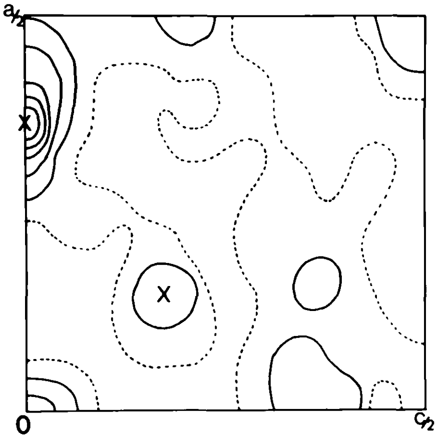
2.6 ANALYSIS OF MOLECULAR VIBRATIONS

The molecular vibrations were analysed in the manner suggested by Cruickshank (1956, 1961a), using the

FIG. 2.1

The Harker sections at $U = \frac{1}{2}$, $V = \frac{1}{2}$, and $W = \frac{1}{2}$. Peaks corresponding to vectors between chromium atoms are indicated by crosses.


c/2
X
X
0
b/2


a/2
X
X
0
c/2

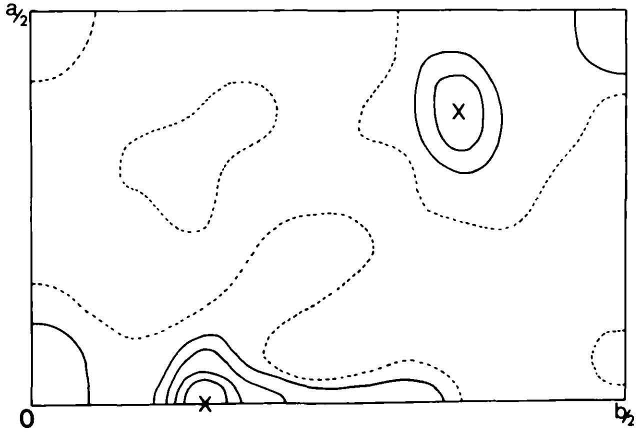

a/2
X
X
0
b/2

FIG. 2.2

The composite final electron density synthesis viewed down the c axis. Contours are at 1 e/Å^3 intervals starting at 2 e/Å^3 except round the chromium atom where the contours are at 10 e/Å^3 intervals starting at 5 e/Å^3.

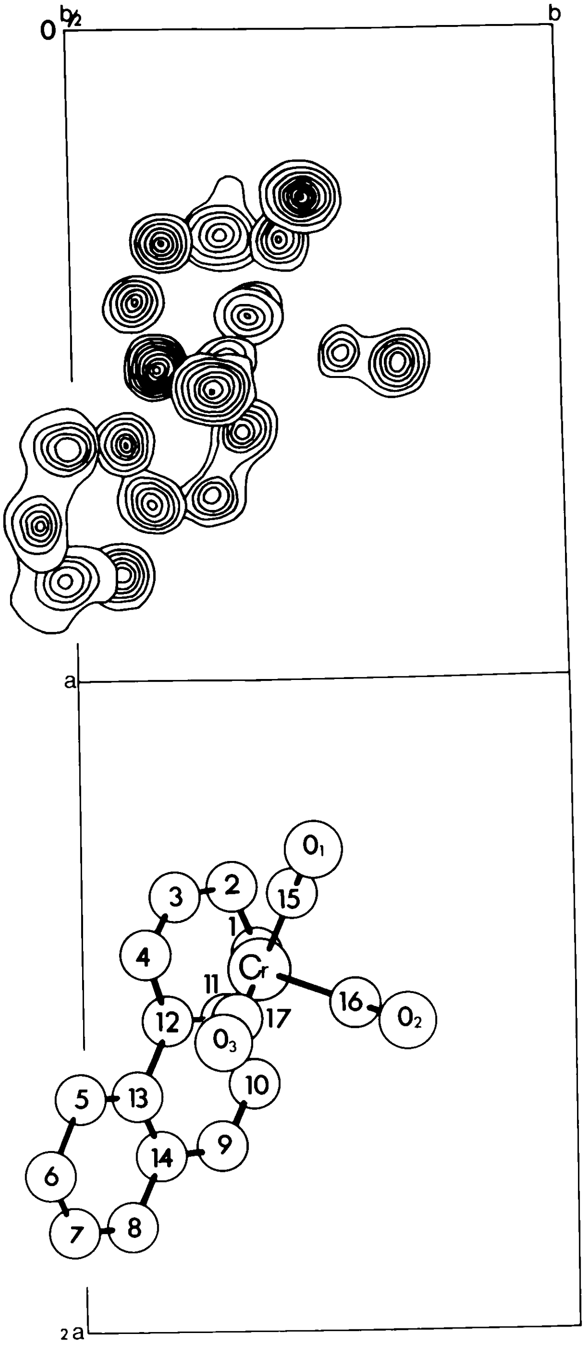

0
b/2
b
a
2a
O1
2
3
15
1
4
Cr
11
16
O2
12
17
O3
10
5
13
9
14
6
7
8

FIG. 2.3

The molecular packing viewed down the c axis. (Roman numerals have the same significance as in Table 2.9).

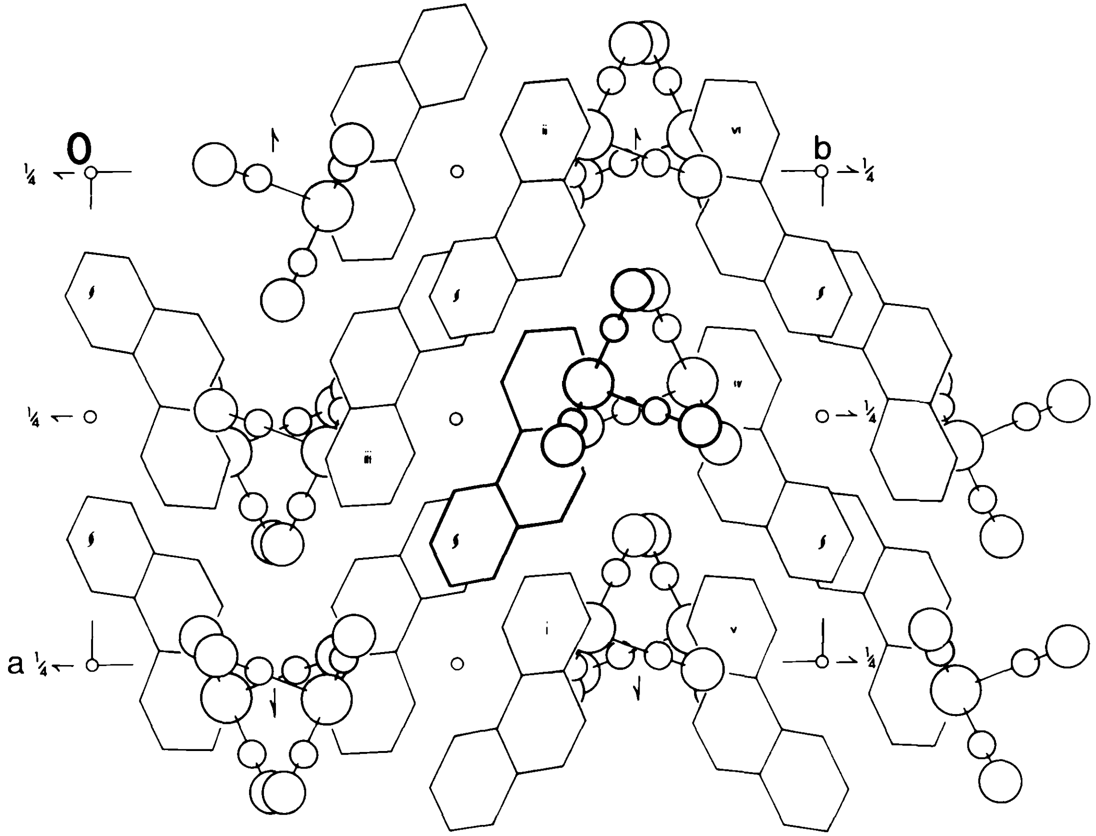

0
¼
b
¼
¼
¼
ii
vi
iii
iv
i
v
a ¼
¼

FIG. 2.4

Molecular diagram showing the numbering of the heavier atoms. (Hydrogen atoms have the same numbers as the carbon atoms to which they are bonded). The bond lengths after libration correction in the phenanthrene ligand are also shown.

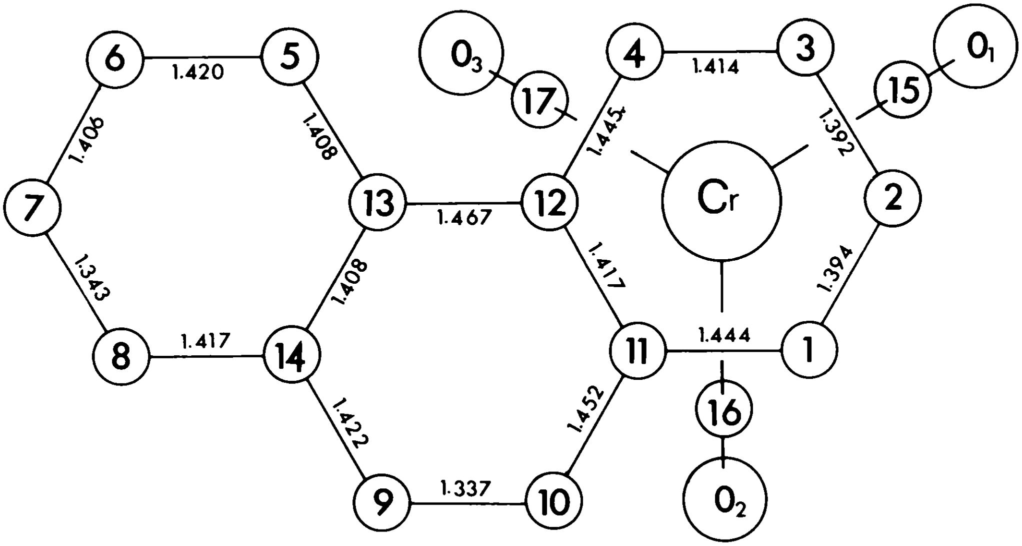
6
5
O3
17
4
3
O1
15
1.420
1.414
1.406
1.408
1.445
1.392
7
13
12
Cr
2
1.467
1.343
1.408
1.417
1.394
1.417
1.444
8
14
11
1
16
1.422
1.452
9
10
O2
1.337

TABLE 2.1

FRACTIONAL COORDINATES AND E.S.D.S.

ATOM	X/a	Y/b	Z/c
Cr(1)	0.43186 ± 4	0.67807 ± 3	0.16117 ± 5
C(1)	0.4120 ± 4	0.6803 ± 3	-0.0170 ± 4
C(2)	0.3166 ± 4	0.6512 ± 3	0.0282 ± 4
C(3)	0.3228 ± 4	0.5909 ± 3	0.0971 ± 4
C(4)	0.4251 ± 4	0.5587 ± 2	0.1236 ± 4
C(5)	0.6468 ± 5	0.4921 ± 3	0.1646 ± 5
C(6)	0.7519 ± 7	0.4590 ± 3	0.1769 ± 6
C(7)	0.8404 ± 5	0.4872 ± 3	0.1169 ± 6
C(8)	0.8281 ± 4	0.5455 ± 3	0.0515 ± 6
C(9)	0.7125 ± 4	0.6410 ± 3	-0.0325 ± 5
C(10)	0.6157 ± 4	0.6737 ± 3	-0.0499 ± 4
C(11)	0.5172 ± 3	0.6462 ± 2	0.0025 ± 3
C(12)	0.5246 ± 3	0.5854 ± 2	0.0737 ± 3
C(13)	0.6324 ± 4	0.5520 ± 2	0.0937 ± 4
C(14)	0.7242 ± 3	0.5797 ± 3	0.0379 ± 4
C(15)	0.3173 ± 4	0.7139 ± 2	0.2417 ± 4
C(16)	0.4882 ± 4	0.7728 ± 3	0.1621 ± 4
C(17)	0.5102 ± 3	0.6566 ± 2	0.2866 ± 4

O(1)	0.2466 ± 3	0.7382 ± 3	0.2948 ± 4
O(2)	0.5189 ± 5	0.8327 ± 2	0.1634 ± 5
O(3)	0.5572 ± 3	0.6422 ± 2	0.3633 ± 3

TABLE 2.2

ASSUMED HYDROGEN ATOM COORDINATES AND TEMPERATURE FACTORS.

ATOM	X/a	Y/b	Z/c	U
H(1)	0.409	0.728	-0.070	0.067
H(2)	0.235	0.677	0.011	0.068
H(3)	0.247	0.566	0.130	0.063
H(4)	0.429	0.513	0.182	0.057
H(5)	0.575	0.470	0.210	0.075
H(6)	0.767	0.413	0.232	0.085
H(7)	0.920	0.459	0.122	0.087
H(8)	0.901	0.568	0.008	0.080
H(9)	0.785	0.663	-0.073	0.071
H(10)	0.610	0.721	-0.104	0.066

TABLE 2.3

ANISOTROPIC TEMPERATURE FACTORS AND E.S.D.S.

ATOM	U11	U22	U33	2U23	2U31	2U12
Cr(1)	0.0286 2	0.0333 2	0.0444 3	-0.0085 4	-0.0067 4	-0.0048 4
C(1)	0.0496 24	0.0622 25	0.0481 22	0.0119 39	-0.0214 35	0.0158 41
C(2)	0.0434 22	0.0681 28	0.0569 25	-0.0415 43	-0.0202 37	0.0003 40
C(3)	0.0388 21	0.0536 24	0.0683 28	-0.0528 41	0.0119 37	-0.0314 36
C(4)	0.0510 23	0.0377 18	0.0569 23	-0.0149 32	0.0099 38	-0.0210 35
C(5)	0.0799 34	0.0427 22	0.0655 30	-0.0242 42	-0.0284 53	0.0234 44
C(6)	0.1120 48	0.0473 26	0.0787 38	-0.0257 49	-0.0778 72	0.0546 58
C(7)	0.0656 32	0.0701 32	0.0917 42	-0.0532 61	-0.0552 61	0.0559 55
C(8)	0.0473 26	0.0718 32	0.0935 42	-0.0659 61	-0.0232 52	0.0206 48
C(9)	0.0464 24	0.0605 27	0.0730 31	-0.0099 46	0.0161 44	-0.0153 42
C(10)	0.0531 24	0.0532 24	0.0570 25	0.0227 39	0.0274 39	0.0056 41
C(11)	0.0417 19	0.0447 19	0.0430 18	-0.0041 29	-0.0048 30	-0.0012 32
C(12)	0.0442 19	0.0342 17	0.0470 19	-0.0206 28	-0.0029 31	-0.0007 30

C(13)	0.0505	0.0370	0.0512	-0.0229	-0.0158	0.0105
	23	18	22	31	35	32
C(14)	0.0383	0.0518	0.0647	-0.0398	-0.0102	0.0096
	21	23	27	39	36	36
C(15)	0.0366	0.0533	0.0584	-0.0137	-0.0267	-0.0050
	19	22	24	39	35	37
C(16)	0.0515	0.0487	0.0656	0.0042	-0.0232	-0.0114
	24	23	27	41	43	38
C(17)	0.0400	0.0450	0.0510	-0.0129	-0.0076	-0.0033
	19	21	22	31	32	32
O(1)	0.0452	0.0973	0.0858	-0.0677	0.0029	0.0175
	17	30	27	46	37	39
O(2)	0.1062	0.0429	0.1381	0.0217	-0.0492	-0.0462
	35	19	45	48	67	43
O(3)	0.0616	0.0774	0.0651	0.0154	-0.0391	-0.0011
	21	24	23	36	36	38

TABLE 2.4

Observed and calculated structure factors.

H	K	L	F OBS	F CALC
4	0	0	100.6	98.1
6	0	0	51.7	-52.1
8	0	0	66.0	-60.2
10	0	0	20.7	-21.5
12	0	0	40.6	45.9
14	0	0	24.4	26.5
16	0	0	26.4	27.0
4	1	0	58.2	-58.7
6	1	0	38.6	-28.9
8	1	0	29.0	29.1
10	1	0	111.1	117.6
12	1	0	23.5	29.5
14	1	0	11.4	11.2
4	2	0	107.8	-97.6
6	2	0	80.0	78.6
8	2	0	20.9	29.0
10	2	0	5.3	-11.1
12	2	0	16.6	-17.7
16	2	0	19.3	-20.0
2	3	0	44.0	44.3
4	3	0	59.9	59.1
6	3	0	52.7	51.9
10	3	0	27.2	30.0
12	3	0	7.2	-7.1
16	3	0	7.3	10.9
0	4	0	77.6	-79.0
2	4	0	148.7	-141.2
4	4	0	67.3	-60.9
6	4	0	44.9	46.2
10	4	0	21.0	-23.7
12	4	0	19.7	11.0
14	4	0	11.0	-10.0
2	5	0	4.0	1.9
4	5	0	11.3	10.8
6	5	0	17.7	-16.4
8	5	0	35.7	-35.6
10	5	0	33.5	-33.0
12	5	0	33.7	-35.0
14	5	0	14.2	-11.0
0	6	0	207.4	214.4
2	6	0	189.3	181.0
4	6	0	59.1	-56.5
6	6	0	34.1	-32.6
8	6	0	69.2	-71.9
10	6	0	7.7	-6.2
12	6	0	10.0	10.7
14	6	0	30.1	32.5
16	6	0	15.0	17.0
2	7	0	93.7	-91.4
4	7	0	117.0	-115.6
6	7	0	67.0	-65.9
8	7	0	40.9	41.5
10	7	0	64.4	67.1
12	7	0	45.3	46.0
16	7	0	18.0	-11.2
0	8	0	151.4	-149.0
2	8	0	92.1	-89.9
4	8	0	50.3	45.0
6	8	0	85.9	83.9
8	8	0	60.0	61.0
12	8	0	10.9	-14.9
14	8	0	22.7	-21.9
2	9	0	76.0	78.6
4	9	0	66.8	67.7
6	9	0	37.5	38.4
8	9	0	11.9	-14.2
10	9	0	38.6	-41.8
12	9	0	16.7	-16.3
0	10	0	87.6	-83.2
4	10	0	56.1	-54.2
6	10	0	23.0	-25.0
10	10	0	7.0	-5.6
12	10	0	5.7	1.2
4	11	0	10.6	11.7
8	11	0	11.9	-12.9
10	11	0	30.8	-34.3
14	11	0	15.3	-15.7
0	12	0	110.7	109.3
2	12	0	64.9	64.9
4	12	0	10.2	14.5
6	12	0	17.6	-17.1
8	12	0	18.5	-21.6
10	12	0	7.9	-7.3
12	12	0	18.9	21.1
2	13	0	50.1	-47.0
4	13	0	56.7	-59.5
6	13	0	17.2	-18.3
8	13	0	19.0	18.5
10	13	0	20.5	20.3
12	13	0	29.9	30.7
0	14	0	34.0	-30.9
2	14	0	36.0	-36.2
4	14	0	18.0	20.7
6	14	0	67.7	68.0
8	14	0	31.4	30.3
10	14	0	14.5	14.0
12	14	0	12.3	-11.5
2	15	0	35.9	36.0
4	15	0	60.9	68.7
6	15	0	42.7	47.9
8	15	0	14.0	-15.9
10	15	0	17.6	-19.3
12	15	0	23.7	-20.6
0	16	0	5.1	6.0
2	16	0	14.0	10.2
4	16	0	40.8	-40.5
6	16	0	49.6	-52.0
8	16	0	20.5	-20.1
10	16	0	16.1	-10.6
4	17	0	25.4	-23.0
6	17	0	11.3	17.9
0	18	0	22.6	23.2
2	18	0	10.0	19.7
4	18	0	16.6	-16.0
6	18	0	7.1	-8.9
10	18	0	7.2	-3.0
2	19	0	22.9	-21.4
4	19	0	43.0	-35.4
6	19	0	19.6	-16.9
8	19	0	9.4	5.4
0	20	0	[illegible]	-23.4
2	20	0	25.7	-25.0
4	20	0	7.1	8.7
6	20	0	27.6	28.6
8	20	0	15.2	18.6
2	21	0	16.0	15.6
4	21	0	22.0	24.0
0	22	0	30.6	30.4
2	22	0	13.1	19.3
4	22	0	7.6	-4.0
6	22	0	15.7	-16.0
2	23	0	12.3	-12.1
4	23	0	15.6	-15.1
2	1	1	44.5	-62.2
3	1	1	30.3	-27.1
4	1	1	18.7	-17.0
5	1	1	[illegible]	-3.7
6	1	1	30.3	-32.7
7	1	1	37.6	-37.0
8	1	1	15.4	16.2
9	1	1	14.0	13.6
10	1	1	46.9	46.9
11	1	1	7.5	-4.0
12	1	1	10.0	10.2
13	1	1	4.9	5.6
14	1	1	4.0	3.2
15	1	1	10.7	7.1
1	2	1	9.0	-12.7
2	2	1	97.3	-93.6
3	2	1	117.7	-110.2
4	2	1	19.9	19.4
5	2	1	53.3	-50.1
6	2	1	53.0	53.6
7	2	1	46.2	-50.1
8	2	1	80.9	79.4
9	2	1	50.1	56.3
10	2	1	20.5	21.2
11	2	1	52.6	51.9
12	2	1	19.9	-19.3
13	2	1	4.9	4.1
14	2	1	28.0	-20.4
15	2	1	9.6	10.5
1	3	1	104.2	-101.1
2	3	1	126.9	115.9
3	3	1	86.3	88.3
4	3	1	66.0	69.3
5	3	1	14.5	15.0
6	3	1	22.7	26.1
7	3	1	60.1	56.0
8	3	1	17.1	-20.4
9	3	1	19.4	20.2
10	3	1	44.1	-41.7
11	3	1	17.5	-19.7
12	3	1	27.7	-29.0

H	K	L	F OBS	F CALC
13	3	1	9.0	-9.5
14	3	1	14.0	-15.1
15	3	1	7.5	-7.6
0	4	1	102.6	99.9
1	4	1	70.5	66.6
2	4	1	5.7	5.5
3	4	1	92.5	89.7
4	4	1	7.9	5.9
5	4	1	59.3	57.2
6	4	1	87.1	-86.6
7	4	1	20.2	20.6
8	4	1	69.3	-68.3
9	4	1	19.2	-20.6
10	4	1	25.0	-25.5
11	4	1	26.1	-25.9
12	4	1	21.1	20.3
13	4	1	11.0	-12.5
14	4	1	21.2	29.3
15	4	1	6.5	5.3
1	5	1	29.7	27.6
2	5	1	51.2	-47.1
3	5	1	5.4	7.1
4	5	1	85.4	-82.6
5	5	1	100.6	-100.3
6	5	1	56.2	-59.6
7	5	1	41.2	-41.0
9	5	1	21.2	-29.2
10	5	1	37.3	36.1
12	5	1	21.1	21.7
13	5	1	9.2	7.7
14	5	1	7.0	7.0
15	5	1	13.5	15.5
0	6	1	26.6	-27.3
1	6	1	4.5	-0.0
2	6	1	19.0	21.4
3	6	1	19.2	-18.7
4	6	1	37.1	33.1
5	6	1	61.5	-59.6
6	6	1	27.2	30.1
7	6	1	12.9	11.6
8	6	1	31.2	34.0
9	6	1	13.6	19.2
10	6	1	6.5	5.0
11	6	1	6.3	8.0
12	6	1	5.9	-7.1
14	6	1	6.5	-0.0
15	6	1	13.1	-11.9
1	7	1	34.3	-31.7
2	7	1	39.3	36.4
3	7	1	13.6	-11.9
4	7	1	7.4	4.3
5	7	1	24.0	24.7
6	7	1	5.0	5.0
7	7	1	13.9	11.7
9	7	1	6.6	7.7
10	7	1	24.1	-23.2
11	7	1	11.5	12.8
12	7	1	6.7	3.3
13	7	1	6.0	-7.9
15	7	1	2.0	2.7
0	8	1	11.1	3.2
1	8	1	18.1	-25.5
2	8	1	104.7	-100.3
3	8	1	30.0	-29.4
4	8	1	13.6	14.0
5	8	1	65.2	-64.1
6	8	1	25.4	26.1
7	8	1	8.9	-7.6
8	8	1	21.3	24.2
10	8	1	3.9	4.2
11	8	1	14.4	15.1
12	8	1	5.5	-2.4
14	8	1	20.5	-21.3
1	9	1	73.6	-68.6
2	9	1	56.9	57.7
3	9	1	3.0	2.2
4	9	1	91.6	91.9
5	9	1	46.2	45.6
6	9	1	32.3	32.8
7	9	1	33.3	31.2
8	9	1	10.2	-10.0
9	9	1	6.7	5.4
10	9	1	23.6	-25.0
11	9	1	5.9	1.3
12	9	1	24.7	-26.0
13	9	1	11.5	-10.1
0	10	1	92.9	92.6
1	10	1	14.0	14.5
2	10	1	55.0	60.5
3	10	1	48.1	47.0
4	10	1	13.4	-13.3
5	10	1	44.3	44.0
6	10	1	39.1	-40.0
7	10	1	9.7	11.1
8	10	1	37.4	-38.6
9	10	1	28.4	-29.5
10	10	1	13.0	-12.9
11	10	1	23.7	-24.7
12	10	1	16.2	15.6
13	10	1	4.6	-3.3
14	10	1	25.4	20.8
1	11	1	66.0	66.6
2	11	1	61.1	-62.6
3	11	1	4.9	10.5
4	11	1	82.3	-82.2
5	11	1	24.1	-23.1
6	11	1	32.6	-32.6
7	11	1	32.0	-32.7
8	11	1	6.2	6.0
9	11	1	22.2	-23.0
10	11	1	22.0	23.6
11	11	1	7.7	7.9
12	11	1	24.2	23.9
13	11	1	18.5	18.6
14	11	1	6.0	4.9
0	12	1	4.0	-4.3
1	12	1	41.0	-38.3
2	12	1	37.4	-30.9
3	12	1	18.5	-19.9
5	12	1	18.9	-19.2
6	12	1	22.9	23.5
7	12	1	6.1	-5.3
8	12	1	27.1	27.7
9	12	1	5.0	3.1
10	12	1	4.6	-1.1
11	12	1	6.3	8.3
12	12	1	7.7	-5.7
13	12	1	8.5	4.5
1	13	1	9.3	-8.7
2	13	1	[illegible]	24.4
3	13	1	23.3	-23.5
4	13	1	24.1	29.6
5	13	1	33.0	34.9
6	13	1	21.1	21.6
7	13	1	6.5	4.6
9	13	1	7.0	5.4
10	13	1	6.3	-6.6
11	13	1	5.6	-6.2
0	14	1	11.7	10.5
1	14	1	13.2	-11.7
2	14	1	13.0	15.1
3	14	1	9.2	1.5
4	14	1	16.5	-20.0
5	14	1	20.9	33.7
6	14	1	7.0	6.9
7	14	1	10.9	-12.1
8	14	1	5.0	1.5
9	14	1	6.3	2.4
11	14	1	9.3	5.3
1	15	1	3.6	-4.0
2	15	1	19.2	24.0
3	15	1	4.4	3.1
4	15	1	17.6	18.1
5	15	1	19.2	22.0
6	15	1	4.6	19.3
7	15	1	10.7	8.9
9	15	1	17.0	17.1
10	15	1	18.5	-10.6
12	15	1	12.2	-11.0
0	16	1	22.0	29.1
1	16	1	5.5	5.2
2	16	1	10.3	0.0
3	16	1	10.9	9.3
4	16	1	21.0	-22.6
5	16	1	62.1	65.6
6	16	1	24.0	-26.5
7	16	1	5.0	4.0
8	16	1	23.0	-22.4
9	16	1	8.0	-9.6
10	16	1	12.3	-14.6
11	16	1	5.5	-2.2
1	17	1	18.3	10.9
2	17	1	26.6	-26.9
3	17	1	7.6	-9.9

H	K	L	F OBS	F CALC
4	17	1	35.0	-39.6
5	17	1	46.3	-42.4
6	17	1	20.6	-21.0
7	17	1	23.1	-23.4
8	17	1	4.0	6.0
9	17	1	13.3	-12.6
10	17	1	14.9	16.2
0	18	1	16.0	-19.3
1	18	1	10.0	-7.7
2	18	1	11.6	-11.7
3	18	1	32.3	-32.1
4	18	1	11.9	-2.7
5	18	1	14.2	-14.3
6	18	1	40.2	42.7
7	18	1	5.5	-4.2
8	18	1	10.1	19.4
9	18	1	4.4	6.7
10	18	1	10.1	10.9
1	19	1	15.1	-15.9
2	19	1	16.6	17.0
3	19	1	12.2	-9.0
4	19	1	14.5	17.0
5	19	1	4.0	2.9
6	19	1	3.7	3.0
7	19	1	12.0	13.1
8	19	1	3.3	-3.6
0	20	1	11.2	12.8
1	20	1	9.0	-8.0
2	20	1	8.4	9.7
3	20	1	7.9	5.6
6	20	1	6.3	-2.6
8	20	1	4.9	-4.6
9	20	1	10.5	-7.7
1	21	1	9.7	8.2
2	21	1	7.2	8.1
3	21	1	8.4	1.8
5	21	1	8.1	7.9
7	21	1	6.6	3.5
3	22	1	3.3	3.5
4	22	1	12.3	-5.0
6	22	1	6.4	-1.2
1	23	1	10.6	12.2
2	23	1	12.6	-12.3
3	23	1	5.3	1.5
4	23	1	12.9	-13.5
5	23	1	2.9	-5.0
0	24	1	14.0	-15.5
1	24	1	4.8	-3.9
2	24	1	12.9	-9.7
3	24	1	9.6	-9.7
2	0	2	66.1	-66.9
3	0	2	200.6	-197.2
4	0	2	72.9	-69.6
5	0	2	130.6	-120.8
6	0	2	51.4	49.8
7	0	2	36.7	-35.6
8	0	2	11.5	10.7
9	0	2	92.1	92.8
10	0	2	29.4	31.0
11	0	2	44.0	43.4
12	0	2	23.0	-23.3
13	0	2	26.9	25.4
14	0	2	11.7	-13.1
15	0	2	4.7	2.2
2	1	2	59.2	56.3
3	1	2	43.1	-37.9
4	1	2	20.2	20.4
5	1	2	12.4	-9.4
6	1	2	30.0	33.0
7	1	2	51.3	51.6
8	1	2	7.0	-8.9
9	1	2	39.7	40.5
10	1	2	4.6	1.7
11	1	2	7.0	-0.0
12	1	2	12.9	-13.7
13	1	2	24.5	-20.1
14	1	2	8.0	-5.0
15	1	2	18.9	-20.1
1	2	2	128.7	139.0
2	2	2	6.1	-3.4
3	2	2	101.4	99.5
4	2	2	62.1	57.2
5	2	2	4.0	-2.5
6	2	2	9.0	6.9
7	2	2	20.3	20.9
8	2	2	13.0	-13.2
9	2	2	2.7	-5.4
10	2	2	13.7	-13.9
11	2	2	20.5	-20.3
12	2	2	15.2	14.0
13	2	2	14.9	-15.4
14	2	2	8.0	3.5
15	2	2	8.2	6.4
1	3	2	10.8	-17.3
2	3	2	25.9	-24.4
3	3	2	62.1	58.4
4	3	2	21.9	21.1
5	3	2	4.7	-0.3
6	3	2	10.4	7.4
7	3	2	11.7	-12.3
8	3	2	18.7	-16.9
9	3	2	9.0	-7.9
10	3	2	37.2	37.5
12	3	2	11.0	-11.0
13	3	2	7.4	6.6
14	3	2	7.6	7.0
15	3	2	6.4	7.1
0	4	2	161.9	-150.2
1	4	2	164.7	155.1
2	4	2	104.1	97.4
3	4	2	21.4	22.2
4	4	2	55.9	-51.0
5	4	2	5.0	4.2
6	4	2	3.4	-3.3
7	4	2	8.7	9.7
8	4	2	13.2	-12.9
9	4	2	6.6	-6.5
10	4	2	5.0	-5.7
11	4	2	19.6	-20.5
13	4	2	7.1	-6.9
14	4	2	10.4	11.1
15	4	2	12.3	-6.9
1	5	2	34.4	-27.7
2	5	2	9.6	-10.1
3	5	2	10.7	10.5
4	5	2	25.2	-25.3
5	5	2	15.0	-15.2
6	5	2	3.9	-5.4
7	5	2	33.7	-32.7
8	5	2	9.2	11.0
9	5	2	34.2	-33.1
10	5	2	6.9	8.0
11	5	2	6.2	6.6
12	5	2	14.0	14.6
13	5	2	5.6	7.7
14	5	2	2.6	2.4
15	5	2	7.3	10.0
0	6	2	55.5	-20.5
1	6	2	43.9	-44.1
2	6	2	92.2	-89.2
3	6	2	74.0	-76.0
4	6	2	5.7	-4.3
5	6	2	114.9	-117.6
6	6	2	8.9	8.9
7	6	2	13.2	12.0
8	6	2	20.0	27.3
9	6	2	25.7	24.0
10	6	2	13.0	14.0
11	6	2	20.7	25.7
12	6	2	3.4	-4.2
13	6	2	23.7	25.1
14	6	2	17.3	-19.0
1	7	2	100.3	-107.9
2	7	2	32.0	33.9
3	7	2	42.5	-40.5
4	7	2	42.9	40.5
5	7	2	63.1	61.0
6	7	2	8.2	-0.1
7	7	2	77.6	77.2
8	7	2	11.6	-13.5
9	7	2	66.0	65.7
10	7	2	18.2	-16.2
11	7	2	9.5	11.2
12	7	2	20.6	-21.0
13	7	2	25.0	-25.5
14	7	2	10.0	-12.3
15	7	2	24.4	-25.7
0	8	2	15.9	-18.0
1	8	2	30.0	43.9
2	8	2	39.5	39.5
3	8	2	66.0	66.0
4	8	2	19.3	18.7
5	8	2	35.5	35.5
7	8	2	8.0	-7.1

H	K	L	F OBS	F CALC
8	8	2	37.9	-36.6
9	8	2	35.2	-35.6
10	8	2	8.7	8.8
11	8	2	47.0	-40.7
13	8	2	13.3	-12.6
14	8	2	12.6	11.9
1	9	2	94.1	93.9
2	9	2	23.6	-24.1
3	9	2	[illegible]	24.1
5	9	2	9.7	-10.7
6	9	2	10.4	-17.7
7	9	2	40.7	-50.1
9	9	2	31.0	-29.9
10	9	2	11.0	11.0
11	9	2	4.0	-1.4
12	9	2	7.0	6.3
13	9	2	10.9	12.7
14	9	2	5.9	1.0
0	10	2	20.2	-17.4
1	10	2	11.2	-9.0
2	10	2	19.3	19.6
3	10	2	20.4	10.0
4	10	2	35.1	34.1
5	10	2	9.2	6.2
6	10	2	23.6	-23.3
7	10	2	14.9	14.3
8	10	2	23.0	24.3
10	10	2	8.9	-5.9
11	10	2	[illegible]	5.0
1	11	2	39.3	35.0
3	11	2	11.2	13.7
4	11	2	18.7	-17.4
5	11	2	6.0	-6.1
6	11	2	4.5	-3.9
7	11	2	12.1	-10.7
8	11	2	10.6	10.5
9	11	2	6.8	-7.0
10	11	2	4.0	-0.2
11	11	2	6.4	-3.0
12	11	2	10.1	10.5
13	11	2	7.4	6.1
0	12	2	8.1	-7.8
1	12	2	27.1	-24.9
2	12	2	29.5	-30.4
3	12	2	[illegible]	-29.5
4	12	2	5.3	[illegible]
5	12	2	13.5	-14.1
6	12	2	5.9	5.5
7	12	2	6.7	6.2
8	12	2	5.0	5.1
9	12	2	[illegible]	24.4
10	12	2	9.0	10.0
11	12	2	21.1	20.9
12	12	2	3.2	-6.0
13	12	2	7.6	8.9
1	13	2	68.9	-65.0
2	13	2	16.0	15.5
3	13	2	29.4	-27.9
4	13	2	32.5	34.2
5	13	2	7.2	-4.5
6	13	2	5.3	-3.6
7	13	2	43.2	43.0
8	13	2	2.6	-3.2
9	13	2	33.9	34.4
10	13	2	13.0	-12.2
12	13	2	13.1	-15.5
13	13	2	10.3	-17.0
0	14	2	34.0	34.0
1	14	2	10.2	13.0
2	14	2	9.4	9.8
3	14	2	46.9	46.9
4	14	2	24.0	26.5
5	14	2	20.2	19.4
6	14	2	22.2	-22.3
8	14	2	9.9	-9.7
9	14	2	17.1	-17.7
10	14	2	7.2	-9.2
11	14	2	23.7	-23.6
12	14	2	6.1	1.6
13	14	2	17.2	-16.4
1	15	2	43.0	43.1
2	15	2	5.2	-5.0
3	15	2	17.2	15.0
4	15	2	20.0	-18.9
5	15	2	39.9	-47.2
7	15	2	37.4	-37.5
8	15	2	4.0	6.1
9	15	2	19.1	-19.7
10	15	2	12.1	13.7
11	15	2	4.3	-7.7
12	15	2	11.7	10.2
1	16	2	11.2	-5.2
3	16	2	25.9	-26.2
4	16	2	7.1	1.0
5	16	2	33.9	-34.0
6	16	2	7.7	7.0
8	16	2	10.0	12.2
9	16	2	14.4	15.4
10	16	2	6.0	9.7
11	16	2	11.6	13.0
2	17	2	5.3	5.1
3	17	2	7.0	4.5
4	17	2	11.0	-9.2
5	17	2	6.1	6.1
6	17	2	6.7	7.0
7	17	2	7.5	9.3
9	17	2	7.0	4.7
0	18	2	24.2	-25.7
2	18	2	6.2	-10.9
3	18	2	9.9	-9.5
4	18	2	19.6	-20.5
5	18	2	20.5	-20.2
6	18	2	7.1	-5.9
8	18	2	6.2	5.4
9	18	2	9.0	9.7
10	18	2	6.3	-3.0
1	19	2	20.0	-27.4
2	19	2	13.3	16.0
3	19	2	17.2	-16.0
4	19	2	3.5	2.0
5	19	2	7.6	5.7
7	19	2	10.5	10.1
8	19	2	3.9	-1.5
9	19	2	10.9	12.9
10	19	2	10.6	-12.1
0	20	2	14.9	15.5
1	20	2	13.0	13.0
2	20	2	10.5	11.1
3	20	2	25.5	25.7
5	20	2	6.7	0.0
6	20	2	3.3	0.9
8	20	2	11.4	-13.4
9	20	2	6.4	-6.9
1	21	2	27.3	27.6
2	21	2	7.4	-9.1
3	21	2	14.4	14.6
4	21	2	9.5	-10.0
5	21	2	5.0	-1.2
6	21	2	9.2	-10.5
7	21	2	13.7	-14.4
1	22	2	6.0	-5.1
2	22	2	6.1	-0.0
3	22	2	13.0	-16.3
5	22	2	10.1	-14.2
6	22	2	10.1	10.9
1	23	2	13.2	-12.9
2	23	2	10.5	5.1
3	23	2	7.2	-0.0
4	23	2	8.5	5.6
5	23	2	6.4	0.0
1	24	2	6.1	6.6
2	1	3	55.5	-53.5
3	1	3	48.2	37.0
4	1	3	46.9	37.7
5	1	3	87.1	83.0
6	1	3	2.2	-3.2
7	1	3	30.5	30.3
8	1	3	2.9	-2.3
9	1	3	43.9	46.0
10	1	3	31.0	31.2
12	1	3	3.5	-4.9
13	1	3	6.6	-11.9
15	1	3	12.5	-13.3
2	2	3	2.2	-2.7
3	2	3	127.1	120.9
4	2	3	4.4	[illegible]
5	2	3	140.0	137.5
6	2	3	6.5	-4.5
7	2	3	33.4	32.0
8	2	3	20.5	26.7
9	2	3	13.6	-16.2
10	2	3	17.7	18.0
11	2	3	20.1	-21.2
12	2	3	3.2	-1.6

H	K	L	F OBS	F CALC
13	2	3	21.7	-22.0
14	2	3	7.1	9.3
15	2	3	8.2	10.5
1	3	3	92.3	-84.7
2	3	3	5.1	-7.4
3	3	3	3.5	-4.9
4	3	3	2.1	5.0
5	3	3	95.1	-91.0
6	3	3	10.1	-9.1
7	3	3	96.3	-93.9
8	3	3	12.4	-10.3
9	3	3	80.9	-81.3
10	3	3	20.1	20.0
11	3	3	11.2	-11.4
12	3	3	7.1	2.9
13	3	3	21.0	24.0
14	3	3	6.4	-5.4
15	3	3	21.0	21.3
1	4	3	40.4	39.0
2	4	3	29.2	27.6
3	4	3	163.2	-154.2
4	4	3	5.3	3.9
5	4	3	77.3	-75.9
6	4	3	22.3	-21.1
7	4	3	31.0	-30.3
8	4	3	17.0	-15.2
9	4	3	25.9	25.6
10	4	3	12.5	-12.2
11	4	3	20.6	27.9
12	4	3	7.9	-3.0
13	4	3	31.0	30.4
14	4	3	7.2	5.3
15	4	3	5.9	-2.0
1	5	3	56.3	-56.5
2	5	3	14.7	-12.5
4	5	3	42.0	-39.6
5	5	3	37.1	36.6
6	5	3	0.0	-1.0
7	5	3	73.9	73.5
8	5	3	5.7	-7.1
9	5	3	30.5	30.2
10	5	3	23.7	-24.7
11	5	3	15.0	16.0
12	5	3	10.5	10.3
13	5	3	21.6	-22.0
14	5	3	4.2	-3.7
15	5	3	16.0	-10.2
1	6	3	46.6	43.7
2	6	3	[illegible]	-3.9
3	6	3	28.0	29.1
4	6	3	9.7	8.2
5	6	3	5.3	-3.0
6	6	3	7.0	10.2
7	6	3	4.5	2.4
8	6	3	12.2	-12.7
9	6	3	20.4	-27.4
10	6	3	7.1	4.6
11	6	3	31.2	-32.1
13	6	3	9.0	-7.4
14	6	3	11.0	-11.6
15	6	3	5.2	-4.2
1	7	3	71.3	66.3
2	7	3	26.7	-26.3
3	7	3	5.6	5.9
4	7	3	41.4	41.5
5	7	3	20.4	20.4
6	7	3	8.1	-9.2
7	7	3	9.0	-7.3
8	7	3	7.9	-6.5
9	7	3	7.4	-6.5
10	7	3	16.7	-19.9
11	7	3	11.3	13.0
12	7	3	9.0	-8.9
13	7	3	8.7	-1.0
0	8	3	18.6	18.1
1	8	3	57.6	55.0
2	8	3	19.2	19.4
3	8	3	64.0	62.3
4	8	3	24.0	21.0
5	8	3	74.0	74.2
6	8	3	11.6	11.0
7	8	3	10.5	13.5
8	8	3	17.3	15.4
9	8	3	7.6	9.6
10	8	3	7.1	10.5
11	8	3	16.4	-14.0
12	8	3	7.9	-8.5
13	8	3	6.4	-6.4
1	9	3	34.7	37.7
2	9	3	16.9	16.1
3	9	3	16.3	19.2
4	9	3	11.0	12.7
5	9	3	44.2	-44.0
6	9	3	17.1	18.9
7	9	3	60.3	-60.9
8	9	3	1.5	-1.0
9	9	3	30.2	-39.9
10	9	3	11.1	-11.2
11	9	3	8.2	-3.7
12	9	3	8.9	9.0
13	9	3	21.1	20.9
14	9	3	5.2	0.3
0	10	3	44.0	44.0
1	10	3	30.5	-36.7
2	10	3	20.2	-18.7
3	10	3	76.0	-74.7
4	10	3	17.5	17.0
5	10	3	74.3	-76.5
6	10	3	1.4	3.1
7	10	3	7.0	-7.0
8	10	3	13.4	-11.0
9	10	3	15.1	16.7
10	10	3	7.0	-5.7
11	10	3	29.2	29.2
12	10	3	6.5	4.3
13	10	3	14.0	15.1
1	11	3	88.4	-82.3
2	11	3	21.1	-21.7
3	11	3	34.0	-34.4
4	11	3	1.3	-2.6
5	11	3	10.5	11.2
6	11	3	19.9	20.1
7	11	3	43.9	43.9
8	11	3	10.4	-6.3
9	11	3	32.3	32.7
10	11	3	7.2	7.0
11	11	3	5.1	-3.6
12	11	3	6.6	2.5
13	11	3	17.1	-19.0
14	11	3	6.3	9.4
0	12	3	10.5	7.9
1	12	3	20.2	27.7
2	12	3	6.9	4.2
3	12	3	34.0	35.3
4	12	3	24.0	-22.5
5	12	3	19.0	18.5
6	12	3	6.0	-4.6
7	12	3	4.0	2.3
8	12	3	6.3	0.0
9	12	3	11.6	-10.9
10	12	3	6.5	-5.9
11	12	3	25.1	-25.4
12	12	3	5.6	-1.9
13	12	3	12.7	-9.1
1	13	3	56.9	56.0
2	13	3	8.7	0.3
3	13	3	30.6	31.2
4	13	3	7.6	6.2
5	13	3	18.0	20.6
6	13	3	14.5	14.7
7	13	3	9.1	-9.0
8	13	3	5.7	-1.6
9	13	3	3.0	0.6
10	13	3	7.1	0.2
11	13	3	7.4	6.0
12	13	3	6.6	-2.6
13	13	3	8.4	9.1
0	14	3	18.5	18.6
1	14	3	8.5	-1.7
2	14	3	1.4	3.3
3	14	3	12.1	12.0
4	14	3	14.3	-12.7
5	14	3	5.5	-5.6
6	14	3	8.0	-6.2
7	14	3	8.6	7.2
8	14	3	7.1	8.9
9	14	3	8.5	6.4
10	14	3	7.5	-2.0
11	14	3	3.3	4.0
2	15	3	7.0	0.9
3	15	3	4.0	-0.0
4	15	3	8.0	-7.0
5	15	3	15.1	-15.6
6	15	3	6.1	4.0

H	K	L	F OBS	F CALC
7	15	3	31.3	-31.2
8	15	3	1.7	4.1
9	15	3	12.6	-10.4
10	15	3	13.6	8.9
11	15	3	6.2	-8.1
1	16	3	[illegible]	-3.7
2	16	3	10.4	-9.5
3	16	3	35.3	-35.6
4	16	3	12.6	-11.3
5	16	3	26.9	-27.2
6	16	3	3.4	5.4
8	16	3	7.1	-7.2
9	16	3	16.3	10.0
10	16	3	5.7	-3.2
11	16	3	21.2	21.5
1	17	3	46.4	-46.6
3	17	3	9.0	-7.9
4	17	3	17.9	-17.9
5	17	3	8.1	6.0
6	17	3	7.6	-7.6
7	17	3	35.4	37.2
8	17	3	7.0	8.5
9	17	3	15.6	21.3
0	18	3	7.0	5.7
1	18	3	17.6	15.4
2	18	3	6.3	-7.2
3	18	3	30.4	40.7
4	18	3	9.4	-0.1
5	18	3	12.4	12.4
6	18	3	1.6	4.2
8	18	3	6.5	3.2
9	18	3	17.2	-10.3
10	18	3	10.0	-2.2
1	19	3	17.7	10.2
2	19	3	6.9	5.1
3	19	3	17.0	15.7
5	19	3	9.7	-8.2
6	19	3	6.4	-7.0
7	19	3	12.0	-11.4
8	19	3	6.4	-8.5
9	19	3	11.2	-11.1
0	20	3	15.2	15.5
1	20	3	9.0	-6.8
3	20	3	5.7	-8.9
4	20	3	5.5	4.4
5	20	3	12.0	-13.0
6	20	3	8.5	11.0
7	20	3	9.1	-8.7
8	20	3	4.9	-2.0
9	20	3	2.0	6.1
1	21	3	7.6	1.0
2	21	3	2.6	-1.0
4	21	3	6.6	9.1
5	21	3	2.7	-6.2
6	21	3	5.2	-7.7
7	21	3	8.5	-3.8
3	22	3	3.9	-4.1
4	22	3	9.6	9.2
5	22	3	9.7	-11.7
6	22	3	2.0	1.0
1	23	3	15.7	-16.6
2	23	3	4.0	1.5
5	23	3	6.1	2.5
0	24	3	9.3	-5.0
1	24	3	12.2	12.7
2	24	3	3.5	-5.1
2	0	4	140.4	-130.6
3	0	4	185.2	170.7
4	0	4	61.3	57.1
5	0	4	69.9	66.6
6	0	4	47.4	45.9
7	0	4	46.7	44.6
8	0	4	59.9	57.9
9	0	4	31.3	-30.3
10	0	4	45.2	45.4
11	0	4	31.0	-31.9
12	0	4	8.0	-6.9
13	0	4	16.7	-16.7
14	0	4	22.0	-23.5
2	1	4	5.9	6.7
3	1	4	30.0	30.1
4	1	4	52.1	51.0
5	1	4	57.7	-54.9
6	1	4	27.7	28.1
7	1	4	58.9	-58.7
8	1	4	1.3	-14.5
8	1	4	16.3	-14.5
9	1	4	22.3	-21.4
10	1	4	3.9	-2.0
11	1	4	3.1	1.0
12	1	4	22.1	-24.0
13	1	4	17.0	19.4
14	1	4	6.1	2.7
1	2	4	14.7	19.6
2	2	4	63.1	60.5
3	2	4	82.0	-79.1
4	2	4	31.9	20.1
5	2	4	33.6	-34.6
6	2	4	35.4	-37.1
7	2	4	16.0	-16.5
8	2	4	21.6	-21.1
9	2	4	32.9	32.5
10	2	4	3.3	-6.2
11	2	4	23.7	24.1
12	2	4	5.0	-4.6
13	2	4	11.4	9.3
14	2	4	13.5	15.0
1	3	4	110.1	-101.6
2	3	4	3.6	1.4
3	3	4	10.7	-10.1
4	3	4	36.7	-35.2
5	3	4	15.9	-15.0
6	3	4	14.3	14.4
8	3	4	13.6	-11.0
9	3	4	3.7	-5.0
10	3	4	6.5	-5.7
12	3	4	9.5	0.0
13	3	4	10.1	-6.0
14	3	4	1.9	4.6
0	4	4	37.2	-33.6
1	4	4	10.5	-14.0
2	4	4	12.5	16.6
3	4	4	6.5	-7.1
4	4	4	2.2	0.2
5	4	4	60.4	-50.0
6	4	4	65.3	-62.4
7	4	4	24.5	25.7
8	4	4	33.2	-30.5
9	4	4	17.4	-17.1
10	4	4	17.1	-10.2
11	4	4	10.9	19.6
12	4	4	2.4	-0.4
13	4	4	5.0	2.0
1	5	4	70.9	-60.9
2	5	4	10.0	-21.2
3	5	4	5.5	-5.4
5	5	4	49.9	50.4
7	5	4	41.0	41.9
8	5	4	7.3	-4.5
9	5	4	6.9	4.0
10	5	4	8.4	-6.9
11	5	4	18.1	19.6
13	5	4	8.0	-10.2
14	5	4	9.0	2.1
0	6	4	37.5	-41.1
1	6	4	3.5	5.2
2	6	4	5.4	-6.5
3	6	4	34.6	33.0
5	6	4	66.1	66.5
6	6	4	53.6	54.1
7	6	4	7.4	-7.1
8	6	4	36.0	35.2
9	6	4	35.0	-37.3
10	6	4	38.7	39.6
11	6	4	50.6	-52.0
13	6	4	11.4	-9.3
14	6	4	13.7	-13.1
1	7	4	109.4	107.0
2	7	4	10.9	11.0
3	7	4	10.9	10.0
4	7	4	77.2	70.0
5	7	4	32.4	-31.5
6	7	4	21.9	20.7
7	7	4	62.9	-61.0
8	7	4	8.1	-7.6
9	7	4	30.2	-30.0
10	7	4	22.9	-22.0
12	7	4	21.4	-22.3
13	7	4	12.9	13.7
0	8	4	56.5	53.0
1	8	4	72.0	-70.2
2	8	4	36.2	37.0
3	8	4	39.7	-30.5
4	8	4	10.4	10.6

H	K	L	F OBS	F CALC
5	8	4	41.0	-39.3
6	8	4	43.2	-42.9
7	8	4	4.7	-4.6
8	8	4	23.3	-23.3
9	8	4	80.0	81.6
10	8	4	9.0	-11.3
11	8	4	30.4	31.6
12	8	4	3.1	5.6
13	8	4	12.1	13.0
14	8	4	13.3	14.0
1	9	4	37.3	-37.2
2	9	4	43.9	-44.9
3	9	4	13.4	-11.6
4	9	4	19.2	-20.0
5	9	4	52.0	49.9
6	9	4	12.4	-13.0
7	9	4	20.4	19.6
8	9	4	6.9	5.0
9	9	4	81.3	81.7
10	9	4	87.3	87.3
11	9	4	4.0	-5.6
12	9	4	10.7	19.9
13	9	4	10.6	-9.6
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

H	K	L	F OBS	F CALC
12	10	0	6.8	3.1
13	10	0	7.8	-1.5
1	11	0	15.4	16.7
2	11	0	10.8	9.0
3	11	0	8.6	7.0
4	11	0	3.9	-7.9
5	11	0	8.1	10.2
6	11	0	5.3	-8.0
7	11	0	6.7	-3.5
9	11	0	6.9	-4.8
10	11	0	5.5	1.4
11	11	0	5.1	3.3
12	11	0	1.9	1.1
13	11	0	3.9	3.4
0	12	0	19.1	-19.3
1	12	0	7.4	-5.4
2	12	0	10.3	-20.4
3	12	0	19.4	-17.0
4	12	0	3.5	-6.0
5	12	0	22.3	-22.0
6	12	0	7.0	6.1
7	12	0	3.9	-5.9
8	12	0	3.3	3.5
9	12	0	10.0	9.4
10	12	0	5.3	-2.1
11	12	0	16.4	15.5
12	12	0	4.3	2.2
1	13	0	35.4	-35.2
2	13	0	8.4	10.3
3	13	0	10.0	-10.0

H	K	L	F OBS	F CALC
2	5	9	10.0	-10.9
3	5	9	6.5	4.0
5	5	9	31.6	31.2
6	5	9	13.0	-14.2
7	5	9	22.4	22.6
8	5	9	4.0	5.0
9	5	9	24 1	23.1
10	5	9	9.0	9.1
12	5	9	6.0	5.4
13	5	9	12.7	-12.9
14	5	9	1.9	6.0
0	6	9	4.0	-3.9
1	6	9	7.0	7.9
2	6	9	5.4	5.5
3	6	9	10.9	11.0
4	6	9	6.1	-6.4
5	6	9	16.4	15.4
6	6	9	5.0	3.4
7	6	9	9.3	-9.7
8	6	9	12.7	11.7
9	6	9	2.6	-1.9
11	6	9	10.0	-8.2
12	6	9	4.0	-1.4
13	6	9	9.7	-11.3
14	6	9	5.4	-2.1
1	7	9	18.7	-19.3
2	7	9	13.5	14.0
3	7	9	20.1	19.2
4	7	9	20.4	20.8
7	7	9	5.7	-4.9

H	K	L	F OBS	F CALC
0	20	9	2.6	-1.0
1	20	9	4.9	-4.5
2	20	9	7.4	2.0
3	20	9	3.3	-4.7
4	20	9	3.3	-0.6
5	20	9	5.4	-6.4
7	20	9	4.5	2.9
8	20	9	6.1	-0.4
1	21	9	6.3	6.2
2	21	9	3.0	-1.2
3	21	9	3.4	0.6
4	21	9	5.5	-2.6
5	21	9	2.0	-0.9
6	21	9	3.5	0.7
1	22	9	5.4	0.3
3	22	9	6.6	-6.9
5	22	9	5.4	-9.2
1	23	9	9.5	-11.0
2	23	9	6.5	-0.0
3	23	9	6.0	-6.1
2	0	10	13.7	-19.5
3	0	10	21.5	25.5
4	0	10	8.4	9.1
5	0	10	20.4	20.2
6	0	10	26.0	20.1
7	0	10	15.9	-14.2
8	0	10	45.1	43.7
9	0	10	20.4	-20.9
10	0	10	7.7	6.7
11	0	10	20.2	-17.7

H	K	L	F OBS	F CALC
1	15	12	8.7	-8.8
2	15	12	6.4	5.5
3	15	12	5.6	-1.4
4	15	12	20.3	18.2
5	15	12	3.4	7.1
7	15	12	10.1	10.3
8	15	12	3.7	-3.7
10	15	12	7.6	-6.9
0	16	12	5.9	3.7
1	16	12	5.9	3.5
2	16	12	4.7	5.1
3	16	12	8.4	8.4
4	16	12	3.8	-5.4
5	16	12	5.5	3.3
6	16	12	6.9	-5.7
7	16	12	2.6	5.6
8	16	12	3.8	-3.5
9	16	12	3.4	-6.2
10	16	12	4.0	-1.6
1	17	12	8.2	5.0
2	17	12	4.9	-3.2
3	17	12	3.9	-2.0
4	17	12	2.5	0.2
5	17	12	6.3	-2.4
6	17	12	5.8	2.3
7	17	12	5.3	-2.3
8	17	12	5.1	3.7
9	17	12	7.7	-0.2
10	17	12	2.9	0.3
0	18	12	6.4	6.1
1	18	12	4.7	3.7
2	18	12	7.1	-3.6
3	18	12	4.4	-8.1
4	18	12	4.5	-1.0
5	18	12	4.9	-2.3
6	18	12	2.7	-1.0
7	18	12	4.0	1.0
8	18	12	6.3	-3.5
1	19	12	4.5	2.4
2	19	12	8.9	-8.4
3	19	12	8.1	-2.7
4	19	12	9.0	-6.0
5	19	12	2.7	0.9
6	19	12	4.4	-4.9
8	19	12	5.7	-0.6
0	20	12	5.7	-9.7
2	20	12	9.7	-10.4
3	20	12	6.1	-7.0
4	20	12	6.5	-1.0
6	20	12	5.3	7.6
7	20	12	6.1	-1.7
1	21	12	8.7	-6.4
2	21	12	9.2	9.5
3	21	12	5.9	-3.6
4	21	12	10.0	10.2
0	22	12	13.0	11.1
2	22	12	7.0	7.0
3	22	12	5.7	4.1
2	1	13	1.2	0.4
3	1	13	7.3	7.7
4	1	13	2.9	-4.5
5	1	13	2.2	-1.9
6	1	13	12.6	-12.9
7	1	13	6.0	5.0
8	1	13	4.0	0.4
9	1	13	8.9	-9.1
10	1	13	7.1	5.0
11	1	13	6.1	0.4
12	1	13	3.6	1.2
13	1	13	5.3	1.9
1	2	13	8.8	-11.2
2	2	13	2.7	4.3
3	2	13	10.0	-11.1
4	2	13	11.4	12.5
5	2	13	11.6	-10.9
6	2	13	3.2	3.4
7	2	13	3.7	4.4
8	2	13	9.6	9.1
9	2	13	9.6	11.0
10	2	13	3.2	0.9
11	2	13	11.0	11.5
12	2	13	4.0	-2.1
13	2	13	8.8	9.2
14	2	13	8.8	-7.5
1	3	13	16.7	-21.6
2	3	13	13.3	18.6
3	3	13	15.2	-15.4
4	3	13	8.7	7.5
5	3	13	9.9	9.7
6	3	13	12.5	17.1
7	3	13	17.7	17.6
8	3	13	3.5	3.3
9	3	13	8.5	10.2
10	3	13	11.9	-10.7
11	3	13	8.4	-8.6
12	3	13	6.2	-6.0
13	3	13	8.0	-6.3
0	4	13	9.4	17.7
1	4	13	13.0	15.0
2	4	13	2.5	8.9
3	4	13	27.0	20.4
4	4	13	3.2	-7.7
5	4	13	16.1	16.6
6	4	13	11.7	-17.6
7	4	13	5.7	2.6
8	4	13	12.6	-13.7
9	4	13	9.4	-7.9
11	4	13	12.0	-13.1
12	4	13	3.0	3.4
14	4	13	5.2	3.0
1	5	13	12.1	13.9
2	5	13	4.1	-1.2
3	5	13	4.5	-5.7
4	5	13	5.8	-6.4
5	5	13	8.2	-9.6
6	5	13	5.6	-5.6
7	5	13	16.5	-17.9
8	5	13	2.1	4.8
9	5	13	11.1	-12.6
10	5	13	5.2	5.7
12	5	13	4.8	5.0
13	5	13	3.8	7.5
0	6	13	5.8	-5.0
1	6	13	6.7	-6.3
2	6	13	8.0	-4.0
3	6	13	6.2	-4.1
4	6	13	4.6	4.0
5	6	13	6.1	-5.6
6	6	13	2.9	0.7
7	6	13	7.2	-3.7
8	6	13	5.0	2.6
9	6	13	2.2	2.4
11	6	13	4.0	3.1
13	6	13	4.3	-8.0
1	7	13	3.4	2.5
2	7	13	4.2	-3.6
3	7	13	4.1	5.3
4	7	13	8.9	-9.1
6	7	13	5.0	-3.4
7	7	13	6.3	2.5
8	7	13	5.7	-1.5
9	7	13	5.6	3.6
12	7	13	5.9	3.1
0	8	13	2.3	-0.6
2	8	13	5.6	-6.0
3	8	13	13.0	-12.2
4	8	13	6.2	6.1
5	8	13	5.7	-5.9
6	8	13	6.0	6.0
8	8	13	2.7	2.1
9	8	13	3.3	1.3
10	8	13	3.0	2.4
11	8	13	4.8	1.6
12	8	13	4.6	0.9
1	9	13	10.1	-10.9
2	9	13	4.1	0.6
3	9	13	11.7	-11.6
4	9	13	9.7	9.0
5	9	13	6.1	5.9
6	9	13	9.6	9.5
7	9	13	8.5	7.2
9	9	13	3.7	5.5
10	9	13	4.3	-4.9
11	9	13	5.0	1.7
13	9	13	4.9	-4.1
0	10	13	10.9	15.7
1	10	13	5.9	6.1
2	10	13	5.2	3.0
3	10	13	16.7	14.9
5	10	13	13.6	11.9
6	10	13	9.8	-8.6
7	10	13	3.0	0.0
8	10	13	5.7	-6.2
9	10	13	8.2	-5.6
10	10	13	6.9	-4.8
11	10	13	7.4	-7.7
12	10	13	3.9	2.5
1	11	13	19.6	18.4
2	11	13	7.9	-8.4
3	11	13	6.6	4.0
4	11	13	7.4	-7.3
5	11	13	7.0	-6.4
6	11	13	3.6	-3.1
7	11	13	16.0	-15.1
8	11	13	6.1	-2.6
9	11	13	10.0	-9.2
10	11	13	7.9	6.1
11	11	13	5.3	0.4
12	11	13	3.9	2.0
0	12	13	8.5	-9.4
1	12	13	7.2	-7.3
2	12	13	6.9	-5.9
3	12	13	19.5	-18.6
4	12	13	7.0	-4.7
5	12	13	9.6	-9.8
6	12	13	5.1	6.6
7	12	13	5.7	-3.3
8	12	13	6.5	5.2
9	12	13	4.0	5.1
11	12	13	3.0	4.7
1	13	13	4.2	-3.6
2	13	13	3.3	-4.3
5	13	13	3.2	3.5
6	13	13	4.0	-1.9
7	13	13	8.7	10.5
10	13	13	3.8	0.5
11	13	13	5.5	-2.3
1	14	13	6.6	-0.9
2	14	13	5.9	4.5
3	14	13	5.3	3.3
5	14	13	2.3	-0.5
6	14	13	4.5	4.7
7	14	13	6.6	3.6
8	14	13	6.3	9.2
9	14	13	5.3	-0.7
11	14	13	4.9	1.6
1	15	13	5.6	-2.2
2	15	13	5.6	1.8
3	15	13	5.4	-0.9
4	15	13	5.0	5.1
5	15	13	6.4	2.0
6	15	13	3.0	4.4
7	15	13	9.2	0.7
8	15	13	8.5	0.6
9	15	13	5.7	4.3
10	15	13	8.8	-4.2
1	16	13	3.7	5.1
2	16	13	6.7	9.3
3	16	13	11.7	11.1
4	16	13	6.3	-6.2
5	16	13	6.4	5.9
6	16	13	5.1	-6.4
7	16	13	6.1	6.0
8	16	13	5.6	-3.6
10	16	13	2.0	-2.4
1	17	13	4.9	5.0
2	17	13	3.9	1.3
3	17	13	6.0	-5.9
4	17	13	3.6	-5.7
5	17	13	4.1	-5.2
6	17	13	4.6	-2.6
7	17	13	9.9	-10.5
8	17	13	5.9	3.4
0	18	13	5.4	-3.4
1	18	13	6.2	-4.8
2	18	13	7.0	-8.1
3	18	13	11.3	-0.5
4	18	13	5.9	-2.2
5	18	13	9.9	-10.3
6	18	13	4.3	4.7
7	18	13	5.5	-0.4
8	18	13	4.8	2.2
9	18	13	5.0	2.7
1	19	13	7.9	-6.3
2	19	13	4.9	3.3
3	19	13	8.0	-7.5
4	19	13	7.9	3.8
5	19	13	3.9	5.6
6	19	13	4.2	-1.6
7	19	13	7.0	7.3
1	20	13	5.7	3.0
2	20	13	8.2	1.0
5	20	13	2.0	3.2
6	20	13	4.0	1.1
7	20	13	7.1	-4.2
1	21	13	6.0	2.9
2	21	13	4.0	2.1
3	21	13	3.4	1.4
4	21	13	6.0	1.3
0	22	13	4.0	5.4
1	22	13	5.3	2.6
2	0	14	8.4	21.0
3	0	14	3.4	-6.4
4	0	14	10.5	11.5
5	0	14	14.1	-15.2
6	0	14	2.4	4.3
7	0	14	11.4	-11.4
8	0	14	4.3	5.1
9	0	14	13.5	12.3
10	0	14	4.3	-0.6
11	0	14	13.9	14.2
13	0	14	4.6	2.6
14	0	14	7.1	-0.5
2	1	14	3.0	5.5
4	1	14	3.4	3.4
5	1	14	2.2	2.5
6	1	14	8.3	7.6
7	1	14	10.9	9.7
8	1	14	6.2	4.9
9	1	14	12.0	10.9
10	1	14	5.0	-1.0
11	1	14	1.7	-1.5
12	1	14	4.4	5.2
13	1	14	7.1	-4.7
14	1	14	4.0	2.0
1	2	14	4.6	10.4
2	2	14	2.5	0.0
3	2	14	9.4	13.1
4	2	14	2.7	-1.4
5	2	14	10.0	9.6
6	2	14	4.1	2.2
8	2	14	3.4	-5.0
9	2	14	6.5	-2.7
10	2	14	4.6	3.2
11	2	14	6.6	-9.0
12	2	14	5.7	-1.4
13	2	14	5.0	-4.1
14	2	14	3.9	-8.7
1	3	14	2.2	4.6
2	3	14	8.0	3.1
3	3	14	2.5	4.6
4	3	14	3.7	5.7
5	3	14	2.0	-2.9
6	3	14	3.3	1.2
7	3	14	7.5	-6.1
8	3	14	6.5	6.2
9	3	14	4.6	-2.5
10	3	14	2.0	-1.3
11	3	14	8.0	2.1
12	3	14	6.0	2.1
14	3	14	5.9	1.2
0	4	14	3.3	-6.9
1	4	14	7.6	2.3
2	4	14	10.3	-12.4
3	4	14	3.5	3.9
6	4	14	5.4	-5.5
7	4	14	3.9	0.6
8	4	14	3.6	-4.9
10	4	14	3.3	0.4
11	4	14	5.5	-3.9
12	4	14	6.1	0.5
1	5	14	9.7	13.9
2	5	14	3.5	-3.4
3	5	14	4.9	6.3
4	5	14	5.2	-5.9
5	5	14	7.1	-7.7
6	5	14	2.0	-2.7
7	5	14	15.1	-13.4
8	5	14	5.2	-8.6
9	5	14	9.6	-9.5
10	5	14	7.0	-0.9
13	5	14	4.3	3.5
1	6	14	3.2	-4.0
3	6	14	14.0	-15.2
4	6	14	8.9	4.5
5	6	14	15.1	-14.0
6	6	14	6.3	2.9
7	6	14	4.3	-4.0
8	6	14	5.5	0.8
9	6	14	6.2	0.4
10	6	14	2.4	1.6
11	6	14	10.9	12.8
13	6	14	6.4	6.7
1	7	14	14.1	-17.5
2	7	14	2.9	-1.3
3	7	14	1.2	-1.7
4	7	14	4.3	-0.4
5	7	14	9.4	9.0
6	7	14	2.0	1.2
7	7	14	13.5	13.2
8	7	14	6.0	-3.0
9	7	14	8.3	0.9
10	7	14	3.4	-2.4
11	7	14	1.8	3.1
12	7	14	2.6	-5.6
13	7	14	3.4	-4.0
0	8	14	2.0	5.0
1	8	14	4.0	4.0
2	8	14	3.1	-1.2
3	8	14	9.3	9.0
5	8	14	11.3	11.6
7	8	14	6.4	6.4
8	8	14	4.5	1.5
9	8	14	7.8	-6.9
10	8	14	1.7	0.3
11	8	14	10.5	-9.4
12	8	14	4.6	2.3
13	8	14	5.2	-5.5
1	9	14	8.1	7.7
2	9	14	2.8	1.7
4	9	14	5.0	3.3
5	9	14	5.0	-5.7
6	9	14	4.2	2.9
7	9	14	7.7	-7.9
8	9	14	2.0	-0.5
9	9	14	7.0	-6.6
10	9	14	2.5	1.3
11	9	14	3.2	0.5
0	10	14	4.5	-2.5
1	10	14	1.3	-2.7
2	10	14	5.1	-3.5
3	10	14	7.6	-7.6
6	10	14	3.4	-3.9
8	10	14	3.7	-3.5
9	10	14	4.9	1.4
10	10	14	6.0	-1.0
11	10	14	5.0	1.7
12	10	14	7.0	-1.4
1	11	14	7.4	6.4
2	11	14	4.0	-4.0
3	11	14	2.0	0.9
4	11	14	4.6	-5.1
5	11	14	5.2	-1.4
6	11	14	8.0	-2.5
7	11	14	3.6	0.0
8	11	14	5.6	-2.3
9	11	14	3.1	-2.4
10	11	14	6.4	1.2
11	11	14	3.3	-1.7
12	11	14	3.4	-1.0
0	12	14	4.9	2.5
1	12	14	5.6	-2.9
2	12	14	3.0	2.0
3	12	14	9.0	-7.7
4	12	14	4.6	5.4
5	12	14	7.8	-9.2
6	12	14	3.2	3.6
7	12	14	6.9	-3.0
8	12	14	2.4	5.1
9	12	14	3.6	4.7
10	12	14	5.3	0.6
11	12	14	8.2	6.3
12	12	14	2.0	-1.1
1	13	14	13.0	-10.0
2	13	14	3.7	-0.4
4	13	14	1.6	2.6
5	13	14	7.1	7.0
6	13	14	2.4	-1.0
7	13	14	16.4	15.3
8	13	14	3.6	-1.0
9	13	14	7.4	6.6
10	13	14	2.7	-0.8
11	13	14	3.4	0.1
0	14	14	3.5	-0.3
2	14	14	6.6	7.9
3	14	14	14.4	13.3
4	14	14	4.0	8.6
5	14	14	11.2	10.3
6	14	14	7.5	-8.9
7	14	14	4.4	4.9
8	14	14	4.5	4.2
9	14	14	3.0	-5.0
10	14	14	3.4	-0.3
11	14	14	8.0	-0.5
1	15	14	9.6	8.1
2	15	14	5.7	6.1
4	15	14	2.4	2.2
5	15	14	4.2	-7.6
6	15	14	3.1	3.0
7	15	14	7.7	-7.2
8	15	14	5.3	5.2
9	15	14	7.2	-4.1
1	16	14	4.1	2.1
2	16	14	4.0	-5.4
3	16	14	6.2	-3.0
4	16	14	4.9	-1.5
5	16	14	7.1	-7.7
7	16	14	7.7	2.4
8	16	14	4.7	-3.6
9	16	14	5.6	2.7
1	17	14	4.9	1.4
2	17	14	4.0	-0.6
3	17	14	6.4	-6.3
4	17	14	3.1	-1.3
5	17	14	4.1	3.1
6	17	14	5.3	-2.9
7	17	14	7.9	1.0
8	17	14	6.5	2.0
0	18	14	3.6	-3.9
1	18	14	3.6	0.4
2	18	14	4.4	-5.6
3	18	14	6.4	6.0
4	18	14	3.2	-0.6
5	18	14	5.6	-5.0
6	18	14	7.7	1.6
7	18	14	5.9	-3.5
8	18	14	7.5	0.6
1	19	14	5.6	-4.6
2	19	14	3.3	1.6
3	19	14	3.3	-4.7
5	19	14	3.9	3.9
6	19	14	5.9	-1.8
7	19	14	5.7	4.0
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1	20	14	5.4	3.5
2	20	14	3.9	2.6
3	20	14	6.5	7.4
5	20	14	7.5	6.5
6	20	14	5.4	-3.1
1	21	14	8.4	0.9
2	21	14	6.3	0.0
4	21	14	5.7	-1.0
5	21	14	3.5	-3.5
1	22	14	4.1	-1.7
2	1	15	2.1	4.6
3	1	15	3.9	0.3
4	1	15	3.2	-0.3
7	1	15	6.7	6.0
8	1	15	3.0	2.3
9	1	15	5.3	5.3
11	1	15	3.0	0.2
12	1	15	6.3	2.0
14	1	15	3.4	2.3
1	2	15	1.9	5.0
2	2	15	4.0	-6.9
3	2	15	9.5	11.0
4	2	15	1.7	-1.0
5	2	15	7.2	0.0
6	2	15	2.0	-1.3
7	2	15	3.0	6.7
8	2	15	3.5	0.7
9	2	15	4.9	-3.6
10	2	15	4.6	2.0
11	2	15	4.9	-5.0
12	2	15	5.4	-0.4
1	3	15	6.5	10.0
2	3	15	3.7	4.0
3	3	15	1.3	0.9
4	3	15	8.1	4.0
5	3	15	6.9	-6.7
6	3	15	5.1	3.1
7	3	15	19.4	-19.1
8	3	15	3.9	3.9
9	3	15	9.6	-10.8
10	3	15	7.9	-6.6
11	3	15	8.8	0.9
12	3	15	7.1	-6.9
13	3	15	1.9	5.9
1	4	15	8.2	-9.9
2	4	15	4.6	7.2
3	4	15	13.1	-14.5
4	4	15	4.2	-8.5
5	4	15	9.5	-10.4
6	4	15	5.8	-5.0
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9	4	15	9.7	8.5
10	4	15	5.0	-2.3
11	4	15	9.0	9.4
12	4	15	5.2	0.9
13	4	15	5.7	4.2
1	5	15	10.9	-12.6
2	5	15	8.6	-9.5
3	5	15	5.0	-2.9
4	5	15	8.3	-9.1
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6	5	15	6.1	-4.9
7	5	15	6.0	6.4
8	5	15	4.2	-1.5
9	5	15	4.0	7.9
10	5	15	4.4	2.2
13	5	15	4.3	-3.7
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1	6	15	2.3	2.5
2	6	15	8.1	-1.0
3	6	15	4.6	0.8
5	6	15	5.1	5.4
6	6	15	5.3	3.9
7	6	15	4.3	-0.4
8	6	15	5.1	-8.7
9	6	15	4.0	-4.6
10	6	15	3.0	4.8
11	6	15	3.6	-5.9
12	6	15	1.9	1.7
13	6	15	3.9	-1.9
1	7	15	4.1	-3.6
2	7	15	2.0	-1.9
3	7	15	4.4	-1.9
4	7	15	2.5	1.4
5	7	15	4.2	-0.1
7	7	15	4.4	3.3
8	7	15	3.5	-1.1
9	7	15	6.0	7.1
10	7	15	4.6	0.9
12	7	15	3.3	-1.2
13	7	15	3.4	-0.3
0	8	15	7.6	-8.3
1	8	15	2.6	1.6
2	8	15	3.0	-1.4
3	8	15	4.1	5.2
4	8	15	4.5	-1.5
5	8	15	6.0	6.0
7	8	15	4.9	-0.6
8	8	15	2.0	-0.1
9	8	15	5.0	-3.0
10	8	15	4.3	-0.1
11	8	15	1.0	-2.3
12	8	15	3.0	-0.9
13	8	15	4.9	-1.6
1	9	15	9.4	10.6
3	9	15	8.1	4.7
4	9	15	3.1	0.3
5	9	15	5.9	-5.8
6	9	15	6.7	6.6
7	9	15	7.1	-7.7
8	9	15	4.3	0.1
10	9	15	3.6	-3.1
11	9	15	4.6	-0.9
12	9	15	3.3	-3.5
0	10	15	8.0	8.5
1	10	15	8.1	-2.9
2	10	15	8.8	5.6
3	10	15	15.6	-15.0
4	10	15	3.2	1.2
5	10	15	11.1	-10.0
6	10	15	4.9	0.3
7	10	15	5.1	-3.4
8	10	15	2.9	-2.9
9	10	15	7.2	6.2
11	10	15	6.0	5.9
12	10	15	4.4	-1.1
1	11	15	9.0	-10.4
2	11	15	5.9	-4.7
3	11	15	5.7	-4.2
4	11	15	6.1	-4.4
5	11	15	5.9	4.5
6	11	15	6.9	-5.6
7	11	15	10.0	9.6
8	11	15	5.9	-0.6
9	11	15	4.6	4.6
10	11	15	4.1	5.1
12	11	15	2.6	4.2
0	12	15	5.2	-6.4
1	12	15	6.3	4.0
2	12	15	4.4	-1.1
3	12	15	9.4	4.9
4	12	15	2.6	0.6
5	12	15	5.9	6.5
6	12	15	3.3	4.7
7	12	15	1.7	0.2
8	12	15	4.6	5.9
9	12	15	4.1	-4.1
10	12	15	4.6	9.1
11	12	15	5.2	-5.3
12	12	15	6.0	-0.5
1	13	15	4.3	5.1
2	13	15	1.5	3.2
3	13	15	7.0	5.1
4	13	15	8.2	4.5
5	13	15	4.9	-2.9
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7	13	15	3.9	1.3
0	14	15	2.2	-3.1
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2	14	15	3.6	-0.6
3	14	15	4.9	4.5
4	14	15	5.5	-1.3
5	14	15	4.0	0.5
7	14	15	4.4	1.7
8	14	15	3.7	0.4
9	14	15	4.6	5.6
10	14	15	5.2	-1.3
1	15	15	2.0	4.0
2	15	15	4.4	3.1
3	15	15	7.5	0.0
4	15	15	5.7	0.2
5	15	15	3.9	-3.5
6	15	15	6.9	2.1
7	15	15	3.2	-4.5
8	15	15	1.9	2.1
9	15	15	8.2	-4.0
1	16	15	5.4	-2.1
3	16	15	5.2	-4.0
5	16	15	10.0	-9.6
9	16	15	6.0	5.3
1	17	15	9.3	-7.6
2	17	15	5.6	0.5
3	17	15	8.6	-6.1
4	17	15	5.1	-3.5
5	17	15	7.4	5.6
6	17	15	4.6	-5.4
7	17	15	5.1	4.1
9	17	15	3.5	2.0
0	18	15	6.3	-2.4
1	18	15	4.0	2.1
2	18	15	3.7	-2.0
3	18	15	6.5	7.2
4	18	15	5.6	2.1
5	18	15	6.6	4.7
6	18	15	5.2	2.7
7	18	15	4.0	-2.2
8	18	15	6.4	3.6
1	19	15	8.4	3.0
2	19	15	7.3	9.0
4	19	15	2.7	3.0
7	19	15	5.7	-5.4
3	20	15	2.0	-1.4
4	20	15	3.4	1.2
5	20	15	4.5	-2.1
1	21	15	2.0	1.5
3	21	15	4.5	3.1
0	22	15	2.9	-0.6
1	22	15	3.5	-1.5
2	0	16	1.6	-7.9
3	0	16	3.3	10.4
5	0	16	3.0	5.3
6	0	16	6.6	6.1
8	0	16	7.1	7.9
9	0	16	3.8	-4.7
10	0	16	6.8	4.0
14	0	16	7.4	-7.2
2	1	16	4.3	9.2
3	1	16	3.1	2.0
4	1	16	8.8	13.3
5	1	16	3.6	-3.0
6	1	16	4.5	7.1
7	1	16	7.2	-7.7
8	1	16	5.1	1.0
9	1	16	5.4	-3.5
10	1	16	4.4	-7.2
11	1	16	5.2	2.9
12	1	16	6.2	-4.2
1	2	16	2.2	-7.1
2	2	16	4.2	0.5
3	2	16	4.1	-4.3
4	2	16	3.7	2.6
5	2	16	2.3	-2.0
6	2	16	7.8	-6.9
7	2	16	3.6	2.5
8	2	16	4.9	-6.9
9	2	16	4.9	1.9
12	2	16	5.2	3.6
2	3	16	3.6	-3.4
3	3	16	1.9	-1.6
4	3	16	3.9	-4.4
6	3	16	3.6	0.7
7	3	16	3.7	-2.1
9	3	16	4.7	1.4
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12	3	16	4.5	4.6
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2	4	16	2.2	-4.4
3	4	16	4.6	-3.3
4	4	16	2.9	-0.9
5	4	16	1.7	0.5
6	4	16	3.5	-2.5
8	4	16	6.7	-6.2
11	4	16	3.9	0.1
12	4	16	9.0	1.1
1	5	16	3.0	-6.3
2	5	16	7.4	-11.7
3	5	16	1.5	-4.4
4	5	16	8.0	-8.1
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7	5	16	5.2	3.9
9	5	16	4.6	3.1
10	5	16	5.6	3.9
11	5	16	3.6	-0.7
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1	6	16	1.3	1.4
2	6	16	6.9	-0.2
3	6	16	5.9	6.2
4	6	16	2.4	1.2
5	6	16	4.5	4.0
6	6	16	6.3	7.7
7	6	16	4.4	-4.6
8	6	16	10.3	10.3
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10	6	16	5.4	3.2
11	6	16	7.0	-2.7
12	6	16	2.0	-1.9
1	7	16	6.4	7.1
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3	7	16	2.1	4.2
4	7	16	10.5	11.3
5	7	16	5.5	-4.0
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7	7	16	8.3	-6.5
8	7	16	4.7	-4.0
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12	7	16	5.7	-6.5
0	8	16	9.0	9.5
1	8	16	3.9	-4.0
2	8	16	6.1	0.8
3	8	16	10.1	-10.7
4	8	16	4.4	-1.1
5	8	16	2.0	-1.0
6	8	16	4.0	-5.4
7	8	16	4.4	0.6
8	8	16	5.6	-5.5
9	8	16	3.4	3.3
10	8	16	4.7	-4.1
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12	8	16	6.4	0.7
1	9	16	3.3	-0.7
2	9	16	3.4	-4.7
3	9	16	2.0	3.0
4	9	16	5.7	-6.5
5	9	16	2.5	2.1
8	9	16	6.6	5.0
9	9	16	3.0	1.0
10	9	16	3.6	4.4
11	9	16	4.2	-2.4
12	9	16	6.4	4.5
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1	10	16	4.2	1.2
2	10	16	4.5	-3.3
3	10	16	2.4	1.0
4	10	16	3.5	-0.2
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7	10	16	3.2	0.9
8	10	16	4.5	2.0
9	10	16	4.3	-0.7
10	10	16	5.2	1.7
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3	11	16	5.4	-1.0
4	11	16	5.2	-0.6
5	11	16	2.2	1.5
6	11	16	5.3	-2.2
7	11	16	1.7	3.5
8	11	16	3.5	-0.1
9	11	16	3.6	0.2
10	11	16	2.6	1.4
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2	12	16	4.4	-1.7
3	12	16	7.9	6.4
4	12	16	2.7	-2.3
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7	12	16	8.9	-1.6
8	12	16	6.0	5.8
11	12	16	2.0	-2.0
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6	14	16	7.2	-6.4
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9	15	16	5.1	0.2
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2	16	16	5.5	-3.4
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7	16	16	2.7	-2.0
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4	18	16	5.0	-0.8
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6	18	16	2.7	-2.2
8	18	16	3.5	-0.9
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2	19	16	6.3	1.9
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4	19	16	7.5	2.4
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2	20	16	5.2	5.6
3	20	16	7.6	-4.9
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3	1	17	2.0	4.6
4	1	17	4.4	6.0
6	1	17	4.6	4.1
7	1	17	2.4	0.3
8	1	17	4.2	-0.5
10	1	17	2.9	-2.7
2	2	17	2.7	3.9
3	2	17	2.4	2.4
4	2	17	3.0	-2.0
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6	2	17	7.6	-7.0
7	2	17	2.4	4.1
8	2	17	5.7	-6.4
9	2	17	3.9	0.1
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4	3	17	9.6	-13.2
6	3	17	6.1	-3.4
7	3	17	3.1	-4.4
8	3	17	4.2	3.7
9	3	17	3.9	-2.7
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3	4	17	3.4	-4.1
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7	4	17	3.2	0.0
8	4	17	9.6	0.2
9	4	17	4.0	-2.0
10	4	17	3.0	2.6
12	4	17	6.9	-3.0
13	4	17	7.5	1.1
3	5	17	4.6	-3.1
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6	5	17	4.3	1.2
7	5	17	2.5	1.4
8	5	17	5.7	-5.9
10	5	17	4.8	-5.3
11	5	17	5.7	1.6
12	5	17	8.2	-5.0
13	5	17	7.5	-8.4
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2	6	17	4.5	3.5
4	6	17	3.8	-1.9
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7	6	17	3.9	-1.0
9	6	17	3.7	-1.4
1	7	17	1.6	3.9
2	7	17	1.1	0.1
3	7	17	2.7	4.6
5	7	17	4.5	-8.0
6	7	17	2.9	1.5
7	7	17	3.7	2.4
8	7	17	3.9	-2.2
9	7	17	4.1	2.4
0	8	17	4.9	7.3
1	8	17	4.2	1.5
2	8	17	4.3	5.8
3	8	17	4.0	-0.2
4	8	17	2.3	1.0
6	8	17	2.1	-2.0
7	8	17	3.0	1.9
9	8	17	3.4	-0.2
11	8	17	7.4	1.4
1	9	17	5.6	-1.2
2	9	17	6.4	-7.1
3	9	17	2.3	-2.4
4	9	17	5.0	-6.8
6	9	17	3.4	-3.3
7	9	17	3.6	0.7
8	9	17	1.7	2.2
9	9	17	3.5	-1.7
11	9	17	6.2	-1.5
0	10	17	9.5	-12.0
1	10	17	1.9	-0.9
2	10	17	4.6	-5.7
3	10	17	2.0	9.5
6	10	17	8.2	7.1
8	10	17	7.2	7.1
1	11	17	4.2	-2.4
2	11	17	9.9	9.2
4	11	17	7.6	10.5
5	11	17	1.5	-1.4
8	11	17	6.3	-2.0
9	11	17	4.4	1.6
10	11	17	6.7	-4.7
0	12	17	5.5	7.5
2	12	17	3.7	5.9
4	12	17	3.5	-0.5
5	12	17	3.2	0.9
6	12	17	7.4	-5.7
7	12	17	4.2	-0.5
8	12	17	5.6	-5.8
9	12	17	4.5	-1.0
1	13	17	3.1	3.7
3	13	17	6.6	2.4
6	13	17	2.4	-1.4
7	13	17	1.7	0.9
8	13	17	9.0	2.4
9	13	17	5.3	-0.6
0	14	17	3.6	-1.7
1	14	17	5.1	0.7
2	14	17	2.0	0.2
3	14	17	4.6	0.9
5	14	17	3.6	-1.7
6	14	17	3.5	-0.6
7	14	17	1.6	0.4
8	14	17	3.7	-1.0
9	14	17	1.9	0.9
10	14	17	7.1	-0.1
2	15	17	5.1	-2.7
3	15	17	6.1	-0.7
4	15	17	8.9	-3.1
6	15	17	6.0	-1.3
7	15	17	6.4	-8.5
8	15	17	2.7	1.6
0	16	17	5.2	-6.6
1	16	17	3.0	-0.1
4	16	17	3.1	0.0
6	16	17	3.2	4.9
8	16	17	3.9	3.3
9	16	17	3.4	0.4
1	17	17	5.4	-1.5
2	17	17	7.9	4.3
3	17	17	3.1	-2.1
4	17	17	8.5	5.4
5	17	17	1.9	-8.7
7	17	17	5.6	-1.9
0	18	17	6.1	5.0
1	18	17	5.0	-1.1
2	18	17	1.9	3.1
3	18	17	5.3	5.1
5	18	17	3.3	1.1
6	18	17	7.0	-5.0
1	19	17	6.0	1.7
2	19	17	6.6	-3.3
3	19	17	6.1	2.3
4	19	17	2.7	-4.4
5	19	17	6.5	0.4
0	20	17	8.0	-2.1
3	20	17	6.5	-2.9
4	20	17	5.2	4.7
1	21	17	2.0	-1.1
2	21	17	2.0	-0.8

TABLE 2.5

STRUCTURE FACTOR AGREEMENT.

(a)Analysis of observed and calculated structure factors as a function of the layer line index. All figures are on absolute scale.

l	$\sum\|Fo\|$	$\sum\|Fc\|$	N	R	$\sum\|\Delta\|/N$
0	5053	5040	133	0.0557	2.11
1	6366	6284	265	0.0814	1.96
2	6376	6236	275	0.0699	1.62
3	5201	4965	263	0.0988	1.95
4	5623	5510	256	0.0709	1.56
5	5118	5018	253	0.0795	1.61
6	4739	4619	269	0.0960	1.69
7	3726	3722	229	0.0846	1.38
8	3236	3014	271	0.1470	1.75
9	2682	2490	242	0.1613	1.79
10	2797	2670	260	0.1443	1.55
11	2248	2029	231	0.1818	1.77
12	1953	1758	243	0.2180	1.75
13	1457	1270	213	0.2563	1.75
14	1260	1013	223	0.3584	2.02
15	1029	800	198	0.3876	2.01
16	984	735	196	0.4201	2.11
17	684	472	149	0.5013	2.30
All	60531	57645	4169	0.1229	1.77

(b) Analysis of observed and calculated structure factors as a function of the magnitude of the observed structure factors. All figures are on absolute scale.

Range of Fo	$\sum\|Fo\|$	$\sum\|Fc\|$	N	R	$\sum\|\Delta\|/N$
0 - 5	3661	3023	1032	0.4953	1.76
5 - 10	10164	8130	1435	0.3113	2.21
10 - 15	6744	6679	551	0.1053	1.29
15 - 20	5721	5759	331	0.0693	1.20
20 - 30	8726	8763	358	0.0482	1.17
30 - 40	6196	6242	179	0.0432	1.49
40 - 60	7089	7006	146	0.0373	1.81
60 - 80	4503	4444	67	0.0304	2.04
80 - 100	3121	3064	35	0.0300	2.67
100 - 150	3030	2987	26	0.0435	5.07
150 - 300	1579	1546	9	0.0378	6.62

TABLE 2.6

PRINCIPAL VALUES OF VIBRATION TENSORS AND THEIR DIRECTION COSINES REFERRED TO CRYSTAL AXES.

ATOM	U $Å^2$	D1	D2	D3
Cr(1)	0.0462	-0.1415	-0.2862	0.9477
	0.0263	0.8523	0.4518	0.2637
	0.0338	-0.5036	0.8450	0.1801
C(1)	0.0347	0.6593	-0.3346	0.6733
	0.0661	0.3957	0.9159	0.0677
	0.0592	-0.6393	0.2218	0.7363
C(2)	0.0850	-0.1540	-0.7672	0.6226
	0.0338	0.6681	0.3834	0.6377
	0.0496	-0.7280	0.5142	0.4535
C(3)	0.0922	0.2634	-0.6148	0.7434
	0.0256	0.6585	0.6777	0.3272
	0.0429	-0.7050	0.4033	0.5834
C(4)	0.0312	0.4265	0.8874	0.1750
	0.0650	0.5611	-0.4113	0.7183
	0.0494	0.7094	-0.2082	-0.6734
C(5)	0.0939	-0.7926	-0.3060	0.5274
	0.0367	-0.1482	0.9357	0.3201
	0.0575	-0.5914	0.1756	-0.7870
C(6)	0.1467	-0.8065	-0.2884	0.5162
	0.0372	0.3695	-0.9273	0.0593
	0.0541	0.4616	0.2385	0.8544
C(7)	0.1321	-0.5045	-0.5221	0.6877
	0.0396	0.7705	-0.6317	0.0857
	0.0556	0.3896	0.5731	0.7210
C(8)	0.1206	-0.2062	-0.5771	0.7902
	0.0435	-0.9263	0.3755	0.0326
	0.0485	-0.3155	-0.7252	-0.6120

C(9)	0.0781	0.3132	-0.3814	0.8697
	0.0420	-0.9244	-0.3325	0.1871
	0.0598	0.2179	-0.8625	-0.4567
C(10)	0.0743	0.5254	0.4569	0.7178
	0.0386	-0.5750	-0.4312	0.6953
	0.0504	0.6272	-0.7780	0.0361
C(11)	0.0393	0.7069	0.3176	0.6320
	0.0463	-0.2362	-0.7362	0.6342
	0.0438	0.6667	-0.5976	-0.4454
C(12)	0.0284	0.0641	0.8708	0.4874
	0.0529	-0.1262	-0.4775	0.8695
	0.0441	0.9899	-0.1172	0.0793
C(13)	0.0641	-0.5702	-0.4105	0.7115
	0.0306	-0.0449	0.8804	0.4720
	0.0440	-0.8203	0.2372	-0.5205
C(14)	0.0803	-0.1632	-0.5829	0.7960
	0.0364	-0.7328	0.6118	0.2978
	0.0381	-0.6606	-0.5347	-0.5270
C(15)	0.0291	0.8683	0.2162	0.4464
	0.0668	-0.3495	-0.3719	0.8599
	0.0524	0.3519	-0.9027	-0.2474
C(16)	0.0730	-0.5044	0.1909	0.8421
	0.0423	0.7580	0.5649	0.3260
	0.0505	-0.4135	0.8027	-0.4297
C(17)	0.0555	-0.1559	-0.4998	0.8520
	0.0368	0.7611	0.4891	0.4262
	0.0437	-0.6297	0.7148	0.3042
O(1)	0.1263	-0.0713	-0.7666	0.6382
	0.0418	-0.9138	0.3067	0.2663
	0.0602	-0.3999	-0.5642	-0.7223
O(2)	0.0353	-0.3006	-0.9533	0.0287
	0.1554	-0.5081	0.1855	0.8411
	0.0966	-0.8071	0.2383	-0.5402
O(3)	0.0430	0.7158	-0.1417	0.6837
	0.0870	-0.5153	0.5536	0.6543
	0.0741	-0.4712	-0.8207	0.3232

TABLE 2.7

BOND LENGTHS (Å) AFTER REFINEMENT OF PHOTOGRAPHIC DATA (I), AFTER REFINEMENT OF COUNTER DATA (II), AND AFTER LIBRATION CORRECTION (III).

	I	II	III
C(1) - C(2)	1.46	1.389 ± 7	1.394
C(2) - C(3)	1.44	1.385 ± 7	1.392
C(3) - C(4)	1.41	1.410 ± 6	1.414
C(4) - C(12)	1.39	1.439 ± 6	1.445
C(11) - C(12)	1.44	1.410 ± 6	1.417
C(1) - C(11)	1.44	1.440 ± 6	1.444
C(5) - C(6)	1.40	1.418 ± 10	1.420
C(6) - C(7)	1.37	1.401 ± 10	1.406
C(7) - C(8)	1.34	1.337 ± 9	1.343
C(8) - C(14)	1.40	1.415 ± 7	1.417
C(13) - C(14)	1.44	1.402 ± 6	1.408
C(5) - C(13)	1.41	1.402 ± 7	1.408
C(9) - C(14)	1.36	1.416 ± 8	1.422
C(9) - C(10)	1.34	1.333 ± 7	1.337
C(10) - C(11)	1.44	1.447 ± 7	1.452
C(12) - C(13)	1.52	1.462 ± 6	1.467

Cr(1) - C(1)	2.25	2.212 ± 5	2.221
Cr(1) - C(2)	2.22	2.210 ± 5	2.217
Cr(1) - C(3)	2.21	2.206 ± 5	2.214
Cr(1) - C(4)	2.22	2.208 ± 4	2.217
Cr(1) - C(11)	2.27	2.289 ± 4	2.298
Cr(1) - C(12)	2.29	2.289 ± 4	2.296
Cr(1) - C(15)	1.83	1.828 ± 5	1.833
Cr(1) - C(16)	1.76	1.844 ± 5	1.853
Cr(1) - C(17)	1.82	1.857 ± 4	1.865
Cr(1) - O(1)	2.97	2.993 ± 4	2.999
Cr(1) - O(2)	2.99	2.989 ± 4	3.000
Cr(1) - O(3)	3.02	2.993 ± 4	3.004
C(15) - O(1)	1.15	1.165 ± 6	1.167
C(16) - O(2)	1.24	1.145 ± 6	1.149
C(17) - O(3)	1.20	1.136 ± 6	1.139

TABLE 2.8

INTERBOND ANGLES AND E.S.D.S.

C(11)- C(1) - C(2)	120.7±5°	C(5) - C(13)- C(12)	122.4±4°
C(1) - C(2) - C(3)	120.0±4	C(5) - C(13)- C(14)	118.8±5
C(2) - C(3) - C(4)	121.0±4	C(12)- C(13)- C(14)	118.8±4
C(3) - C(4) - C(12)	120.1±4	C(8) - C(14)- C(9)	120.2±5
C(13)- C(5) - C(6)	120.4±5	C(8) - C(14)- C(13)	119.7±5
C(5) - C(6) - C(7)	118.7±6	C(9) - C(14)- C(13)	120.1±4
C(6) - C(7) - C(8)	121.3±6	C(15)- Cr(1)- C(16)	87.1±2
C(7) - C(8) - C(14)	121.0±5	C(16)- Cr(1)- C(17)	89.9±2
C(14)- C(9) - C(10)	122.3±5	C(17)- Cr(1)- C(15)	90.6±2
C(9) - C(10)- C(11)	120.3±5	O(1) - Cr(1)- O(2)	85.5±1
C(1) - C(11)- C(10)	120.7±4	O(2) - Cr(1)- O(3)	90.9±2
C(1) - C(11)- C(12)	119.7±4	O(3) - Cr(1)- O(1)	90.1±1
C(10)- C(11)- C(12)	119.6±4	Cr(1)- C(15)- O(1)	177.8±4
C(4) - C(12)- C(11)	118.4±4	Cr(1)- C(16)- O(2)	177.1±5
C(4) - C(12)- C(13)	122.7±4	Cr(1)- C(17)- O(3)	178.7±4
C(11)- C(12)- C(13)	118.9±4		

TABLE 2.9

INTERMOLECULAR CONTACTS BELOW 4 Å.

C(16)....O(1)	i	3.24 Å	C(3).....C(7)	iii	3.59 Å
O(1).....O(2)	ii	3.29	C(8).....C(17)	i	3.59
C(2).....C(6)	iii	3.33	C(4).....C(7)	ii	3.60
C(17)....O(1)	i	3.38	C(2).....O(1)	iv	3.61
C(3).....O(3)	ii	3.39	C(3).....C(6)	iii	3.61
C(1).....O(1)	iv	3.41	C(2).....C(7)	iii	3.62
C(4).....C(13)	iii	3.42	C(4).....C(12)	iii	3.62
C(2).....O(3)	ii	3.43	C(12)....C(12)	iii	3.63
C(9).....O(1)	i	3.44	C(15)....O(3)	ii	3.65
C(8).....O(3)	i	3.45	C(1).....C(5)	iii	3.68
O(1).....O(3)	ii	3.48	C(4).....C(14)	iii	3.68
C(3).....C(13)	iii	3.54	C(4).....C(6)	ii	3.71
C(14)....O(1)	i	3.54	C(1).....C(15)	iv	3.72
C(2).....C(5)	iii	3.55	C(10)....O(1)	i	3.72
C(3).....C(14)	iii	3.55	C(10)....O(2)	iv	3.73
C(10)....O(3)	iv	3.57	C(12)....C(13)	iii	3.75
C(3).....C(8)	iii	3.58	O(2).....O(3)	iv	3.76
C(3).....C(5)	iii	3.58	C(1).....C(6)	iii	3.77

C(3).....C(6)	ii	3.77	C(10)....C(17)	iv	3.89
C(10)....O(1)	v	3.77	C(13)....O(1)	i	3.89
C(4).....C(5)	iii	3.78	C(9).....O(1)	v	3.93
C(5).....C(11)	iii	3.80	C(1).....O(3)	iv	3.95
C(14)....C(15)	i	3.82	C(2).....C(9)	vi	3.96
C(7).....O(3)	i	3.85	C(8).....C(15)	i	3.97
C(5).....C(12)	iii	3.86	C(10)....C(15)	v	3.97
C(7).....C(17)	i	3.88	C(1).....C(17)	iv	4.00
C(15)....C(17)	ii	3.88	C(10)....C(16)	iv	4.00
C(9).....C(15)	v	3.89			

Roman numerals refer to the following transformations of the fractional coordinates given in Table 2.1.

i	1/2 + x,	y,	1/2 - z;
ii	-1/2 + x,	y,	1/2 - z;
iii	1 - x,	1 - y,	- z;
iv	x,	3/2 - y,	-1/2 + z;
v	1/2 + x,	3/2 - y,	- z;
vi	-1/2 + x,	3/2 - y,	- z;

TABLE 2.10

MEAN MOLECULAR PLANES.

PLANE NO.	ATOMS DEFINING PLANE
1	C(15),C(16), and C(17)
2	O(1),O(2), and O(3)
3	C(1),C(2),C(3),C(4),C(11), and C(12)
4	C(9),C(10),C(11),C(12),C(13), and C(14)
5	C(5),C(6),C(7),C(8),C(13), and C(14)
6	The fourteen atoms of the phenanthrene ligand

PLANE EQUATIONS

PLANE NO.	P	Q	R	S	RMS D*
1	-0.0739	-0.5949	-0.8004	-10.3504	-
2	-0.0904	-0.5878	-0.8039	-11.0402	-
3	-0.1206	-0.6206	-0.7748	-8.0484	0.018
4	-0.1643	-0.6264	-0.7620	-8.3776	0.010
5	-0.2043	-0.6264	-0.7540	-8.6842	0.009
6	-0.1553	-0.6218	-0.7676	-8.2393	0.043

* P,Q, and R are the direction cosines on the crystal axes of the plane normal, S is the plane to origin distance, and RMS D is the root mean square deviation from the plane (in Å)

of the atoms defining it. The plane equation is

$$PX + QY + RZ = S$$

where X, Y, and Z are coordinates in Å s referred to crystal axes.

DIHEDRAL ANGLES

PLANE A	PLANE B	∠ AB	PLANE A	PLANE B	∠ AB
1	2	1.05°	2	6	4.69°
1	3	3.39	3	4	2.63
1	4	5.91	3	5	4.95
1	5	8.12	3	6	2.03
1	6	5.26	4	5	2.34
2	3	3.05	4	6	0.66
2	4	5.35	5	6	2.92
2	5	7.43			

DEVIATIONS FROM PLANES (Å)

PLANE NO. ATOM	1	2	3	4	5	6
Cr(1)	1.078	1.761	-1.733	-1.679	-1.540	-1.725
C(1)	2.832	3.526	-0.026	0.011	0.142	-0.025
C(2)	2.783	3.491	0.008	0.105	0.286	0.054
C(3)	2.747	3.443	0.018	0.129	0.311	0.068
C(4)	2.738	3.409	-0.025	0.039	0.173	-0.015
C(5)	2.852	3.468	0.006	-0.034	-0.006	-0.072
C(6)	2.993	3.583	0.107	0.017	-0.007	-0.013
C(7)	3.202	3.781	0.234	0.085	0.013	0.071
C(8)	3.232	3.823	0.223	0.064	-0.006	0.058
C(9)	3.138	3.768	0.124	0.002	-0.016	-0.003
C(10)	3.046	3.700	0.066	-0.010	0.018	-0.022
C(11)	2.912	3.581	0.017	0.006	0.085	-0.024
C(12)	2.856	3.512	0.008	0.009	0.090	-0.029
C(13)	2.920	3.549	0.032	-0.017	0.013	-0.047
C(14)	3.092	3.709	0.122	0.012	-0.007	-0.002
C(15)	-	0.707	-2.737	-2.613	-2.409	-2.675
C(16)	-	0.683	-2.887	-2.872	-2.757	-2.904
C(17)	-	0.659	-2.806	-2.771	-2.658	-2.819
O(1)	-0.722	-	-3.413	-3.246	-3.002	-3.317
O(2)	-0.685	-	-3.617	-3.624	-3.521	-3.648
O(3)	-0.644	-	-3.446	-3.422	-3.326	-3.472

TABLE 2.11

ANALYSIS OF RIGID BODY VIBRATIONS.

(a) Centre of mass, referred to crystal axes in Å s.

X	Y	Z
6.3611	11.5090	1.6059

(b) Principal moments of inertia, I, and direction cosines D1, D2, D3, of inertial axes referred to crystal axes.

$I\ (\mathrm{gmcm}^2 \times 10^{-40})$	D1	D2	D3
1504	-0.7935	0.5717	0.2087
3728	0.5993	0.6744	0.4313
3517	0.1058	0.4074	-0.8777

(c) T and W and their e.s.d.s, referred to inertial axes.

$$T(\text{Å}^2) = \begin{bmatrix} 0.0344 & 0.0020 & -0.0027 \\ 8 & 15 & 15 \\ & 0.0241 & -0.0049 \\ & 11 & 18 \\ & & 0.0377 \\ & & 14 \end{bmatrix}$$

$$W(^{\circ 2}) = \begin{bmatrix} 24.0 & 0.8 & -2.3 \\ 2.2 & 1.8 & 1.2 \\ & 14.4 & -4.7 \\ & 1.1 & 1.4 \\ & & 6.4 \\ & & 1.0 \end{bmatrix}$$

(d) U obs - U calc, with respect to inertial axes.

ATOM	U11	U22	U33	2U23	2U31	2U12
Cr(1)	-0.0013	-0.0002	-0.0005	0.0000	0.0010	0.0013
C(1)	0.0060	0.0055	-0.0033	-0.0049	0.0018	0.0119
C(2)	0.0103	-0.0004	-0.0025	-0.0015	0.0174	-0.0048
C(3)	0.0050	-0.0018	0.0010	0.0001	0.0227	-0.0162
C(4)	0.0073	0.0081	-0.0022	0.0080	0.0096	-0.0161
C(5)	0.0112	-0.0021	0.0049	0.0242	0.0095	-0.0228
C(6)	0.0258	-0.0141	-0.0120	0.0211	-0.0180	-0.0379
C(7)	0.0096	-0.0089	-0.0173	-0.0108	-0.0139	-0.0132
C(8)	0.0068	-0.0051	0.0032	-0.0120	-0.0207	-0.0170
C(9)	-0.0013	-0.0046	0.0102	-0.0075	-0.0202	-0.0066
C(10)	-0.0114	0.0058	0.0026	-0.0 94	-0.0080	-0.0052
C(11)	0.0018	0.0012	0.0050	0.0013	0.0032	-0.0022
C(12)	0.0037	0.0081	0.0073	0.0077	0.0051	-0.0164
C(13)	0.0062	0.0053	0.0031	0.0114	-0.0020	-0.0170
C(14)	-0.0013	-0.0012	0.0075	0.0032	-0.0124	-0.0123
C(15)	0.0108	-0.0085	-0.0143	-0.0063	-0.0276	0.0077
C(16)	0.0156	0.0066	-0.0074	0.0139	0.0004	0.0226
C(17)	0.0010	-0.0036	0.0087	-0.0099	-0.0037	-0.0022
O(1)	0.0063	0.0026	0.0033	-0.0054	-0.0030	0.0002
O(2)	0.0550	0.0089	0.0081	-0.0148	-0.0404	0.0159
O(3)	0.0216	-0.0031	0.0095	-0.0249	-0.0287	0.0208

programme described in Part II. The main results of this analysis are presented in Table 2.11. The bond lengths after librational correction are given in Table 2.7 and in Fig. 2.4 (which also explains the atomic numbering).

The molecular motions suggested by this analysis are qualitatively reasonable. The tensor of translational motion is almost isotropic while the librational tensor is markedly anisotropic, with the axis of maximum libration coinciding closely with the axis of minimum inertia. The agreement between the atomic vibration tensors obtained from the least-squares refinement, U_{obs}, and those calculated from the molecular vibration tensors, U_{calc}, is, however, disappointingly poor. The root mean square difference between U_{obs} and U_{calc} is 0.0130 $\mathring{A}^2$ and this must be considered significant in terms of the estimated standard deviations of the U_{obs} (Table 2.2). Schomaker and Trueblood (1966) have shown that Cruickshank's (1956) treatment should be extended to include "helical" motions in the case of a non-centrosymmetric molecule. This may be the reason for the poor agreement between U_{obs} and U_{calc}. The agreement is also somewhat worse than average for the atoms in the carbonyl groups and there may well be additional wagging motion in these groups.

In view of this it has seemed safer to take the bond lengths before librational correction as the final values, while bearing in mind that they are subject to a systematic error of which the quoted standard deviations take no account.

2.7 DISCUSSION OF THE RESULTS

The gross molecular structure of phenanthrene-chromium tricarbonyl obtained from this analysis is basically the same as that described by Deuschl and Hoppe (1964). In the free hydrocarbon the side rings have greater overall aromatic character than the centre ring and it is to a side ring that the chromium tricarbonyl moiety is bonded. The linear carbonyl groups point roughly towards the midpoints of the ring C-C bonds which have greater double bond character in phenanthrene itself. The planes defined by the phenanthrene system, by the three carbonyl carbons, and by the three carbonyl oxygens are roughly parallel. The carbonyl groups are approximately perpendicular to each other (Table 2.8).

Three aspects of the molecular structure merit detailed comment, namely, the effect of the chromium atom on the hydrocarbon ligand, the relationship of the chromium atom to the ring to which it is bonded, and the geometry of the carbonyl groups.

A simple valence bond treatment (Trotter, 1963) leads to the prediction of 1.399 Å for the mean C-C bond in a side ring of phenanthrene. The latest x-ray analysis of this hydrocarbon gave 1.405 Å for the corresponding mean (Trotter, 1963). The comparable means obtained in this analysis are 1.412 Å for the ring bonded to chromium and 1.396 Å for the non-bonded side ring. For the means of the two sets of three alternate bond lengths in a side ring of phenanthrene the V.B. predictions are 1.388 and 1.409 Å. The comparable figures in this analysis are 1.386 and 1.406 Å for the non-bonded ring and 1.403 and 1.421 Å for the bonded ring. This suggests that the main effect of the chromium atom has been to increase the mean C-C bond length in the ring to which it is bonded by about 0.016 Å without inducing any further bond length alternation. The mean values for the non-bonded ring agree within experimental error with the V.B. predictions for phenanthrene, but the agreement with Trotter's x-ray study is not so good. The changes in individual bond lengths in the bonded ring, compared either with the

V.B. predictions or with the bond lengths in the non-bonded ring, show no obvious pattern and it is probable that little weight should be attached to them.

The bond lengths in the middle ring agree with the V.B. predictions except for the C(9)-C(14) bond which is more than three standard deviations shorter; it is, however, still longer than Trotter's x-ray value.

As in Trotter's analysis, the phenanthrene nucleus is significantly non-planar, the root mean square deviation being 0.043 Å. This is at least partly due to the intramolecular overcrowding of H(4) and H(5), which is also shown by significant distortions of the interbond angles at C(12) and C(13). When the three rings of the phenanthrene ligand are considered separately, however, (Table 2.10 planes, 3,4,&5) the deviations of the atoms from the ring bonded to chromium are found to be rather larger than the deviations of the atoms from the other two rings. This seems to be due to a slight folding of the bonded ring about a line through C(1) and C(4).

A possible explanation for this distortion of the bonded ring presents itself when the Cr-C(ring) distances are considered. The Cr-C(1), Cr-C(2), Cr-C(3), and Cr-C(4) distances are equal within experimental error, with a mean of 2.209 Å. The Cr-C(11) and Cr-C(12) distances are equal at 2.289 Å and the difference between these two means cannot possibly be covered by the standard deviations. Of the bonds opposite carbonyl groups the C(11)-C(12) bond is the one with least double bond character in the free hydrocarbon. The orbitals of C(11) and C(12) might therefore be less capable of forming a strong bond to the metal atom than those of the other ring carbon atoms. Such an asymmetry in the bonding could be responsible for small distortions in the planarity of the bonded ring.

The Cr-O distances are equal within experimental error with a mean value of 2.992 Å. The Cr-C(carbonyl) and C(carbonyl)-O distances are a little less regular; the mean values are 1.843 Å and 1.149 Å and the root mean square deviation from each of these means is 0.012 Å, which is about twice the standard deviation of an individual measurement. The carbonyl groups all show small but significant departures from linearity. The mean $\angle$Cr-C-O is 177.9°. Kettle (1965) has suggested on theoretical grounds that such departures from linearity might be expected. In this case crystal packing forces provide an adequate explanation for the effect. Packing forces are also the likely explanation of the low

O(1)-Cr-O(2) angle of 85.5 °.

The molecular packing (Fig. 2.3) involves pairs of molecules arranged round centres of symmetry with the phenanthrene units parallel to each other. The interplanar spacing between phenanthrene units so related is 3.35 Å. This is close to the interplanar spacing found in graphite and in many analyses of aromatic hydrocarbons. None of the intermolecular atomic distances are significantly less than the sum of the van der Waals radii (Pauling 1960) of the atoms involved. A rather similar packing arrangement was found in Deuschl and Hoppe's analysis of the monoclinic polymorph.

A detailed comparison of the structural features of the molecule with those of related compounds is postponed until Chapter IV.

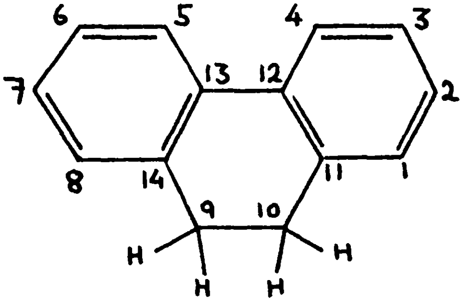
CHAPTER III

9,10 - DIHYDROPHENANTHRENECHROMIUM TRICARBONYL

3.1 INTRODUCTION

The structure analysis of dihydrophenanthene-chromium tricarbonyl was undertaken for reasons similar to those which motivated the analysis of the phenanthrene compound.

In 9,10-dihydrophenanthrene (I) four of the bonds in the centre ring are single and only the C(11)-C(12) and C(13)-C(14) bonds have double bond character. The requirement that the sp^3 carbon atoms C(9) and C(10) should have normal valency angles can only be met if the planes of the two side rings are not parallel. It therefore seems unlikely that there is much interaction between the aromatic systems in the two side rings. If the chromium tricarbonyl fragment bonds to one side ring the bonding in the other side ring should be relatively unaffected.



I

3.2 EXPERIMENTAL

Crystal Data

9,10-Dihydrophenanthrenechromium Tricarbonyl

$C_{14}H_{12}Cr(CO)_3$

F.W. 316.3

Monoclinic $a = 10.50$, $b = 12.73$, $c = 11.98$ Å, $\beta = 118.9°$

$U = 1404$ Å^3 $F(000) = 648$

$D_m = 1.48$ gmcm^{-3} $Z = 4$ $D_x = 1.502$ gmcm^{-3}

Linear absorption coefficient (Mo Kα x-rays, wavelength 0.7107 Å) = 8.6 cm^{-1}.

Systematic Absences

$h0\ell$ when ℓ is odd

$0k0$ when k is odd

Space Group $P2_1/c$ (No. 14)

When the present writer started work on this problem the space group had already been determined as $P2_1$ or $P2_1/m$. Moving film photographs of the three equatorial reciprocal lattice nets and preliminary values of the cell dimensions were available. A redetermination of the cell dimensions from an $h0\ell$ Weissenberg photograph (copper Kα radiation, $\lambda = 1.5418$ Å) and from $hk0$ and $0k\ell$ precession photographs (molybdenum Kα radiation, $\lambda = 0.7107$ Å) gave $a = 5.99$, $b = 12.73$, $c = 9.24$ Å, and $\beta = 95.7°$, which were in good agreement with the previous values. These cell dimensions yield a calculated density of 1.502 $gmcm^{-3}$ (D_m = 1.48 $gmcm^{-3}$) for two molecules per unit cell. The space group $P2_1/m$ was thus incompatible with an ordered molecular packing and therefore the space group $P2_1$ was assumed.

Intensity data were measured from a crystal mounted about the b axis, using a Hilger-Watts linear diffractometer equipped with balanced SrO-ZrO_2 Ross filters (see Appendix I). Molybdenum Kα radiation was employed. Each reflection was measured at least four times with each filter, using a one minute oscillation cycle and a 3° oscillation angle. About thirty reflections had to be set by hand. The maximum recording angle was $\theta = 30^\circ$. Lorentz and polarisation factors appropriate to equi-inclination Weissenberg geometry were applied to the data using programmes devised by Dr. J.G. Sime for the KDF9 computer. In this manner 2353 independent structure amplitudes on the reciprocal lattice nets $h0\ell$ to $h16\ell$ were obtained. Of these, 382 reflections on the nets $h14\ell$ to $h16\ell$ were used only in the last stages of refinement.

As described in Section 3.3, work on the structure led to the conclusion that the space group had been wrongly determined and $h0\ell$ and $h1\ell$ Weissenberg photographs allowed the true space group to be determined as $P2_1/c$. Using subscripts 1 and 2 to denote respectively the $P2_1$ and $P2_1/c$ unit cells, the relationship between the two cells can be expressed in terms of the vector equations:

$$\begin{aligned} \underline{a}_2 &= \underline{a}_1 + \underline{c}_1 \\ \underline{b}_2 &= \underline{b}_1 \\ \underline{c}_2 &= -2\underline{a}_1 \end{aligned} \qquad (1)$$

The first set of data collected corresponds only to the reflections with ℓ even in the correct space group. The missed reflections (with ℓ odd) were therefore collected, using the same crystal and diffractometer settings as before, and were reduced to structure amplitudes using the same programmes. In this way a further 2037 reflections on the nets $h1\ell$ to $h16\ell$ were obtained, giving a total of 4390 independent reflections.

The data were initially set on an approximately absolute scale by correlation with the calculated structure amplitudes. In the final refinement a scale factor was obtained by least-squares for each of the two sets of data.

3.3 STRUCTURE SOLUTION AND REFINEMENT

A sharpened three-dimensional Patterson function was calculated using the first set of data. The sections at U = 0 and V = ½ through this function are shown in Fig. 3.1. On the Harker section at V = ½ there is a large peak which was attributed to a vector between chromium atoms related by the two-fold screw axis along b. On the section at U = 0 there is a peak of comparable height, on the line (0,V,0). This peak was initially attributed to unresolved vectors between a chromium atom and the carbon and oxygen atoms of a carbonyl group pointing almost exactly along the b axis. This interpretation did not lead to a successful solution of the structure and it was necessary to consider another interpretation, namely that the peak at (0,V,0) was due to a vector between chromium atoms related by a mirror plane normal to the b axis. Such an interpretation could be accepted only if the space group were $P2_1/m$, with a disordered molecular packing. It fitted, however, with the presence in the Patterson function of a peak which was half the height of the peak on the Harker section at V = ½, and which had the same U and W coordinates as the Harker peak. In the space group $P2_1/m$ such a peak is to be expected due to vectors between heavy atoms related by a centre of symmetry. The coordinates of the chromium atom were therefore worked out from the Patterson function on the assumption that the space group was $P2_1/m$.

An electron density synthesis based on the phases of structure factors calculated from these coordinates contained peaks corresponding to a dihydrophenanthrene-chromium tricarbonyl molecule of acceptable stereochemistry. Inclusion of the atoms of the aromatic ring bonded to chromium and of the atoms of the carbonyl groups in the structure factor calculations reduced R from 0.45 to 0.38. A second electron density synthesis allowed all the atoms to be reliably located and reduced R to 0.27. A further cycle of Fourier refinement by means of F_o and F_c maps reduced R to 0.24. The computer programmes described in Part II Chapter II were used throughout the Fourier refinement.

The model of the structure, as it stood at this stage of the analysis, gave satisfactory structure factor agreement, but it required a very unusual packing disorder. For this reason the space group was checked and was found to be in error. To complete the refinement further data collection was therefore necessary. While this was being done the structure was refined in the space group $P2_1/m$.

Two cycles of full matrix least-squares refinement with isotropic temperature factors, and five cycles of block-diagonal least-squares with anisotropic temperature factors, were calculated using the KDF9 computer programme written by Cruickshank and Smith. As a result R fell from 0.24 to 0.101.

When the complete set of data became available the indices of the reflections, the fractional atomic coordinates, and the anisotropic temperature factors were transformed to correspond with the true space group. The transformed parameters of the seventh least-squares cycle were used to calculate structure factors for all 4390 reflections; the resulting R-factor was 0.110, indicating that the structure was essentially correct.

A difference synthesis was then calculated using only the 483 reflections with $\sin\theta/\lambda < 0.35$ Å^{-1}. Peaks corresponding to the expected positions of eleven of the twelve hydrogen atoms could be located. The hydrogen bonded to C(2) lay in a region of positive density but not on a peak. The mean hydrogen peak height was 0.4e/Å^3. All the hydrogen atoms were then included in the structure factor calculations, assuming positions consistent with those of the carbon atoms adjacent to them. An isotropic temperature parameter 1·5 times greater than that of the carbon atom to which it was bonded was applied to each hydrogen. R dropped from 0.110 to 0.102.

At this stage seven reflections for which $\sin\theta/\lambda < 0.10\ \mathring{A}^{-1}$ were excluded from the analysis. Each had $|F_o|$ much smaller than $|F_c|$ and this was ascribed to extinction or to partial interposition of the beamstop.

A weighting scheme of the form

$$w = \left\{ 1-\exp(-15s^2) \right\} /(1+0.0015\ |F_o|^2);\ (s = \sin\theta/\lambda)$$

was applied and two further cycles of refinement were done, reducing R to 0.094.

The weighting scheme was then changed to

$w = w_1 \times w_2$ where

$w_1 = 1$ if $\sin\theta/\lambda > 0.4$ otherwise $w_1 = (\sin\theta/\lambda)^2/0.16$

$w_2 = 1$ if $|F_o| < 40$ otherwise $w_2 = 40/|F_o|$.

Three further cycles reduced R to 0.086. In the final cycle coordinate shifts were all less than 0.001 Å and the scale and temperature factor shifts were also insignificant. The change in the weighting scheme again affected mainly the scale and temperature factors. R' was reduced to 0.0081 and the standard deviations were reduced by about 10%. It was not found necessary in this case to assign zero weight to any of the weak reflections. This, and also the lower R-factor as compared with the phenanthrene compound, is probably due to the longer counting time used in collecting the data. R,' however, is about the same for both analyses and so are the parameter standard deviations.

The atomic scattering curves used in this analysis were for chromium those of Freeman and Watson (1963), for oxygen those of Berghuis et al. (1955), for carbon those of Hoerni and Ibers (1954), and for hydrogen those of Stewart, Davidson, and Simpson (1965).

The structure factors from the last least-squares cycle were used to calculate electron density and difference syntheses. A composite view of the final electron density synthesis is shown in Fig. 3.2 which also explains the atomic numbering. The maximum and minimum function values in the final difference synthesis were respectively $+0.4e/\overset{o}{A}^3$ and $-0.7e/\overset{o}{A}^3$.

In Tables 3.1 and 3.2 the final values of the coordinates of the heavier atoms and the assumed coordinates of the hydrogen atoms are respectively presented. Hydrogen atoms have been assigned the numbers of the carbon atoms to which they are bonded, except that H(10) is bonded to C(9) and H(11) and H(12) are

Course of the Analysis

(1) Refinement of Partial Data (1971 reflections)

S.F. Cycle No.	Atoms Included	R
1	Cr	0.45
2	Cr+3O+9C	0.38
3	Cr+3O+17C	0.27
4	Cr+3O+17C	0.24

S.F.L.S. Cycle No.	R	S.F.L.S. Cycle No.	R
1	0.24	5	0.113
2	0.164	6	0.105
3	0.148	7	0.101
4	0.122		

(2) Refinement of Complete Data (4390 reflections)

S.F.L.S. Cycle No.	Comment	R'	$\Sigma w \Delta^2$	R
8	Same parameters as cycle 7	0.0144	15820	0.110
9	Hydrogen atoms included	0.0110	12071	0.102
10	Weighting scheme changed	0.0097	9930	0.096
11		0.0096	9817	0.095
12	Weighting scheme changed	0.0088	5324	0.092
13		0.0082	4792	0.087
14		0.0081	4762	0.086

bonded to C(10). Table 3.3 contains the anisotropic temperature parameters of the heavier atoms. Table 3.4 contains the final observed and calculated structure factors. Orthogonal coordinates of the heavier atoms and of the hydrogen atoms are given respectively in Tables 3.5 and 3.6. Table 3.7 contains some results from a molecular vibrations analysis and Tables 3.8, 3.9, 3.10, and 3.11 present respectively bond lengths, interbond angles, intermolecular contacts, and the deviations from least-squares planes through various sets of atoms. Standard deviations, where quoted, are in units of the last place of the quantity to which they refer. The quantities in Tables 3.5 to 3.11 were calculated using the programmes described in Part II and the equations given there apply. A view of the molecular packing is given in Fig. 3.3.

3.4 ANALYSIS OF MOLECULAR VIBRATIONS

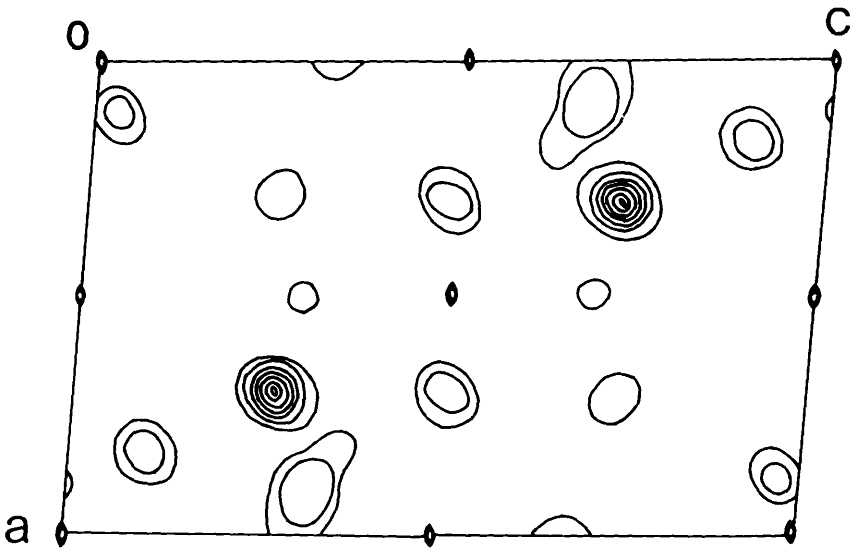
An analysis of the molecular vibrations was carried out in the manner suggested by Cruickshank (1956, 1961a). The results (Table 3.7 and Fig. 3.4) are very similar to those obtained for phenanthrene-chromium tricarbonyl. The translational vibration tensor is almost isotropic. The tensor of librational motion is anisotropic and almost diagonal; the principal values correspond to root mean square amplitudes of oscillation of 5½, 2 and 3° and the principal directions make angles of 10°, on average, with the molecular axes.

Though these results seem quite acceptable, the root mean square difference between the observed atomic vibration tensors, U_{obs}, and those calculated from the molecular vibration tensors, U_{cal}, is 0.0130 $\mathring{A}^2$. In terms of the standard deviations of the U_{obs} (Table 3.2) this difference is large, even allowing for the approximate nature of the rigid-body hypothesis. There is not any obvious reason for suspecting large systematic errors in the U_{obs}, and the poor agreement may therefore be due to deficiencies in the model used to describe the molecular vibrations (Schomaker and Trueblood, 1966). This view is supported by the similarity of these results with those for the corresponding phenanthrene compound.

Because of these difficulties, the libration corrections can only be accepted with reservations, and therefore the detailed discussion of the molecular structure has been conducted mainly in terms of the uncorrected coordinates. Correction for libration results in an average increase of 0.005 Å in the bond lengths and does not alter any of the main conclusions of the analysis.

FIG. 3.1

The sections at $V = \frac{1}{2}$ and $U = 0$ of the sharpened three-dimensional Patterson function corresponding to the $P2_1/m$ unit cell.


0
c
a

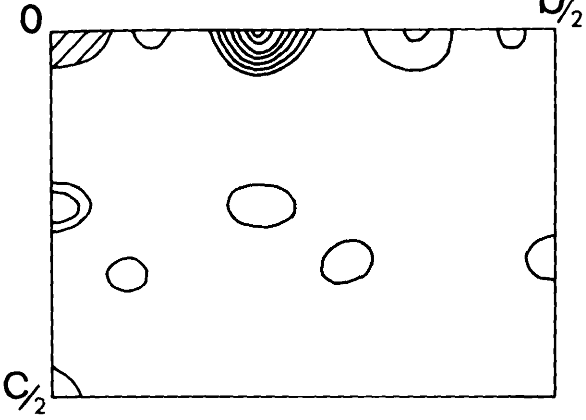

0
b/2
c/2

FIG. 3.2

The composite final electron density synthesis viewed down the b axis. Contours are at 1 e/Å^3 intervals starting at 2 e/Å^3 except round the chromium atom where the contours are at 5 e/Å^3 intervals starting at 5 e/Å^3. Some symmetry elements have been omitted for clarity.

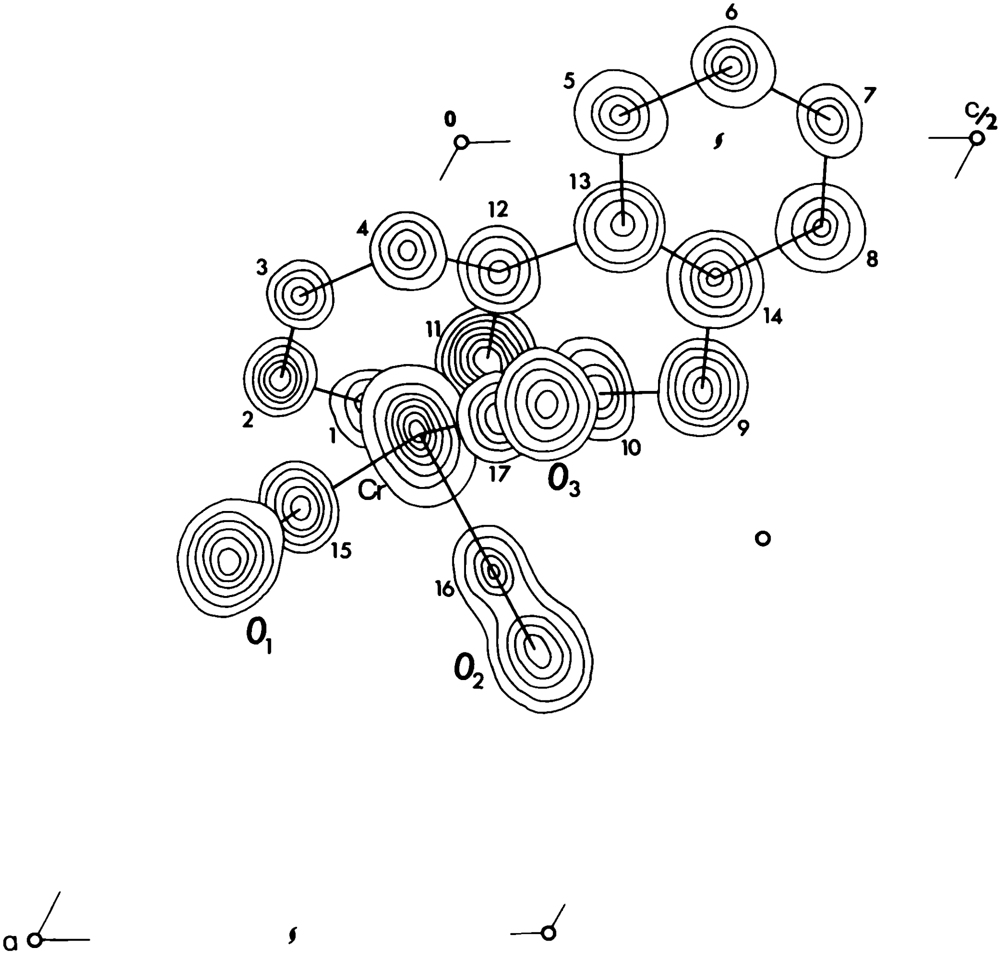

6
5
7
0
c/2
13
12
4
3
8
14
11
2
1
10
9
17
O_3
Cr
15
16
O_1
O_2
a

FIG. 3.3

The molecular packing viewed down the b axis. (Roman numerals have the same significance as in Table 3.10). Some symmetry elements have been omitted for the sake of clarity.

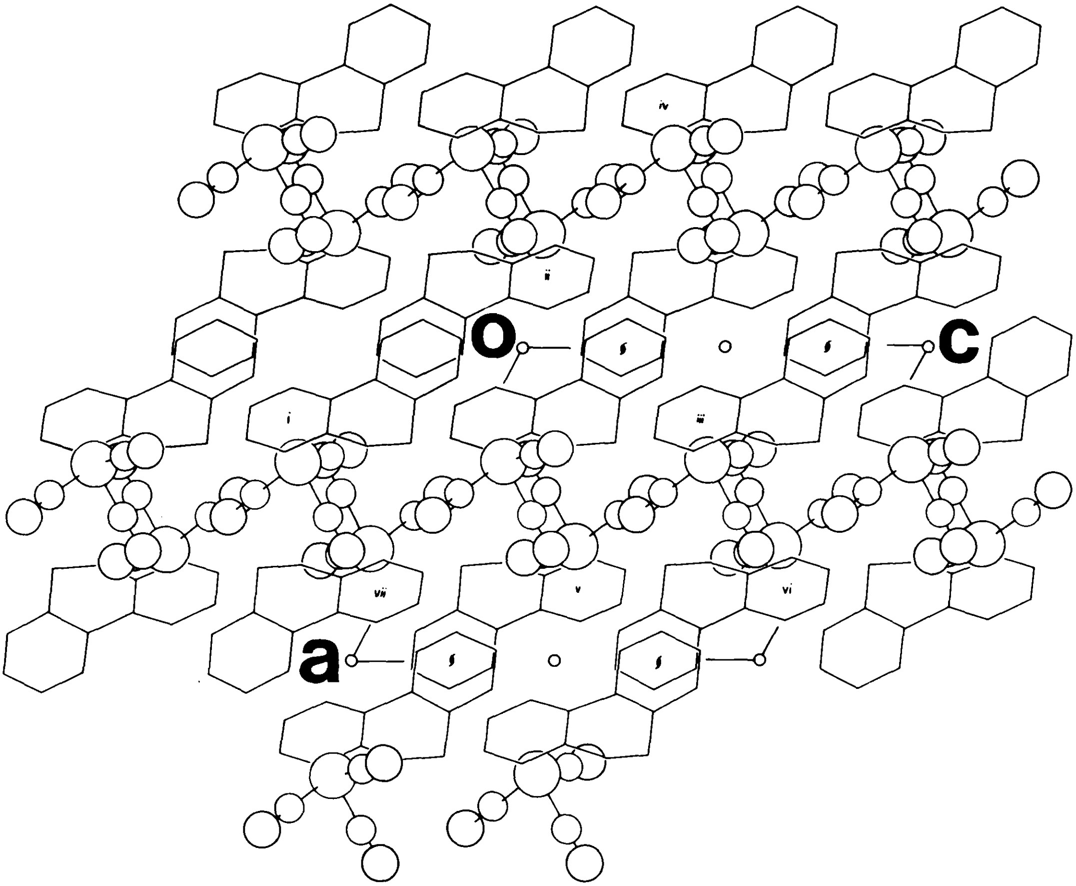

iv
ii
O
c
i
iii
a
vii
v
vi

FIG. 3.4

Molecular diagram showing the numbering of the heavier atoms and the bond lengths after libration correction in the dihydrophenanthrene ligand.

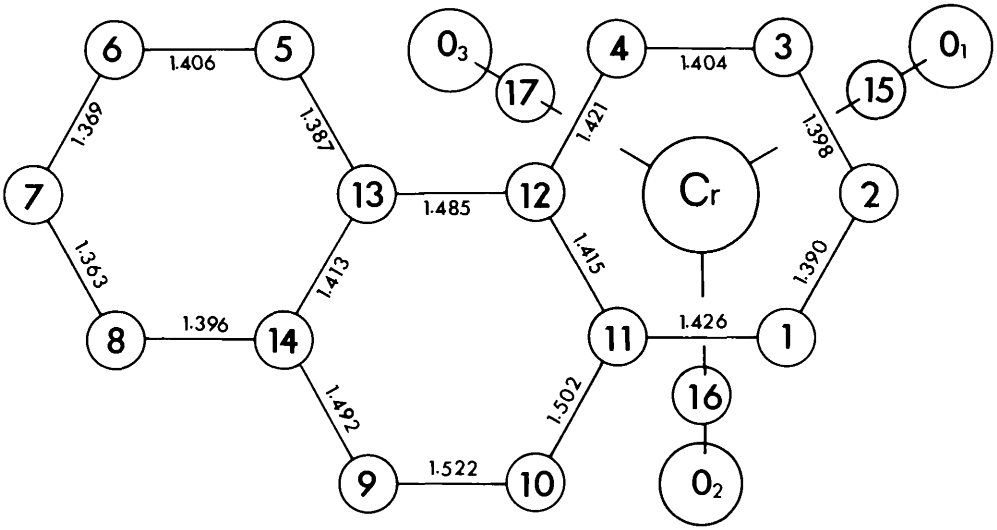

O3
17
O1
15
Cr
16
O2
1
2
3
4
5
6
7
8
9
10
11
12
13
14
1.406
1.369
1.387
1.363
1.413
1.396
1.485
1.492
1.522
1.502
1.415
1.421
1.404
1.398
1.390
1.426

TABLE 3.1

FRACTIONAL COORDINATES AND E.S.D.S.

ATOM	X/a	Y/b	Z/c
Cr(1)	0.36213 ± 6	0.14786 ± 4	0.10478 ± 5
C(1)	0.3306 ± 5	-0.0211 ± 3	0.0573 ± 4
C(2)	0.2883 ± 5	0.0348 ± 4	-0.0542 ± 4
C(3)	0.1837 ± 5	0.1132 ± 4	-0.0885 ± 4
C(4)	0.1239 ± 4	0.1371 ± 3	-0.0094 ± 4
C(5)	-0.0296 ± 4	0.1563 ± 4	0.1442 ± 5
C(6)	-0.0927 ± 5	0.1666 ± 5	0.2235 ± 6
C(7)	-0.0308 ± 6	0.1200 ± 5	0.3406 ± 6
C(8)	0.0961 ± 6	0.0664 ± 5	0.3842 ± 5
C(9)	0.3058 ± 5	0.0005 ± 4	0.3589 ± 4
C(10)	0.3130 ± 5	-0.0636 ± 4	0.2554 ± 5
C(11)	0.2697 ± 4	0.0008 ± 3	0.1381 ± 3
C(12)	0.1641 ± 4	0.0801 ± 3	0.1042 ± 3
C(13)	0.0982 ± 4	0.1002 ± 3	0.1870 ± 4
C(14)	0.1637 ± 5	0.0552 ± 4	0.3094 ± 3
C(15)	0.4635 ± 4	0.2177 ± 3	0.0403 ± 4
C(16)	0.5364 ± 4	0.1262 ± 4	0.2510 ± 4
C(17)	0.3401 ± 4	0.2711 ± 3	0.1730 ± 4

O(1)	0.5285 ± 4	0.2617 ± 3	0.0006 ± 3
O(2)	0.6454 ± 3	0.1138 ± 4	0.3405 ± 3
O(3)	0.3239 ± 4	0.3483 ± 3	0.2131 ± 4

TABLE 3.2

ASSUMED HYDROGEN ATOM FRACTIONAL COORDINATES AND TEMPERATURE FACTORS.

ATOM	X/a	Y/b	Z/c	U
H(1)	0.411	-0.084	0.082	0.070
H(2)	0.338	0.021	-0.115	0.076
H(3)	0.148	0.155	-0.179	0.067
H(4)	0.045	0.201	-0.035	0.064
H(5)	-0.080	0.192	0.048	0.079
H(6)	-0.192	0.215	0.192	0.099
H(7)	-0.083	0.122	0.401	0.115
H(8)	0.146	0.031	0.479	0.102
H(9)	0.393	0.058	0.393	0.078
H(10)	0.321	-0.052	0.436	0.078
H(11)	0.423	-0.093	0.291	0.078
H(12)	0.239	-0.130	0.233	0.078

TABLE 3.3

ANISOTROPIC TEMPERATURE FACTORS AND E.S.D.S.

ATOM	U11	U22	U33	2U23	2U31	2U12
Cr(1)	0.0383	0.0434	0.0356	-0.0033	0.0384	-0.0086
	2	3	2	4	4	4
C(1)	0.0620	0.0467	0.0708	-0.0165	0.0794	-0.0097
	22	19	24	33	40	31
C(2)	0.0730	0.0661	0.0544	-0.0343	0.0807	-0.0435
	25	24	21	35	40	39
C(3)	0.0595	0.0763	0.0355	-0.0048	0.0264	-0.0392
	22	27	17	32	32	39
C(4)	0.0402	0.0639	0.0482	0.0142	0.0191	-0.0088
	17	22	19	32	29	29
C(5)	0.0408	0.0699	0.0914	-0.0479	0.0577	-0.0133
	18	27	32	47	40	34
C(6)	0.0465	0.0859	0.1260	-0.0947	0.0952	-0.0367
	21	34	44	64	53	42
C(7)	0.0760	0.1016	0.1076	-0.0863	0.1320	-0.0576
	31	40	41	66	63	57
C(8)	0.0778	0.1067	0.0755	-0.0553	0.1097	-0.0653
	30	41	29	56	53	57
C(9)	0.0619	0.0856	0.0546	0.0361	0.0611	0.0050
	23	31	22	42	39	43
C(10)	0.0639	0.0632	0.0708	0.0438	0.0799	0.0176
	23	24	25	39	42	37
C(11)	0.0444	0.0457	0.0490	0.0008	0.0466	-0.0070
	16	17	17	26	29	25
C(12)	0.0370	0.0489	0.0480	-0.0056	0.0382	-0.0094
	15	17	17	26	27	24

C(13)	0.0351	0.0524	0.0546	-0.0151	0.0424	-0.0144
	14	18	19	29	28	25
C(14)	0.0548	0.0679	0.0649	-0.0203	0.0761	-0.0352
	20	24	23	37	38	35
C(15)	0.0572	0.0566	0.0457	-0.0156	0.0588	-0.0165
	20	20	18	29	32	31
C(16)	0.0467	0.0750	0.0498	0.0067	0.0561	-0.0017
	18	25	19	34	32	33
C(17)	0.0501	0.0616	0.0464	-0.0070	0.0501	-0.0153
	18	21	18	30	31	31
O(1)	0.0895	0.0784	0.0711	-0.0135	0.1114	-0.0507
	23	21	19	32	36	35
O(2)	0.0486	0.1338	0.0556	0.0259	0.0384	0.0281
	16	34	17	38	27	37
O(3)	0.0963	0.0613	0.0795	-0.0445	0.1021	-0.0021
	24	19	21	31	39	33

TABLE 3.4

Observed and calculated structure factors.

H	K	L	F OBS	F CALC
0	0	-14	10.0	-10.5
0	0	-12	4.6	3.6
0	0	-10	16.7	17.2
0	0	-8	23.6	-23.7
0	0	-6	11.7	-13.3
0	0	-4	61.0	-60.9
0	0	-2	14.9	-15.0
1	0	-14	9.4	6.7
1	0	-12	12.2	11.4
1	0	-10	15.3	-14.6
1	0	-8	35.0	-34.8
1	0	-6	2.6	-3.3
1	0	-4	30.8	-25.7
1	0	2	99.0	-105.2
1	0	4	5.2	2.1
1	0	6	47.4	45.9
1	0	8	1.6	1.4
1	0	10	4.9	-3.6
1	0	12	9.2	-9.5
2	0	-14	5.4	-6.1
2	0	-12	10.0	-10.1
2	0	-10	9.0	-8.6
2	0	-8	36.1	38.5
2	0	-6	42.3	42.7
2	0	-4	40.3	38.9
2	0	0	34.1	-33.4
2	0	2	123.4	132.8
2	0	4	44.2	44.3
2	0	6	2.4	-2.0
2	0	8	12.6	-12.7
2	0	12	11.4	10.6
3	0	-14	4.4	-5.4
3	0	-12	6.6	5.6
3	0	-10	10.5	-11.9
3	0	-8	1.9	-4.0
3	0	-6	22.9	-23.1
3	0	-4	74.6	-78.0
3	0	-2	4.0	-2.8
3	0	0	87.3	93.9
3	0	2	61.4	-63.0
3	0	4	65.8	-69.1
3	0	6	4.9	-4.4
3	0	8	11.4	12.0
3	0	10	3.4	3.2
3	0	12	7.0	-6.6
4	0	-14	10.7	19.2
4	0	-12	9.2	8.6
4	0	-10	54.0	-56.4
4	0	-8	18.7	-19.0
4	0	-6	41.9	41.9
4	0	-4	24.9	24.4
4	0	-2	44.4	44.0
4	0	0	83.3	-87.6
4	0	2	22.7	-23.7
4	0	4	47.2	47.8
4	0	6	18.7	18.5
4	0	8	2.3	1.5
4	0	10	12.5	-11.4
5	0	-14	10.5	-10.8
5	0	-12	10.1	-12.0
5	0	-10	15.2	15.0
5	0	-8	28.0	29.9
5	0	-6	18.2	19.4
5	0	-4	73.0	-75.6
5	0	-2	53.3	-56.7
5	0	0	46.9	-39.3
5	0	2	54.0	55.3
5	0	4	16.8	-16.2
5	0	6	25.0	-26.7
5	0	8	10.9	-10.5
6	0	-14	4.2	-4.0
6	0	-12	23.3	22.8
6	0	-10	14.0	16.5
6	0	-8	16.7	-17.2
6	0	-6	30.3	-30.9
6	0	-4	8.5	-8.7
6	0	-2	47.2	49.3
6	0	0	55.1	55.6
6	0	2	18.4	-27.0
6	0	4	21.2	-20.7
6	0	6	5.2	4.3
6	0	8	6.7	8.0
7	0	-14	15.0	15.3
7	0	-12	8.4	-7.5
7	0	-10	24.0	-23.5
7	0	-8	8.7	-7.8
7	0	-6	40.0	39.5
7	0	-4	37.9	38.5
7	0	-2	6.0	-7.1
7	0	0	38.3	-31.2
7	0	2	5.9	6.0
7	0	4	12.6	13.2
7	0	6	2.6	2.2
7	0	8	2.3	-3.8
8	0	-14	5.5	-6.9
8	0	-12	6.7	-9.1
8	0	-10	20.4	18.2
8	0	-8	17.0	17.7
8	0	-6	8.3	-9.5
8	0	-4	26.0	-27.6
8	0	-2	17.7	-17.1
8	0	0	12.0	12.1
8	0	2	27.1	27.1
8	0	4	9.5	-9.4
8	0	6	1.7	0.8
9	0	-14	4.7	2.7
9	0	-12	14.1	13.9
9	0	-10	3.3	4.3
9	0	-8	14.0	-16.7
9	0	-6	18.1	-19.2
9	0	-4	27.4	28.4
9	0	-2	29.2	29.6
9	0	0	3.5	5.2
9	0	2	23.6	-24.0
9	0	4	8.7	8.1
10	0	-14	6.7	7.4
10	0	-10	21.5	-21.7
10	0	-8	2.7	1.2
10	0	-6	25.4	25.9
10	0	-4	7.8	7.4
10	0	-2	19.0	-19.6
10	0	0	14.7	-13.4
10	0	2	6.1	7.7
10	0	4	18.5	9.9
11	0	-14	10.2	-15.1
11	0	-12	2.3	6.3
11	0	-10	14.7	14.3
11	0	-8	10.4	9.9
11	0	-6	6.3	-6.7
11	0	-4	19.3	-20.3
11	0	-2	8.0	-9.2
11	0	0	18.0	19.1
11	0	2	5.2	5.3
12	0	-14	6.1	6.0
12	0	-10	3.2	8.6
12	0	-8	15.0	-13.4
12	0	-6	7.2	-7.1
12	0	-2	5.2	6.0
12	0	0	5.1	-4.0
13	0	-10	7.7	-7.9
13	0	-8	13.1	12.6
13	0	-6	5.3	4.9
13	0	-4	5.4	5.0
13	0	-2	6.0	-4.0
14	0	-10	7.7	7.0
14	0	-8	3.4	-2.2
14	0	-6	7.2	-7.2
15	0	-10	9.6	-9.4
0	1	-15	3.7	-3.9
0	1	-14	4.6	-0.3
0	1	-13	5.3	-5.3
0	1	-12	12.9	12.5
0	1	-11	8.8	7.7
0	1	-10	7.1	7.7
0	1	-9	14.0	14.8
0	1	-8	25.2	-24.5
0	1	-7	13.5	-13.2
0	1	-6	8.5	-8.4
0	1	-5	57.3	-55.5
0	1	-4	3.6	2.9
0	1	-3	40.7	38.3
0	1	-2	75.8	77.9
1	1	-15	3.4	-1.0
1	1	-14	6.1	5.8
1	1	-13	7.7	7.9
1	1	-12	9.9	-10.0
1	1	-11	8.9	9.4
1	1	-10	29.2	-29.0
1	1	-9	7.1	-5.8
1	1	-8	8.7	9.9
1	1	-7	29.0	-25.5
1	1	-6	26.2	27.3
1	1	-5	21.1	21.3
1	1	-4	12.0	12.9
1	1	-3	38.7	37.0
1	1	-2	72.3	-75.5
1	1	1	78.6	-78.7
1	1	2	28.4	-22.2
1	1	3	45.8	-45.1
1	1	4	59.9	-62.1
1	1	5	47.1	46.5
1	1	6	5.7	-12.1
1	1	7	29.5	28.6
1	1	8	14.9	14.1
1	1	9	6.1	-6.4
1	1	10	13.7	13.9
1	1	11	9.0	-8.5
1	1	12	6.7	-7.7
2	1	-15	3.4	-0.8
2	1	-14	10.1	-10.4
2	1	-13	4.4	-4.1
2	1	-12	9.2	-8.0
2	1	-11	4.9	-6.2
2	1	-10	14.7	14.2
2	1	-9	4.0	-4.5
2	1	-8	15.0	15.5
2	1	-7	37.3	37.6
2	1	-6	25.1	-25.4
2	1	-5	18.8	17.4
2	1	-4	27.7	-27.4
2	1	-3	73.4	-69.4
2	1	-2	17.6	-18.4
2	1	-1	47.3	-43.9
2	1	0	41.2	-40.5
2	1	0	40.9	40.5
2	1	1	32.9	-29.7
2	1	2	14.4	11.4
2	1	3	30.7	32.0
2	1	4	41.6	42.4
2	1	5	36.4	32.1
2	1	6	30.2	29.2
2	1	7	28.2	-21.2
2	1	8	0.6	1.5
2	1	9	2.8	-1.1
2	1	10	9.7	-9.1
2	1	12	2.4	1.7
3	1	-15	4.5	-5.9
3	1	-14	12.2	11.1
3	1	-13	2.3	-5.7
3	1	-12	19.1	19.0
3	1	-11	15.1	14.8
3	1	-10	8.9	-8.7
3	1	-9	12.2	-12.7
3	1	-8	30.3	-39.0
3	1	-7	20.7	-20.8
3	1	-6	8.9	-7.9
3	1	-5	20.7	-21.0
3	1	-4	20.5	29.1
3	1	-3	70.5	67.4
3	1	-2	20.3	29.3
3	1	-1	6.1	7.5
3	1	0	10.0	-10.7
3	1	1	18.8	17.7
3	1	2	61.6	61.6
3	1	3	14.0	-15.7
3	1	4	10.4	-11.2
3	1	5	23.7	-23.3
3	1	6	19.4	-19.7
3	1	7	1.3	-0.2
3	1	8	13.3	-13.6
3	1	9	12.3	14.1
3	1	10	9.0	8.4
3	1	12	5.3	5.0
4	1	-15	5.9	5.0
4	1	-14	8.7	8.2
4	1	-13	8.3	8.0
4	1	-12	18.5	-17.8
4	1	-11	17.0	-17.1
4	1	-10	16.2	-16.9
4	1	-9	15.2	-15.9
4	1	-8	20.4	20.0
4	1	-7	20.2	-20.6
4	1	-6	10.6	10.2
4	1	-5	32.3	32.2
4	1	-4	49.0	-70.5
4	1	-3	2.8	4.4
4	1	-2	38.5	-39.0
4	1	-1	15.2	-14.9
4	1	0	6.6	-10.0
4	1	1	27.5	-26.5
4	1	2	34.2	-35.0
4	1	3	14.5	-13.8
4	1	4	4.6	-4.6
4	1	5	11.0	12.9
4	1	6	11.6	11.8
4	1	7	13.1	13.9
4	1	8	18.2	17.9
4	1	9	11.1	-12.2
4	1	10	1.4	2.6
5	1	-15	2.3	2.6
5	1	-14	9.5	-9.6
5	1	-13	7.6	-8.9
5	1	-12	14.4	13.7
5	1	-11	5.9	-4.8
5	1	-10	30.8	30.7
5	1	-9	32.1	32.2
5	1	-8	22.1	21.9
5	1	-7	33.7	33.9
5	1	-6	40.6	-40.3
5	1	-5	55.4	-52.8
5	1	-4	4.1	0.9
5	1	-3	45.7	-43.6
5	1	-2	2.0	1.0
5	1	-1	24.7	-21.7
5	1	0	60.7	71.6
5	1	1	26.4	26.0
5	1	2	3.5	3.0
5	1	3	10.2	9.0
5	1	4	26.3	26.3
5	1	5	10.3	-10.5
5	1	6	2.0	0.1
5	1	7	13.0	-12.0
5	1	8	10.0	-10.3
5	1	9	2.7	2.0
6	1	-15	18.4	-18.7
6	1	-14	10.6	9.9
6	1	-13	8.6	1.7
6	1	-12	8.6	8.9
6	1	-11	10.9	10.8
6	1	-10	17.5	-17.6
6	1	-9	3.3	3.8
6	1	-8	39.5	-40.6
6	1	-7	27.9	-28.9
6	1	-6	20.1	20.9
6	1	-5	21.6	-20.3
6	1	-4	21.8	22.5
6	1	-3	34.9	33.1
6	1	-2	14.2	13.8
6	1	-1	8.4	4.6
6	1	0	15.6	-16.6
6	1	1	13.6	17.8
6	1	2	14.3	14.0
6	1	3	1.4	1.7
6	1	4	4.6	-5.2
6	1	5	24.9	-25.9
6	1	6	28.8	-20.5
6	1	7	4.9	4.4
6	1	8	2.0	1.8
7	1	-15	5.1	5.6
7	1	-14	3.8	-1.1
7	1	-13	3.1	4.8
7	1	-12	8.4	-7.9
7	1	-11	18.9	-12.7
7	1	-10	2.2	-1.1
7	1	-9	13.2	-13.3
7	1	-8	43.8	44.5
7	1	-7	19.8	19.8
7	1	-6	20.2	20.6
7	1	-5	32.8	31.7
7	1	-4	12.9	-13.8
7	1	-3	4.3	4.8
7	1	-2	21.5	-22.8
7	1	-1	18.8	-17.2
7	1	0	8.4	8.9
7	1	1	2.3	2.4
7	1	2	19.7	-19.3
7	1	3	5.7	6.4
7	1	4	4.6	-5.3
7	1	5	5.1	6.8
7	1	6	3.5	2.7
7	1	8	0.8	2.1
8	1	-15	3.1	1.8
8	1	-14	9.0	-9.8
8	1	-13	3.3	-4.5
8	1	-12	5.7	5.3
8	1	-11	1.6	-2.4
8	1	-10	7.8	6.5
8	1	-9	22.8	22.3
8	1	-8	21.6	-21.7
8	1	-7	6.7	6.1
8	1	-6	20.7	-22.4
8	1	-5	8.1	-8.1
8	1	-4	12.6	-12.8
8	1	-3	33.8	-32.9
8	1	-2	19.0	19.8
8	1	-1	12.4	11.4
8	1	0	12.6	12.9
8	1	1	7.1	7.5
8	1	2	6.5	8.6
8	1	3	3.3	3.4
8	1	4	13.9	14.3
8	1	5	2.2	-0.6
8	1	6	5.0	-5.3
9	1	-15	0.7	8.4
9	1	-14	13.6	12.6
9	1	-13	3.8	2.3
9	1	-12	6.2	6.7
9	1	-11	18.9	19.5
9	1	-10	18.2	-18.8
9	1	-9	19.8	-20.8
9	1	-8	3.7	-3.3
9	1	-7	10.5	-19.2
9	1	-6	33.3	39.8
9	1	-5	20.6	21.7
9	1	-4	2.2	3.1
9	1	-3	22.1	21.4
9	1	-2	2.1	-4.6
9	1	-1	4.6	-4.6
9	1	0	10.6	-10.9
9	1	1	2.9	-2.9
9	1	2	7.8	7.4
9	1	3	6.3	-6.6
9	1	4	7.9	-7.3
9	1	5	2.2	0.0
10	1	-15	3.5	3.7
10	1	-14	9.9	-10.3
10	1	-13	8.7	-8.9
10	1	-12	15.5	-15.9
10	1	-11	18.5	-18.6
10	1	-10	0.6	-0.9
10	1	-9	11.4	-11.4
10	1	-8	10.1	9.6
10	1	-7	1.1	0.4
10	1	-6	3.9	9.7
10	1	-5	30.5	34.6
10	1	-4	30.4	-34.3
10	1	-3	9.9	-10.9
10	1	-2	6.5	-6.8
10	1	-1	12.6	-12.5
10	1	0	8.3	6.7
10	1	1	8.9	8.4
10	1	2	9.2	-9.1
10	1	3	4.9	5.9
10	1	4	1.7	2.7
11	1	-15	2.4	-2.4
11	1	-14	1.7	0.3
11	1	-13	1.9	-3.3
11	1	-12	17.9	17.0
11	1	-11	4.8	3.9
11	1	-10	7.5	7.1
11	1	-9	10.3	11.9
11	1	-8	6.7	-6.5
11	1	-7	1.0	-2.8
11	1	-6	3.1	-3.6
11	1	-5	14.1	-12.1
11	1	-4	3.1	8.6
11	1	-3	11.4	-12.1
11	1	-2	6.1	7.1
11	1	-1	4.2	6.9
11	1	0	2.8	4.1
11	1	1	7.4	8.0
11	1	2	9.4	8.9
12	1	-15	3.9	-2.8
12	1	-14	8.3	8.3
12	1	-11	5.9	6.7
12	1	-10	15.7	-14.9
12	1	-8	8.7	-2.8
12	1	-7	7.5	-7.4
12	1	-6	14.9	13.9
12	1	-5	8.6	-8.7
12	1	-4	8.1	-8.7
12	1	-3	6.4	4.6
12	1	-2	5.9	-6.9
12	1	-1	2.0	-0.8
12	1	0	5.4	-5.5
13	1	-10	7.5	6.8
13	1	-8	10.8	10.4
13	1	-7	7.9	7.4
13	1	-6	4.9	-3.9
13	1	-4	2.8	-3.4
13	1	-3	3.9	-1.9
13	1	-2	6.8	9.6
14	1	-10	4.9	-4.2
14	1	-6	3.1	-3.1
0	2	-14	5.7	3.9
0	2	-13	6.4	6.9
0	2	-12	2.9	-2.9
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H	K	L	F OBS	F CALC
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6	5	-7	8.5	-8.9
6	5	-6	41.3	-41.4
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6	5	-2	3.7	-3.9
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7	5	-14	12.6	11.7
7	5	-13	2.4	-1.5
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H	K	L	F OBS	F CALC
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6	7	-12	4.2	1.5
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3	9	-10	3.9	-4.2
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3	9	-5	22.3	21.6
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11	9	-4	7.8	5.9
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H	K	L	F OBS	F CALC
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2	11	3	9.6	-9.9
2	11	4	3.4	-3.5
2	11	5	2.6	-1.7
2	11	6	5.1	-5.1
2	11	7	7.5	0.2
2	11	8	0.6	-1.6
2	11	9	3.2	2.5
2	11	10	4.1	4.5
2	11	12	2.7	2.8
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3	11	-12	2.0	-2.0
3	11	-11	7.0	-7.5
3	11	-10	3.4	-0.1
3	11	-9	0.0	-9.4
3	11	-8	7.7	6.3
3	11	-7	6.2	6.6
3	11	-6	6.7	-6.5
3	11	-5	17.4	18.0
3	11	-4	12.2	-12.1
3	11	-3	7.7	-8.2
3	11	-2	19.0	-18.6
3	11	-1	15.1	-15.9
3	11	0	6.2	6.3
3	11	1	4.2	-4.8
3	11	2	19.0	-18.9
3	11	3	15.9	15.9
3	11	4	3.0	3.0
3	11	5	9.2	9.7
3	11	6	6.0	5.8
3	11	7	3.7	-3.2
3	11	8	0.6	-0.2
3	11	9	3.9	-4.1
3	11	10	3.2	-3.2
4	11	-14	0.7	2.2
4	11	-13	3.2	-3.5
4	11	-12	4.0	4.7
4	11	-11	2.8	1.4
4	11	-10	7.3	6.9
4	11	-9	12.7	12.6
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4	11	-5	17.0	-17.3
4	11	-4	5.2	5.5
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4	11	-2	21.1	21.1
4	11	-1	14.7	15.2
4	11	0	4.7	5.3
4	11	1	6.2	5.5
4	11	2	2.3	2.9
4	11	3	1.5	1.5
4	11	4	11.7	11.8
4	11	5	5.7	-5.7
4	11	6	2.2	-2.4
4	11	7	3.5	-3.2
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5	11	-14	3.3	2.9
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6	11	2	14.3	-14.3
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6	11	4	2.5	0.4
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6	11	7	4.0	-5.0
6	11	8	0.7	1.2
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7	11	1	2.3	1.2
7	11	2	9.9	9.6
7	11	3	5.6	-5.4
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7	11	6	2.8	-3.0
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9	11	-13	2.0	-2.4
9	11	-12	4.9	3.7
9	11	-11	5.0	-5.1
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1	13	10	2.9	-1.6
1	13	12	3.6	2.4
2	13	-14	0.7	1.9
2	13	-13	3.2	-2.2
2	13	-12	1.9	1.3
2	13	-11	5.1	-4.2
2	13	-10	3.1	-2.7
2	13	-9	4.1	-4.1
2	13	-8	1.6	0.3
2	13	-7	6.3	6.4
2	13	-6	3.7	2.9
2	13	-5	3.1	3.8
2	13	-4	8.7	8.3
2	13	-3	10.0	-10.2
2	13	-2	1.2	-1.6
2	13	-1	7.0	-8.1
2	13	0	7.1	-7.3
2	13	1	4.8	5.7
2	13	2	4.4	5.1
2	13	3	8.9	9.5
2	13	4	9.5	-7.8
2	13	5	1.9	1.3
2	13	6	2.6	-1.9
2	13	7	7.3	-7.9
2	13	8	1.4	-1.6
2	13	9	1.9	-2.2
2	13	10	2.7	2.3
2	13	12	0.7	-5.3
3	13	-14	0.7	-4.7
3	13	-13	1.7	1.2
3	13	-12	2.8	-3.9
3	13	-11	6.6	7.1
3	13	-10	2.6	1.3
3	13	-9	3.6	4.2
3	13	-8	0.8	8.3
3	13	-7	2.3	-2.4
3	13	-6	2.8	-2.3
3	13	-5	9.5	-9.6
3	13	-4	3.4	-2.9
3	13	-3	1.6	1.6
3	13	-2	4.8	-4.5
3	13	-1	0.5	8.7
3	13	0	6.9	6.7
3	13	1	5.9	6.4
3	13	2	13.0	-13.6
3	13	3	6.2	-6.1
3	13	4	0.9	0.5
3	13	5	0.1	-0.2
3	13	6	3.3	2.5
3	13	7	3.2	3.7
3	13	8	0.6	-0.3
3	13	9	4.3	5.4
3	13	10	3.6	-2.6
4	13	-14	2.9	0.6
4	13	-13	1.9	2.3
4	13	-12	1.2	1.5
4	13	-11	4.4	-4.6
4	13	-10	1.9	1.6

H	K	L	F OBS	F CALC
4	13	-9	7.4	-7.2
4	13	-8	6.1	-3.5
4	13	-7	1.0	0.1
4	13	-6	9.9	-9.4
4	13	-5	6.3	6.2
4	13	-4	1.6	0.4
4	13	-3	2.9	3.3
4	13	-2	5.7	4.9
4	13	-1	9.8	-9.2
4	13	0	1.9	-0.7
4	13	1	6.5	-7.4
4	13	2	2.5	2.0
4	13	3	3.7	-4.1
4	13	4	5.0	5.6
4	13	5	8.4	9.0
4	13	6	3.0	-2.4
4	13	7	2.0	3.0
4	13	8	3.0	-2.5
4	13	9	3.7	-3.0
5	13	-14	2.4	0.9
5	13	-13	5.4	-5.0
5	13	-12	2.7	-2.7
5	13	-11	3.5	-4.4
5	13	-10	3.1	-3.6
5	13	-9	5.4	5.0
5	13	-8	3.5	3.3
5	13	-7	11.9	11.9
5	13	-6	5.9	5.4
5	13	-5	0.6	0.4
5	13	-4	6.9	6.1
5	13	-3	14.9	-14.9
5	13	-2	3.0	-2.7
5	13	-1	0.4	1.5
5	13	0	6.4	-6.5
5	13	1	9.0	9.2
5	13	2	2.7	-3.4
5	13	3	5.1	5.1
5	13	4	3.1	-1.0
5	13	5	2.0	-2.3
5	13	6	8.4	0.5
5	13	7	5.1	-5.9
5	13	8	3.0	2.2
6	13	-14	0.7	-2.0
6	13	-13	1.5	0.9
6	13	-12	1.7	-0.6
6	13	-11	7.7	7.6
6	13	-10	3.1	1.3
6	13	-9	2.7	-2.5
6	13	-8	4.4	4.1
6	13	-7	9.4	-9.1
6	13	-6	6.0	-6.2
6	13	-5	6.0	-6.9
6	13	-4	7.7	-6.9
6	13	-3	6.7	4.0
6	13	-2	7.2	-7.0
6	13	-1	4.0	4.9
6	13	0	4.0	2.6
6	13	1	1.2	1.7
6	13	2	6.0	-1.2
6	13	3	5.0	-6.0
6	13	4	2.9	3.3
6	13	5	1.7	-2.9
6	13	6	1.7	-1.0
7	13	-14	0.7	1.0
7	13	-13	2.7	4.6
7	13	-12	2.0	1.5
7	13	-11	3.7	-3.9
7	13	-10	0.0	-0.3
7	13	-9	3.2	-4.1
7	13	-8	9.2	-0.0
7	13	-7	1.7	1.9
7	13	-6	0.5	1.7
7	13	-5	12.1	11.0
7	13	-4	3.9	4.1
7	13	-3	1.5	1.2
7	13	-2	6.9	6.1
7	13	-1	4.0	-5.1
7	13	0	1.5	-0.9
7	13	1	2.9	-2.9
7	13	2	3.0	3.3
7	13	3	2.1	0.0
7	13	4	3.2	1.0
7	13	5	3.1	2.7
7	13	6	3.0	-3.2
8	13	-14	1.7	0.1
8	13	-13	3.1	-4.1
8	13	-12	3.0	-1.4
8	13	-11	2.1	-1.9
8	13	-10	2.6	-1.1
8	13	-9	4.0	5.2
8	13	-8	4.1	2.4
8	13	-7	3.9	4.7
8	13	-6	6.0	5.9
8	13	-5	6.7	-6.7
8	13	-3	7.2	-7.2
8	13	-2	7.5	-5.7
8	13	-1	5.0	4.9
8	13	0	2.3	-1.5
8	13	1	4.3	4.3
8	13	2	0.9	0.0
8	13	3	6.9	-0.3
8	13	4	0.7	-0.9
8	13	5	3.7	-3.3
9	13	-14	2.4	-1.5
9	13	-13	4.9	3.0
9	13	-11	3.9	4.0
9	13	-10	5.2	4.4
9	13	-9	2.0	-2.7
9	13	-8	1.7	0.9
9	13	-7	7.1	-6.7
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9	13	-5	0.5	0.0
9	13	-4	3.2	-2.4
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9	13	-2	2.3	2.4
9	13	-1	2.0	3.0
9	13	0	0.9	4.6
9	13	1	3.2	-3.9
9	13	2	2.5	-1.4
9	13	3	2.9	-0.9
9	13	4	2.5	0.0
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10	13	-11	4.1	-4.4
10	13	-10	2.4	-2.1
10	13	-9	2.0	-3.4
10	13	-8	4.1	-2.3
10	13	-7	2.9	4.5
10	13	-6	1.6	1.7
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10	13	-4	3.0	2.3
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10	13	-2	3.4	1.2
10	13	-1	7.2	-7.7
10	13	0	3.7	-2.6
10	13	1	2.0	-0.9
10	13	2	2.1	0.5
11	13	-11	1.7	-0.4
11	13	-10	1.9	-0.6
11	13	-9	4.3	5.5
11	13	-8	4.9	3.9
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11	13	0	2.1	0.2
12	13	-11	0.7	1.7
12	13	-10	1.9	1.7
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12	13	-4	2.5	-0.6
12	13	-3	4.2	4.7
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13	13	-10	2.0	-2.7
13	13	-7	1.4	0.5
13	13	-6	1.0	0.6
13	13	-3	1.9	-0.7
0	14	-12	3.6	-1.1
0	14	-10	3.4	4.1
0	14	-9	1.3	-0.0
0	14	-8	7.7	7.5
0	14	-7	5.0	-6.3
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0	14	-3	2.9	6.7
0	14	-2	1.7	1.9
0	14	-1	0.4	1.9
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1	14	-4	10.6	10.9
1	14	-3	2.0	-1.1
1	14	-1	1.3	0.1
1	14	1	0.0	4.0
1	14	2	11.1	-11.0
1	14	3	6.2	-4.5
1	14	4	1.7	1.3
1	14	5	1.1	-2.0
1	14	6	0.7	0.0
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1	14	8	3.2	3.0
1	14	9	2.9	3.0
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1	14	12	2.0	-1.5
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2	14	-11	1.1	1.6
2	14	-10	3.6	-3.6
2	14	-9	4.0	3.6
2	14	-8	2.0	1.0
2	14	-7	0.2	6.0
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2	14	-4	1.2	0.6
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2	14	-1	1.2	2.4
2	14	0	3.0	-3.0
2	14	1	1.3	-1.0
2	14	2	13.4	13.0
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2	14	9	1.6	-1.7
2	14	10	3.2	0.6
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3	14	-2	1.4	-6.6
3	14	-1	0.3	-0.6
3	14	0	9.0	9.4
3	14	1	1.2	3.2
3	14	2	3.0	-3.6
3	14	3	2.9	0.6
3	14	4	9.2	-9.5
3	14	5	3.0	-2.4
3	14	6	1.2	-1.0
3	14	7	4.6	-4.9
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3	14	9	0.6	0.5
4	14	-14	3.4	2.7
4	14	-13	2.0	-1.2
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4	14	-10	7.7	-6.5
4	14	-9	2.6	0.6
4	14	-8	7.2	-7.5
4	14	-7	4.5	4.1
4	14	-6	7.1	6.0
4	14	-5	3.9	3.1
4	14	-4	6.3	6.1
4	14	-3	0.3	-4.2
4	14	-2	3.5	-3.7
4	14	-1	2.2	-0.3
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4	14	7	2.6	2.9
4	14	8	0.6	-2.9
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5	14	-14	3.3	-3.0
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5	14	1	4.7	-2.1
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5	14	8	4.2	-4.2
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6	14	-4	1.5	1.1
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7	14	-11	2.7	-3.6
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7	14	-8	3.5	-2.2
7	14	-7	2.0	2.9
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7	14	-4	5.5	4.7
7	14	-3	0.5	-4.1
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7	14	4	3.9	3.1
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7	14	6	2.4	1.3
7	14	8	3.2	-1.3
8	14	-14	3.7	-3.0
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8	14	-9	1.5	1.7
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11	14	-2	0.9	1.1
11	14	-1	1.0	1.7
11	14	1	0.7	0.4
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13	14	-6	0.7	1.2
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2	15	-7	2.3	-1.5
2	15	-6	3.3	-3.1
2	15	-5	2.7	1.4
2	15	-4	6.6	-5.9
2	15	-3	1.0	2.0
2	15	-2	1.9	-2.2
2	15	-1	2.4	-2.9
2	15	0	11.7	11.3
2	15	1	2.5	3.3
2	15	2	2.0	-2.0
2	15	3	3.5	3.7
2	15	4	6.5	6.2
2	15	5	1.4	-1.2
2	15	6	6.2	5.4
2	15	7	0.5	-0.6
2	15	8	6.6	-0.2
2	15	9	1.3	-0.2
2	15	10	2.5	-2.7
3	15	-12	3.1	2.9
3	15	-10	2.2	-1.0
3	15	-9	0.7	-0.4
3	15	-8	6.2	-5.9
3	15	-7	2.1	-2.7
3	15	-6	3.0	-3.3
3	15	-5	0.7	-0.7
3	15	-4	2.9	2.4
3	15	-3	3.3	-3.1
3	15	-2	3.1	2.0
3	15	-1	2.4	-2.0
3	15	0	7.7	-6.6
3	15	1	1.0	0.5
3	15	2	8.2	7.6
3	15	3	3.3	-3.4
3	15	4	2.6	-2.6
3	15	5	1.3	0.1
3	15	6	7.4	-6.4
3	15	7	1.4	1.4
3	15	8	4.3	-1.4
3	15	9	1.7	0.9
4	15	-14	3.1	-0.5
4	15	-12	5.7	-4.7
4	15	-11	2.7	-1.0
4	15	-10	3.9	-3.2
4	15	-9	3.1	2.6
4	15	-8	8.0	7.1
4	15	-7	1.5	-1.7
4	15	-6	8.1	7.1
4	15	-5	2.1	3.1
4	15	-4	0.4	-0.4
4	15	-3	1.9	-2.2
4	15	-2	6.4	-5.6
4	15	-1	1.4	1.2
4	15	0	2.2	-1.9
4	15	1	3.5	-2.9
4	15	2	9.2	-0.5
4	15	3	0.4	-0.3
4	15	4	4.1	-4.7
4	15	5	1.0	1.0
4	15	6	4.1	3.5
4	15	7	1.5	0.2
4	15	8	4.3	4.4
4	15	9	1.7	-2.3
5	15	-14	2.0	-2.2
5	15	-13	3.4	-3.0
5	15	-12	1.5	1.6
5	15	-11	1.0	-0.5
5	15	-10	8.5	7.0
5	15	-9	1.5	0.5
5	15	-8	0.5	2.0
5	15	-7	1.5	-1.2
5	15	-6	9.1	-7.9
5	15	-5	1.7	-1.3
5	15	-4	7.6	-6.5
5	15	-3	0.4	-1.0
5	15	-2	5.4	4.7
5	15	-1	0.0	-0.4
5	15	0	8.0	7.2
5	15	1	2.0	2.6
5	15	2	3.7	3.8
5	15	3	2.2	-3.1
5	15	4	7.7	6.6
5	15	5	0.5	-0.6
5	15	6	2.3	1.6
5	15	7	2.1	-1.3
5	15	8	4.3	-3.1
5	15	9	2.1	-0.2
6	15	-14	3.4	3.3
6	15	-13	1.2	1.5
6	15	-12	3.5	3.2
6	15	-11	2.0	2.9
6	15	-10	4.1	-3.0
6	15	-9	0.5	-0.5
6	15	-8	7.0	-6.3
6	15	-7	1.1	-1.6
6	15	-6	1.5	1.7
6	15	-5	1.4	1.4
6	15	-4	6.7	6.9
6	15	-3	0.4	1.0
6	15	-2	0.0	4.0
6	15	-1	1.5	1.1
6	15	0	3.7	-3.5
6	15	1	1.3	-0.1
6	15	2	7.2	5.0
6	15	3	0.5	-1.5
6	15	4	4.4	-4.4
6	15	5	1.7	1.3
6	15	6	5.9	-4.3
6	15	7	2.7	0.4
7	15	-14	0.0	-0.9
7	15	-13	1.9	0.9
7	15	-12	2.6	-3.6
7	15	-11	1.0	-1.0
7	15	-10	0.0	-1.1
7	15	-9	1.5	0.1
7	15	-8	3.0	4.3
7	15	-7	2.4	1.9
7	15	-6	4.9	4.6
7	15	-5	1.4	0.2
7	15	-4	3.6	-3.0
7	15	-3	0.5	-1.6
7	15	-2	3.0	-4.0
7	15	-1	0.0	-6.3
7	15	0	3.5	0.2
7	15	1	1.5	-0.5
7	15	2	4.0	-3.9
7	15	3	2.0	0.9
7	15	4	0.7	-0.9
7	15	5	0.6	0.3
7	15	6	2.5	2.1
8	15	-14	2.0	-1.3
8	15	-11	0.0	0.1
8	15	-10	5.1	4.4
8	15	-9	1.7	1.7
8	15	-8	2.1	-1.0
8	15	-7	1.0	1.7
8	15	-6	5.0	-4.0
8	15	-5	0.5	-1.5
8	15	-4	1.5	1.2
8	15	-3	1.0	0.7
8	15	-2	4.0	4.6
8	15	-1	3.3	4.2
8	15	0	5.4	4.4
8	15	1	1.2	1.1
8	15	2	3.4	2.9
8	15	3	2.1	-0.6
8	15	4	2.5	2.7
8	15	5	0.6	-0.4
9	15	-13	0.9	0.5
9	15	-11	0.2	1.2
9	15	-10	3.4	-3.3
9	15	-9	2.2	-2.6
9	15	-8	3.0	-2.1
9	15	-7	0.5	0.4
9	15	-6	4.3	3.9
9	15	-5	1.2	-0.7
9	15	-4	4.1	2.9
9	15	-3	2.6	2.2
9	15	-2	2.9	-2.9
9	15	-1	1.0	-0.6
9	15	0	7.3	-5.3
9	15	1	2.2	-1.6
9	15	2	3.5	0.5
9	15	3	2.7	0.4
10	15	-13	1.7	0.4
10	15	-11	2.0	-1.3
10	15	-10	0.7	0.4
10	15	-9	1.9	0.6
10	15	-8	5.6	4.9
10	15	-7	0.6	1.0
10	15	-6	0.7	-0.4
10	15	-5	1.6	0.4
10	15	-4	5.6	-4.6
10	15	-3	0.6	-1.2
10	15	-2	3.2	-2.1
10	15	-1	0.6	-1.5
10	15	0	2.0	2.1
10	15	1	2.1	0.7
10	15	2	4.1	-3.9
11	15	-11	2.1	-0.0
11	15	-10	3.7	2.9
11	15	-8	1.4	-2.1
11	15	-7	0.6	-0.4
11	15	-6	3.5	-2.9
11	15	-5	0.0	-1.2
11	15	-4	2.7	1.0
11	15	-3	1.9	0.4
11	15	-2	4.0	3.6
11	15	-1	1.6	0.6
11	15	0	1.0	0.3
11	15	1	2.5	0.4
12	15	-10	2.7	-3.1
12	15	-7	1.6	-0.7
12	15	-6	0.7	2.2
12	15	-4	0.0	0.0
12	15	-3	2.3	0.9
12	15	-2	3.3	-1.5
12	15	-1	1.0	-0.4
13	15	-6	1.3	-0.9
0	16	-12	3.1	0.5
0	16	-10	3.0	-2.6
0	16	-9	0.5	-1.4
0	16	-8	2.2	1.0
0	16	-7	5.4	-6.5
0	16	-6	2.9	3.5
0	16	-5	1.0	-3.6
0	16	-4	2.2	3.3
0	16	-3	5.5	6.9
0	16	-2	2.4	-2.9
0	16	-1	1.1	3.6
1	16	-12	2.7	-2.6
1	16	-10	3.7	1.6
1	16	-9	3.1	-2.6
1	16	-8	2.6	3.4
1	16	-7	0.4	1.0
1	16	-6	2.1	-1.5
1	16	-5	3.9	5.2
1	16	-4	3.7	-3.7
1	16	-3	0.0	-0.1
1	16	-2	1.1	-1.9
1	16	0	1.1	3.6
1	16	1	0.9	0.4
1	16	2	7.6	7.9
1	16	3	4.4	-4.6
1	16	4	1.0	-1.3
1	16	5	1.3	-2.4
1	16	6	2.4	-2.1
1	16	7	2.9	3.2
1	16	8	3.5	-3.6
1	16	9	3.1	3.4
1	16	10	2.9	1.7
1	16	12	2.0	1.4
2	16	-12	2.2	1.7
2	16	-10	2.9	2.4
2	16	-9	2.4	2.4
2	16	-8	3.0	-4.1
2	16	-7	2.0	2.3
2	16	-6	4.1	-4.6
2	16	-5	4.2	-4.9
2	16	-4	3.4	3.7
2	16	-3	4.4	-5.3
2	16	-2	4.3	5.5
2	16	-1	1.1	1.7
2	16	0	1.4	-0.5
2	16	1	1.6	-3.3
2	16	2	3.2	-3.0
2	16	3	1.7	1.5
2	16	4	2.4	-2.0
2	16	5	4.5	5.3
2	16	6	2.3	1.0
2	16	7	0.5	1.1
2	16	8	2.3	1.6
2	16	9	1.2	-1.2
2	16	10	1.5	0.2
3	16	-12	2.7	-1.6
3	16	-10	2.9	-3.9
3	16	-9	2.9	-3.7
3	16	-8	1.7	0.1
3	16	-7	1.0	-1.5
3	16	-6	3.6	4.1
3	16	-5	1.0	1.0
3	16	-4	2.6	1.7
3	16	-3	2.1	2.4
3	16	-2	5.4	-5.5
3	16	-1	1.5	-1.9
3	16	0	6.1	-6.1
3	16	1	5.1	5.4
3	16	2	2.9	3.0
3	16	3	1.0	1.1
3	16	4	4.1	4.1
3	16	5	3.2	-4.0
3	16	6	2.3	1.9
3	16	7	2.0	-2.4
3	16	8	2.2	-1.1
3	16	9	0.9	1.2
4	16	-12	1.0	-0.2
4	16	-11	4.9	-3.6
4	16	-10	3.3	2.5
4	16	-9	1.1	-0.3
4	16	-8	5.9	5.2
4	16	-7	4.6	4.0
4	16	-6	1.7	-2.3
4	16	-5	2.6	3.0
4	16	-4	4.1	-4.0
4	16	-3	5.0	-5.7
4	16	-2	2.6	-2.0
4	16	-1	3.1	-2.6
4	16	0	5.4	5.4
4	16	1	2.7	-3.6
4	16	2	2.0	0.7
4	16	3	2.6	-3.4
4	16	4	3.0	-3.6
4	16	5	0.5	0.6
4	16	6	2.6	-2.6
4	16	7	3.6	4.0
4	16	8	2.6	-0.3
4	16	9	0.6	1.0
5	16	-13	0.6	-0.2
5	16	-11	4.5	4.4
5	16	-10	1.2	0.6
5	16	-9	2.0	2.6
5	16	-8	6.7	-6.6
5	16	-7	1.5	-0.6
5	16	-6	2.2	-2.6
5	16	-5	2.0	-4.0
5	16	-3	1.4	0.4
5	16	-2	0.2	7.5
5	16	-1	7.6	7.4
5	16	0	2.2	-0.6
5	16	1	2.1	-2.6
5	16	2	6.0	-5.6
5	16	3	2.7	3.6
5	16	4	1.6	0.9
5	16	5	1.3	2.6
5	16	6	3.0	2.5
5	16	7	0.6	-1.4
5	16	8	0.7	0.5
5	16	9	1.6	-2.9
6	16	-13	2.2	3.6
6	16	-11	1.5	-0.2
6	16	-10	2.5	-1.7
6	16	-9	4.1	-4.2
6	16	-8	1.7	1.6
6	16	-7	2.3	-2.9
6	16	-6	4.4	4.0
6	16	-5	2.7	2.7
6	16	-4	1.5	0.9
6	16	-3	3.5	3.6
6	16	-2	4.5	-4.0
6	16	-1	2.2	-1.5
6	16	0	3.4	-3.6
6	16	1	4.6	4.6
6	16	2	2.5	1.2
6	16	3	0.5	-0.6
6	16	4	4.3	4.1
6	16	5	3.2	-3.0
6	16	6	2.1	-0.9
6	16	7	1.0	-1.3
6	16	8	2.6	-1.0
7	16	-13	2.5	-1.0
7	16	-11	2.6	-2.3
7	16	-10	2.2	2.0
7	16	-9	2.0	2.1
7	16	-8	2.7	2.4
7	16	-7	2.7	3.4
7	16	-6	3.5	-2.0
7	16	-5	0.9	0.3
7	16	-4	4.6	-4.0
7	16	-3	2.5	-2.4
7	16	-2	0.5	-0.5
7	16	-1	0.5	-0.7
7	16	0	5.5	5.0
7	16	1	3.0	-3.3
7	16	2	1.1	0.4
7	16	3	3.1	-2.6
7	16	4	2.4	-1.5
7	16	5	1.1	0.0
7	16	6	1.0	-1.0
8	16	-13	2.4	0.6
8	16	-11	2.5	1.6
8	16	-10	2.9	-1.3
8	16	-9	1.6	-0.0
8	16	-8	0.5	-2.3
8	16	-7	2.3	-2.2
8	16	-6	0.5	0.6
8	16	-5	0.9	-1.7
8	16	-4	3.1	2.0
8	16	-3	1.4	2.1
8	16	-2	3.1	4.0
8	16	-1	1.7	2.5
8	16	0	2.2	-1.6
8	16	1	1.6	1.4
8	16	2	3.2	-3.1
8	16	3	1.0	2.0
8	16	4	2.0	2.5
9	16	-13	0.9	1.6
9	16	-11	2.2	-2.3
9	16	-10	1.6	-0.6
9	16	-9	2.2	-2.3
9	16	-8	4.0	3.4
9	16	-7	1.4	1.6
9	16	-6	1.0	0.7
9	16	-5	1.7	2.0
9	16	-4	1.6	-1.5
9	16	-3	1.1	-0.3
9	16	-2	1.7	-1.7
9	16	-1	3.0	-3.6
9	16	0	1.0	-1.6
9	16	1	0.6	1.7
9	16	2	2.9	2.0
9	16	4	3.0	2.1
10	16	-11	1.4	-0.6
10	16	-10	0.6	1.2
10	16	-9	0.6	2.5
10	16	-8	1.6	0.4
10	16	-7	1.1	0.2
10	16	-6	2.4	-3.3
10	16	-5	2.6	-2.1
10	16	-4	2.0	-1.6
10	16	-3	2.0	-2.0
10	16	-2	2.7	1.7
10	16	-1	0.6	-0.2
10	16	0	0.7	1.2
10	16	2	1.2	0.2
11	16	-11	3.2	2.3
11	16	-10	3.5	-2.0
11	16	-8	1.3	-1.1
11	16	-7	2.0	-2.6
11	16	-6	2.3	1.2
11	16	-5	0.6	0.2
11	16	-4	2.0	1.6
11	16	-2	2.0	0.0
11	16	-1	0.6	1.1
11	16	0	3.1	-1.5
12	16	-10	1.7	0.6
12	16	-7	0.6	0.6
12	16	-6	1.2	0.1
12	16	-4	2.6	-1.6
12	16	-2	1.4	-0.6
13	16	-6	2.7	-1.9

TABLE 3.5

ORTHOGONAL COORDINATES AND E.S.D.S.

ATOM	X	Y	Z
Cr(1)	3.329 ± 1	1.882 ± 1	-0.582 ± 1
C(1)	3.039 ± 4	-0.269 ± 4	-0.991 ± 4
C(2)	2.650 ± 5	0.442 ± 5	-2.112 ± 4
C(3)	1.689 ± 4	1.441 ± 5	-1.992 ± 4
C(4)	1.139 ± 4	1.746 ± 4	-0.741 ± 4
C(5)	-0.272 ± 4	1.989 ± 5	1.877 ± 6
C(6)	-0.852 ± 5	2.120 ± 6	3.148 ± 7
C(7)	-0.283 ± 6	1.528 ± 7	4.237 ± 6
C(8)	0.884 ± 5	0.845 ± 6	4.115 ± 5
C(9)	2.811 ± 5	0.006 ± 5	2.748 ± 4
C(10)	2.878 ± 5	-0.810 ± 5	1.472 ± 4
C(11)	2.480 ± 3	0.010 ± 4	0.286 ± 4
C(12)	1.508 ± 3	1.020 ± 4	0.415 ± 4
C(13)	0.903 ± 3	1.275 ± 4	1.742 ± 4
C(14)	1.505 ± 4	0.703 ± 5	2.875 ± 3
C(15)	4.261 ± 4	2.772 ± 4	-1.870 ± 4
C(16)	4.931 ± 4	1.607 ± 5	0.286 ± 4
C(17)	3.127 ± 4	3.451 ± 4	0.347 ± 4

O(1)	4.859 ± 4	3.331 ± 4	-2.675 ± 3
O(2)	5.933 ± 3	1.448 ± 5	0.805 ± 3
O(3)	2.978 ± 4	4.434 ± 3	0.909 ± 3

TABLE 3.6

ORTHOGONAL HYDROGEN ATOM COORDINATES.

ATOM	X	Y	Z
H(1)	3.78	-1.07	-1.10
H(2)	3.11	0.26	-3.09
H(3)	1.36	1.97	-2.89
H(4)	0.41	2.56	-0.65
H(5)	-0.74	2.44	0.98
H(6)	-1.77	2.73	3.27
H(7)	-0.76	1.56	5.23
H(8)	1.34	0.40	5.00
H(9)	3.61	0.73	2.71
H(10)	2.95	-0.67	3.59
H(11)	3.89	-1.18	1.34
H(12)	2.19	-1.65	1.58

TABLE 3.7

MOLECULAR VIBRATIONS ANALYSIS.

(a) Principal values of vibration tensors and their direction cosines referred to standard orthogonal axes.

ATOM	U $\mathring{A}^2$	D1	D2	D3
Cr(1)	0.0458	-0.4947	0.8691	0.0029
	0.0335	-0.3217	-0.1863	0.9283
	0.0362	0.8073	0.4583	0.3717
C(1)	0.0751	0.6797	-0.2775	0.6790
	0.0440	0.0420	0.9389	0.3416
	0.0508	-0.7323	-0.2037	0.6498
C(2)	0.0933	0.7428	-0.6447	0.1804
	0.0401	0.0358	0.3073	0.9509
	0.0480	-0.6685	-0.6999	0.2514
C(3)	0.0953	-0.5766	0.7419	0.3422
	0.0342	0.6454	0.1569	0.7475
	0.0542	0.5009	0.6519	-0.5693
C(4)	0.0774	-0.2906	0.6461	0.7057
	0.0356	0.9257	0.0030	0.3783
	0.0542	0.2423	0.7632	-0.5990
C(5)	0.1116	0.1720	-0.5068	0.8447
	0.0386	-0.9849	-0.1056	0.1372
	0.0557	0.0197	-0.8556	-0.5173
C(6)	0.1594	0.2888	-0.5436	0.7881
	0.0362	-0.9554	-0.1103	0.2740
	0.0554	-0.0620	-0.8321	-0.5512
C(7)	0.1510	0.5019	-0.6659	0.5520
	0.0445	-0.6983	0.0647	0.7129
	0.0624	-0.5104	-0.7433	-0.4325
C(8)	0.1341	0.5518	-0.7903	0.2664
	0.0418	-0.5460	-0.1008	0.8317
	0.0617	-0.6304	-0.6044	-0.4871

C(9)	0.0945	0.0789	0.9091	0.4090
	0.0429	0.0194	-0.4116	0.9111
	0.0617	0.9967	-0.0639	-0.0501
C(10)	0.0896	0.4657	0.6295	0.6219
	0.0420	-0.0800	-0.6700	0.7381
	0.0569	0.8813	-0.3935	-0.2617
C(11)	0.0402	-0.6993	-0.6098	0.3729
	0.0496	-0.0263	0.5433	0.8391
	0.0484	-0.7143	0.5770	-0.3960
C(12)	0.0353	-0.9435	-0.3222	0.0770
	0.0513	0.3032	-0.7464	0.5924
	0.0491	-0.1334	0.5823	0.8020
C(13)	0.0321	-0.9431	-0.3030	0.1365
	0.0613	0.3046	-0.6239	0.7197
	0.0493	-0.1329	0.7203	0.6808
C(14)	0.0831	0.6022	-0.7341	0.3138
	0.0363	-0.7501	-0.3857	0.5371
	0.0567	-0.2733	-0.5588	-0.7830
C(15)	0.0659	0.6972	-0.6962	0.1708
	0.0389	0.0017	0.2398	0.9708
	0.0489	-0.7169	-0.6766	0.1683
C(16)	0.0756	-0.0001	0.9910	0.1341
	0.0384	-0.6069	-0.1066	0.7876
	0.0515	0.7948	-0.0813	0.6015
C(17)	0.0654	0.4472	-0.8944	0.0107
	0.0438	-0.3308	-0.1543	0.9310
	0.0467	-0.8310	-0.4199	-0.3648
O(1)	0.1108	0.7929	-0.5967	0.1234
	0.0390	-0.4309	-0.4061	0.8058
	0.0679	-0.4308	-0.6921	-0.5791
O(2)	0.1366	0.1526	0.9847	0.0842
	0.0444	0.9355	-0.1714	0.3090
	0.0646	0.3187	0.0316	-0.9473
O(3)	0.0398	-0.0457	0.7538	0.6555
	0.0988	0.8843	-0.2746	0.3775
	0.0877	0.4646	0.5969	-0.6541

(b) Centre of mass, referred to orthogonal axes.

X	Y	Z
2.5364	1.5566	0.5076

(c) Principal moments of inertia, I, and direction cosines D1, D2, D3, of inertial axes referred to orthogonal axes.

I ($\mathrm{gmcm}^2 \times 10^{-40}$)	D1	D2	D3
1516	-0.6052	-0.1561	0.7727
3615	0.5252	0.6499	0.5494
3489	-0.5879	0.7439	-0.3179

(d) T and W and their e.s.d.s, referred to inertial axes.

$$T(\mathrm{\AA}^2) = \begin{bmatrix} \begin{matrix}0.0354\\8\end{matrix} & \begin{matrix}0.0003\\16\end{matrix} & \begin{matrix}0.0009\\16\end{matrix} \\ & \begin{matrix}0.0348\\15\end{matrix} & \begin{matrix}0.0041\\19\end{matrix} \\ & & \begin{matrix}0.0357\\12\end{matrix} \end{bmatrix}$$

$$W({}^{\circ 2}) = \begin{bmatrix} \begin{matrix}29.13\\2.32\end{matrix} & \begin{matrix}-2.34\\1.61\end{matrix} & \begin{matrix}0.04\\1.60\end{matrix} \\ & \begin{matrix}15.57\\1.12\end{matrix} & \begin{matrix}1.46\\1.21\end{matrix} \\ & & \begin{matrix}4.52\\1.20\end{matrix} \end{bmatrix}$$

(e) U obs - U calc, with respect to inertial axes.

ATOM	U11	U22	U33	2U23	2U31	2U12
Cr(1)	-0.0013	-0.0006	-0.0002	-0.0009	0.0010	-0.0007
C(1)	0.0070	0.0046	-0.0072	0.0032	0.0059	0.0048
C(2)	0.0053	0.0040	-0.0073	-0.0076	0.0162	0.0012
C(3)	0.0149	-0.0052	-0.0061	-0.0089	0.0123	0.0160
C(4)	0.0138	0.0039	-0.0007	-0.0096	-0.0006	0.0236
C(5)	0.0211	-0.0117	0.0126	-0.0185	-0.0256	0.0175
C(6)	0.0232	-0.0205	0.0099	-0.0169	-0.0424	0.0288
C(7)	0.0134	-0.0021	0.0008	-0.0055	-0.0298	0.0072
C(8)	0.0033	0.0016	0.0179	0.0045	-0.0286	0.0041
C(9)	-0.0042	0.0088	0.0097	0.0098	-0.0167	-0.0012
C(10)	-0.0096	0.0077	0.0053	0.0213	-0.0031	-0.0004
C(11)	0.0021	0.0021	0.0008	0.0119	0.0014	0.0061
C(12)	0.0058	0.0072	0.0052	-0.0062	-0.0071	0.0102
C(13)	0.0064	0.0016	0.0022	-0.0030	-0.0117	0.0139
C(14)	0.0003	0.0046	0.0143	-0.0088	-0.0203	0.0151
C(15)	0.0071	-0.0075	-0.0154	0.0034	-0.0111	-0.0126
C(16)	-0.0081	0.0104	0.0052	-0.0057	0.0158	-0.0131
C(17)	0.0017	0.0020	0.0071	0.0320	-0.0010	-0.0044
O(1)	0.0058	0.0012	-0.0138	0.0035	0.0044	-0.0054
O(2)	-0.0012	0.0195	0.0017	0.0134	0.0077	-0.0336
O(3)	0.0261	-0.0046	0.0058	0.0239	-0.0130	-0.0424

TABLE 3.8

BOND LENGTHS (Å) AT COMPLETION OF LEAST-SQUARES REFINEMENT (I) AND AFTER LIBRATION CORRECTION (II).

	I	II
C(1) - C(2)	1.383 ± 6	1.390
C(2) - C(3)	1.392 ± 7	1.398
C(3) - C(4)	1.400 ± 6	1.404
C(4) - C(12)	1.415 ± 6	1.421
C(11) - C(12)	1.407 ± 5	1.415
C(1) - C(11)	1.422 ± 6	1.426
C(5) - C(6)	1.404 ± 8	1.406
C(6) - C(7)	1.364 ± 9	1.369
C(7) - C(8)	1.358 ± 8	1.363
C(8) - C(14)	1.394 ± 6	1.396
C(14) - C(13)	1.405 ± 5	1.413
C(13) - C(5)	1.381 ± 5	1.387
C(14) - C(9)	1.485 ± 6	1.492
C(9) - C(10)	1.517 ± 7	1.522
C(10) - C(11)	1.495 ± 6	1.502
C(12) - C(13)	1.480 ± 5	1.485

Cr(1) - C(1)	2.209 ± 4	2.218
Cr(1) - C(2)	2.208 ± 4	2.216
Cr(1) - C(3)	2.207 ± 4	2.217
Cr(1) - C(4)	2.200 ± 4	2.209
Cr(1) - C(11)	2.232 ± 4	2.241
Cr(1) - C(12)	2.248 ± 3	2.255
Cr(1) - C(15)	1.821 ± 4	1.826
Cr(1) - C(16)	1.843 ± 4	1.852
Cr(1) - C(17)	1.834 ± 4	1.843
Cr(1) - O(1)	2.970 ± 3	2.975
Cr(1) - O(2)	2.982 ± 3	2.995
Cr(1) - O(3)	2.976 ± 4	2.988
C(15) - O(1)	1.148 ± 5	1.150
C(16) - O(2)	1.140 ± 5	1.143
C(17) - O(3)	1.142 ± 5	1.145

TABLE 3.10

INTERMOLECULAR CONTACTS BELOW 4 Å.

O(1).....O(2)	i	3.16 Å	C(5).....C(11)	ii	3.68 Å
C(2).....C(6)	ii	3.30	C(9).....O(2)	vi	3.68
C(2).....O(3)	i	3.34	C(6).....O(2)	iv	3.70
C(16)....O(1)	iii	3.35	C(9).....O(1)	iii	3.70
O(1).....O(3)	i	3.36	C(10)....C(15)	v	3.70
C(1).....C(5)	ii	3.38	C(3).....C(5)	ii	3.71
C(3).....O(3)	i	3.38	C(1).....O(3)	v	3.72
C(7).....O(2)	iv	3.40	C(2).....C(7)	ii	3.74
C(10)....O(1)	v	3.40	C(12)....C(12)	ii	3.74
C(2).....C(5)	ii	3.41	C(3).....C(13)	ii	3.76
C(17)....O(1)	iii	3.46	C(6).....O(1)	iv	3.76
O(2).....O(3)	v	3.48	C(16)....O(3)	v	3.77
C(9).....O(1)	v	3.50	C(4).....C(13)	ii	3.78
C(4).....C(7)	i	3.55	C(8).....C(17)	iii	3.78
C(15)....O(3)	i	3.56	C(10)....O(3)	v	3.81
C(1).....C(6)	ii	3.59	C(4).....C(6)	i	3.82
C(1).....O(1)	vii	3.61	C(1).....C(15)	vii	3.84
C(8).....O(3)	iii	3.65	C(3).....C(6)	ii	3.84

C(4).....C(12)	ii	3.84	C(3).....C(14)	ii	3.95
C(9).....C(9)	vi	3.84	C(4).....C(8)	i	3.95
C(8).....O(2)	vi	3.85	C(2).....C(13)	ii	3.96
C(3).....C(6)	i	3.88	C(12)....C(13)	ii	3.97
C(10)....C(17)	v	3.92	C(3).....C(7)	ii	3.98
C(3).....C(7)	i	3.93	C(5).....C(12)	ii	3.98
C(15)....C(17)	i	3.94	C(4).....C(5)	ii	4.00

Roman numerals refer to the following transformations of the fractional coordinates given in Table 3.1.

i	x,	1/2 - y,	-1/2 + z;
ii	- x,	- y,	- z;
iii	x,	1/2 - y,	1/2 + z;
iv	-1 + x,	y,	z;
v	1 - x,	-1/2 + y,	1/2 - z;
vi	1 - x,	- y,	1 - z;
vii	1 - x,	- y,	- z;

TABLE 3.11

MEAN MOLECULAR PLANES.

PLANE NO.	ATOMS DEFINING PLANE
1	C(1),C(2),C(3),C(4),C(11), and C(12)
2	C(5),C(6),C(7),C(8),C(13), and C(14)
3	C(15),C(16), and C(17)
4	O(1),O(2), and O(3)

PLANE EQUATIONS

PLANE NO.	P	Q	R	S	RMS D*
1	-0.7250	-0.6670	-0.1715	-1.8523	0.006
2	-0.5210	-0.8382	-0.1613	-1.8291	0.009
3	-0.7092	-0.6885	-0.1518	-4.6461	-
4	-0.7047	-0.6920	-0.1568	-5.3093	-

* These symbols are defined in Table 2.10. The plane equation is

$$PX + QY + RZ = S$$

where X,Y, and Z refer to orthogonal axes.

DIHEDRAL ANGLES

PLANE A	PLANE B	∠ AB	PLANE A	PLANE B	∠ AB
1	2	15.3°	2	3	13.8°
1	3	1.9	2	4	13.5
1	4	2.0	3	4	0.4

DEVIATIONS FROM PLANES (Å)

PLANE NO. ATOM	1	2	3	4
Cr(1)	-1.717	-1.389	1.078	1.752
C(1)	-0.002	0.631	2.826	3.509
C(2)	-0.002	0.418	2.783	3.467
C(3)	0.008	0.063	2.759	3.434
C(4)	-0.011	-0.108	2.749	3.415
C(5)	0.401	0.001	-	-
C(6)	0.516	-0.012	-	-
C(7)	0.312	0.013	-	-
C(8)	-0.058	-0.003	-	-
C(9)	-0.661	-0.084	-	-
C(10)	0.054	0.771	2.940	3.611
C(11)	-0.001	0.483	2.838	3.510
C(12)	0.007	0.121	2.811	3.475
C(13)	0.048	0.009	2.864	3.518
C(14)	-0.201	-0.008	-	-
C(15)	-2.765	-2.413	-	0.682
C(16)	-2.843	-2.133	-	0.678
C(17)	-2.776	-2.749	-	0.663
O(1)	-3.433	-3.063	-0.687	-
O(2)	-3.553	-2.606	-0.681	-
O(3)	-3.420	-3.586	-0.657	-

3.5 DISCUSSION

The molecular structure of 9,10-dihydrophenanthrenechromium tricarbonyl is extremely similar to that of the corresponding phenanthrene compound. The chromium atom, as would be expected, is bonded to a side ring. Three linear carbonyl groups are disposed at right angles to one another and point approximately at the midpoints of the C(1)-C(2), C(3)-C(4), and C(11)-C(12) bonds. The possible Kekule structures of 9,10-dihydrophenanthrene indicate that the orders of the side ring bonds are equal, so that this configuration in 9,10-dihydrophenanthrenechromium tricarbonyl is presumably adopted to minimise intramolecular repulsions between the chromium tricarbonyl fragment and the hydrocarbon ligand.

No structural studies on 9,10-dihydrophenanthrene itself have been reported. However, an inspection of a Dreiding molecular model of the hydrocarbon suggests that there should be a two-fold symmetry axis passing through the midpoints of the C(9)-C(10) and C(12)-C(13) bonds, and also that the two side rings should be rotated about an axis passing through the C(12)-C(13) bond out of the plane defined by the symmetry axis, C(12) and C(13). To a first approximation this is found to be the case in 9,10-dihydrophenanthrenechromium tricarbonyl. The dihedral angle between the planes of the two side rings is 15.3°.C(8), C(14), and C(9) are displaced from the plane of the bonded side ring in the same direction as the chromium atom and C(5) and C(6) are displaced in the opposite direction.

As in the case of phenanthrenechromium tricarbonyl, three aspects of the molecular structure require detailed comment, namely, the effect of the chromium tricarbonyl moiety on the hydrocarbon ligand, the relationship of the chromium atom to the aromatic ring, and the stereochemistry of the chromium tricarbonyl fragment.

In the side ring of the hydrocarbon ligand bonded to chromium (ring A) the mean bond length is 1.403 Å, which is comparable with the 1.401 Å found in benzenechromium tricarbonyl by Bailey and Dahl (1965). One bond, C(1)-C(2), differs from this mean at the 0.1% significance level. In the non-bonded side ring (ring C) the mean bond length is 1.384 Å which is slightly shorter than the 1.394 Å found in benzene (Sutton, 1965), and again one bond, C(13)-C(14), differs from the mean at the 0.1% significance level. These results suggest that in each side ring the bond lengths are almost equal to each other and that the effect of the chromium atom has been to increase the mean bond length in ring A by about 0.02 Å. This conclusion is strengthened by comparison of the individual bonds in ring A with those in ring C which are related by the assumed two-fold symmetry axis; four are longer by, on average, 0.028 Å and two are equal within experimental error.

The bonds in the central ring (ring B) are in fair agreement with the literature values. The formally single C(12)-C(13) bond of 1.480 Å is between 1.497 Å found in biphenyl (Hargreaves and Rizvi, 1962) and 1.471 Å found in perylene (Camerman and Trotter, 1964) for similar bonds. The C(9)-C(14) and C(10)-C(11) bonds are equal within experimental error, with an average of 1.490 Å, which is slightly shorter than the expected value (Sutton, 1965) of 1.505 Å; libration correction increases this mean to 1.497 Å. The C(9)-C(10) bond is 1.517 Å, which is slightly less than the literature value of 1.537 Å (Sutton, 1965).

Ring A and ring C are planar, the respective root mean square deviations being 0.006 and 0.009 Å. In the dihydrophenanthrene ligand there is some distortion of the assumed two-fold symmetry of the free hydrocarbon.

This is shown by the displacements of the other atoms in the ligand from the plane of ring A. Atoms C(10) and C(13) have small but significant positive displacements (i.e. in the direction opposite from the chromium). A similar displacement of the methyl groups was found in hexamethylbenzenechromium tricarbonyl (Bailey and Dahl, 1965). Atom C(7) has a positive displacement of 0.312 Å, and the positive displacements of C(5) and C(6) are greater than the negative displacements of C(8) and C(14). Ring C is thus placed below ring A in the direction opposite to that of the chromium, as well as being rotated relative to ring A about the C(12)-C(13) bond. Such a distortion could be due to intramolecular repulsions or to packing forces; the closest approaches to C(9), C(10), and C(13) of the chromium atom and the atoms of the carbonyl groups are all greater than 3.4 Å.

The distances from the chromium atom to C(1), C(2), C(3) and C(4) are equal within the accuracy of the results, with a mean value of 2.206 Å. The Cr-C(11) and Cr-C(12) distances are significantly longer, with a mean of 2.240 Å. A similar, though more marked, effect was found in the phenanthrene compound, the long Cr-C bonds averaging 2.289 Å, and was ascribed to the low double bond order of the C(11)-C(12) bond. Such an explanation is not valid in the case of dihydrophenanthrenechromium tricarbonyl and therefore intramolecular repulsions or crystal packing forces must presumably play a part.

The means of the Cr-C, C-O, and Cr-O distances in the tricarbonyl moiety are respectively 1.833, 1·143, and 2.976 Å. These means are in good agreement with comparable values for the phenanthrene compound. The average Cr-C-O angle of 178.9° indicates smaller departures from linearity than were found in the phenanthrene compound. The O(1)-Cr-O(2) angle is again slightly less than 90°, presumably due to crystal packing forces.

The molecular packing (Fig. 3.3) is similar to that of the phenanthrene compound (Fig. 2.3). There are no intermolecular contacts significantly less than the sum of the van der Waals radii (Pauling, 1960) of the participating atoms.

A comparison of the molecular structure with those of related compounds is postponed until Chapter IV.

CHAPTER IV

ARENECHROMIUM TRICARBONYLS: A REVIEW

4.1 INTRODUCTION

This review covers structural studies on compounds with the general formula ArCrX, where Ar is a benzenoid aromatic ring and CrX is a chromium tricarbonyl fragment; in addition, a few compounds in which Ar is not benzenoid have been included. Structural work on dibenzenechromium and chromium hexacarbonyl is also discussed.

4.2 DIBENZENECHROMIUM

The crystal structure of dibenzenechromium, $(C_6H_6)_2Cr$, was first described by Weiss and Fischer (1956). In an apparently accurate analysis of the structure, Jellinek (1960, 1963) found that the benzene rings were significantly distorted, with long bonds of 1.436±12 Å alternating with short ones of 1.366±12 Å. However, in an independent analysis by Cotton, Dollase, and Wood (1963) the bond lengths in the benzene rings were found to be equal within experimental error, with a mean value of 1.387 Å. Jellinek (1963) suggested that disorder in the crystals used by Cotton would explain the discrepancies between the results of the two analyses. Ibers (1964) undertook a rigid-body refinement of the structure, using Cotton's data, and confirmed that they were not consistent with any distortion of the benzene rings from D_{6h} symmetry. These analyses were complicated by the high crystallographic point group symmetry (C_{3i}) required of the molecule.

An electron diffraction study of the molecule by Haaland (1965) provided no evidence for bond length alternation. An x-ray investigation of the crystal structure at low temperature, by Keulen and Jellinek (1966), gave results which, after libration correction, were in very good agreement with the electron diffraction study. The interatomic distances found by Keulen and Jellinek were C-C 1.420±3 Å and 1.419±3 Å, Cr-C 2.147±2 and 2.144±2 Å. The Cr-ring distance was 1.609±1 Å.

From these results it appears that sandwich bonding to chromium results in an increase of 0.02-0.03 Å in the mean benzene ring C-C bond length, without lowering the symmetry of the ring. This is in agreement with the most recent theoretical study of dibenzenechromium (den Boer et al., 1962) which suggests that distortion of the benzene ring symmetry is unlikely.

4.3 CHROMIUM HEXACARBONYL

This molecule has been the subject of x-ray and electron diffraction studies, both of rather limited accuracy. Using x-ray methods, Rudorff and Hofmann (1935) found the Cr-C distance to be1.80 Å; they assumed the C-O distance to be 1.15 Å, which gave, by addition, a Cr-O distance of 2.95 Å. Brockway et al. (1938) did an electron diffraction study, which gave 1.92±4 Å for the Cr-C distance, 1.16±5 Å for the C-O bond, and 3.08±5 Å for the Cr-O distance. Octahedral coordination of the chromium was assumed.

4.4 ARENECHROMIUM TRICARBONYLS

Prior to 1965 only the structures of benzenechromium tricarbonyl, $C_6H_6Cr(CO)_3$(Corradini and Allegra, 1959), of biphenyl bis(chromium tricarbonyl), $C_{12}H_{10}(Cr(CO)_3)_2$ (Corradini and Allegra, 1960), and of a monoclinic modification of phenanthrenechromium tricarbonyl, $C_{14}H_{10}Cr(CO)_3$ (Deuschl and Hoppe, 1964), had been published. In each of these compounds linear carbonyl groups, disposed at right angles to one another, were found to point approximately towards the midpoints of ring C-C bonds; to within the accuracy of the results the arene rings were planar, and parallel to the planes defined by the carbon atoms and by the oxygen atoms of the carbonyl groups. No reliable conclusions could be drawn about the effect of the chromium atom on the arene ring, since projection data only were used in these analyses.

More recently, Bailey and Dahl (1965a, 1965b) have described analyses of hexamethylbenzenechromium tricarbonyl, $C_6Me_6Cr(CO)_3$, and of benzenechromium tricarbonyl, both based on three-dimensional data. The structures of an orthorhombic modification of phenanthrenechromium tricarbonyl and of 9,10-dihydrophenanthrenechromium tricarbonyl, $C_{14}H_{12}Cr(CO)_3$, have been described in the two previous chapters of this thesis (a preliminary note on this work has been published by Muir, Ferguson, and Sim, 1966). These four analyses allow fairly firm conclusions to be drawn about the effect of a bonded chromium atom on an arene ring.

No evidence for an alternation of the arene ring bond lengths due to the chromium atom has been found in any of these compounds.

Some molecular dimensions of these compounds are given in Table 4.1. The first column contains the mean arene ring C-C bond length, together with the standard deviation of an individual measurement, estimated from the least-squares totals (in brackets). The second column gives the root mean square difference

TABLE 4.1

Molecular Dimensions (Å) in some $ArCr(CO)_3$ Complexes

Ar	Mean C-C	RMSD	RMS	Cr-Ring
C_6H_6	1.401(11)	0.018	0.007	1.724
$C_{14}H_{12}$	1.403(7)	0.013	0.006	1.717
$C_{14}H_{10}$	1.412(7)	0.022	0.018	1.733
C_6Me_6	1.417(14)	0.033	0.009	1.726
C_7H_8O	1.39	0.02	-	-

TABLE 4.2

Mean Dimensions of Carbonyl Groups in some Chromium Carbonyls (in Å and °)

Compound	Cr-C	C-O	Cr-O	Cr-C-O
$Cr(CO)_6$	1.92(4)	1.16(5)	3.08(5)	180(ass.)*
	1.80	1.15(ass)	2.95	-
$C_6H_6Cr(CO)_3$	1.842(10)	1.142(8)	2.984(11)	179.2(6)
$C_{14}H_{12}Cr(CO)_3$	1.833(4)	1.143(5)	2.976(4)	178.9(4)
$C_{14}H_{10}Cr(CO)_3$	1.843(5)	1.149(6)	2.992(4)	177.9(5)
$C_6Me_6Cr(CO)_3$	1.814(13)	1.163(12)	2.977(9)	177.6(12)
$C_7H_8OCr(CO)_3$	1.79	1.19(2)	-	176(2)
$C_4H_4SCr(CO)_3$	1.769(25)	1.210(25)	2.978(24)	175.0(22)

* Electron diffraction results

(Figures in brackets are e.s.d.s of individual measurements estimated from least-squares totals.)

from these means. The results suggest, but do not conclusively prove that the mean C-C bond length is a little greater in the complex than in the free hydrocarbon. In benzenechromium tricarbonyl the mean C-C bond length of 1.401 Å differs only by 0.007 Å from the accepted benzenoid C-C bond length of 1.394 Å (Sutton, 1965), but libration correction would probably increase this difference. In the phenanthrene and dihydrophenanthrene compounds the means of the C-C bond lengths in the bonded side rings are respectively 0.016 and 0.019 Å greater than the comparable means for the non-bonded side rings. The mean value of 1.417 Å in hexamethylbenzenechromium tricarbonyl is probably longer than the comparable mean in the free hydrocarbon, for which a projection study gave 1.39 Å (Robertson and Brockway, 1939).

The third column of Table 4.1 gives the root mean square deviations from the planes of the bonded rings. Only in the case of phenanthrenechromium tricarbonyl, in which special circumstances seem to exist, are the deviations significant.

The mean Cr-ring distances (Table 4.1, column 4) are all close to one another and rather greater than the corresponding values for dibenzenechromium. As pointed out previously, however, the chromium is not symmetrically placed with respect to the ring carbon atoms either in phenanthrenechromium tricarbonyl or in the related dihydrophenanthrene compound.

The mean dimensions of the chromium tricarbonyl fragments in each of these compounds are included in Table 4.2. The results are in general agreement with one another. The departures from linearity of the carbonyl groups are uniformly small. The mean interatomic distances are in fair agreement with the x-ray study of chromium hexacarbonyl and in rather worse agreement with the electron diffraction study of the same compound. In view of the limited accuracy with which the bond lengths in chromium hexacarbonyl have been determined, these disagreements have little significance.

In the arenechromium tricarbonyl compounds so far discussed, the carbonyl groups have invariably pointed towards the midpoints of ring C-C bonds. However, in anisolechromium tricarbonyl, $C_7H_8OCr(CO)_3$ (Carter, McPhail, and Sim, 1966a, 1966b), the carbonyls point towards ring carbon atoms. This is also the case in p-toluidinechromium tricarbonyl, $C_7H_9NCr(CO)_3$ (Carter, McPhail, and Sim, 1966c). These authors suggest that this configuration is due to the presence of ortho-para directing substituents.

In anisolechromium tricarbonyl the Cr-C(carbonyl) distances are shorter on average, and the C-O distances are longer, than in other arenechromium tricarbonyls (see Table 4.2). The departures from linearity of the carbonyl groups are also greater. No structural details have yet been published for the toluidine complex.

4.5 RELATED STRUCTURES

Brown, McPhail, and Sim (1966) have described the structure of a substituted cycloheptatrienechromium tricarbonyl, $C_{18}H_{16}Cr(CO)_3$; their results suggest that alternation of double and single bonds is retained on complexing to chromium. A preliminary report suggests that this is also true of phenylcycloheptatrienechromium tricarbonyl, $C_{13}H_{12}Cr(CO)_3$ (Baikie et al., 1965). Retention of single and double bond character was also found in cycloheptatrienemolybdenum tricarbonyl, $C_7H_8Mo(CO)_3$ (Dunitz and Pauling, 1960). In each of these compounds the carbonyls are trans to the midpoints of the double bonds of the ligand. However, the ring bond lengths were found to be irregular and without marked alternation in cyclooctatrienechromium tricarbonyl,

$C_8H_{10}Cr(CO)_3$ (Armstrong and Prout, 1962).

In 1,6-methanocyclodecapentaenechromium tricarbonyl, $C_{11}H_{10}Cr(CO)_3$ (Baikie and Mills, 1966), four Cr-C(ring) distances are equal to one another, with a mean of 2.20 Å, and two are longer and also about equal to one another (2.54 and 2.57 Å). It is possible that the chromium does not attain a formally inert gas electron structure in this molecule.

In thiophenechromium tricarbonyl, $C_4H_4SCr(CO)_3$ (Bailey and Dahl, 1966c), the thiophene ring proved to be disordered. In the chromium tricarbonyl moiety the mean Cr-C distance is shorter and the mean C-O distance is longer than in benzenechromium tricarbonyl and similar compounds (Table 4.2). The differences are significant, at least at the 1% probability level.

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APPENDIX I

THE LINEAR DIFFRACTOMETER

Appendix 1

The Linear Diffractometer

The Hilger-Watts linear diffractometer (Arndt and Phillips, 1961) is a device for automatic measurement of the integrated intensities of diffracted x-ray beams. Its main components are a stabilised x-ray generator, counter equipment for measuring the intensities of x-ray beams, an analogue computer which positions the counter and crystal, and an output printer and tape punch.

Molybdenum radiation is most often used, in conjunction with balanced SrO-ZrO_2 Ross filters. With this radiation a scintillation counter is normally employed and monochromatization is improved by arranging the counting system so as to accept only pulses within a given energy range.

The analogue computer consists of three slides on which the counter is mounted. The counter is also constrained to be at a constant distance from the crystal. The crystal is set so that each of its reciprocal axes is parallel to one of the slides and its rotation is coupled to the movement of the counter. By moving the slides the crystal can be rotated to bring a predetermined crystal plane into the Bragg reflection condition, while simultaneously the counter is positioned so as to measure the diffracted beam.

The integrated reflection is measured by first rotating the crystal by a small angle out of the reflection condition and measuring the background for t seconds, then by rotating the crystal at constant speed through the reflection condition and counting for 2t seconds, and finally by counting background again for t seconds. For phenanthrenechromium tricarbonyl 2t was thus 15 seconds while for the dihydrophenanthrene compound it was 30 seconds. The intensity is the difference between the second count and the sum of the first and third. This process is repeated at least once for each filter.

The diffractometer automatically measures each reflection in a given reciprocal net. Upper layers are brought into the reflecting condition in the equi-inclination Weissenberg setting.

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APPENDIX II

ALGOL TEXT

ALGOL TEXT

The programmes presented in this Appendix are written in the computer language KDF9 ALGOL. This language is defined in a manual by Green (1964).

DBX016000KP4 is part of the molecular functions system; it is used to write unit cell dimensions, fractional coordinates etc. on to magnetic tape at the start of a run.

DBX016100KP4 is the contacts-seeking distance and angle programme described in Part II Section 1.4.

Reference

1. Green,J.S. (1964). "KDF9 ALGOL Programming", English Electric-Leo Computers Limited,Kidsgrove, England.

```
DBX016000KP4→
  begin
    library A0,A6,A7,A9,A13;
    integer  DV 1,D IN,MT 1,i,j,nat;
    real  pi,angle,a;
    array  cell[1:6],N,M[1:3,1:3],title[1:200],index[1:20];
    boolean array key[1:20];
    procedure pack four (d in,x); value d in;
      integer d in; real x;
    begin
      integer i,j;
      integer array SYM [-2:5];
      SYM[-2] := SYM[-1] := SYM[0] := 158;
      for i := 1 step 1 until 5 do
      begin
   in:  SYM[i] := in basic symbol (d in);
        if SYM[1] = 158 or SYM[1] = 160 or SYM[1] =
          174 or SYM[1] = 209 or SYM[1] = 152
          then goto in;
        if SYM[i] ≠ 132 and SYM[i] ≠ 158 and
          SYM[i]≠ 160 and SYM[i] ≠ 209 then goto next;
        for j := 4 step -1 until 1 do
          SYM[j] := SYM[i + j - 5];
        goto form x;
 next:
      end;
form x:
      i := 256×(256×(256×SYM[1] + SYM[2]) + SYM[3])
        + SYM[4];
      x := i;
    end  procedure pack four;
    procedure form integer(x,failure); real x;
      label failure;
    begin
      integer y,i,symbol;
      y := 0;
      for i := 1 step 1 until 3 do
      begin
   in:  symbol := in basic symbol (D IN);
        if symbol = 158 then goto in;
        if symbol = 148 then goto out;
        if symbol >  9 then
        begin
          write text (DV 1,[[2c]PUNCHING*ERROR*IN*
            BRACKETED*INTEGER]);
          goto failure;
        end;
        y := y×10 + symbol
```

```
      end;
      write text (DV 1,[[2c]BRACKETED*INTEGER*TOO*LARGE]);
      goto failure;
out:  x := y;
    end  of form integer;
    procedure orthog(cell,matrix); value cell;
      array cell,matrix;
    begin
      real one;
      matrix[1,2] := matrix[1,3] := matrix[2,3] := 0.0;
      matrix[3,3] := cell[3];
      matrix[3,2] := cell[2] × cos(cell[4]);
      matrix[3,1] := cell[1] × cos(cell[5]);
      matrix[2,2] := cell[2] × sin(cell[4]);
      one := (cos(cell[6]) - cos(cell[5]) ×
        cos(cell[4]))/sin(cell[4]);
      matrix[2,1] := one × cell[1];
      matrix[1,1] := cell[1] × sqrt(sin(cell[5])↑2
        - one↑2);
    end  procedure orthog;
    procedure inverse(matrix,inv); value matrix;
      array matrix,inv;
    begin
      integer i;
      inv[1,2] := inv[1,3] := inv[2,3] := 0.0;
      for i := 1 step 1 until 3 do
        inv[i,i] := 1.0/matrix[i,i];
      inv[2,1] := -matrix[2,1]/(matrix[1,1] × matrix[2,2]);
      inv[3,1] := -matrix[3,1]/(matrix[1,1] ×
        matrix[3,3]) + matrix[2,1] ×
        matrix[3,2]/(matrix[1,1] ×  matrix[2,2] ×
        matrix[3,3]);
      inv[3,2] := -matrix[3,2]/(matrix[2,2] × matrix[3,3]);
    end  procedure inverse;
    D IN := 20;   DV 1 := 30;   open(D IN);   open(DV 1);
    MT 1 := 100;   find(MT 1,[DG030003]);
    interchange(MT 1);   pi := 3.141 592 6536;
    angle := pi/180.0;
caption:
    for i := 1 step 1 until 200 do
    begin
      j := in basic symbol(D IN);   title[i] := j;
      if j = 152 then goto unit cell;
      if i = 200 then goto failure;
    end;
unit cell:
    for i := 1 step 1 until 3 do cell[i] := read(D IN);
    for i := 4 step 1 until 6 do
```

```
      cell[i] := read(D IN) × angle;
    orthog(cell,N);   inverse(N,M);
data:
    for i := 1 step 1 until 4 do index[i] := read(D IN);
    nat := index[1];
    for i := 2 step 1 until 4 do
      key[i - 1] := index[i] > 0.5;
    begin
      array ch[1:nat,1:2],at[1:nat,1:3]
        ,vib[1:nat,0:6],sigma[1:nat,1:3],corr[1:nat,1:3];
sf tape:
      for i := 1, 2 do j := read(D IN);
      for i := 1 step 1 until j do a := read(D IN);
      key[20] := read(D IN) > 0.5;
      for i := 1 step 1 until nat do
      begin
        pack four(D IN,ch[i,1]);
        form integer(ch[i,2],failure);
        for j := 1 step 1 until 3 do at[i,j] := read(D IN);
        if not key[1] then goto exit;
        a := read(D IN);
        if a > 0.5 and a < 1.5 then goto aniso;
        for j := 1 step 1 until 6 do vib[i,j] := -999;
        vib[i,0] := read(D IN);   goto exit;
aniso:  for j := 1 step 1 until 6 do
          vib[i,j] := read(D IN);
        vib[i,0] := -999;
        if key[20] then a := read(D IN);
 exit:
      end;
      if read(D IN) < 998 then goto failure;
sdevs:
      if not key[2] then goto load;
      for i := 1 step 1 until nat do
        for j := 1 step 1 until 3 do
          sigma[i,j] := read(D IN);
      if read(D IN) < 998 then goto failure;
correln:
      if not key[3] then goto load;
      if index[4] > 3.5 then
      begin
        for i := 1 step 1 until nat do
          for j := 3 step -1 until 1 do
            corr[i,j] := read(D IN);
      end
        else
      begin
        integer row;
```

```
        if index[4] < 1.5 then row := 3 else
          if index[4] < 2.5 then row := 2 else row := 1;
        for i := 1 step 1 until nat do
        begin
          for j := 1 step 1 until 3 do corr[i,j] := 0.0;
          corr[i,row] := read(D IN);
        end;
      end;
      if read(D IN) < 998 then goto failure;
load:
      write binary(MT 1,title,[TITLE]);
      write binary(MT 1,cell,[CELL]);
      write binary(MT 1,N,[N]);   write binary(MT 1,M,[M]);
      write binary(MT 1,index,[INDEX]);
      write binary(MT 1,ch,[CH]);
      write binary(MT 1,at,[X]);
      if key[1] then write binary(MT 1,vib,[U]);
      if key[2] then write binary(MT 1,sigma,[SIGMA]);
      if key[3] then write binary(MT 1,corr,[CORRELATION]);
      goto terminate;
    end;
failure:
    write text(00,[[c]ERROR*IN*DATA*TERMINATE*RUN[c]]);
terminate:
    interchange(MT 1);   close(D IN);   close(DV 1);
    close(MT 1);
  end→
```

```
DBX016100KP4→
  begin
    library A0,A6,A12,A7,A8,A13;
    boolean lineprint,axes orthogonal,restrictions;
    real d max,a max,a,b,c,alpha,beta,gamma,pi,
      pibytwo,radian,angle,t,S,D;
    integer i,j,k,l,m,n,CKEY,KEY 1,KEY 2,KEY 3,FORM
      1,FORM 2, LT,C,P,LP,SN,Z,D IN,DV 1,DV 2, num,M;
    integer array C1[1:27,1:3];
    array TEST[1:30,1:3],N[1:3,1:3],F,G[1:3],C2[1:27,1:3];
    procedure  out equivalent positions ( d out,sym
      no,vector); value d out, sym no;
      integer d out, sym no; array vector;
    begin
      integer i;
      procedure out coordinate (d out,a1,a2,a3,t);
        value d out, a1,a2,a3,t; integer d out;
        real a1,a2,a3,t;
      begin
        array OUT[1:3];
        integer j,k,F;
        F := format([d]);   OUT[1] := a1;   OUT[2] := a2;
        OUT[3] := a3;
        if t ≠ 0 then
        begin
          k := entier(12×t + 0.5);
          for j := 6, 4, 3, 2, 1 do
            if abs(k/j - k÷j) < 0.000 000 1
            then goto number;
 number:  write (d out,format([s≠nd]),k/j);
          out basic symbol (d out,161);
          write (d out,F,12/j);
          out basic symbol (d out,158);
        end;
        for j := 1 step 1 until 3 do
        begin
          if OUT[j] = 0 then goto exit;
          out basic symbol (d out,158);
          if OUT[j] > 0 then
            out basic symbol (d out,193) else
            out basic symbol (d out,209);
          out basic symbol (d out,158);
          if abs(OUT[j]) ≠ 1 then
            write (d out,F,abs(OUT[j]));
          out basic symbol (d out,60 + j);
   exit:
        end;
      end  procedure out coordinate;
```

```
      write text (d out,[[2c]EQUIVALENT*POSITION*
        NUMBER***]);
      write (d out,format([nddsssss]),sym no);
      for i := 1 step 1 until 3 do
      begin
        out coordinate(d out,vector[3×i -
          2],vector[3×i - 1], vector[3×i],vector[9 + i]);
        out basic symbol (d out,(if i ≠ 3 then 166
          else 152));
      end;
      out basic symbol (d out,160);
    end procedure out equivalent positions;
    procedure skip char(d in,char);
      value d in,char; integer d in,char;
    begin
      integer symbol;
in:   symbol := in basic symbol (d in);
      if symbol ≠ char then goto in;
    end procedure skip char;
    procedure orthogonalise (in vector,out
      vector,matrix,mode);
      value in vector,matrix,mode; boolean mode;
      array in vector,out vector,matrix;
    begin
      procedure axes only (in vector,out vector,matrix);
        value in vector,matrix;
        array in vector,out vector,matrix;
      begin
        integer numb;
        for numb := 1 step 1 until 3 do
          out vector[numb] := in vector[numb]
          ×matrix[numb,numb];
      end procedure axes only;
      procedure full matrix (in vector,out vector,matrix);
        value in vector, matrix;
        array in vector,out vector,matrix;
      begin
        integer numb;
        for numb := 1 step 1 until 3 do
          out vector[numb] := in vector
          [1]×matrix[numb,1] + in vector
          [2]×matrix[numb,2] + in vector
          [3]×matrix[numb,3];
      end procedure full matrix;
      if mode then
        axes only (in vector,out vector,matrix)
        else full matrix (in vector,out vector,matrix);
    end procedure orthogonalise;
```

```
   procedure out name(d out,f dev,a,b,failure);
     value a,b,d out,f dev; integer d out,f dev;
     real a,b; label failure;
   begin
     integer y,i,f,spaces;
     integer array SYMBOL[1:4];
     y := a;   spaces := 0;
     for i := 4 step - 1 until 1 do
     begin
       f := y÷256;   SYMBOL[i] := y - 256×f;   y := f;
     end;
     for i := 1 step 1 until 4 do
       if SYMBOL[i] = 158 then
       spaces := spaces + 1 else
       out basic symbol (d out,SYMBOL[i]);
     y := b;
     for i := 3 step - 1 until 1 do
     begin
       f := y÷10;   SYMBOL[i] := y - 10×f;   y := f;
     end;
     if y ≠0 then
     begin
       write text(f dev,[[2c]INTEGER*FOR*OUTPUT*
         GREATER*THAN*999]);
       goto failure;
     end;
     out basic symbol(d out,132);   f := 0;
     for i := 1 step 1 until 3 do
     begin
       if f = 0 and SYMBOL[i] =0 then
       begin
         spaces := spaces + 1;   goto next;
       end;
       out basic symbol (d out,SYMBOL[i]);   f := 1;
next:
     end;
     out basic symbol (d out,148);
     for i := 0 step 1 until spaces do
       out basic symbol (d out,158);
   end  procedure out name;
   procedure out symmetry (d out,sym,cell,no);
     value d out,sym,no; integer d out,sym,no;
     integer array cell;
   begin
     integer i;
     write (d out,format([ndsss]),sym);
     out basic symbol (d out,132);
     for i := 1 step 1 until 3 do
```

```
      begin
        write (d out,format([-d]),cell[no,i]);
        if i ≠ 3 then out basic symbol (d out,166);
      end;
      out basic symbol (d out,148);
    end  procedure out symmetry;
    procedure in equiv pos(d in, d out, vector, failure);
      value d in, d out; integer d in, d out;
      array vector; label failure;
    begin
      integer i;
      boolean semicolon;
      procedure coordinate(a1, a2, a3, t, termin);
        real a1, a2, a3, t; boolean termin;
      begin
        integer char a, char b, num, sig;
        real number;
        boolean first;
        a1 := a2 := a3 := t := 0.0;   first := true;
set sig:
        sig := 1;   num := 0;
clear b:
        char b := 0;
 next:  char a := in basic symbol(d in);
        goto if char a = 158 or char a = 160 or
          char a = 174 then next else
          if char a = 193 or char a = 209 then
          signs else if char a ≤9 then digits
          else
          if char a = 61 or char a = 62 or char a = 63
          then xyz else if char a = 161 then
          slash else terminator;
digits:
        char b := char b × 10 + char a;   first := false;
        goto next;
slash:  num := char b;   goto clear b;
  xyz:  number := if num ≠ 0 then
          sig × num/char b else if char b ≠ 0
          then sig × char b else sig;
        if char a = 61 then a1 := number else
          if char a = 62 then a2 := number else
          a3 := number;
        goto set sig;
signs:  if first then
        begin
          sig := if char a = 193 then +1 else -1;
          first := false
        end;
```

```
        if char b ≠ 0 then
        begin
          t := if num ≠ 0 then
            sig × num/char b else sig × char b;
          sig := if char a = 193 then +1 else -1
        end;
        num := 0;   goto clear b;
terminator:
        if char a ≠ 166 and  char a ≠ 152 then
          write text(d out, [[2c]Wrong*terminator.]);
        termin := char a = 152;
        if num ≠ 0 or char b ≠ 0 then
            t := if num ≠ 0 then
            sig × num/char b else sig × char b
      end  procedure coordinate;
      for i := 0, 1, 2 do
      begin
        coordinate(vector[3 × i + 1], vector[3 × i
          + 2], vector[3 × i + 3], vector[10 + i],
          semicolon);
        if semicolon and i ≠ 2 or not semicolon and
          i = 2 then
        begin
          write text(d out, [[2c]Equivalent*
            positions*are*out*of*phase]);
          goto failure
        end
      end
    end  procedure in equiv pos;
    procedure pack four (d in,x); value d in;
      integer d in; real x;
    begin
      integer i,j;
      integer array SYM [-2:5];
      SYM[-2] := SYM[-1] := SYM[0] := 158;
      for i := 1 step 1 until 5 do
      begin
   in:  SYM[i] := in basic symbol (d in);
        if SYM[1] = 158 or SYM[1] = 160 or SYM[1] =
          174 or SYM[1] = 209 or SYM[1] = 152
          then goto in;
        if SYM[i] ≠ 132 and SYM[i] ≠ 158 and
          SYM[i]≠ 160 and SYM[i] ≠ 209 then goto next;
        for j := 4 step -1 until 1 do
          SYM[j] := SYM[i + j - 5];
        goto form x;
 next:
      end;
```

```
form x:
      i := 256x(256x(256xSYM[1] + SYM[2]) + SYM[3])
        + SYM[4];
      x := i;
    end  procedure pack four;
    procedure SORT (n, t, p, in); value n, t, p;
      integer n, t, p; real array  in;
    begin
      integer h, i, j, flag;
      real  C;
      for j:= 1 step 1 until entier (n/2) do
      begin
        flag:=0;
        for i:= j+1 step 1 until n-j+1 do
        begin
          if in [i,p]> in [i-1,p] then goto L1;
          flag:= 1;
          for h:= 1 step 1 until t do
          begin
            C:=in [i,h];   in [i,h]:= in [i-1,h];
            in [i-1,h]:=C;
          end;
     L1:  if in [n-i+1,p]< in [n-i+2,p] then goto L2;
          flag:=1;
          for h:= 1 step 1 until t do
          begin
            C:=in[n-i+1,h];   in [n-i+1,h]:= in [n-i+2,h];
            in [n-i+2,h]:=C;
          end;
     L2:
        end;
        if flag=0 then goto finish;
      end;
finish:
    end  procedure SORT;
    D IN := 20;   DV 1 := DV 2 := 30;   lineprint := false;
    open (D IN);   open (DV 1);   pi := 3.141 592 653 6;
    pibytwo := pi/2;   radian := pi/180;
    angle := 1/radian;   find(100,[DG030003]);
    begin
      array  title[1:200],cell[1:6],index[1:20];
      read binary (100,title,[TITLE]);
      read binary (100,cell,[CELL]);
      read binary (100,index,[INDEX]);   M := index[1];
      for i := 1 step 1 until 200 do
      begin
        j := entier(title[i] + 0.5);
        if j = 152 then goto unit cell;
```

```
        out basic symbol(DV 2,j);
      end;
unit cell:
      a := cell[1];   b := cell[2];   c := cell[3];
      alpha := cell[4];   beta := cell[5];
      gamma := cell[6];
    end;
    d max := read (D IN);   a max := read (D IN);
    skip char (D IN,160);
    if a max > d max or d max > 10 then
    begin
      write text (DV 1,[[2c]D*MAX*OR*A*MAX*INAPPROPRIATE]);
      goto end;
    end;
    d max := d max↑2;   num := 0;   restrictions := false;
enter:
    i := in basic symbol (D IN);
    if i = 158 or i = 160 or i = 174 then goto enter;
    if i = 25 then goto next else if i = 29 then
    begin
      num := read (D IN);
      if num > 30 then
      begin
        write text (DV 1,[[2c]TOO*MANY*RESTRICTIONS]);
        goto end;
      end;
      restrictions := true;
      for j := 1 step 1 until  num do
      begin
        pack four (D IN,TEST[j,1]);
        pack four (D IN,TEST[j,2]);
        TEST[j,3] := read (D IN)↑2;   skip char (D IN,160);
      end;
      goto enter;
    end
      else
    begin
      write text (DV 1,[[2c]NUMBER*OF*CELLS*NOT*
        SPECIFIED]);
      goto end;
    end;
next:
    CKEY := read (D IN);
    if CKEY ≠ 0 and CKEY ≠ 1 and CKEY ≠ 27 then
    begin
      write text (DV 1,[[2c]WRONG*NUMBER*OF*CELLS]);
      goto end;
    end;
```

```
    if CKEY > 0.5 then goto lattice;
    LT := C := P := Z := 1;   goto evaluate matrices;
lattice:
    LT := read (D IN);   C  := read (D IN);
    P  := read (D IN);   Z  := P×C;
evaluate matrices:
    begin
      array R[1:Z,1:12],A[1:12];
      if CKEY > 0.5 then
      begin
        i := in basic symbol (D IN);
        for i := 1 step 1 until P do
        begin
          in equiv pos (D IN,DV 1,A,end);
          for j := 1 step 1 until 12 do R[i,j] := A[j];
        end;
      end
        else
      begin
        for i := 1 step 1 until 12 do R[1,i] := 0.0;
        R[1,1] := R[1,5] := R[1,9] := +1;
      end;
      KEY 1 := KEY 2 := KEY 3 := 0;
print:
      i := in basic symbol (D IN);
      if i = 152 or i = 158 or i = 160 or i = 174
        then goto print else if i =  16 then
        goto cpr finished else if i =  27 then
      begin
        KEY 1 := 1;   skip char (D IN,160);   goto print;
      end
        else if i = 26 then
      begin
        KEY 2 := 1;   skip char (D IN,160);   goto print;
      end
        else if i = 30 then
      begin
        KEY 3 := 1;   skip char (D IN,160);   goto print;
      end
        else
      begin
        write text (DV 1,[[2c]OPTIONAL*OUTPUT*
          INSTRUCTIONS*NOT*UNDERSTOOD]);
        goto end;
      end;
cpr finished:
      begin
        array X[1:M,1:3],Ch[1:M,1:2];
```

```
        read binary (100,Ch,[CH]);
        read binary (100,X,[X]);   rewind (100);
        axes orthogonal := abs(pibytwo - alpha) <
          0.000 000 1 and abs(pibytwo - beta) <
          0.000 000 1 and abs(pibytwo - gamma) <
          0.000 000 1;
        if axes orthogonal then
        begin
          N[1,1] := a;   N[2,2] := b;   N[3,3] :=  c;
          N[1,2] := N[1,3] := N[2,1] := N[2,3] :=
            N[3,1] := N[3,2] := 0.0;
        end
          else
        begin
          N[1,2] := N[1,3] := N[2,3] := 0.0;
          N[1,1] := a × sqrt((sin(beta))↑2 -
            ((cos(gamma) - cos(alpha)×cos(beta))
            /sin(alpha))↑2);
          N[2,1] := a × (cos(gamma) -
            cos(alpha)×cos(beta))/sin(alpha);
          N[2,2] := b × sin(alpha);
          N[3,1] := a × cos(beta);
          N[3,2] := b × cos(alpha);   N[3,3] := c;
        end;
        if C > 1.5 then
        begin
          for i := 1 step 1 until P do
            for j := 1 step 1 until 12 do
              R[P + i,j] := - R[i,j];
        end;
        LP := (if LT ≤ 4 then LT - 1 else 1);
        SN := Z × (LP + 1);
        begin
          array T[0:LP,1:3];
          T[0,1] := T[0,2] := T[0,3] := 0.0;
          if LP = 0 then goto generate;
          if LT = 2 then goto I lattice else
            if LT = 3 then goto R lattice else
            if LT = 4 then goto F lattice else
            if LT = 5 then goto A lattice else
            if LT = 6 then goto B lattice else
            if LT = 7 then goto C lattice else
          begin
            write text (DV 1,[[2c]LATTICE*NUMBER*WRONG]);
            goto end;
          end;
I lattice:T[1,1] :=T[1,2] := T[1,3] := 0.5;
```

```
          goto generate;
R lattice:
          T[1,1] := T[2,2] := T[2,3] := 1/3;
          T[1,2] := T[1,3] := T[2,1] := 2/3;
          goto generate;
F lattice:
          T[1,1] := T[2,2] := T[3,3] := 0.0;
          T[1,2] := T[1,3] := T[2,1] := T[2,3] :=
            T[3,1] := T[3,2] := 0.5;
          goto generate;
A lattice:
          T[1,1] := 0.0;    T[1,2] := T[1,3] := 0.5;
          goto generate;
B lattice:
          T[1,2] := 0.0;    T[1,1] := T[1,3] := 0.5;
          goto generate;
C lattice:
          T[1,3] := 0.0;    T[1,1] := T[1,2] := 0.5;
generate:
          begin
            array Y[1:M,1:SN,1:3];
            for i := 0 step 1 until LP do
              for j := 1 step 1 until Z do
                for k := 1 step 1 until M do
                  for l := 1 step 1 until 3 do
                    Y[k,j + Z × i,l] := R[j,3 ×l -
                    2] × X[k,1] + R[j,3 × l - 1] ×
                    X[k,2] + R[j,3 ×l]×X[k,3] +
                    R[j,9 + l] + T[i,l];
            for i := 1 step 1 until SN do
              for j := 1 step 1 until  M do
            begin
              for k := 1 step 1 until 3 do
                F[k] := Y[j,i,k];
              orthogonalise (F,G,N,axes orthogonal);
              for k := 1 step 1 until 3 do
                Y[j,i,k] := G[k];
            end;
            if CKEY < 1.5 then
            begin
              C1[1,1] := C1[1,2] := C1[1,3] := 0.0;
              CKEY := 1;   goto jump;
            end;
            i := 1;
            for j := 1, 2, 3, 10, 11, 12, 19, 20, 21 do
              C1[j,i] := 0;
            for j := 4, 5, 6, 13, 14, 15, 22, 23, 24 do
              C1[j,i] :=  +1;
```

```
          for j := 7, 8, 9, 16, 17, 18, 25, 26, 27 do
           C1[j,i] := -1;
         i := 2;
         for j := 1, 4, 7, 10, 13, 16, 19, 22, 25 do
          C1[j,i] := 0;
         for j := 2, 5, 8, 11, 14, 17, 20, 23, 26 do
          C1[j,i] := +1;
         for j := 3, 6, 9, 12, 15, 18, 21, 24, 27 do
          C1[j,i] := -1;
         i := 3;
         for j := 1 step 1 until 9 do C1[j,i] := 0;
         for j := 10 step 1 until 18 do C1[j,i] := +1;
         for j := 19 step 1 until 27 do C1[j,i] := -1;
jump:    for i := 1 step 1 until CKEY do
         begin
          for j := 1 step 1 until 3 do F[j] := C1[i,j];
          orthogonalise (F,G,N,axes orthogonal);
          for j := 1 step 1 until 3 do C2[i,j] := G[j];
         end;
         if KEY 1 < 0.5 then goto out orthog;
         FORM 1 := format ([nd.dddd]);
         FORM 2 := format ([ndd.dd]);
         write text (DV 2,[[3c]a*=**]);
         write (DV 2,FORM 1,a);
         write text (DV 2,[[2s]ANGSTROMS[8s]alpha*=**]);
         write (DV 2,FORM 2,alpha × angle);
         write text (DV 2,[[2s]DEGREES[2c]b*=**]);
         write (DV 2,FORM 1,b);
         write text (DV 2,[[2s]ANGSTROMS[8s]beta**=**]);
         write (DV 2,FORM 2,beta × angle);
         write text (DV 2,[[2s]DEGREES[2c]c*=**]);
         write (DV 2,FORM 1,c);
         write text (DV 2,[[2s]ANGSTROMS[8s]gamma*=**]);
         write (DV 2,FORM 2,gamma × angle);
         write text (DV 2,[[2s]DEGREES[5c]]);
         for i := 0 step 1 until LP do
          for j := 1 step 1 until Z do
         begin
          for k := 1 step 1 until 9 do A[k] := R[j,k];
          for k := 1 step 1 until 3 do
           A[9 + k] := R[j,9 + k] + T[i,k];
          out equivalent positions (DV 2,j + Z × i,A);
         end;
         write text (DV 2,[[5c]FRACTIONAL*
          COORDINATES[3c]]);
         gap (DV 2,100);
         for i := 1 step 1 until M do
         begin
```

```
       out name (DV 2,DV 1,Ch[i,1],Ch[i,2],end);
       for j := 1 step 1 until 3 do
        write (DV 2,format([sss≠n.ddddd;
        s]),X[i,j]);
       out basic symbol (DV 2,160);
      end;
      gap (DV 2,100);
out orthog:
      if KEY 2 < 0.5 then goto begin;
      write text (DV 2,[[5c]ORTHOGONAL*
       COORDINATES[3c]]);
      gap (DV 2,100);
      for i := 1 step 1 until M do
      begin
       out name (DV 2,DV 1,Ch[i,1],Ch[i,2],end);
       for j := 1 step 1 until 3 do
        write (DV 2,format([sss≠ndd.dddd;
        s]),Y[i,1,j]);
       out basic symbol (DV 2,160);
      end;
      gap (DV 2,100);
  begin:  for i := 1 step 1 until M do
      begin
       integer COUNT;
       array RES[1:500,1:(7 + KEY 3)];
       COUNT := 0;
       for j := 1 step 1 until CKEY do
        for k := (if KEY 3 > 0.5 and j = 1
        then 2 else 1) step 1 until  SN do
         for l := 1 step 1 until  M do
       begin
        for m := 1 step 1 until 3 do
         F[m] := Y[l,k,m] + C2[j,m] - Y[i,1,m];
        S := F[1]↑2 + F[2]↑2 + F[3]↑2;
        D := d max;
        if not restrictions then goto out;
        begin
         boolean check 1,check 2;
         for m := 1 step 1 until num do
          for n := 1 step 1 until  2 do
         begin
          check 1 := abs(Ch[i,1] -
           TEST[m,n]) < 0.1;
          check 2 := abs(Ch[l,1] -
           TEST[m,(if n = 1 then 2 else
           1)]) < 0.1;
          if check 1 and check 2 then
           D := TEST[m,3];
```

```
                 end;
               end  testing block;
         out:  if S > D or S = 0 then goto not required;
               COUNT := COUNT + 1;
               if COUNT = 500 then
                 write text (DV 1,[[2c]
                 TOO*MANY*BOND*LENGTHS*ASKED*FOR]);
               RES[COUNT,1] := 1;   RES[COUNT,2] := k;
               RES[COUNT,3] := j;
               for m := 4 step 1 until 6 do
                 RES[COUNT,m] := F[m - 3];
               RES[COUNT,7] := sqrt(S);
not required:
             end;
             SORT(COUNT,(7 + KEY 3),7,RES);
             write text (DV 2,[[2c]ATOM*A[7s]
               ATOM*B[4s]EP[6s]CELL[6s]
               A-B*ANGSTROMS[2c]]);
             for j := 1 step 1 until COUNT do
             begin
               out name (DV 2,DV 1,Ch[i,1],Ch[i,2],end);
               for k := 1 step 1 until 3 do
                 out basic symbol (DV 2,158);
               out name (DV 2,DV 1,Ch[RES[j,1],1]
                 ,Ch[RES[j,1],2],end);
               out symmetry (DV 2,RES[j,2],C1,RES[j,3]);
               write (DV 2,format
                 ([ssnd.ddddc]),RES[j,7]);
             end;
             if a max ≠ 0 and COUNT > 1.5  then
             begin
               write text (DV 2,[[2c]ATOM*A[4s]
                 EP[6s]CELL[13s]ATOM*B[8s]
                 ATOM*C[4s]EP[6s]CELL[4s]ANGLE*ABC[2c]]);
               for j := 1 step 1 until COUNT do
                 for k := j + 1 step 1 until COUNT do
               begin
                 if RES[j,7] > a max or RES[k,7] >
                   a max then goto one more;
                 t := (RES[j,4]xRES[k,4] +
                   RES[j,5]xRES[k,5] +
                   RES[j,6]xRES[k,6])/(RES[j,7]xRES[k,7]);
                 if t = 0 then
                 begin
                   t := 90.0;   goto case;
                 end
                   else if t ≥ +1 then
                 begin
```

```
                    t := 0.0;   goto case;
                  end
                    else if t ≤ -1 then
                  begin
                    t := 180.0;   goto case;
                  end;
                  t := arctan(sqrt(1 - t↑2)/t)×angle;
                  if t < 0 then t := 180.0 + t;
           case:  out name (DV 2,DV
                    1,Ch[RES[j,1],1],Ch[RES[j,1],2],end);
                  out symmetry (DV 2,RES[j,2],C1,RES[j,3]);
                  write text (DV 2,[[10s]]);
                  out name (DV 2,DV 1,Ch[i,1],Ch[i,2],end);
                  write text (DV 2,[[4s]]);
                  out name (DV 2,DV
                    1,Ch[RES[k,1],1],Ch[RES[k,1],2],end);
                  out symmetry (DV 2,RES[k,2],C1,RES[k,3]);
                  write (DV 2,format([sssndd.ddc]),t);
       one more:
                end  angle calculation;
              end  angle searching loop;
            end  loop through atom list;
          end  cell coordinate block;
        end  block lattice type;
      end  atom list block;
    end  block equivalent positions;
end:
    close (D IN);   close (DV 1);   close(100);
  end→
```