this method to know the upper limit of integration precisely, and that is why the calculated structure factors of the unobserved reflexions within the Cu $K\alpha$ reciprocal-lattice sphere were included in the Fourier synthesis.) The profile obtained in this way does have diffraction ripples and is likely to give a truer value for the correction for series-termination errors.

The $(h0l)$ zone F_o synthesis (Fig. 1(*a*)) was computed at intervals of $a/60$ (= 0·140 Å) and $c/240$ (= 0·105 Å).

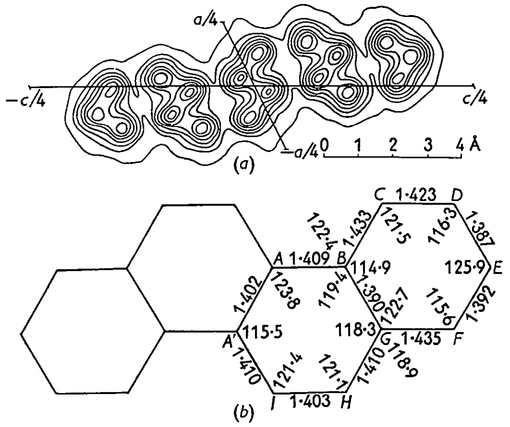

Fig. 1. (*a*) Chrysene ($C_{18}H_{10}$): electron-density map of projection on (010). (*b*) Bond lengths (Å) and angles (°).

Every atom gives a resolved peak in this projection, and the correct positions for the electron-density maxima can be determined with considerable accuracy.

The observed and calculated structure factors agree very well if McWeeny's (1951) scattering curve for carbon is used with a temperature factor (B) of 3·97 Å^2. The reliability indices $R\ (= \Sigma|F_o|-|F_c|\div\Sigma|F_o|)$, including only those planes actually observed, are, $R(0kl) = 13{\cdot}1\,\%$, $R(h0l) = 9{\cdot}3\,\%$.

Referring the coordinates to orthogonal axes x', y and z', where x' and y are parallel to a and b respectively, and z' is perpendicular to the plane (001), the mean plane of the molecule is given by the equation

$$0{\cdot}8559x'+0{\cdot}4789y+0{\cdot}1952z' = 0\,.$$

The crystals are monoclinic with

$$a = 8{\cdot}39,\ b = 6{\cdot}20,\ c = 25{\cdot}20\ \text{Å},\ \beta = 116{\cdot}2°;$$

space group, $I2/c$; 4 molecules per unit cell. The maximum, mean and r.m.s. values for the distances of the atoms from the mean plane are, respectively, 0·031, 0·012, 0·0145 Å.

The bond lengths and bond angles are shown in Fig. 1(*b*). The mean bond length is $1{\cdot}408_5$ Å and the maximum deviation from this mean is $0{\cdot}026_5$ Å, which is not statistically significant if we take the r.m.s. value of the deviation of the atoms from the mean plane as a measure of the accuracy of the atomic coordinates.

Pritchard & Sumner (1954) have recently calculated the bond lengths in chrysene using a self-consistent molecular-orbital approximation, and Table 1 gives a comparison of the experimental and the two theoretical values, M.O. and S.C.M.O., quoted from their paper.

Table 1. *Bond lengths in chrysene*

Bond	Expt. (Å)	M.O. (Å)	S.C.M.O. (Å)
A–B	1·409	1·426	1·438
B–C	1·433	1·404	1·423
C–D	1·423	1·381	1·363
D–E	1·387	1·398	1·423
E–F	1·392	1·380	1·363
F–G	1·435	1·407	1·424
G–H	1·410	1·417	1·439
H–I	1·403	1·372	1·355
A–A′	1·402	1·413	1·438
B–G	1·390	1·414	1·388

The agreement between experimental and theoretical values is not very good but it is perhaps significant that there is a wider range of values in the calculated bond lengths than in those found experimentally.

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Polarization correction for crystal-monochromatized X-radiation.

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In a previous publication bearing the above title (Azaroff, 1955), it was stated that the polarization correction for the equi-inclination method would have to be determined, individually, for each reflection. In a recent publication, Whittaker (1953) has derived a straightforward equation using reciprocal-lattice coordinates, μ, ν, and γ, for performing these calculations for an entire level at a time. A new calculation, however, should be made for each new crystal. The purpose of this note is to correct the omission of this reference from the original paper.

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