choice since their prominent faces are $\{hk0\}$ faces, terminated by large $\{\bar{1}01\}$ faces. However, a smaller crystal on which most of the X-ray work was done showed only $\{hk0\}$ and $\{001\}$ faces.

Glycine has the lattice constants

$$a = 5{\cdot}10,\ b = 11{\cdot}96,\ c = 5{\cdot}45\ \text{Å};\ \beta = 111^\circ\ 38'$$

and the crystals have good cleavage parallel to (010). The nearly flat glycine molecules lie in sheets, parallel to (010), with four molecules to the unit cell (Albrecht & Corey, 1939). That the sheet-like structure is also present in the glycine sulfate described here is indicated by the good (010) cleavage and is suggested by the optical properties.

When crystals are grown from a solution containing glycine and sulfuric acid in equal molecular proportions, they are orthorhombic with the formula

$$(CH_2NH_2COOH)_2H_2SO_4\ .$$

These crystals are not ferroelectric and may correspond to an orthorhombic glycine sulfate listed by Groth (1909). Crystals of the orthorhombic

$$(CH_2NH_2COOH)_2H_2SO_4\ ,$$

the orthorhombic $(CH_2NH_2COOH)_2H_2SeO_4$, and the monoclinic $(CH_2NH_2COOH)_3H_2SeO_4$ have all been grown and are currently under investigation. The selenates and the sulfates are isomorphous.

The writers wish to thank Mr Val Bala for assistance in obtaining the data reported.

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Atomic form-factor curves for carbon and oxygen of $>$C=O bond of anthraquinone (25–35° C.).

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The crystal structure of anthraquinone, $C_{14}H_8O_2$, was determined by Banerjee & Sen (1938) and by Sen (1945) by the two-dimensional Fourier synthesis method. In deriving F_c, Sen (1948) used the carbon scattering-factor curve of benzoquinone (Robertson, 1935) and the oxygen scattering-factor curve of magnesium oxide (Wollan, 1930). The agreement between F_o and F_c was not very satisfactory: the R value was 21% for the ($h0l$) projection, which is very well resolved. In spite of careful intensity measurements at temperatures ranging between 25° C. and 35° C., and refinement of the atomic positions by a difference synthesis, F_c's being calculated by Hartree curves corrected for temperature, it was still found that the R value remained quite high (R was 23% before refinement and 24% after refinement). This necessitated the determination of f curves for carbon and oxygen in anthraquinone. The publication of f curves for oxygen where it is bonded to a carbon atom of an aromatic benzene ring is expected to be useful for the determination of structures of aromatic compounds with C=O bonds.

Considering a particular atom, its scattering factor in any direction is given by

$$f = \int_{-r_0}^{+r_0} \varrho(r) \exp\left[i\mu r\right] dr\ ,$$

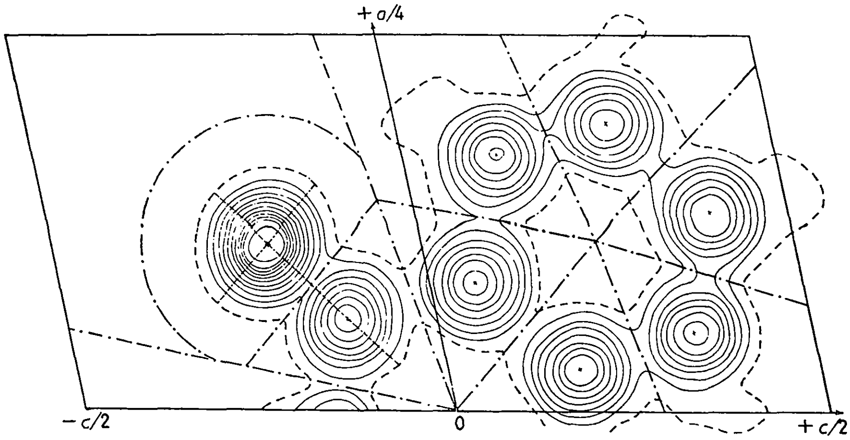

Fig. 1. The ($h0l$) projection of anthraquinone. Contours are drawn at intervals of 1 e.Å^{-2}, the 1-electron line being broken. The division lines for different atoms, the projected $>$C=O bond and the major axis of the oxygen atom are shown as chain lines.

where $\varrho(r)$ is the projection of electron density on a line at distance (r) from the centre of the atom along that line and $\mu = 4\pi \sin \theta/\lambda$.

Thus

$$f = \int_{-r_0}^{+r_0} \varrho(r) \cos \mu r dr + i \int_{-r_0}^{+r_0} \varrho(r) \sin \mu r dr .$$

On carrying out the integrations by summations it is found that the second term on the right-hand side is negligibly small compared with the first term, and so may be neglected. At $\sin \theta/\lambda = 0$, however, f (the total number of electrons in the atom) is precisely equal to

$$\int_{-r_0}^{+r_0} \varrho(r) \cos \mu r dr .$$

In applying the above method the whole area of projection is divided into parts containing different atoms through their points of contact, as shown in Fig. 1.

In carrying out the integration the influence of an atom is considered up to 1·3 Å from its peak in free space, after which the electron density is observed to be negligibly small; in the direction of the bond with another atom it is considered up to the contact between the two.

The contour diagram of the $F_o(h0l)$ synthesis in the case of oxygen indicated appreciable ellipticity with its minor axis along the projected $>\mathrm{C}=\mathrm{O}$ bond, which makes a very small angle (3·8°) with the actual bond direction in the plane of the molecule; thus the f values derived from this projection may be taken as equal to those along the bond itself. The electron density may be regarded to have rotational symmetry for the oxygen atom about the bond axis so that the f curve along one direction normal to this axis is enough. The scattering-factor curves along the minor and major axis are separately deduced and are given (along with Hartree's curves for oxygen ion and atom) in Fig. 2(*a*). The carbon atoms are found to have more or less circular symmetry in this projection, indicating the spherical symmetry of atoms, and so the scattering factor along one direction only is deduced, that one direction being the projected bond for the carbon of $>\mathrm{C}=\mathrm{O}$. From the results it appears that oxygen is in a partially ionized condition and the total number of electrons in it is found to be approximately nine. The carbon atom bonded with it has been found to have a total number of roughly five electrons. Thus the extra electrons required by the oxygen for this partial ionization may be considered as supplied by the adjacent carbon atom. This carbon atom therefore itself suffers ionization and differs from the other carbon atoms, which show in general a total electron count of roughly six. The f curves for this atom and one of the other carbon atoms, all of which gave identical values within experimental limits, are given (along with Hartree's curves) in Fig. 2(*b*). It is of special interest to note that all the experimental curves for $0{\cdot}1 < \sin \theta/\lambda < 0{\cdot}35$ are higher than the corresponding Hartree curves.

R value calculated with these f values after one refinement of the co-ordinates came down to roughly 14%. Further refinement is in progress.

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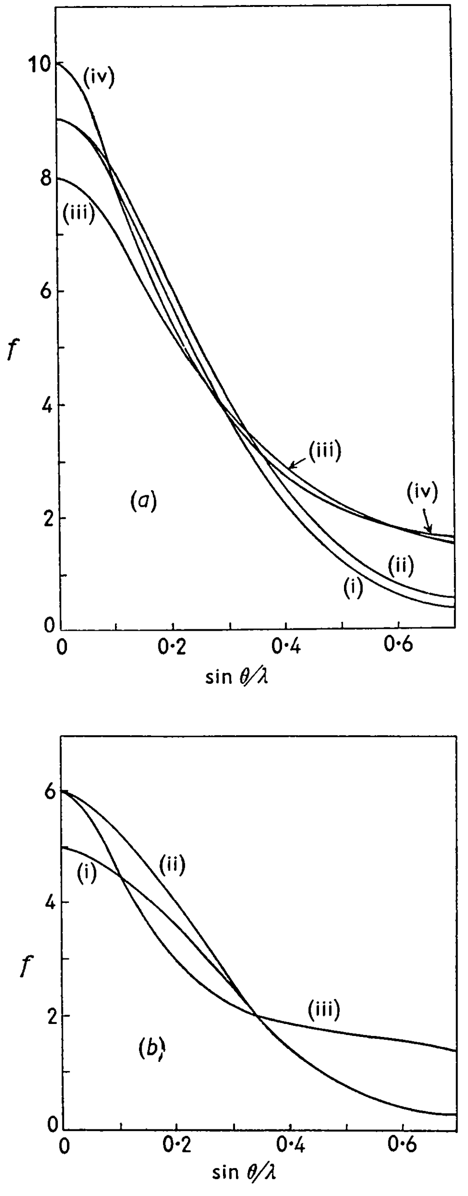

Fig. 2. (*a*) The f curves of oxygen of $>\mathrm{C}=\mathrm{O}$ in anthraquinone (25–35° C.). (i) Major axis; (ii) minor axis; (iii) Hartree atom; (iv) Hartree ion. (*b*) The f curves of carbon of $>\mathrm{C}=\mathrm{O}$ and of the general carbon atom in anthraquinone (25–35° C.). (i) Carbon of $>\mathrm{C}=\mathrm{O}$; (ii) general carbon atom; (iii) Hartree atom.

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