Acta Cryst. (1961). **14**, 553

p-Benzoquinone: mean-plane Fourier.

By J. Trotter, *Department of Chemistry, University of British Columbia, Vancouver 8, Canada*

(*Received* 6 *December* 1960)

In a three-dimensional refinement of the crystal structure of *p*-benzoquinone (Trotter, 1960), the author did not have access to facilities for computing the electron-density in the plane of the molecule. Recently, however, a program for computing the electron-density in any general plane in a crystal was made available; this program takes the equation of the plane as

$$Z' = aX' + bY + d$$

and computes z to the nearest 1/3600th of the cell edge for any predetermined x, y grid of points. The maximum error in z is therefore 1/7200th of the c-axis; for *p*-benzoquinone this error is of the order of 0·001 Å, and therefore quite negligible. The electron density is then computed at each point (x, y, z).

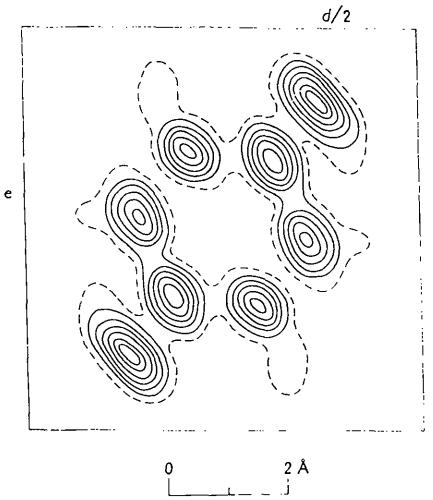

Fig. 1. Section through the plane of the *p*-benzoquinone molecule. Contours at intervals of 1 e.Å^{-3}, with the one-electron line broken.

The electron-density in the mean molecular plane of *p*-benzoquinone, computed with measured structure amplitudes and calculated signs, is shown in Fig. 1. On this diagram the boundary line d is the line of intersection of the molecular plane and (010), and e is the intersection of the molecular plane and (100). The lengths of the lines d and e are

$$d = 13{\cdot}220,\ e = 6{\cdot}798 \text{ Å}$$

and the angle between them is 91° 25′.

On this electron-density map the carbon and oxygen atoms are of course very clearly resolved, but the map as a whole is not as striking as the corresponding diagrams for naphthalene and anthracene (Abrahams, Robertson & White, 1949; Mathieson, Robertson & Sinclair, 1950). This is mainly due to the elongation of the contours, particularly for the oxygen atom, as a result of the anisotropic thermal motion. The shape of the one-electron line provides evidence for the presence of the hydrogen atoms.

A corresponding $(F_o - F_c)$ map was computed, but showed no really significant features. We should not of course expect to be able to detect such fine detail as bonding electrons in this case, since the criterion for determining the anisotropic temperature factors (Cochran, 1951) attributes all the differences between observed and calculated electron-density peaks to the thermal motion, and does not allow for possible changes in the peak shapes due to the formation of bonds. In addition such detailed electron-density studies are very difficult and the results are very susceptible to the effects of systematic errors in the F_o's; it was considered that the data were not sufficiently accurate to warrant further electron-density studies.

The author thanks the University of Glasgow for an I.C.I. Research Fellowship during the tenure of which some of this work was carried out. He is indebted also to Prof. J. M. Robertson for his interest, and to Dr J. G. Syme for kindly making available his DEUCE mean-plane Fourier program.

References

Abrahams, S. C., Robertson, J. M. & White, J. G. (1949*a*). *Acta Cryst.* **2**, 233.

Abrahams, S. C., Robertson, J. M. & White, J. G. (1949*b*). *Acta Cryst.* **2**, 238.

Cochran, W. (1951). *Acta Cryst.* **4**, 408.

Mathieson, A. McL., Robertson, J. M. & Sinclair, V. C. (1950*a*). *Acta Cryst.* **3**, 245.

Mathieson, A. McL., Robertson, J. M. & Sinclair, V. C. (1950*b*). *Acta Cryst.* **3**, 251.

Trotter, J. (1960). *Acta Cryst.* **13**, 86.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (D. W. Smits, Mathematisch Instituut, University of Groningen, Reitdiepskade 4, Groningen, The Netherlands).

International Union of Crystallography

Prices of Union Publications

By a formal decision of the Executive Committee in 1954, the fundamental prices of the main publications of the Union are those expressed in the currency of the country of publication: Danish Crowns for *Acta Crystallographica*, Netherlands Guilders for *Structure Reports*, and Pounds Sterling for the *International Tables*. For convenience approximate equivalents have been quoted in other currencies, subject to changes in the official rates of exshange.

The recent action of the Netherlands Government in