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***p*-Benzoquinone: mean-plane Fourier.** By J. TROTTER, *Department of Chemistry, University of British Columbia, Vancouver 8, Canada*

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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).

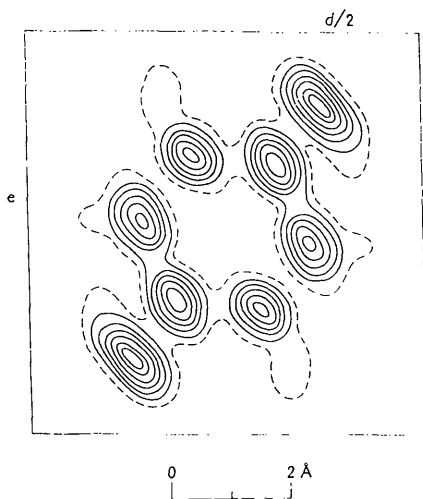


Fig. 1. Section through the plane of the *p*-benzoquinone molecule. Contours at intervals of $1 \text{ e} \cdot \text{Å}^{-3}$, with the one-electron line broken.

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

$$d = 13.220, \quad e = 6.798 \text{ Å}$$

and the angle between them is $91^\circ 25'$.

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.

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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, Reithdiepskade 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 exchange.

The recent action of the Netherlands Government in

revaluing the Guilder has made necessary a revision of the equivalent prices for *Structure Reports* in other currencies. The Executive Committee has consequently approved the prices in the following table. The prices of *Structure Reports* in Guilders (*f*) are, of course, unchanged.

Selling prices of Structure Reports

Vol.	Regular prices		Reduced personal prices			
	<i>f</i>	U.S. \$	U.K. shillings	<i>f</i>	U.S. \$	U.K. shillings
8	80	22.50	160	45	12.50	90
9	70	19.50	140	40	11.50	80
10	55	15.50	110	35	10.00	70
11	100	28.00	200	55	15.50	110
12	70	19.50	140	40	11.50	80
13	100	28.00	200	55	15.50	110
14	35	10.00	70	20	6.00	40
15	110	31.00	220	60	17.00	120
16	120	33.50	240	70	19.50	140

Naturally, the revaluation of the Netherlands Guilder does not affect the prices of *Acta Crystallographica* and the *International Tables*.

International Union of Crystallography Commission on Crystallographic Computing

A meeting of the Commission on Crystallographic Computing and its consultants and correspondents will take place at Frankfurt, Germany, from 7 to 9 June 1961. The following three items will be the main business for discussion at this meeting:

- Recommendations for the publication of crystallographic computing procedures.
- Plans for the collection of data for a World List of Crystallographic Computing Programs.
- Plans for a Computing Symposium, to be held in 1962 or 1963.

Anyone wishing to suggest further topics for discussion by the Commission on Crystallographic Computing at its meeting should communicate directly with the Chairman, Professor G. A. Jeffrey, University of Pittsburgh, Pittsburgh, Pa., U.S.A.

International Union of Crystallography International Conference on Magnetism and Crystallography

An International Conference on Magnetism and Crystallography will be held in Kyoto, Japan, 25-30 September 1961, by invitation of the Science Council, the Physical Society and the Crystallographic Society of Japan. The Conference will consist of two Parts: (I) an International Conference on Magnetism; and (II) an International Symposium on Electron and Neutron Diffraction.

The International Conference on Magnetism, which is sponsored by the International Union of Pure and Applied Physics, will be one of the regular conferences on magnetism which are promoted by the Commission on Magnetism of this Union. It will be devoted to all current topics of magnetism except those which are primarily of technical interest.

The International Symposium on Electron and Neutron Diffraction is sponsored by the International Union of

Crystallography, and the Commission on Electron Diffraction of this Union is participating in the organization of this Symposium. It will deal with methods, phenomena and important applications of electron and neutron diffraction.

The two series of meetings will run parallel, and joint sessions will be arranged for papers on magnetic scattering of neutrons. Proceedings of the Conference will be published as a Supplement to the Journal of the Physical Society of Japan.

The meetings are open to all scientists who are interested in the topics. Further details can be found in the Second Circular which was issued recently, and copies of which can be obtained from the Organizing Committee, c/o Science Council of Japan, Ueno Park, Tokyo, Japan.

1961 Summer Schools on Crystallography

The I.U.Cr. Commission on Crystallographic Teaching has collected the following information about Summer Schools to be held in 1961:

Gent (Belgium). July 24-August 5

Electrical, optical and mechanical properties of lattice defects.

Information and registration: Laboratorium voor Kristallografie en Studie van Vaste Stoffen, Rozier 6, Gent (Belgium).

Chicago (U. S. A.). Illinois Institute of Technology. June 12-23

X-Ray diffraction analysis.

Course I

The powder method, June 12-16; designed to familiarize beginners with the method. [Elementary X-ray diffraction theory, procedure for preparing powder diagrams, interpretation and indexing, identification of polycrystalline substances, quantitative analysis, precision lattice-constant determination.]

Attendance limited to 12 students.

Course II

Advanced methods in X-ray analysis, June 19-23; designed for those already familiar with the fundamentals of X-ray diffraction (the equivalent of the content of course I). Topics covered: the reciprocal lattice concept, advanced indexing methods, preferred orientation determination, particle-size determination, single-crystal orientation, crystal-symmetry determination.

Attendance limited to 12 students. Preference will be given to those who also enroll in course I.

Information and registration: Prof. Leonid V. Azaroff, Metall. Eng. Dept., Illinois Institute of Technology, Technology Center, Chicago 12, Ill. (U.S.A.).

Brooklyn (U. S. A.). Beginning of June

A two-week Summer School organized by Prof. I. Fankuchen.

Information and registration: Prof. I. Fankuchen, Polytechnic Institute of Brooklyn, 333 Jay Street, Brooklyn 1, N.Y. (U.S.A.).