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The accuracy of atomic co-ordinates derived from Fourier syntheses.

By G. J. Dickins,* *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England*

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During the refinement of the tetragonal structure of σ-CoCr (Dickins, Douglas & Taylor, 1956) it was found that the statistical method of calculating peak positions, due to Ladell & Katz (1954), gave positions which did not always agree with those found graphically. The purpose of this note is to illustrate the accuracy with which the atomic co-ordinates are determined.

The electron density values were determined at intervals of 1/120th (0·0083) of the cell edge. The values (arbitrary units) near the peak corresponding to an atom I_2 of this structure are shown in projection on (001) in Fig. 1(*a*). In Fig. 1(*b*) are shown the four positions for the peak, calculated from four sets of figures centred on the four points nearest the peak, together with the resulting mean calculated peak position and the graphically determined position; thus (for example) A^{645} is the peak position determined by the method of Ladell & Katz from the set of nine electron-density values centred by 645. The cross locates the position of the centre of the inner square of co-ordinates corresponding to electron densities 645, 616, 634, 627, as in Fig. 1(*a*).

The four calculated positions do not exactly superpose on account of the deviation of the shape of the atomic peak from a true paraboloid, but nevertheless the circle centred at A^{mean}, and of radius equivalent to 0·001 of the cell edge (i.e. ~ 0·01 Å), encloses all the co-ordinates determined graphically or statistically.

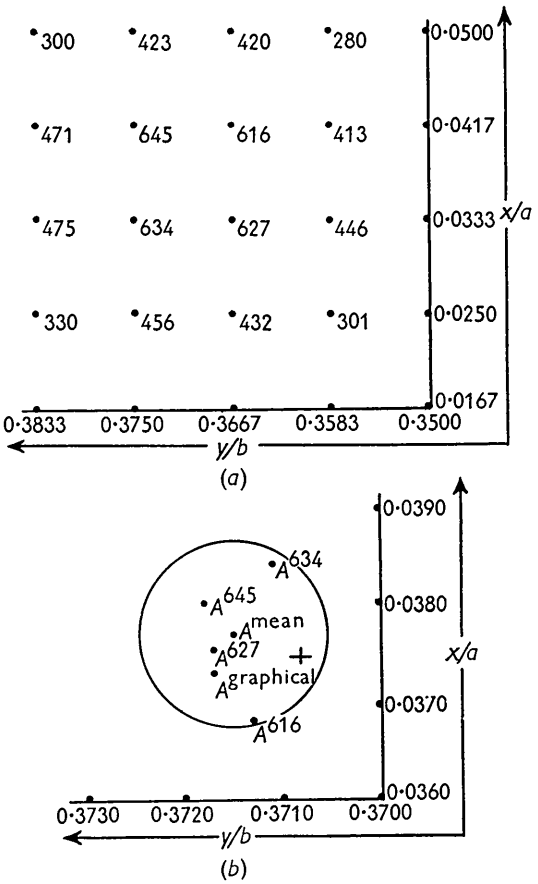

Fig. 1. Projections on (001) of atom I_2. (*a*) Electron-density values. (*b*) Position of electron-density peaks calculated in several ways from the data given in (*a*).

References

Dickins, G. J., Douglas, A. M. B. & Taylor, W. H. (1956). *Acta Cryst.* In the Press.

Ladell, J. & Katz, J. L. (1954). *Acta Cryst.* **7**, 460.

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Crystal data on cinchonine, $C_{19}H_{22}N_2O$.

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Precession photographs were taken with the crystal mounted parallel to the needle (*b*) axis, giving a monoclinic unit cell of the dimensions:

$a = 11{\cdot}20 \pm 0{\cdot}03$, $b = 7{\cdot}20 \pm 0{\cdot}02$, $c = 10{\cdot}80 \pm 0{\cdot}03$ Å, $\beta = 108°$.

The density, measured by flotation, is $1{\cdot}20 \pm 0{\cdot}06$ g.cm.$^{-3}$; that determined by X-rays is 1·18 g.cm.$^{-3}$. There are two molecules per unit cell. Systematic absences were observed only for $0k0$ with k odd, making the space group $P2_1$ or $P2_1/m$.

Powder data were obtained with a cylindrical camera

Table 1. *Indexed lines.*

d (Å)	*I*	*hkl*	*d* (Å)	*I*	*hkl*
10·66 *	70	100	4·32	40	210, 11$\bar{2}$
10·44		001	3·77	20	21$\bar{2}$
9·02	10	10$\bar{1}$	3·62	60	211, 020
5·93 *	100	110	3·31	10	31$\bar{1}$
5·85		011	3·09	10	013
5·30 *	40	200	2·96	20	30$\bar{3}$
5·25		10$\bar{2}$	2·82	10	311
5·13	30	002	2·72	10	122
4·78	40	111	2·55	10	203

* Lines resolved only on diffractometer.

of 114·6 mm. diameter, and with a diffractometer, using filtered copper radiation. The first few lines were indexed to ensure correspondence of the single-crystal and powder data. Intensities were estimated visually. The indexed lines are listed in Table 1. No structure determination is contemplated.

Letters to the Editor

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The need for determination of structures at different temperatures.

From KATHLEEN LONSDALE.
Department of Chemistry, University College, Gower Street, London W.C. 1, England

(*Received* 29 *December* 1955)

May I put in a plea that wherever possible structures for which diffraction measurements are made at more than one temperature shall be accurately determined *at each temperature* for which data are available. At present if measurements at low temperatures are made, this is only in order to minimize thermal vibrations, and the structure is usually refined only at the low temperature, and not also at room temperatures.

But there is an intrinsic interest in the changes of atomic parameters, if any, that take place with temperature change. There is also, from the point of view of crystal physics, an intrinsic interest in the thermal anisotropy of the atoms and molecules. And certain changes of physical properties of crystals with temperature, for example, diamagnetic anisotropy, can be adequately interpreted only if any changes of molecular orientation are known.

In the case of two organic structures (urea and benzil) that have been examined recently in this laboratory, it appears that although the size and shape of the unit cell changes considerably with a 200° C. drop in temperature, the atomic parameters do not change. This result is so unexpected that we would like to know whether there is any evidence for a similar invariance of parameters in other molecular compounds.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Structure Reports for 1942–44

The above volume of *Structure Reports*, the fifth to be prepared under the auspices of the International Union of Crystallography, is now ready. It is the aim of these *Reports* to give a critical account of crystal-structure investigations so complete that only those in need of minute detail will find it profitable to consult the original papers.

The volume now published has been prepared under the general editorship of A. J. C. Wilson, with N. C. Baenziger (Metals), J. M. Bijvoet (Inorganic Compounds) and J. M. Robertson (Organic Compounds) as section editors.

Orders may be placed direct with the publisher:

N.V. A. Oosthoek's Uitgevers Mij.
Domstraat 1–3, Utrecht,
Holland,

with the Polycrystal Book Service, 84 Livingston Street, Brooklyn 1, N.Y., U.S.A., or with any bookseller. The price is 65 Dutch florins, £6. 6*s*., or $17·50, post free. A remittance should accompany all orders.

The above volume is the last but one of those required to fill the war-time gap; it is expected that the last (Vol. 8 for 1940–41) will appear in the course of 1956. Further volumes covering the years 1951 onwards are also in course of preparation.

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Readers are reminded that arrangements have been made with Messrs Easibind Ltd, 84 Newman Street, London W. 1, England, for the provision of self-binders for *Acta Crystallographica*. The binder for Vols. 1–2 is designed to carry the twelve parts of the two volumes, which are held without damage by steel wires; it is lettered with title, volume numbers and years (e.g. Vols 1 and 2, 1948–9).

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