Acta Cryst. (1956). **9**, 201

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

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(*Received* 14 *November* 1955)

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. $\sim$ 0·01 Å), encloses all the co-ordinates determined graphically or statistically.

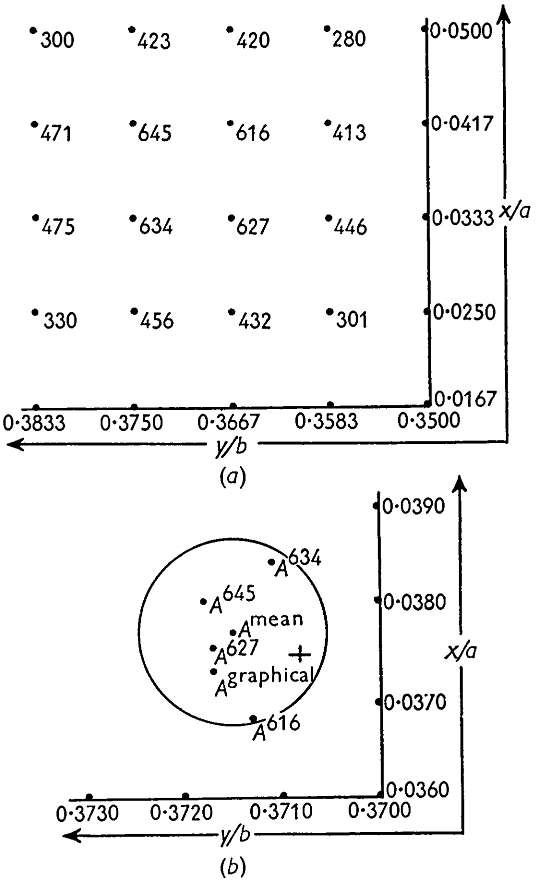

Fig. 1. Projections on (001) of atom I_2. (*a*) Electron-density values. (*b*) Position of electron-density peaks calculated in several ways from the data given in (*a*).

References

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Acta Cryst. (1956). **9**, 201

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

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(*Received* 23 *August* 1955 *and in revised form* 24 *October* 1955)

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

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

The density, measured by flotation, is 1·20 ± 0·06 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 0*k*0 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.