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The errors in the measurement of intensities from X-ray photographs.

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Attention is drawn to the θ-dependence of errors due to absorption.

Monahan, Schiffer & Schiffer (1967) state that the most reasonable estimate of errors in intensity measurements is that 'the fractional error in each determination is constant'.

This is true only for crystals of low absorption. Reference to Fig. 4 of Jeffery & Rose (1964) shows that, for near-spherical crystals, the proportional error is independent of θ only up to $\mu r = 0{\cdot}4$ and that at $\mu r = 3$ the error for reflexions in the forward direction is roughly three times that in the back-reflexion region.

The example of fluoromalic acid, quoted by Monahan *et al.*, probably comes in the low absorption category, but serious errors could arise from ignoring the θ-dependence in more highly absorbing crystals.

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The crystal and molecular structure of D(+)-barium uridine-5′-phosphate.

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A correction to *Acta Cryst.* (1965) **18**, 1067.

In Table 1 of the article under the above title (Shefter & Trueblood, 1965), the atom in line 7 [below O(III) and above C(5′)] should be O(5′), not O(2′). [Correct O(2′) is given later in the table.]

Reference

SHEFTER, E. & TRUEBLOOD, K. N. (1965). *Acta Cryst.* **18**, 1067.

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A four-dimensional view of some cubic lattices.

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The face-centred cubic lattice and the diamond 'lattice' can be regarded as derived from a four-dimensional simple hyper-cubic lattice.

The treatment of the face-centred cubic (f.c.c.) lattice outlined below is analogous to the well-known description of the plane hexagonal lattice as a section on the plane (111) of the simple cubic lattice. For this two-dimensional lattice we use, not a pair of integers, but a set of three integers, i, j, k satisfying $i+j+k=0$ to represent a lattice point. This idea is widely used in crystallography in the form of the Miller–Bravais 4-indices for crystals of the hexagonal system, where it has the advantage over a 3-index description of not obscuring the symmetry of the lattice. Frank (1965) has emphasized the usefulness of regarding the Miller–Bravais indices in terms of a four-dimensional model.

For the f.c.c. lattice we start from the simple hyper-cubic lattice (I) given by the set of four integers i, j, k, l, and consider the section (II) defined by $i+j+k+l=0$. The form of the resulting three-dimensional structure is apparent when we rotate the axes by the transformation

$$w=\tfrac{1}{2}\,(i+j+k+l) \qquad y=\tfrac{1}{2}\,(i+j-k-l)$$
$$x=\tfrac{1}{2}\,(i-j+k-l) \qquad z=\tfrac{1}{2}\,(-i+j+k-l)$$

Then for the section II, the coordinates w, x, y, z take the form $0,\ i+k,\ i+j,\ j+k$; thus the coordinates x, y, z have $x+y+z$ even and form a f.c.c. lattice with a cube edge of length 2 units.

The construction is extended to the diamond 'lattice' by adding to the f.c.c. lattice additional points constructed as follows: take those points of I lying in the section (III) defined by $i+j+k+l=-1$, and project them onto section II along the direction $[\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}]$, *i.e.* parallel to the w axis. In this way a second f.c.c. lattice is obtained, displaced through $x,y,z=\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}$ from the first, and the two lattices together give the diamond 'lattice'.

To gain some familiarity with this representation, one may consider simple features of the lattices such as the number of nearest neighbours. In the f.c.c. lattice we find a nearest neighbour of a point i, j, k, l by adding $+1$ to one index and -1 to another, the changes in two indices being necessary to avoid leaving the section II. There are twelve ways of doing this. In the diamond 'lattice' a point from section II (III) has as nearest neighbours four points from section III (II) obtained by adding -1 $(+1)$ to one of the four indices. For such questions one may ignore the step of projecting the section III points onto section II.

In the conventional description of the f.c.c. lattice the advantages of orthogonal axes and of retaining the symmetry of the lattice are achieved by adopting a non-primitive unit cell. In the present description the set of four indices retains the symmetry of the lattice and uses orthogonal axes, whilst by dropping any one of the four indices we have an indexing of the lattice using a primitive unit cell.

Many numerical studies have been made using the diamond 'lattice' to throw light on the problems of conformation of flexible polymer molecules (*e.g.* Wall, Windwer & Gans, 1963). The four-dimensional description of the diamond 'lattice' could well be useful in such studies, particularly when it is required to store an array in the computer representing the points of the 'lattice,' as in the study by Martin (1962).

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Crystal data for some halogenated steroids.

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The lattice parameters and space groups of eight kinds of halogenated steroid have been determined.

Recently Nagata (1962, 1964, 1966) carried out a study of the structure of 8β-substituted steroids on the basis of chemical evidence. In connexion with his study, the present authors and others in the Shionogi X-ray group have determined the crystal structure of some halogenated steroids. The crystal data for these substances, which are given in Table 1, were obtained from Weissenberg and precession photographs with Cu $K\alpha$ radiation. Densities were determined by the flotation method.

The crystal structures of 8β-methyltestosterone 17β-monobromoacetate (Shiro, Sato, Tsukuda & Koyama, 1967), testosterone 17β-*p*-bromobenzoate (Sato, Shiro, Tsukuda & Koyama, 1967), 8β-methylestradiol 3-methyl ether 17-monobromoacetate (Tsukuda, Shiro, Sato & Koyama, 1967*a*) and estradiol 3-*p*-bromobenzoate (Tsukuda, Shiro, Sato & Koyama, 1967*b*) have already been determined, and will be published in the near future.

No further work is being undertaken on the other four halogenated steroids.

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Table 1. *Crystal data for some halogenated steroids*

	1	2	3	4	5	6	7	8
Formula	$C_{22}H_{31}O_3Br$	$C_{21}H_{29}O_3I$	$C_{26}H_{31}O_3Br$	$C_{21}H_{27}O_3Br$	$C_{22}H_{29}O_3Br$	$C_{21}H_{27}O_3I$	$C_{26}H_{29}O_3Br$	$C_{25}H_{27}O_3Br$
Mol.wt.	423·4	456·4	471·4	407·4	421·4	454·4	469·4	455·4
D_m (g.cm^{-3})	1·378	1·476	1·385	1·352	1·397	1·560	1·377	1·412
D_x (g.cm^{-3})	1·381	1·481	1·385	1·373	1·406	1·567	1·379	1·413
Space group	$P2_12_12_1$	$P2_12_12_1$	$C2$	$P2_1$	$P2_1$	$P2_1$	$P2_12_12_1$	$P2_12_12_1$
Z	4	4	4	4	2	2	8	4
a (Å)	18·509	16·060	17·788	9·027	11·842	21·237	37·428	20·508
b (Å)	10·355	10·285	7·081	30·713	8·081	7·326	7·349	9·541
c (Å)	10·626	12·394	18·050	7·484	10·474	6·217	16·440	10·942
β (°)	—	—	95·02	108·25	96·65	95·55	—	—
V (Å^3)	2036·6	2047·2	2261·0	1970·6	995·5	962·7	4521·8	2140·9
Solvent	Ether–light petroleum	Ether	Methylene chloride–methanol	Ether–light petroleum	Ether–light petroleum	Ether	Ether–light petroleum	Acetone

1. 8β-Methyltestosterone 17-monobromoacetate
2. Testosterone 17-monoiodoacetate
3. Testosterone 17-*p*-bromobenzoate
4. Estradiol 3-methyl ether 17-monobromoacetate
5. 8β-Methylestradiol 3-methyl ether 17-monobromoacetate
6. Estradiol 3-methyl ether 17-monoiodoacetate
7. Estradiol 3-methyl ether 17-*p*-bromobenzoate
8. Estradiol 3-*p*-bromobenzoate