

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 conforma-

tion 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. By H. NAKAI and H. KOYAMA, *Shionogi Research Laboratory, Shionogi & Co., Ltd, Fukushima-ku, Osaka, Japan*

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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 17 β -monobromoacetate (Shiro, Sato, Tsukuda & Koyama, 1967), testosterone 17 β -*p*-bromobenzoate (Sato, Shiro, Tsukuda & Koyama, 1967), 8β -methyl estradiol 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 ₃ Br	C ₂₁ H ₂₉ O ₃ I	C ₂₆ H ₃₁ O ₃ Br	C ₂₁ H ₂₇ O ₃ Br	C ₂₂ H ₂₉ O ₃ Br	C ₂₁ H ₂₇ O ₃ I	C ₂₆ H ₂₉ O ₃ Br	C ₂₅ H ₂₇ O ₃ Br
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	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>C</i> 2	<i>P</i> 2 ₁	<i>P</i> 2 ₁	<i>P</i> 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>Z</i>	4	4	4	4	2	2	8	4
<i>a</i> (Å)	18.509	16.060	17.788	9.027	11.842	21.237	37.428	20.508
<i>b</i> (Å)	10.355	10.285	7.081	30.713	8.081	7.326	7.349	9.541
<i>c</i> (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	—	—
<i>V</i> (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 -Methyl estradiol 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