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## A note on the elastic properties of pentaerythritol.

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Srivastava & Chakraborty (1960) published theoretical relationships connecting the rekha constants (using the nomenclature of Ramachandran & Wooster, 1951) corresponding to simple and elementary directions of reciprocal lattice and the thermal wave vector in terms of the elastic constants for crystals belonging to tetragonal crystal classes 4, $\bar{4}$ and $4/m$. They also suggested a method of 'successive approximations' to obviate the difficulty arising in the evaluation of the elastic constants due to the presence of the constant $C_{16}$ in the elastic matrix of the above crystals. It may be mentioned here that the elastic constants of any crystal belonging to 4, $\bar{4}$, or $4/m$ class have not yet been determined. It is expected, therefore, that the elastic constants of such crystals may prove to be of interest.

Pentaerythritol belongs to $\bar{4}$ crystal class. Its (200), (202) and (004) diffuse reflections with [010] axis and, (200) and (220) with [001] axis perpendicular to the direction of incidence of X-rays have been studied. The choice of the reflections was made according to the criterion given by Ramachandran & Wooster (1951). For evaluating the elastic constants from the experimentally determined rekha constants the method suggested by Srivastava & Chakraborty (1960) has been employed.

The value of the constants is given below in units of $10^{10}$ dynes/cm.$^2$:

$$C_{11}=6{\cdot}1,\ C_{33}=8{\cdot}0,\ C_{44}=3{\cdot}5,\ C_{66}=4{\cdot}6,$$
$$C_{16}=-0{\cdot}39,\ C_{13}=0{\cdot}50,\ C_{12}=-2{\cdot}50.$$

The discussion of the accuracy of the method has been done in detail by Ramachandran & Wooster (1951) and Chakraborty & Sen (1958). The accuracy of the determination of the constants $C_{11}$, $C_{33}$, $C_{44}$, $C_{66}$, $C_{16}$ is estimated to be $\pm 4\%$ whereas that of $C_{12}$ and $C_{13}$ $\pm 6\%$.

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### References

Chakraborty, S. C. & Sen, R. K. (1958). *Proc. of the Symposium on Crystal Physics. Nat. Inst. Sci., India*, Bull. No. 14, 20.

Ramachandran, G. N. & Wooster, W. A. (1951). *Acta Cryst.* **4**, 335.

Srivastava, R. C. & Chakraborty, S. C. (1960). *Indian J. Phys.* **34**, 253.

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## The morphology and space groups of some halogen substituted derivatives of 5α-cholestane.

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In connection with investigations in one of our laboratories (L.O.C.), concerning the stereochemical features of 1,2 dihalogenocyclohexane and dioxane compounds (Kwestroo, Meyer & Havinga, 1954; Altona, Romers & Havinga, 1959; Van der Linden, 1958; Wessels, 1960) and of steroids (Van Moorselaar, 1962), a morphological survey and an X-ray analysis of some dihalogenosteroids was undertaken.

Single crystals of

I 2β, 3α [*a*, *a*] dibromo-cholestane
II 2β, 3α [*a*, *a*] chloro-bromo-cholestane
III 2β, 3α [*a*, *a*] dichloro-cholestane (two forms α and β)
IV 2α, 3β [*e*, *e*] dibromo-cholestane
V 2α, 3β [*e*, *e*] dichloro-cholestane

were obtained by slow crystallization from ethylacetate.

### Morphology and optics

I. 2, 3 [*a*, *a*] Br, Br

$$a:b:c=4{\cdot}214:1:0{\cdot}5810;\ \beta=90^\circ;\ \text{orthorhombic.}$$

Crystals are tablets {100} of varying thickness and with a rectangular outline. In the zone [010] the form {101} is always present and sometimes {001}. In [001] occur {110}, {210} and {310} of which the latter is always very small.

Barker angles, omitting {310}:

$$cr=82^\circ\ 9',\ am=30^\circ\ 9',\ bq=13^\circ\ 21'.$$

Transformations: old → new $001/010/\bar{1}00$; new → old $00\bar{1}/010/100$.

Barker angles for combinations without {110}, but with {210} present:

$$cr=16^\circ\ 12',\ am=25^\circ\ 23',\ bq=82^\circ\ 9'.$$

Transformations: old → new $020/\bar{1}00/001$; new → old $0\bar{2}0/100/002$.

II. 2, 3 [*a*, *a*] Cl, Br

$$a:b:c=1{\cdot}285:1:0{\cdot}949;\ \beta=112^\circ\ 26';\ \text{monoclinic.}$$

Crystals are tablets {100}, elongated along the *c*-axis.

Observed forms: {100} large, {110} and $\{1\bar{1}0\}$ small; sometimes {010} and $\{0\bar{1}0\}$. The tablets are terminated by {001}, {101}, $\{0\bar{1}1\}$, {011}, $\{1\bar{1}1\}$ and {111}. Of these $\{0\bar{1}1\}$ is always larger than {011}, while {111} always larger than $\{1\bar{1}1\}$. The latter six forms are not always all present, but various combinations occur.