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The crystal structure of B_2O_3.

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The structure of B_2O_3 prepared by the method of McCulloch (1937), has been determined. As it was impossible to obtain single crystals, use was made of powder photographs taken with monochromatized Cu $K\alpha$ radiation. The unit cell containing $3\ B_2O_3$ is hexagonal, as found by H. F. McMurdie. The axial lengths are

$$a = 4{\cdot}325,\ c = 8{\cdot}317\ \text{Å}$$

and the space group is C_3^2–$C3_1$(C_3^3–$C3_2$).

The structure had to be determined by trial-and-error methods. The only position in the above space group is general and threefold. The atoms are distributed in five such positions with the parameters:

$3\ O_I$:	0·20, 0·15, 0·00,
$3\ O_{II}$:	0·46, 0·79, 0·07,
$3\ O_{III}$:	0·51, 0·23, 0·56,
$3\ B_I$:	0·54, 0·15, 0·02,
$3\ B_{II}$:	0·59, 0·77, 0·26.

The agreement between calculated and observed $p|F|^2_{hkl}$ values is quite satisfactory.

The structure is built up of two sets (a and b) of BO_4 tetrahedra (Fig. 1). Each of these shares corners with others. Three of the corners are divided between three and the fourth between two tetrahedra.

The interatomic distances calculated from the parameters given above are:

a tetrahedra	b tetrahedra
O_I'–O_{II}' = 2·47 Å	O_I –O_{II} = 2·43 Å
O_I'–O_{III}' = 2·36	O_I –O_{III} = 2·42
O_{II}'–O_{III}' = 3·05	O_{II} –O_{III} = 2·37
O_{II}–O' = 2·65	O_{III}'–O_I = 2·74
O_{II}–O_I' = 2·92	O_{III}'–O_{II} = 2·98
O_{II}–O_{III}' = 2·45	O_{III}'–O_{III} = 2·96

a tetrahedra	b tetrahedra
B –O_I' = 1·31	B –O_I = 1·48
B –O_{II}' = 2·03	B –O_{II} = 1·50
B –O_{III}' = 1·59	B –O_{III} = 1·36
B –O_{II} = 1·69	B –O_{III}' = 2·12 .

Pauling's electrostatic valence rule is fulfilled if the strength of the bond B–O_I is 1 and the strengths of the other B–O bonds are $\frac{2}{3}$. These bond strengths are in accord with the short distance B–O_I' in the tetrahedron (a), which has practically the same value as the B–O distance corresponding to the strength 1 in the BO_3 triangles of known borate structures. In the tetrahedron (b), O_I forms part of a highly contracted oxygen triangle with the edges 2·37, 2·42 and 2·43 Å. The boron atom is placed only 0·40 Å from the plane of this triangle. Its distance to the fourth oxygen, O_{III}', is as long as 2·12 Å. The distribution of the bond strengths is evidently not so simple as could be supposed from Pauling's rule.

On account of the fact that B_2O_3 tends to crystallize spontaneously from a highly viscous liquid of partially dehydrated H_3BO_3 in the presence of crystals of cubic HBO_2 (designated HBO_2(I) by Kracek, Morey & Merwin (1938)), it seems reasonable to suppose a structural relationship to exist between B_2O_3 and HBO_2(I).

There also exist certain interesting analogies between the structure of B_2O_3 and the structures of α- and β-quartz.

A detailed report with refined parameters and atomic distances will be given later.

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A correction and note on the relation of the β-uranium and σ-phase structures.

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Owing to an unfortunate slip in my paper on the crystal structure of the β-phase of uranium (Tucker, 1951), the reference to the work of Shoemaker & Bergman on the structure of the σ-phase in the Fe–Cr system was given as 1951 rather than 1950. The complete reference should be *J. Amer. Chem. Soc.* **72**, 5793, (1950).

This slip was most regrettable. Furthermore, that part of my paper dealing with the relation of the β-uranium and σ-phase structures, as the paragraph heading indicated, was intended to discuss that subject alone, and presents the discovery and verification of this similarity just as it came to my attention. It was not intended to infer anything regarding the history of σ-phase investigation in any part of my paper nor from a connection of anything in my paper with the misdating, as this history was considered outside the scope of my paper.

A detailed answer to the criticisms of the β-uranium structure by Bergman & Shoemaker (1951) and by Thewlis (1951) is being prepared and will be submitted as a separate note.

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