Financial support from NSERC (M. H. Benn) is gratefully acknowledged. We also wish to thank Dr K. A. Kerr for providing access to the diffractometer.

References

CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee.

RICHARDSON, J. F. & CULVENOR, C. C. J. (1985). *Acta Cryst.* C**41**, 1475–1477.

STEWART, J. M. (1976). Editor. *XRAY76*. Tech. Rep. TR-446. Computer Science Center, Univ. of Maryland, College Park, Maryland.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

WALKER, N. & STUART, D. (1983). *Acta Cryst.* A**39**, 158–166.

YADAV, V. K., RÜEGER, H. & BENN, M. H. (1984). *Heterocycles*, **22**, 2735–2738.

SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1985). C**41**, 1689–1690

New description of the $Ca_3(BO_3)_2$ structure.

By A. VEGAS, *Instituto de Química Inorgánica 'Elhúyar', CSIC, Serrano* 113, 28006 *Madrid, Spain*

(*Received* 22 *February* 1985; *accepted* 29 *July* 1985)

Abstract

The structure of $Ca_3(BO_3)_2$ [and isostructural $Sr_3(BO_3)_2$] is difficult to describe using the traditional cation-centered polyhedra model. However, the structure can be described in a simple and more elegant way as anticorundum Ca_3X_2 ($X = BO_3$), by considering the alternative model of an anion-stuffed cation array [White & Hyde (1982). *Phys. Chem. Miner.* **8**, 55–63].

From a comparison of their powder patterns, $Ca_3(BO_3)_2$ and $Sr_3(BO_3)_2$ have been reported as isostructural (Richter & Müller, 1980). However, only the structure of the Ca compound has been determined from single-crystal data. It is trigonal, $R\bar{3}c$, with cell dimensions $a = 8{\cdot}6377\,(8)$, $c = 11{\cdot}849\,(2)$ Å and $Z = 6$. The structure was first solved by Schuckmann (1970), who observed a slight deviation from planarity, in the BO_3 group, which was confirmed in a redetermination carried out by Vegas, Cano & Garcia-Blanco (1975).

In both cases, the structure was described as built up of cation-centered anion polyhedra, with eight-coordinated Ca at the center of a distorted square antiprism and BO_3 triangles, but the structure could not be related to any known structural type. It is our aim to offer an alternative and clearer description, regarding this structure as an anion-stuffed cation array, as proposed by White & Hyde (1982) and applied successfully to describe and relate the structures of the humite and leucophoenicite families (White & Hyde, 1983).

The structure, projected on the *ab* plane, is represented in Fig. 1. The cation array is clearly related to the corundum structure, *i.e.* Ca with slightly distorted h.c.p. and B occupying pairs of face-sharing octahedra. As does Al in corundum, the B atoms deviate towards the opposite faces of these octahedra. The model is represented in Fig. 2.

The structure should be stuffed with O atoms, occupying tetrahedral holes of the Ca h.c.p., but, if so, they could not bond to B atoms. So, the BO_3 groups, as a whole, are inserted into the Ca_6 octahedra and the structure is better described as anticorundum Ca_3X_2 ($X = BO_3$).

O atoms are pentacoordinated by four Ca [at $2{\cdot}347\,(1)$, $2{\cdot}431\,(1)$, $2{\cdot}440\,(1)$ and $2{\cdot}732\,(1)$ Å] and one B [$1{\cdot}384\,(1)$ Å], forming an irregular triangular bipyramid,

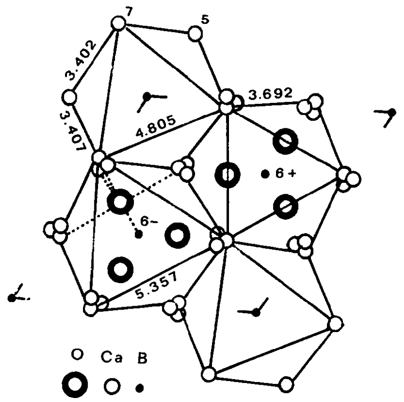

Fig. 1. Cation array of $Ca_3(BO_3)_2$ projected on the *ab* plane, showing a sheet of BCa_6 octahedra. Heights are expressed in twelfths (5 and 7 for Ca, 6+ and 6– for B). Ca–Ca distances are given in Å (e.s.d.'s ~0·001 Å).

0108-2701/85/111689-02$01.50

with B in the equatorial plane. These bonds are marked with dotted lines in Figs. 1 and 2.

Looking at Fig. 2, one has the impression that the Ca_6 octahedra are highly compressed along the triad axes. What really happens is that, to satisfy the Ca—O bond lengths and also owing to the shape and orientation of the BO_3 groups, Ca atoms expand markedly, in the close-packed layers, up to a distance of 5·36 Å.

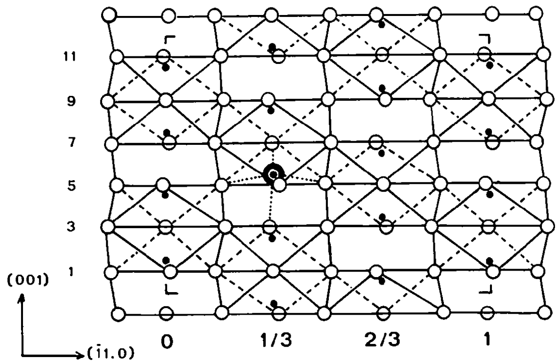

Fig. 2. A sheet of BCa_6 octahedra projected on ($\bar{1}$1.0) to show the similarity with corundum. Heights along **c** are in twelfths. The dotted lines represent the coordination polyhedron around O; it corresponds to that drawn in Fig. 1.

References

Richter, L. & Müller, F. (1980). *Z. Anorg. Allg. Chem.* **467**, 123–125.

Schuckmann, W. (1970). *Neues Jahrb. Mineral. Monatsh.* pp. 142–144.

Vegas, A., Cano, F. H. & García-Blanco, S. (1975). *Acta Cryst.* B**31**, 1416–1419.

White, T. J. & Hyde, B. G. (1982). *Phys. Chem. Miner.* **8**, 55–63.

White, T. J. & Hyde, B. G. (1983). *Acta Cryst.* B**39**, 10–17.

Acta Cryst. (1985). C**41**, 1690

A comparison of two independent determinations of the crystal structure of sodium aqua[ethylenediaminetetraacetato(4—)]ferrate(III) dihydrate.

By X. Solans, *Departamento Cristalografía y Mineralogía, Universidad de Barcelona, Gran Via* 585, 08007-*Barcelona, Spain*

(*Received* 20 *June* 1985; *accepted* 5 *August* 1985)

Abstract

The crystal structure of the title compound has been independently determined by Solans, Font-Altaba & García-Oricain [*Acta Cryst.* (1984). C**40**, 635–638] and López-Alcalá, Puerta-Vizcaino, González-Vilchez, Duesler & Tapscott [*Acta Cryst.* (1984). C**40**, 939–941]. A normal probability-plot comparison of 75 non-hydrogen coordinates shows that 71 deviate by $\le 2(\sigma_1^2 + \sigma_2^2)^{1/2}$, σ_i being the e.s.d. in the coordinates for each structure, and a half-normal probability-plot comparison of 143 non-hydrogen interatomic lengths <4 Å shows that 137 deviate by $\le 2(\sigma_1^2 + \sigma_2^2)^{1/2}$.

The main differences between the two crystal structure determinations are in the diffractometer measurements. The ranges of the 25 reflections used in the cell-parameter determination are $4 \le \theta \le 12°$ in structure *A* (Solans *et al.*, 1984) and $5 \le \theta \le 17{\cdot}5°$ in structure *B* (López-Alcalá *et al.*, 1984). This fact, the different sample size and the centring of the crystal lead to cell parameters $a = 8{\cdot}896$ (1), $b = 11{\cdot}931$ (2), $c = 15{\cdot}065$ (2) Å, $\beta = 100{\cdot}15$ (2)° for *A* and $a = 8{\cdot}895$ (1), $b = 11{\cdot}924$ (2), $c = 15{\cdot}043$ (2) Å, $\beta = 100{\cdot}06$ (1)° for *B*, showing the typical underestimation of standard deviations in cell parameters. The ranges of intensity collected were $2 \le \theta \le 25°$ in *A* and $0{\cdot}5 \le \theta \le 30°$ in *B*, so the number of independent reflections used in the refinements were 1403 and 2370, respectively. As the H atoms in *B* were computed and included with fixed C—H distances, while those in *A* were refined, the ratios of number of reflections/number of parameters are 5·1 in *A* and 10·6 in *B*. The final *R* values are 0·047 and 0·027, respectively, in the same absolute configuration in space group *Cc*.

A normal probability-plot comparison of the atomic coordinates has been carried out (Abrahams & Keve, 1971). The residual variance was 1·30, slope 2·2 (2) and intercept −0·8 (2). Only two coordinates differ by $> 3(\sigma_1^2 + \sigma_2^2)^{1/2}$: the *x* and *z* coordinates of the Na^+ ion. In the range $2–3(\sigma_1^2 + \sigma_2^2)^{1/2}$ are *y* of O(22) and *z* of C(22). A half-normal probability-plot comparison between the interatomic distances less than 4 Å leads to a residual variance of 0·174, slope 1·33 (6) and intercept −0·31 (6). The four distances that deviate by $> 3(\sigma_1^2 + \sigma_2^2)^{1/2}$ are Na···O(11) 3·500 (7), 3·526 (2); Na···C(42) 2·781 (9), 2·745 (3); Na···O(41) 2·507 (7), 2·466 (2); and Na···O(*W*1) 3·824 (7), 3·775 (2) Å, respectively, for *A* and *B*.

References

Abrahams, S. C. & Keve, E. T. (1971). *Acta Cryst.* A**27**, 157–165.

López-Alcalá, J. M., Puerta-Vizcaino, M. C., González-Vilchez, F., Duesler, E. N. & Tapscott, R. E. (1984). *Acta Cryst.* C**40**, 939–941.

Solans, X., Font-Altaba, M. & García-Oricain, J. (1984). *Acta Cryst.* C**40**, 635–638.

0108-2701/85/111690-01$01.50