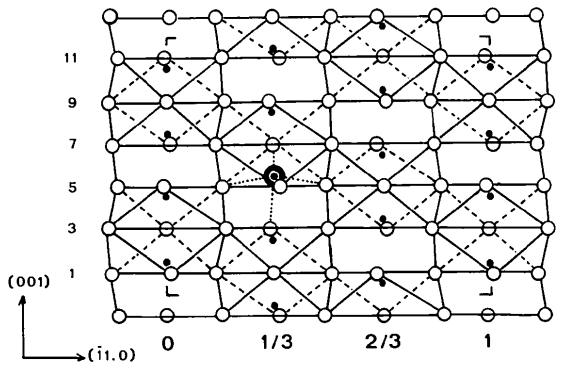

Fig. 2. A sheet of BCa_6 octahedra projected on ($\bar{1}$1.0) to show the similarity with corundum. Heights along **c** are in twelfths. The dotted lines represent the coordination polyhedron around O; it corresponds to that drawn in Fig. 1.

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.

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 $\leq 2(\sigma_1^2 + \sigma_2^2)^{1/2}$, 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 $\leq 2(\sigma_1^2 + \sigma_2^2)^{1/2}$.

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 $4 \leq \theta \leq 12°$ in structure *A* (Solans *et al.*, 1984) and $5 \leq \theta \leq 17{\cdot}5°$ 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 $2 \leq \theta \leq 25°$ in *A* and $0{\cdot}5 \leq \theta \leq 30°$ 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 $2\text{–}3(\sigma_1^2 + \sigma_2^2)^{1/2}$ 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