

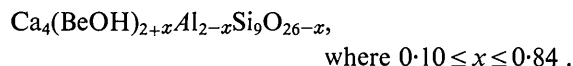
$T(4)$: some evidence arises from the short average Al–O distance. The specimens richer in beryllium have about one half of the aluminum replaced by beryllium; this substitution does not result in a variation of the electrostatic field around the oxygen atoms involved, O(3) and O(4), only if the hydrogen that accompanies beryllium distributes itself statistically between them. There is also much room around O(2) suitable for occupancy by hydrogen, without any need of a statistical distribution among more than one position; this could be a likely way because in many respects O(2) and O(8), or $T(3)$ and Be play similar roles in the structure, as pointed out above in this discussion. In this case the beryllium to aluminum substitution would result in a clear improvement of the sum of the electrostatic valences around O(2) quoted in Table 5, because the hydrogen that accompanies the beryllium excess would add its contribution to the latter sum. An increase of the distances $T(3)$ –O(2) and Ca–O(2) parallel to the increase of the beryllium to aluminum substitution would strengthen this hypothesis, as an evidence that the shortness of these distances is less and less necessary to obtain the balance of the electrostatic valences around O(2).

There is no clear evidence to choose between these hypotheses; the diadochy could be even more complicated and involve also the silicon atoms: for example, diadochy between $T(1)$ and Al cannot be excluded to a small extent, owing to the long average $T(1)$ –O distance and to the short Al–O one. However these open

questions have been discussed here to point out that a comparison of the structure of this bavenite with that of a beryllium-rich one would be of interest in order to understand the details of diadochy between the tetrahedrally coordinated cations.

Chemical formula

The up-to-date more reasonable chemical formula of bavenite appears to be:



We wish to thank Professor F. Sgarlata who kindly made available to us his program for three-dimensional refinement by the least-squares method.

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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. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1966). **20**, 309

Crystal data for (–)-threo-12,13-dihydroxyoleic acid. By DAVID A. LUTZ and WILLIAM E. SCOTT, *Eastern Utilization Research and Development Division, Agricultural Research Service, U.S. Department of Agriculture, Philadelphia, Pa.* 19118, U.S.A.

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The present study was undertaken to obtain crystal data on (–)-threo-12,13-dihydroxyoleic acid, $\text{C}_{18}\text{H}_{34}\text{O}_4$, which was prepared by acetolysis of the seed oil of *Vernonia anthelmintica* (L.) Willd. (Scott, Krewson & Riemenschneider, 1962). The compound was further purified [as evidenced by chemical analysis (C 68.5, H 10.8%) and melting point (63–63.5°C)] and single crystals were produced by a series of slow crystallizations from acetone at room temperature. Cell constants were determined from various oscillation and Weissenberg photographs, using Cu $K\alpha$ radiation ($\lambda = 1.5418 \text{ \AA}$). The density was measured by flotation. The space group was determined from systematic extinctions ($h00$, $0k0$ and $00l$ absent for h , k or l odd). The crystal data are

as follows: $a = 8.05 \pm 0.01$, $b = 8.51 \pm 0.02$, $c = 44.66 \pm 0.05 \text{ \AA}$, $U = 1920 \text{ \AA}^3$, $z = 4$, $D_x = 1.088 \text{ g.cm}^{-3}$, $D_m = 1.085 \text{ g.cm}^{-3}$; space group, $P2_12_12_1$.

No further work on this compound is contemplated at present.

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References

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