Cryst.Struct.Comm. (1978). *7*, 33.

MORINITE, $Ca_2NaAl_2(OH)(H_2O)_2F_4(PO_4)_2$

F. C. Hawthorne*

Department of Earth Sciences, University of Manitoba, Winnipeg, Manitoba, Canada, R3T 2N2.

Preliminary information. Morinite is a pegmatitic phosphate mineral, typically associated with montebrasite, apatite, augelite and wardite. Crystals from the Hugo Mine, Keystone, S. Dakota were used for the structure determination.

Crystal data. (From single crystal X-ray diffractometry, MoKα , λ = 0.71069Å): a = 9.454(3), b = 10.692(4), c = 5.444(2)Å, β = 105.46(2)°, Z = 2, space group: $P2_1/m$.

Intensity data, structure determination and refinement. Intensities of 1252 independent intensities with $2\theta < 60^\circ$ were measured with C monochromated MoKα radiation on a Syntex $P\bar{1}$ automatic four-circle single-crystal diffractometer operating in the θ-2θ scan mode with variable scan rates. Standard data reduction procedures resulted in 1095 observed (3σ) reflections. The structure was solved by three-dimensional Patterson and Fourier methods and refined by full-matrix least-squares to a final conventional R-value of 2.8% for an anisotropic thermal model.

Atomic coordinates ($x10^4$).

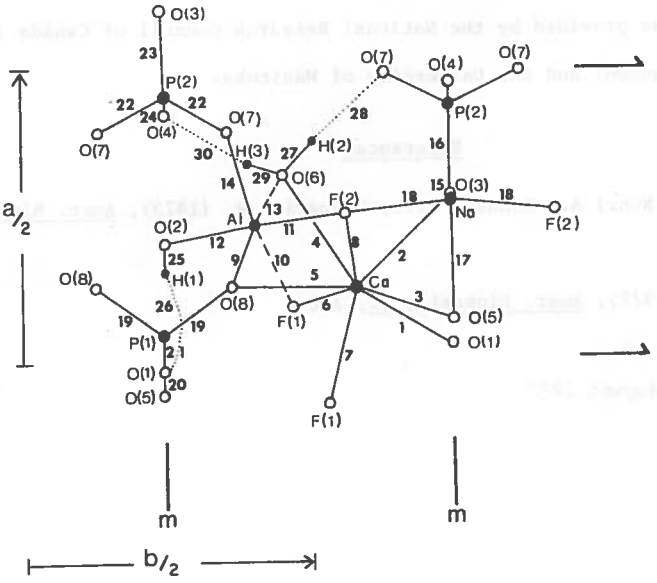
Ca	1452(1)	5829(1)	2400(1)	O(5)	9292(3)	1/4	5248(6)
Al	2576(1)	4062(1)	7733(2)	O(6)	3554(2)	419(2)	1304(4)
Na	6885(2)	1/4	2083(4)	O(7)	4423(2)	1340(2)	7364(4)
P(1)	438(1)	1/4	3715(2)	O(8)	1433(2)	1320(2)	4416(4)
P(2)	5087(1)	1/4	6415(2)	F(1)	968(2)	328(2)	8605(3)
O(1)	9699(3)	1/4	854(6)	F(2)	7150(2)	587(2)	3392(3)
O(2)	2287(3)	1/4	8962(6)	H(1)	1688(76)	1/4	9846(134)
O(3)	6754(3)	1/4	7650(6)	H(2)	4255(51)	-75(51)	1616(87)
O(4)	4748(4)	1/4	3535(6)	H(3)	3824(50)	1125(50)	2182(88)

Bond distances and angles.

1	2.545(2)	9	1.886(2)	17	2.463(4)	25	0.84(7)
2	2.468(2)	10	1.830(2)	18	2.156(2)	26	2.09(7)
3	2.408(2)	11	1.782(2)	19	1.558(2)	27	0.83(5)
4	2.591(2)	12	1.844(2)	20	1.534(3)	28	1.82(5)
5	2.545(2)	13	1.996(2)	21	1.528(3)	29	0.89(5)
6	2.344(2)	14	1.862(2)	22	1.539(2)	30	1.77(5)
7	2.272(2)	15	2.383(4)	23	1.541(3)		
8	2.334(2)	16	2.359(4)	24	1.514(3)		

1,2	69.8(1)	5,6	76.7(1)	11,14	87.0(1)	19,20	109.6(1)
1,3	73.7(1)	5,7	83.3(1)	12,13	88.4(1)	19,21	109.4(1)
1,6	79.0(1)	5,8	62.9(1)	12,14	93.7(1)	20,21	110.9(2)
1,7	77.3(1)	6,7	73.5(1)	13,14	87.9(1)	22,22	107.2(2)
2,3	76.7(1)	9,10	91.2(1)	15,16	121.4(1)	22,23	108.4(1)
2,4	78.3(1)	9,11	88.1(1)	15,17	119.8(1)	22,24	110.8(1)

2,8	83.1(1)	9,12	92.8(1)	16,17	118.8(1)	23,24	111.2(1)
3,6	83.3(1)	9,14	99.4(1)	15,18	107.7(1)	25,26	161(7)
3,8	74.3(1)	10,11	88.4(1)	16,18	85.7(1)	27,29	109(4)
4,5	74.3(1)	10,12	90.8(1)	17,18	76.4(1)	27,28	169(5)
4,6	60.6(1)	10,13	81.4(1)	19,19	107.9(2)	29,30	165(4)
4,8	84.2(1)	11,13	90.5(1)				



Comments. Equivalent $Ca(O_p)_4(H_2O)F_3$ polyhedra are fused by face-sharing across the mirror plane, and these doublets are repeated by the 2_1 operation to form a staggered edge-sharing chain parallel to the y axis. Chain linkage occurs through the $Na(O_p)_3F_2$ trigonal bipyramid and an $\left[Al_2(OH)F_4(H_2O)_2(PO_4)_2\right]$ polyhedral cluster. This cluster is formed from a corner-sharing octahedral dimer $\left[Al_2(OH)F_4(H_2O)_2(O_p)_4\right]$ that is further

linked by two (PO_4) tetrahedra; it is topologically identical to the $\left[Fe_2^{3+}(OH)(H_2O)_4(SO_4)_2(O_S)_2\right]$ and $\left[Al_2F(H_2O)_4(PO_4)_2(O_p)_2\right]$ clusters in copiapite (Fanfani, Nunzi, Zanazzi and Zanzari, 1973) and minyulite (Kampf, 1977).

Acknowledgments. I thank R. Faggiani and the Materials Research Institute, McMaster University, Hamilton for data collection facilities. Financial assistance was provided by the National Research Council of Canada (grant to R. B. Ferguson) and the University of Manitoba.

References

Fanfani L., Nunzi A., Zanazzi P.F., Zanzari A.R. (1973), Amer. Mineral., 58, 314.

Kampf A.R. (1977), Amer. Mineral., 62, 256.

Received: 31 August 1977