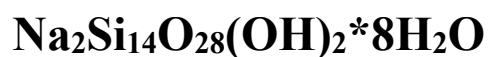


# **The crystal structure of mineral magadiite,**



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## **SUPPLEMENTAL DATA**

**Table S1:** Experimental and crystallographic parameters for the structure refinements of magadiite.

Diffractometer	Siemens D5000 with 6 ° PSD
Wavelength	1.54059 Å
Sample	0.3 mm glass capillary
Range of data used [°]	4.0 - 90.0
Step size [°2θ]	0.007902
No. steps	10886
No. contributing reflections	715
No. geometric restraints	84
No. structural parameters	79
No. profile parameters	18
FWHM at ca. 24.2 °2θ	0.17 - 0.47
R <sub>Bragg</sub>	0.031
R <sub>F</sub>	0.026
R <sub>wp</sub>	0.087
R <sub>exp</sub>	0.030
χ <sup>2</sup>	8.52
Space group	F2dd (No. 43)
a <sub>0</sub> [Å]	10.5035(9)
b <sub>0</sub> [Å]	10.0262(9)
c <sub>0</sub> [Å]	61.9608(46)
VUC [Å <sup>3</sup> ]	6525.13(93)
Density (calc.) [g cm <sup>-3</sup> ]	2.169
Unit cell content	Na <sub>16</sub> [Si <sub>112</sub> O <sub>224</sub> (OH) <sub>16</sub> ]*64H <sub>2</sub> O

**Table S2:** Fractional coordinates, displacement parameters and occupancy factors of magadiite.

Estimated standard deviations are given in brackets. The occupancy factors of the oxygen atoms representing water molecules are increased to represent the scattering power of the hydrogen atoms, as well. The presented e.s.d.s have to be multiplied by a factor of 5.8 to generate reliable values.

atom	Wyck off	scatt. factor	x	y	z	B <sub>iso</sub>	occ. factor
Si1	16b	Si	0.3775(4)	0.2349(3)	0.50100(6)	1.18(3)	1.00
Si2	16b	Si	0.2529(4)	0.3827(4)	0.46483(5)	1.18(3)	1.00
Si3	16b	Si	0.0483(3)	0.6209(4)	0.46539(6)	1.18(3)	1.00
Si4	16b	Si	0.4847(4)	0.5778(4)	0.46444(6)	1.18(3)	1.00
Si5	16b	Si	0.7147(3)	0.3828(4)	0.46426(6)	1.18(3)	1.00
Si6	16b	Si	0.3426(3)	1.0075(4)	0.32041(6)	1.18(3)	1.00
Si7	16b	Si	0.1454(4)	0.2447(4)	0.32009(5)	1.18(3)	1.00
O1	16b	O	0.1402(8)	0.4914(8)	0.47053(15)	1.73(5)	1.00
O2	16b	O	0.2659(6)	0.2969(9)	0.48625(11)	1.73(5)	1.00
O3	16b	O	0.9485(8)	0.6034(7)	0.44680(12)	1.73(5)	1.00
O4	16b	O	0.3271(7)	0.1319(7)	0.51896(12)	1.73(5)	1.00
O5	16b	O	0.4981(8)	0.3426(10)	0.55735(11)	1.73(5)	1.00
O6	16b	O	0.6153(7)	0.4995(9)	0.47172(13)	1.73(5)	1.00
O7	16b	O	0.4418(9)	0.6470(8)	0.48588(11)	1.73(5)	1.00
O8	16b	O	0.7791(7)	0.4203(10)	0.44196(10)	1.73(5)	1.00
O9	16b	O	0.4740(9)	0.8578(9)	0.51256(11)	1.73(5)	1.00
O10	16b	O	0.2127(6)	0.6978(10)	0.55575(11)	1.73(5)	1.00
O11	16b	O	0.3809(7)	0.4624(8)	0.45815(13)	1.73(5)	1.00
O12	16b	O	0.1403(10)	0.7455(7)	0.45903(12)	1.73(5)	1.00
O13	16b	O	0.2566(8)	0.1373(8)	0.32748(14)	1.73(5)	1.00
O14	16b	O	0.9137(9)	0.4470(10)	0.34133(11)	1.73(5)	1.00
O15	16b	O	0.6014(10)	0.7995(11)	0.34322(9)	1.73(5)	1.00
Na1	16b	Na	1.0105(11)	0.8799(13)	0.36995(19)	3.8(2)	1.00
OW1	16b	O-2	1.0188(10)	0.8575(13)	0.33425(20)	1.73(5)	1.00
OW2	16b	O-2	1.0250(10)	0.8517(11)	0.41327(20)	1.73(5)	1.00
OW3	16b	O-2	1.0062(14)	0.6071(12)	0.3768(2)	1.73(5)	1.00
OW4	16b	O-2	0.5066(15)	0.6144(13)	0.3756(2)	1.73(5)	1.00