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The location of H in the high-pressure synthetic $Al_2SiO_4(OH)_2$ topaz analogue

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For deposit: Tables 1b and 2b

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Table 1b. Anisotropic thermal parameters ($U_{(i,j)}$ *1000).

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Al*	4.4(2)	4.0(2)	4.4(2)	0.2(1)	-0.1(1)	-0.1(1)
	4.9(3)	4.0(3)	3.9(3)	0.4(2)	0.1(2)	0.0(2)
Si	3.5(2)	3.4(2)	3.9(2)	0.0(1)	0	0
	4.0(4)	3.5(3)	4.3(3)	0.2(2)	0	0
O1	4.1(5)	5.3(4)	4.9(4)	-1.5(4)	0	0
	5.0(8)	4.5(8)	4.4(7)	-0.9(6)	0	0
O2	6.6(5)	4.2(4)	4.0(4)	0.6(4)	0	0
	5.3(8)	4.6(8)	4.5(7)	1.0(6)	0	0
O3	5.0(3)	4.5(3)	4.6(3)	0.9(3)	-1.0(3)	-0.2(2)
	5.0(6)	4.9(6)	4.5(5)	0.2(4)	-1.1(5)	0.2(4)
F	6.3(3)	6.8(3)	6.4(3)	1.9(2)	-1.0(2)	1.1(2)
OH	6.2(6)	8.2(6)	5.9(6)	1.6(5)	0.2(5)	0.7(5)

*Upper value for each entry refers to fluor-topaz; the second line refers to topaz-OH; errors apply to the last digit printed.

Table 2b. Al-O and Si-O angles (°).

Angle	Fluor-topaz	Topaz-OH	Angle	Fluor-topaz	Topaz-OH
O1-Al-O2	83.38(4)	84.67(5)	OH-Al-OHa	88.71(2)	90.85(4)
O1-Al-O3	92.05(4)	89.81(7)	O1-Al-OHa	171.64(4)	173.79(8)
O1-Al-O3a	100.64(4)	98.12(5)	O2-Al-O3a	175.61(6)	175.44(6)
O1-Al-OH	88.81(4)	86.85(6)	O3-Al-OH	173.75(2)	175.06(7)
O2-Al-O3	95.31(4)	92.59(5)			
O2-Al-OH	90.94(4)	90.94(7)	O1-Si-O2	109.71(6)	110.8 (1)
O2-Al-OHa	88.68(3)	89.36(4)	O1-Si-O3 (x2)	109.38(4)	110.10(6)
O3-Al-O3a	82.85(4)	83.85(5)	O2-Si-O3 (x2)	110.41(4)	110.24(6)
O3-Al-OHa	91.28(3)	92.82(6)	O3-Si-O3	107.52(5)	105.19(8)
O3a-Al-OH	90.91(4)	92.96(6)			
O3a-Al-OHa	87.38(3)	87.75(5)	Al-F/OH-Ala	145.22(4)	139.60(7)