

Crystals

Supporting Information for

Investigation of the high-pressure behaviors of Amblygonite by Single-crystal X-ray diffraction, Raman Spectroscopy, and DFT calculations

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Tables S1 to S2

Table S1 Lattice parameters of amblygonite at various pressures.

Pressure (GPa)	a (Å)	b (Å)	c (Å)	α	β	γ	V (Å ³)
0.00001	5.0338(3)	5.191(1)	7.0160(6)	106.63(1)	109.26(1)	97.933(1)	160.3(1)
1.0(1)	5.030(1)	5.185(3)	7.011(2)	106.65(1)	109.33(1)	97.83(1)	159.8(3)
2.5(1)	5.012(3)	5.164(3)	6.984(1)	106.62(2)	109.33(1)	97.89(2)	158.0(3)
4.7(1)	4.983(1)	5.135(3)	6.940(1)	106.61(2)	109.36(1)	97.90(2)	155.1(3)
7.3(1)	4.952(1)	5.109(1)	6.894(1)	106.65(3)	109.39(3)	97.85(3)	152.4(3)
9.9(1)	4.925(1)	5.081(3)	6.853(1)	106.65(3)	109.39(3)	97.75(3)	149.8(3)
12.8(1)	4.893(2)	5.052(2)	6.803(3)	106.66(2)	109.47(1)	97.72(2)	146.9(3)
15.0(1)	4.874(4)	5.033(4)	6.777(1)	106.70(3)	109.55(1)	97.75(3)	145.1(3)
17.4(1)	4.8532(3)	5.011(3)	6.746(9)	106.72(2)	109.51(1)	97.63(2)	143.3(2)
20.0(1)	4.8334(3)	4.9834(4)	6.715(1)	106.71(2)	109.50(8)	97.63(2)	141.3(2)
23.0(1)	4.8101(3)	4.960(3)	6.679(1)	106.70(2)	109.51(1)	97.56(2)	139.2(2)
25.2(2)	4.7928(7)	4.939(5)	6.653(2)	106.54(5)	109.45(2)	97.77(5)	137.1(1)
27.7(2)	4.778(2)	4.922(4)	6.636(3)	106.76(2)	109.52(1)	97.47(2)	136.3(2)
30.1(2)	4.760(1)	4.900(4)	6.608(3)	106.60(8)	109.52(3)	97.61(8)	134.8(2)
32.1(2)	4.748(1)	4.887(4)	6.590(3)	106.60(7)	109.52(3)	97.57(7)	133.7(2)
34.4(2)	4.7350(4)	4.866(3)	6.569(1)	106.76(3)	109.59(1)	97.28(3)	132.3(2)

Table S2 Bond length (\AA), Polyhedral Volume (\AA^3), Distortion index (D), Quadratic (λ) and Bond angle variance (σ^2) for various polyhedra in Amblygonite at pressures up to 28.4 GPa.

Pressure (GPa)	1.9	5.4	9.5	14.1	19.2	22.1	25.1	28.3
AlIO₄F₂								
Mean bond length (\AA)	1.8706	1.8566	1.8428	1.8289	1.8159	1.8094	1.8027	1.7966
Volume (\AA^3)	8.7017	8.5041	8.3134	8.1240	7.9518	7.8637	7.7787	7.6975
Distortion index (D)	0.01203	0.01445	0.01618	0.01745	0.01848	0.01926	0.01946	0.01984
Quadratic (λ)	1.0022	1.0025	1.0027	1.0030	1.0031	1.0033	1.0033	1.0034
Bond angle variance (σ^2)	6.5702	7.3839	7.8161	8.2673	8.3230	9.0099	8.6873	9.0863
Al₂O₄F₂								
Mean bond length (\AA)	1.8744	1.8615	1.8489	1.8361	1.8243	1.8181	1.8125	1.8067
Volume (\AA^3)	8.7681	8.5768	8.3888	8.1994	8.0195	7.9258	7.8407	7.7517
Distortion index (D)	0.00239	0.00394	0.00529	0.00575	0.00646	0.00736	0.00747	0.00823
Quadratic (λ)	1.0010	1.0019	1.0030	1.0044	1.0064	1.0074	1.0084	1.0096
Bond angle variance (σ^2)	3.4997	6.5055	10.6753	15.645	22.5465	26.3130	29.8821	34.1880
PO₄								
Mean bond length (\AA)	1.5467	1.5421	1.5375	1.5327	1.5282	1.5251	1.5225	1.5201
Volume (\AA^3)	1.8900	1.8737	1.8571	1.8399	1.8232	1.8122	1.8024	1.7933
Distortion index (D)	0.00646	0.0064	0.00532	0.00698	0.00575	0.0054	0.00525	0.0050
Quadratic (λ)	1.0032	1.0031	1.0030	1.0029	1.0031	1.0031	1.0033	1.0035
Bond angle variance (σ^2)	12.2521	11.730	11.420	11.2516	11.911	12.2085	12.8149	13.9570
LiO₄F								
Mean bond length (\AA)	2.0776	2.0551	2.0333	2.0099	1.9913	1.9785	1.9672	1.9578
Volume (\AA^3)	6.5523	6.3168	6.0919	5.8754	5.6651	5.5618	5.4665	5.3770
Distortion index (D)	0.03921	0.04171	0.05073	0.05815	0.06679	0.06895	0.07257	0.07611