Atomic-scale deformation mechanisms at high-pressure in inderborite, $CaMg[B^3O^3(OH)^5]^2(H^2O)^4 \cdot 2H^2O$

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Table S1: Ca-O, Mg-O and B-O interatomic distances (in Å) in inderborite (average distance, < d >, in Å; volume, *V*, in $Å^3$; bond angle variance, σ^2; distortion index, *D*; quadratic elongation <λ>), with pressure. Data are referred to the first experimental dataset (see Table 1). Average $\Delta\%_{Ca\text{-}O} \sim 4\%$, $\Delta\%_{Mg\text{-}O} \sim 2\ \%$, $\Delta\%_{B\text{-}O} \sim 1.6\%$ [Δ% defined as $100\cdot(X\text{-}O_{0.0001GPa} - X\text{-}O_{P8.11(5)GPa}) / X\text{-}O_{0.0001GPa}$, where X-O is the cation-oxygen bond length].

***P*(GPa)**	**0.0001**	**0.43(5)**	**0.61(5)**	**1.19(5)**	**1.80(5)**	**2.35(5)**	**2.82(5)**	**3.33(5)**	**3.84(5)**	**4.54(5)**	**6.23(5)**	**7.08(5)**	**7.80(5)**	**8.11(5)**
Ca1-O1 x2	2.394(3)	2.387(4)	2.385(4)	2.371(4)	2.356(4)	2.350(4)	2.342(4)	2.330(4)	2.327(4)	2.316(4)	2.292(5)	2.283(5)	2.280(5)	2.276(5)
Ca1-O3 x2	2.438(7)	2.437(3)	2.439(3)	2.436(3)	2.433(3)	2.438(3)	2.432(3)	2.437(3)	2.438(4)	2.435(3)	2.433(4)	2.431(4)	2.430(4)	2.423(4)
Ca1-O10 x2	2.450(8)	2.442(3)	2.441(3)	2.434(3)	2.427(3)	2.420(3)	2.415(3)	2.408(3)	2.402(3)	2.394(3)	2.382(4)	2.375(4)	2.373(4)	2.369(4)
Ca1-O6 x2	2.520(6)	2.496(4)	2.494(4)	2.471(4)	2.450(4)	2.440(4)	2.424(4)	2.409(4)	2.401(4)	2.390(4)	2.366(5)	2.350(5)	2.353(5)	2.352(5)
<Ca1-O>*	2.451	2.441	2.440	2.428	2.417	2.412	2.403	2.396	2.392	2.384	2.368	2.360	2.359	2.355
***V* (Å^3)**	26.23	25.89	25.87	25.50	25.15	25.01	24.75	24.52	24.39	24.15	23.67	23.41	23.44	23.30
D	0.014	0.012	0.011	0.012	0.012	0.013	0.013	0.014	0.013	0.014	0.017	0.018	0.018	0.017

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Mg1-O9 x2	2.091(5)	2.095(5)	2.094(5)	2.090(5)	2.089(5)	2.078(5)	2.088(6)	2.084(6)	2.087(6)	2.087(6)	2.081(6)	2.064(6)	2.060(6)	2.053(6)
Mg1-O8 x2	2.102(5)	2.103(3)	2.100(3)	2.101(3)	2.098(3)	2.096(3)	2.095(3)	2.088(3)	2.082(3)	2.048(3)	2.033(4)	2.025(4)	2.023(4)	2.019(4)
Mg1-O2 x2	2.072(8)	2.077(3)	2.076(3)	2.072(3)	2.066(3)	2.066(3)	2.063(3)	2.054(3)	2.052(3)	2.081(3)	2.068(4)	2.060(5)	2.051(5)	2.047(4)
<Mg1-O>*	2.088	2.092	2.090	2.088	2.084	2.080	2.082	2.075	2.074	2.072	2.061	2.045	2.045	2.040
***V* (Å^3)**	12.12	12.17	12.14	12.09	12.02	11.93	11.97	11.83	11.80	11.76	11.54	11.35	11.28	11.17
D	0.005	0.005	0.004	0.005	0.006	0.005	0.006	0.007	0.007	0.008	0.009	0.008	0.007	0.007
<λ>	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.1	10.1	10.1	10.1	10.1	10.1	10.1
σ^2	52.0	66.8	69.0	86.4	104.7	125.8	140.2	167.6	188.1	211.8	257.7	283.5	298.5	309.2

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***P*(GPa)**	**0.0001**	**0.43(5)**	**0.61(5)**	**1.19(5)**	**1.80(5)**	**2.35(5)**	**2.82(5)**	**3.33(5)**	**3.84(5)**	**4.54(5)**	**6.23(5)**	**7.08(5)**	**7.80(5)**	**8.11(5)**
B3-O5	1.406(18)	1.364(5)	1.361(5)	1.357(5)	1.359(5)	1.361(5)	1.357(5)	1.359(5)	1.364(6)	1.364(6)	1.356(7)	1.358(7)	1.362(7)	1.365(6)
B3-O4	1.334(13)	1.369(6)	1.371(7)	1.363(7)	1.368(7)	1.377(7)	1.372(7)	1.367(7)	1.362(7)	1.362(7)	1.367(8)	1.364(9)	1.357(9)	1.358(8)
B3-O6	1.389(7)	1.366(8)	1.361(8)	1.368(8)	1.365(8)	1.357(8)	1.363(8)	1.364(8)	1.360(8)	1.360(8)	1.363(10)	1.360(10)	1.356(10)	1.339(10)
<B3-O>*	1.3764	1.3665	1.3642	1.3628	1.3642	1.3648	1.364	1.3635	1.362	1.362	1.3619	1.3609	1.358	1.3539

***P*(GPa)**	**0.0001**	**0.43(5)**	**0.61(5)**	**1.19(5)**	**1.80(5)**	**2.35(5)**	**2.82(5)**	**3.33(5)**	**3.84(5)**	**4.54(5)**	**6.23(5)**	**7.08(5)**	**7.80(5)**	**8.11(5)**
B1-O1	1.42(2)	1.434(5)	1.432(5)	1.435(5)	1.435(5)	1.432(5)	1.466(8)	1.466(8)	1.434(5)	1.438(5)	1.431(6)	1.431(6)	1.434(6)	1.430(6)
B1-O4	1.498(6)	1.476(7)	1.475(8)	1.471(8)	1.468(8)	1.467(8)	1.480(6)	1.480(6)	1.472(8)	1.455(8)	1.459(9)	1.459(9)	1.468(10)	1.47(1)
B1-O2	1.493(5)	1.492(5)	1.489(5)	1.485(5)	1.486(5)	1.482(5)	1.476(5)	1.476(5)	1.473(5)	1.473(5)	1.465(6)	1.465(6)	1.452(6)	1.459(6)
B1-O3	1.483(9)	1.469(6)	1.471(6)	1.478(6)	1.480(6)	1.477(6)	1.435(5)	1.435(5)	1.470(6)	1.476(6)	1.479(7)	1.479(7)	1.475(7)	1.475(7)
<B1-O>*	1.474	1.468	1.467	1.467	1.467	1.465	1.464	1.464	1.462	1.461	1.459	1.459	1.457	1.458
***V* (Å^3)**	1.640	1.620	1.616	1.618	1.618	1.609	1.608	1.608	1.603	1.596	1.591	1.591	1.587	1.590
D	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
<λ>	10.023	10.016	10.016	10.015	10.016	10.014	10.013	10.013	10.011	10.012	10.010	10.010	10.008	10.007
σ^2	64.701	46.040	43.795	46.909	50.335	42.762	41.931	41.931	31.850	39.810	31.542	31.542	23.173	18.264

***P*(GPa)**	**0.0001**	**0.43(5)**	**0.61(5)**	**1.19(5)**	**1.80(5)**	**2.35(5)**	**2.82(5)**	**3.33(5)**	**3.84(5)**	**4.54(5)**	**6.23(5)**	**7.08(5)**	**7.80(5)**	**8.11(5)**
B2-O5	1.496(7)	1.484(7)	1.487(7)	1.482(7)	1.480(7)	1.476(7)	1.466(7)	1.464(7)	1.467(8)	1.460(7)	1.462(9)	1.467(9)	1.459(9)	1.449(6)
B2-O1	1.443(10)	1.451(6)	1.456(6)	1.453(6)	1.456(6)	1.449(6)	1.451(6)	1.456(6)	1.449(6)	1.446(6)	1.438(7)	1.438(8)	1.430(8)	1.460(9)
B2-O8	1.500(4)	1.502(4)	1.506(4)	1.504(4)	1.500(4)	1.497(4)	1.497(4)	1.492(4)	1.491(5)	1.487(4)	1.474(5)	1.470(5)	1.476(5)	1.476(5)
B2-O7	1.448(13)	1.455(5)	1.449(5)	1.452(5)	1.456(5)	1.456(5)	1.454(5)	1.452(5)	1.454(5)	1.449(5)	1.448(6)	1.449(6)	1.453(6)	1.431(8)
<B2-O>*	1.472	1.473	1.474	1.473	1.473	1.470	1.467	1.466	1.465	1.461	1.456	1.456	1.454	1.454
***V* (Å^3)**	1.635	1.638	1.643	1.638	1.638	1.627	1.619	1.616	1.613	1.597	1.581	1.583	1.576	1.576
D	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
<λ>	10.010	10.006	10.007	10.007	19.919	10.007	10.007	10.006	10.007	10.008	10.009	10.009	10.010	10.008
σ^2	32.217	21.942	24.203	22.855	39.780	24.737	24.998	25.169	26.133	31.218	34.508	33.921	41.427	31.449

*In the *P*-range considered, the <Ca-O>, <Mg-O>, <B1-O>, <B2-O> and <B3-O> distances decrease of about 3.9, 2.3, 1.1, 1.2 and 1.6%, respectively.

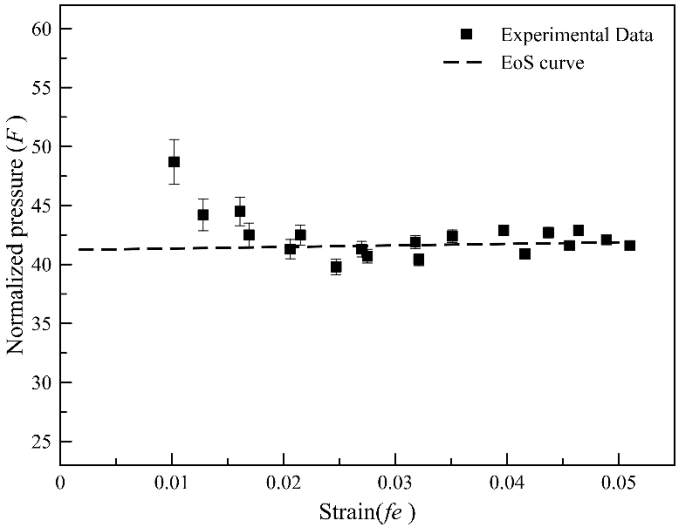

Figure S1: Normalized pressure $F = P/\left[3fe(1+2fe)^{5/2}\right]$ *vs.* Eulerian finite strain $fe = \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]/2$ plot, based on the first data set collected at high pressure.

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Figure S2: Interatomic angles O8···$\widehat{O11}$···O9, O6···$\widehat{O3}$ ···O7, O5···$\widehat{O10}$ ···O4, due to the H-bond interaction in inderborite.

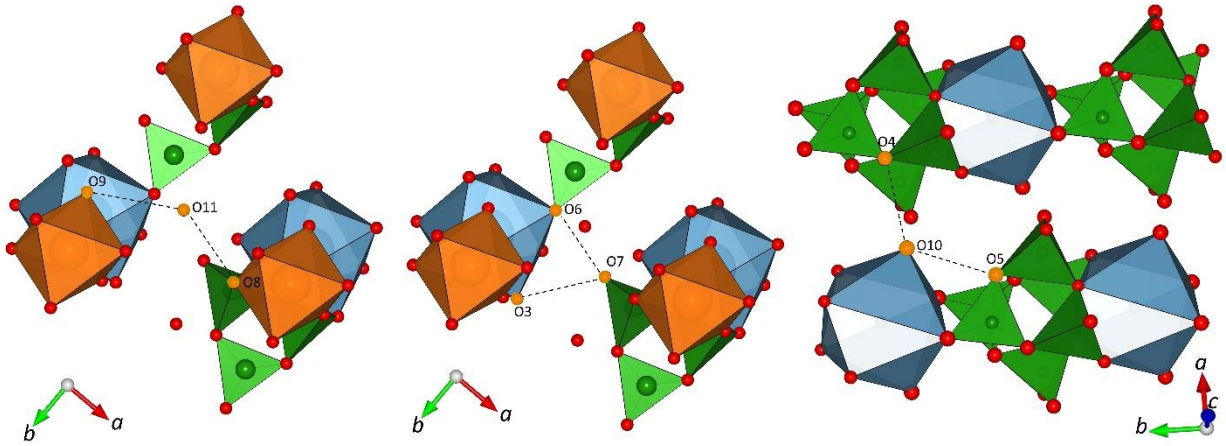
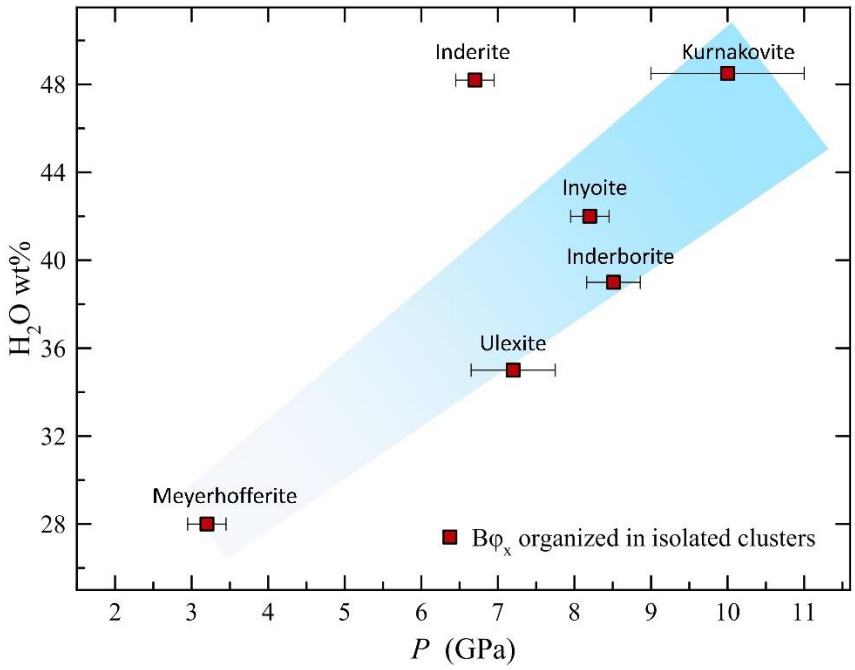


Figure S3: H_2O content *vs.* pressure at which the phase transition occurs in borate structures characterized by isolated polyions. A qualitative linear correlation is represented by the sky-blue shade (modified from Comboni *et al.*, 2023)



Comboni D., Poreba T., Battiston T., Hanfland M. and Gatta G.D. (2023) On the anomalous high-pressure phase transition of inderite, MgB3O3(OH)5·5H2O. *Solid State Sciences*, **140**, 107187. Elsevier Masson SAS.

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Figure S4: Evolution of the O···O interatomic distances with pressure (O9, O10, O11 represent H_2O molecules, O3, O6, O7, O8 are OH^- groups, O4 and O5 are oxygen hinges; O3, O6, O10 and O11 are *donors*).