Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Table S1. Crystallographic data and refinement parameters for reedmergnerite (reedmergnerite-I) and $NaBSi_3O_8$ modifications obtained as a result of its transformation

Crystal data	0.0001 GPa	1.8(1) GPa	4.9(1) GPa	8.2(1) GPa	11.9(1) GPa	16.2(1) GPa	24.8(1) GPa	27.8(1) GPa	32.3(1) GPa	35.1(1) GPa
	P00	P01	P02	P03	P04	P05	P07	P08	P09	P10
	Reedmergnerite-I					Reedmergnerite-II	Reedmergnerite-III			
Space group					*P*–1					
a, Å	6.802(4)	6.7686(19)	6.7152(8)	6.6565(9)	6.5869(15)	6.7571(19)	6.3777(14)	6.350(2)	6.245(7)	6.27(3)
b, Å	7.196(4)	7.1398(19)	7.0429(17)	6.944(2)	6.8464(17)	7.109(2)	6.4083(13)	6.351(2)	6.324(8)	6.21(3)
c, Å	7.435(4)	7.3847(8)	7.3048(15)	7.234(2)	7.1774(8)	11.921(2)	6.6321(6)	6.5954(10)	6.544(7)	6.52(3)
α, º	115.306(10)	115.761(17)	116.50(2)	117.19(3)	117.906(17)	97.574(18)	103.787(12)	115.664(19)	116.01(13)	115.8(5)
β, °	100.789(12)	100.558(15)	100.246(13)	99.971(17)	99.654(13)	90.949(18)	115.708(15)	103.664(19)	103.12(11)	103.2(4)
γ, º	106.907(11)	106.86(2)	106.716(15)	106.418(18)	106.06(2)	118.25(3)	102.068(18)	101.84(3)	101.56(11)	100.0(4)
Volume, Å^3	293.6(3)	287.09(13)	276.56(11)	266.79(14)	257.50(10)	498.0(3)	221.55(8)	218.04(12)	212.5(5)	211.4(19)
Z	2	2	2	2	2	4	2	2	2	2
d, g/cm^3	2.783	2.847	2.955	3.063	3.174	3.282	3.689	3.748	3.845	
Data collection										
Wavelength, Å	0.71073	0.2896								
Max. *θ*°	31.184	17.339	17.461	17.154	17.816	17.958	17.204	17.250	17.840	17.539
Index ranges	-9≤*h*≤9	-9≤*h*≤8	-12≤*h*≤13	-12≤*h*≤13	-10≤*h*≤8	-8≤*h*≤8	-9≤*h*≤8	-8≤*h*≤7	-8≤*h*≤7	-8≤*h*≤7
	-10≤*k*≤10	-9≤*k*≤9	-8≤*k*≤5	-8≤*k*≤5	-8≤*k*≤9	-6≤*k*≤9	-7≤*k*≤8	-8≤*k*≤9	-7≤*k*≤9	-7≤*k*≤8
	-9≤*l*≤10	-14≤*l*≤15	-9≤*l*≤10	-8≤*l*≤9	-13≤*l*≤15	-22≤*l*≤23	-11≤*l*≤10	-10≤*l*≤11	-10≤*l*≤10	-10≤*l*≤10
No.meas.refl.	5554	1117	1000	771	907	1824	776	761	633	354
No.uniq.refl.	1891	731	689	560	631	1276	528	521	434	280
No. obs.refl ($I > 2\sigma(I)$)	1433	681	607	493	595	915	504	448	214	
Refinement of the structure										
No.of variables	119	119	69	54	79	135	68	63	63	
R_{int}	0.0417	0.0193	0.0193	0.0251	0.0325	0.0337	0.0121	0.0286	0.0832	
R_1, all data	0.0597	0.0294	0.0583	0.1183	0.0868	0.1222	0.0898	0.0874	0.2070	
R_1, $I > 2\sigma(I)$	0.0380	0.0267	0.0487	0.0875	0.0829	0.0890	0.0800	0.0741	0.1374	
wR_2, all data	0.0854	0.0790	0.1374	0.2510	0.2266	0.3088	0.3070	0.2268	0.3799	
wR_2, $I > 2\sigma(I)$	0.0783	0.0754	0.1187	0.2037	0.2192	0.2403	0.2650	0.2004	0.3223	
GooF	1.057	1.131	1.146	1.194	1.081	1.065	2.691	1.157	0.933	

Table S2. Bond distances and polyhedral parameters in reedmergnerite-I $NaBSi_3O_8$

Pressure	**0.0001 GPa**	**1.8(1) GPa**	**4.9(1) GPa**	**8.2(1) GPa**	**11.9(1) GPa**
	P00	**P01**	**P02**	**P03**	**P04**
			SiO_4 polyhedra		
Si1–O4, Å	1.644(3)	1.640(4)	1.634(10)	1.582(18)	1.628(13)
Si1–O5, Å	1.603(3)	1.601(5)	1.587(8)	1.623(15)	1.594(14)
Si1–O6, Å	1.614(3)	1.615(4)	1.615(7)	1.609(13)	1.574(13)
Si1–O8, Å	1.608(3)	1.607(3)	1.584(5)	1.592(9)	1.588(8)
<Si1–O>, Å	1.618	1.616	1.605	1.601	1.596
Volume, Å^3	2.164	2.157	2.109	2.099	2.082
Si2–O1, Å	1.595(3)	1.589(5)	1.580(7)	1.530(14)	1.584(16)
Si2–O2, Å	1.621(3)	1.623(5)	1.589(11)	1.60(3)	1.604(15)
Si2–O3, Å	1.6168(19)	1.620(4)	1.616(6)	1.619(11)	1.599(10)
Si2–O6, Å	1.606(3)	1.599(4)	1.594(7)	1.607(13)	1.612(12)
<Si2–O>, Å	1.610	1.608	1.595	1.588	1.600
Volume, Å^3	2.134	2.125	2.073	2.040	2.093
Si3–O2, Å	1.618(3)	1.618(3)	1.633(8)	1.62(3)	1.609(10)
Si3–O3, Å	1.613(3)	1.611(3)	1.607(5)	1.597(10)	1.580(9)
Si3–O4, Å	1.636(3)	1.636(5)	1.632(10)	1.633(17)	1.609(16)
Si3–O7, Å	1.587(3)	1.592(5)	1.594(7)	1.588(13)	1.581(15)
<Si3–O>, Å	1.613	1.614	1.617	1.609	1.595
Volume, Å^3	2.143	2.144	2.158	2.126	2.065
			BO_4 polyhedra		
B1–O1, Å	1.487(4)	1.477(6)	1.474(10)	1.44(3)	1.441(17)
B1–O5, Å	1.446(5)	1.451(7)	1.449(15)	1.32(4)	1.44(3)
B1–O7, Å	1.470(5)	1.452(9)	1.441(13)	1.53(3)	1.42(4)
B1–O8, Å	1.480(3)	1.481(4)	1.491(9)	1.57(3)	1.475(12)
<B1–O>, Å	1.471	1.465	1.464	1.464	1.445
Volume, Å^3	1.625	1.607	1.601	1.586	1.540
			NaO_7 polyhedra		
Na1–O1, Å	2.453(3)	2.408(4)	2.335(9)	2.328(18)	2.219(12)
Na1–O1, Å	2.483(3)	2.452(6)	2.395(9)	2.401(17)	2.27(3)
Na1–O2, Å	2.809(4)	2.765(6)	2.740(10)	2.65(3)	2.601(17)
Na1–O3, Å	2.861(4)	2.836(5)	2.800(10)	2.774(18)	2.832(16)
Na1–O4, Å	2.399(3)	2.332(3)	2.259(7)	2.175(13)	2.141(8)
Na1–O7, Å	2.403(3)	2.365(5)	2.323(7)	2.304(13)	2.257(15)
Na1–O8, Å	2.373(3)	2.342(4)	2.294(8)	2.262(16)	2.229(12)
<Na1–O>, Å	2.540	2.500	2.449	2.414	2.364
Volume, Å^3	20.980	20.149	19.206	18.414	17.491

Table S3. Bond distances and polyhedral parameters in reedmergnerite-II $NaBSi_3O_8$ at 16.2 GPa

Pressure	**16.2 GPa**		
	P05		
SiO_4 polyhedra			
Si1–O1, Å	1.570(16)	**Si4–O6, Å**	1.595(13)
Si1–O4, Å	1.592(9)	**Si4–O12, Å**	1.515(12)
Si1–O7, Å	1.533(15)	**Si4–O15, Å**	1.598(12)
Si1–O15, Å	1.608(11)	**Si4–O16, Å**	1.603(15)
<Si1–O>, Å	1.576	**<Si4–O>, Å**	1.578
Volume, Å^3	1.984	**Volume, Å^3**	2.007
Si2–O2, Å	1.601(11)	**Si5–O1, Å**	1.625(11)
Si2–O3, Å	1.640(15)	**Si5–O8, Å**	1.622(16)
Si2–O4, Å	1.580(12)	**Si5–O13, Å**	1.582(11)
Si2–O11, Å	1.545(13)	**Si5–O16, Å**	1.580(14)
<Si2–O>, Å	1.592	**<Si5–O>, Å**	1.602
Volume, Å^3	2.059	**Volume, Å^3**	2.106
Si3–O2, Å	1.621(11)	**Si6–O3, Å**	1.630(13)
Si3–O5, Å	1.586(15)	**Si6–O5, Å**	1.643(11)
Si3–O6, Å	1.575(9)	**Si6–O9, Å**	1.572(16)
Si3–O14, Å	1.546(15)	**Si6–O10, Å**	1.580(10)
<Si3–O>, Å	1.582	**<Si6–O>, Å**	1.606
Volume, Å^3	2.004	**Volume, Å^3**	2.119
BO_4 polyhedra			
B1–O9, Å	1.442(18)	**B2–O7, Å**	1.46(3)
B1–O11, Å	1.393(16)	**B2–O8, Å**	1.428(18)
B1–O13, Å	1.45(3)	**B2–O10, Å**	1.46(3)
B1–O14, Å	1.59(3)	**B2–O12, Å**	1.512(19)
<B1–O>, Å	1.469	**<B2–O>, Å**	1.464
Volume, Å^3	1.613	**Volume, Å^3**	1.603
NaO_7 polyhedra			
Na1–O2, Å	2.505(18)	**Na2–O1, Å**	2.126(16)
Na1–O3, Å	2.562(13)	**Na2–O6, Å**	2.501(14)
Na1–O5, Å	2.147(14)	**Na2–O7, Å**	2.220(11)
Na1–O11, Å	2.211(14)	**Na2–O10, Å**	2.183(11)
Na1–O11, Å	2.241(18)	**Na2–O12, Å**	2.157(12)
Na1–O13, Å	2.234(11)	**Na2–O12, Å**	2.304(17)
Na1–O14, Å	2.282(11)	**Na2–O15, Å**	2.645(18)
<Na1–O>, Å	2.312	**<Na2–O>, Å**	2.305
Volume, Å^3	16.435	**Volume, Å^3**	16.661

Table S4. Bond distances and polyhedral parameters in reedmergnerite-III $NaBSi_3O_8$

Pressure	**24.8(1) GPa**	**27.8(1) GPa**	**32.3(1) GPa**
	P07	**P08**	**P09**
		SiO_n polyhedra	
		SiO_4	
Si1–O2, Å	1.619(17)	1.610(17)	1.56(5)
Si1–O5, Å	1.582(17)	1.591(17)	1.56(4)
Si1–O6, Å	1.570(10)	1.559(10)	1.48(3)
Si1–O8, Å	1.615(16)	1.605(18)	1.64(4)
<Si1–O>, Å	1.596	1.591	1.561
Volume, Å^3	2.053	2.028	1.912
		SiO_4	
Si2–O1, Å	1.550(14)	1.577(16)	1.48(5)
Si2–O2, Å	1.619(11)	1.627(12)	1.62(4)
Si2–O4, Å	1.51(3)	1.56(3)	1.44(5)
Si2–O5, Å	1.594(10)	1.585(11)	1.63(3)
<Si2–O>, Å	1.569	1.588	1.541
Volume, Å^3	1.965	2.045	1.854
		SiO_5	
Si3–O3, Å	1.726(14)	1.753(14)	1.80(4)
Si3–O4, Å	1.688(16)	1.670(16)	1.67(4)
Si3–O6, Å	1.655(15)	1.697(16)	1.70(4)
Si3–O7, Å	1.675(19)	1.676(18)	1.67(3)
Si3–O7, Å	1.688(11)	1.682(11)	1.71(5)
<Si3–O>, Å	1.825	1.695	1.710
Volume, Å^3	5.007	3.761	3.817
		BO_4 polyhedra	
B1–O1, Å	1.51(4)	1.35(5)	1.92(12)
B1–O3, Å	1.47(3)	1.49(3)	1.47(4)
B1–O3, Å	1.521(13)	1.522(18)	1.54(7)
B1–O8, Å	1.323(17)	1.39(2)	1.06(5)
<B1–O>, Å	1.456	1.439	1.497
Volume, Å^3	1.537	1.479	1.525
		NaO_9 polyhedra	
Na1–O1, Å	2.535(14)	2.467(16)	2.45(5)
Na1–O2, Å	2.38(3)	2.36(3)	2.37(6)
Na1–O4, Å	2.225(8)	2.172(8)	2.19(2)
Na1–O4, Å	2.637(11)	2.617(13)	2.65(4)
Na1–O5, Å	2.37(3)	2.40(3)	2.45(5)
Na1–O6, Å	2.758(18)	2.647(19)	2.53(5)
Na1–O7, Å	2.189(14)	2.219(14)	2.28(4)
Na1–O8, Å	2.119(8)	2.100(9)	2.08(2)
Na1–O8, Å	2.32(3)	2.33(3)	2.37(5)
<Na1–O>, Å	2.394	2.368	2.372
Volume, Å^3	24.604	23.900	23.885

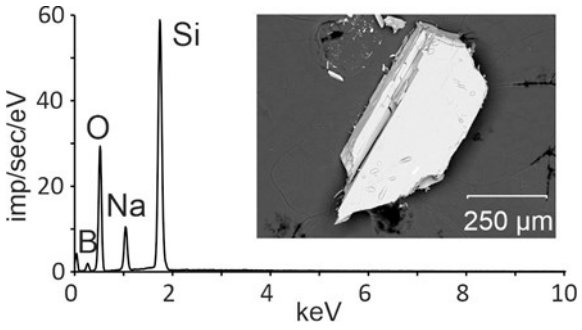

Figure S1. Scanning electron microscopy image and experimental energy dispersive spectrum of reedmergnerite crystal.

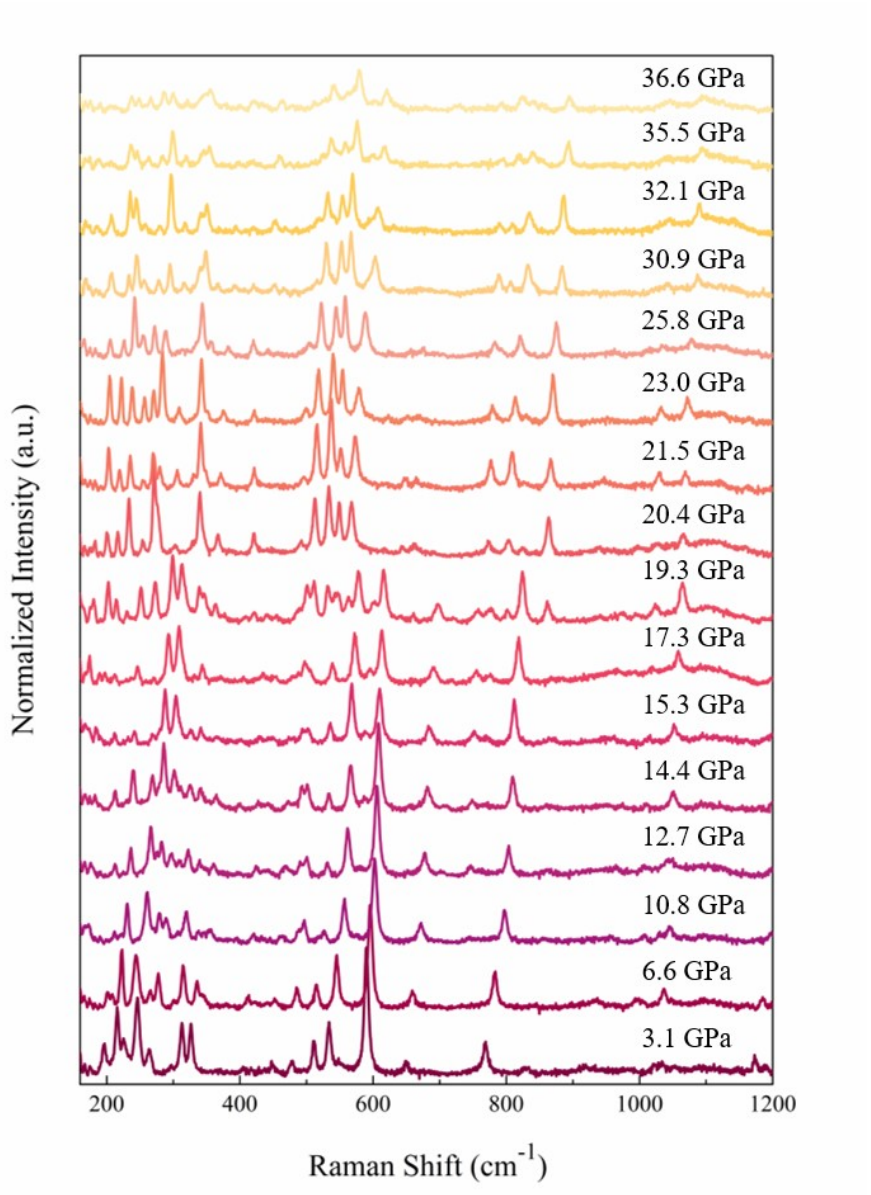

Figure S2. Evolution of the Raman spectrum of reedmergnerite from 150 to 1200 cm^{-1} during isothermal (T = 25 ºC) compression.

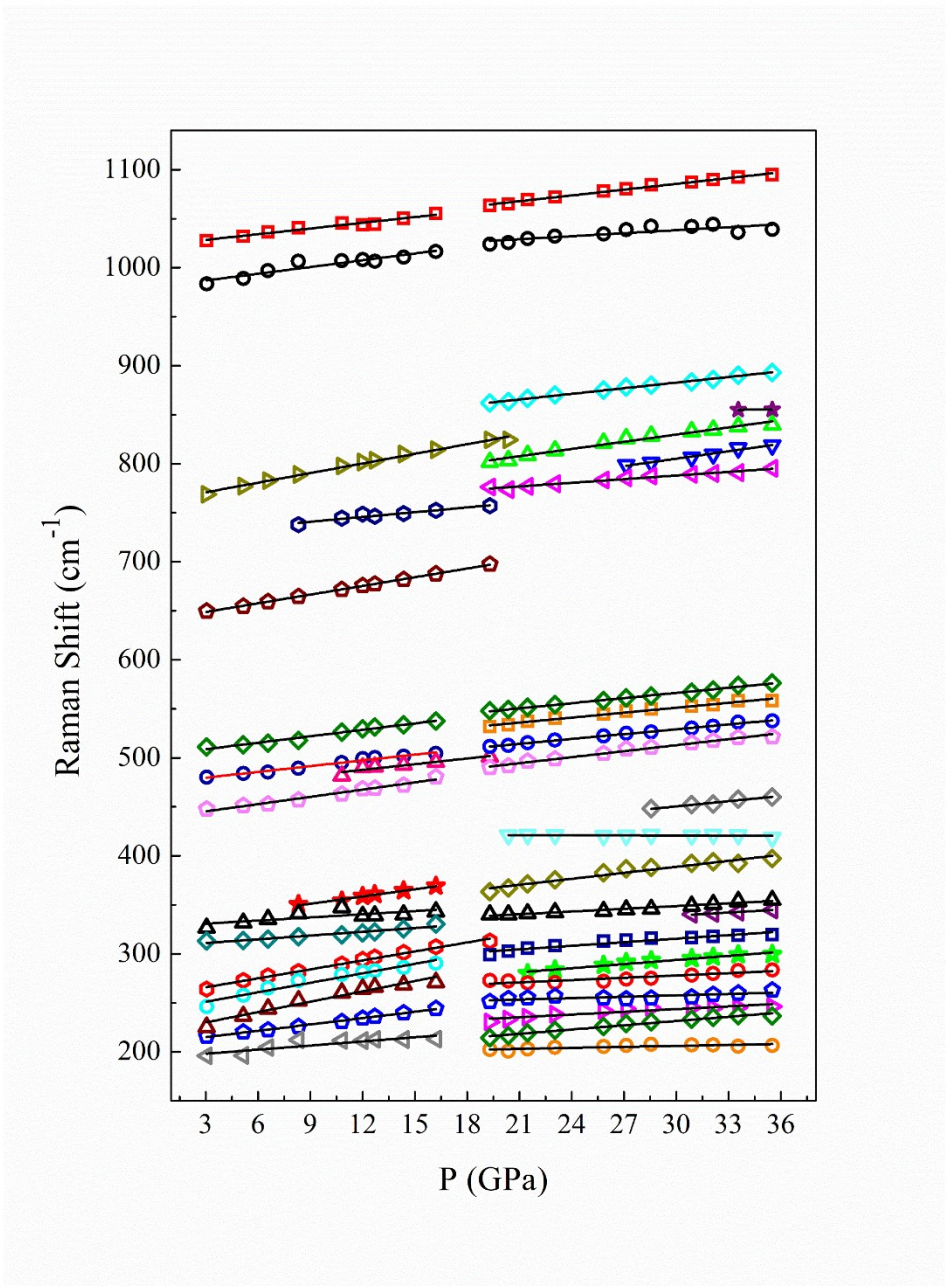

Figure S3. Pressure evolution of some selected Raman bands of reedmergnerite. The errors are smaller than size of the symbols.

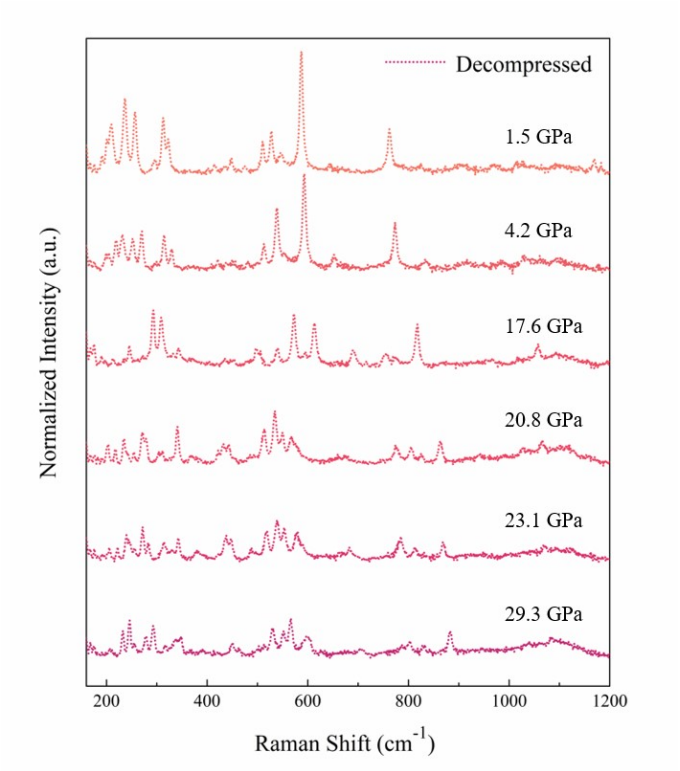

Figure S4. Evolution of the Raman spectrum from 150 to 1200 cm^{-1} during isothermal (T = 25 °C) decompression.

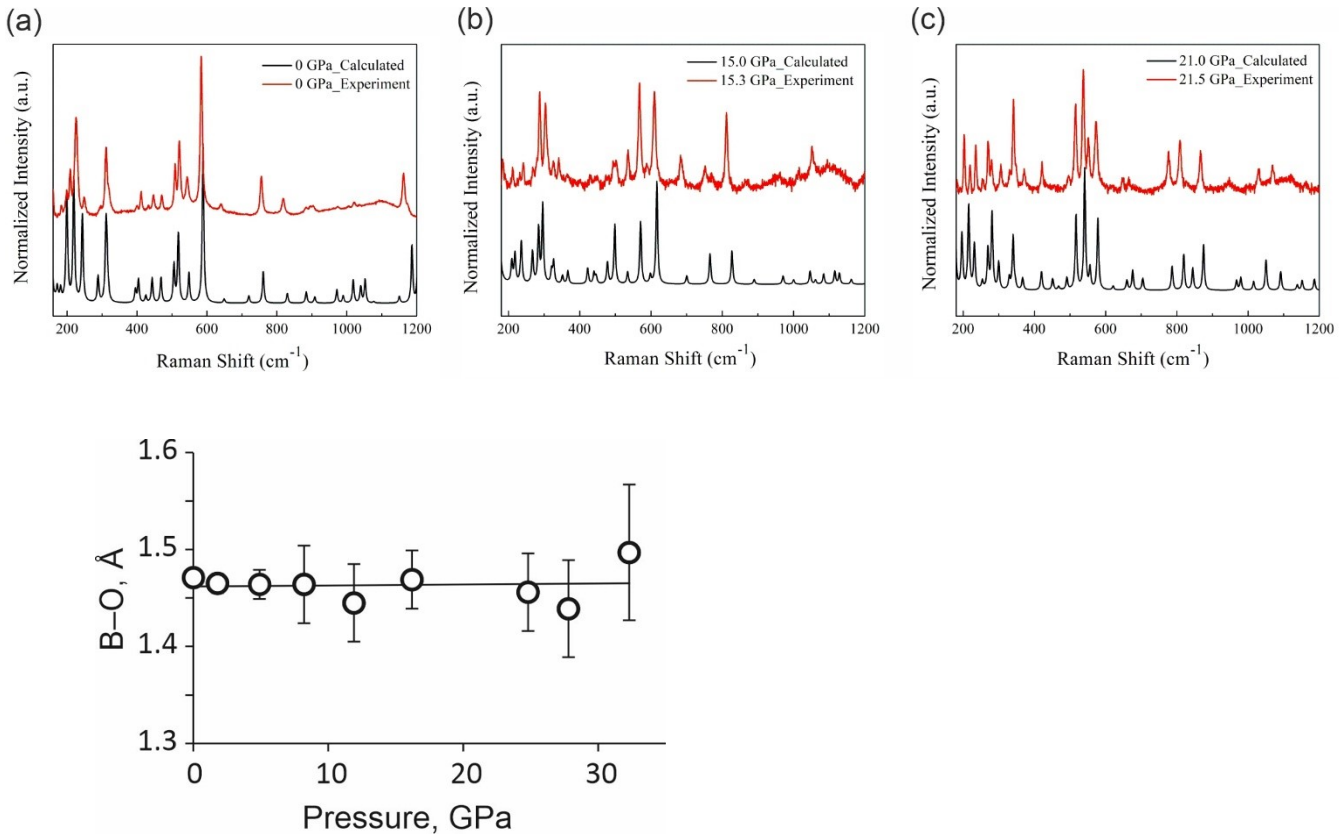

Figure S5. Comparison of the experimentally determined Raman spectrum of reedmergnerite at different pressures to results of DFPT calculations.

Figure S6. Pressure dependence of the <B–O> distances in the crystal structure of reedmergnerite.

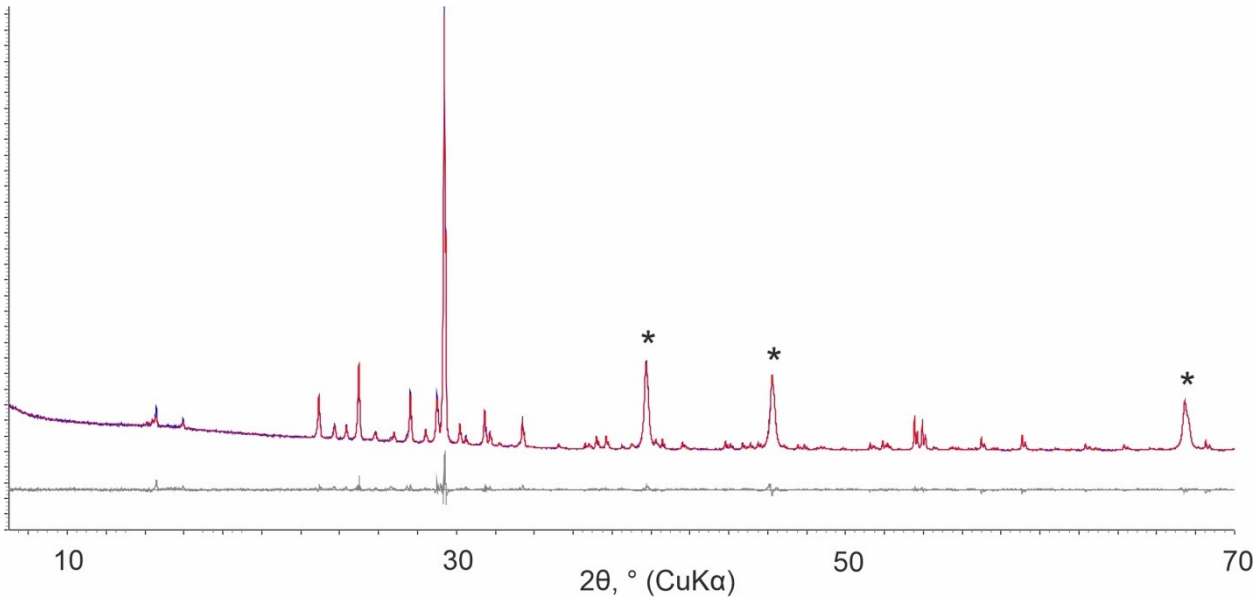

Figure S7. Experimental powder X-ray diffraction pattern of studied reedmergnerite $NaBSi_3O_8$ (blue line), Rietveld-simulated pattern (red line), the difference between experimental and calculated patterns (grey line at the bottom). * - Pt (Pt holder).