Supplementary Material for:

Synthesis, structure refinement and single-crystal elasticity of Al-bearing superhydrous phase B

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Table S1. Frequency, integral absorbance and band width of FTIR absorption OH bands observed on the thin films

		Peak position cm^{-1}	A_{int} cm^{-2}	FWHM cm^{-1}
MA-399	ν_1	3407	210.000	36
	ν_2	3346	130.000	35
	ν_3	3261	60.000	174
	ν_4	3524	10.000	139
MA-575	ν_1	3406	280.000	64
	ν_2	3344	130.000	49
	ν_3	3243	130.000	129
	ν_4	3553	>10.000	51
MA-576	$\nu_1+\nu_2$	3397	410.000	118
	ν_3	3246	520.000	199
	ν_4	3554	20.000	71

Table S2. FTIR data lattice vibrations observed on thin films

MA-399 Peak position (cm^{-1})	MA-575 Peak position (cm^{-1})	MA-576 Peak position (cm^{-1})	Assignment after Hofmeister et al. 1999
	1220	1220	
1158	1156	1153	O-Mg stretching
	1034	1034	
966	967	968	tetrahedral Si
883	888	895	tetrahedral Si
695	696	710	octahedral Si
		679	octahedral Al
		627	octahedral Al
645	640		
599	606		
560	565	579	Mg-O-Mg bending
533	539	543	

Table S3. Raman modes frequency, assignment and line width based on our measurements

	MA-399		MA-575		MA-576	
peak position cm^{-1}	assignment Hofmeister et al. 1999	FWHM cm^{-1}	peak position cm^{-1}	FWHM cm^{-1}	peak position cm^{-1}	FWHM cm^{-1}
845 (wshd)		20	850	15	858	35
831 (vst)	SiO_4 stretching	9	833	14	836	23
					708	20
683 (st)	SiO_4 stretching	20	686	19	689	19
603 (w)	Mg-O-Mg?	7	604	13	607	19
554 (w)		10	555	11	560	19
536 (w)	octahed. Si?	13	536	10	539	19
496 (w)	octahed. Si?	7	495	13	492	17
					444	16
433 (w)	octahed. Si[1]	11	435	19	431	41
277 (vw)	Mg trans	9	280	17	287	37

wshd weak shoulder; vst very strong; st strong; w weak; vw very weak
[1]As the FWHM increases with increasing Al content, we assign this band to octahedral Si.

Table S4. Cell parameters for MA-399, MA-575 and MA-576

Run No.	a(Å)	error(Å)	b(Å)	error(Å)	c(Å)	error(Å)	V($Å^3$)	error($Å^3$)
MA-399	5.10219	0.00006	13.99498	0.00012	8.71843	0.00006	622.54	0.01
MA-575	5.09776	0.00004	13.97829	0.00014	8.70539	0.00008	620.329	0.01
MA-576	5.08655	0.00006	13.94165	0.00013	8.6983	0.00008	616.839	0.011

Figure S1

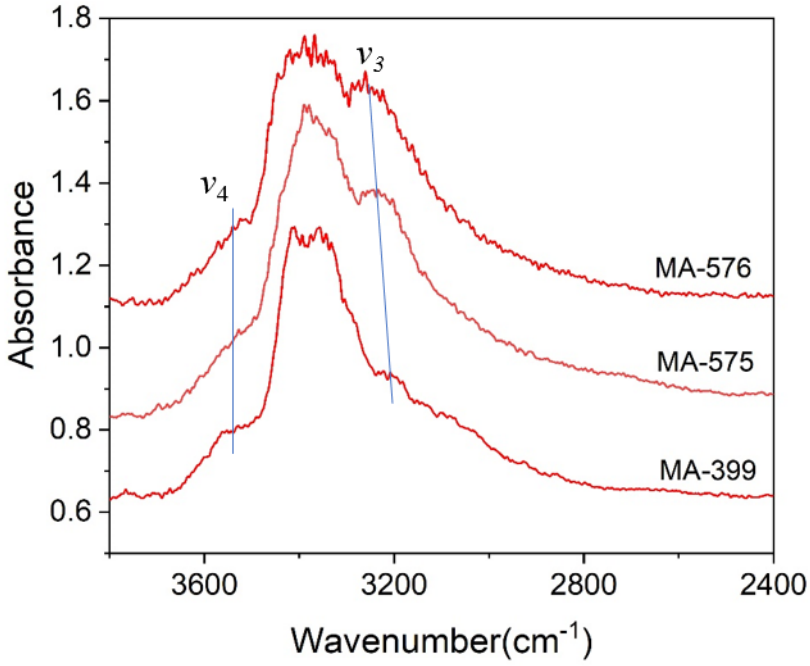

Figure S1. Infrared spectra of shy-B crystals with different Al content in the frequency range of the OH stretching vibration. The spectra are oversaturated in the range of 3450 to 3300 cm^{-1}and only shown for the defect-H bands ν_3 and ν_4.

Figure S2

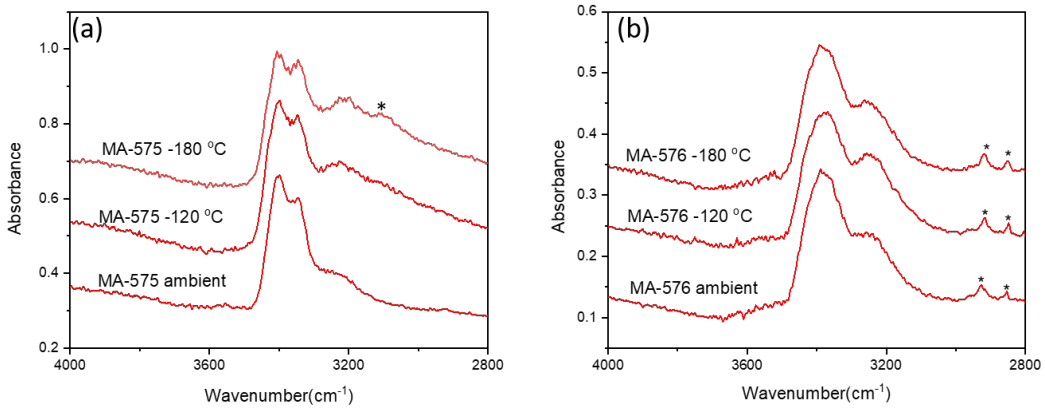

Figure S2. Low temperature Infrared spectra of shy-B prepared as thin films with different Al content in the frequency range of the OH stretching vibrations. (a) MA-575 shy-B at ambient condition, -120ºC and -180ºC, respectively. The asterisk in S2a shows the position of an ice-band (see main text) (b) MA-576 shy-B at ambient condition, -120ºC and -180ºC, respectively. The asterisks in S2b represent impurities of C-H components on the sample surface which disappeared during annealing to 300 °C (not shown). The high temperature spectra were taken within the same cooling/heating stage directly after the cooling experiments.

Figure S3

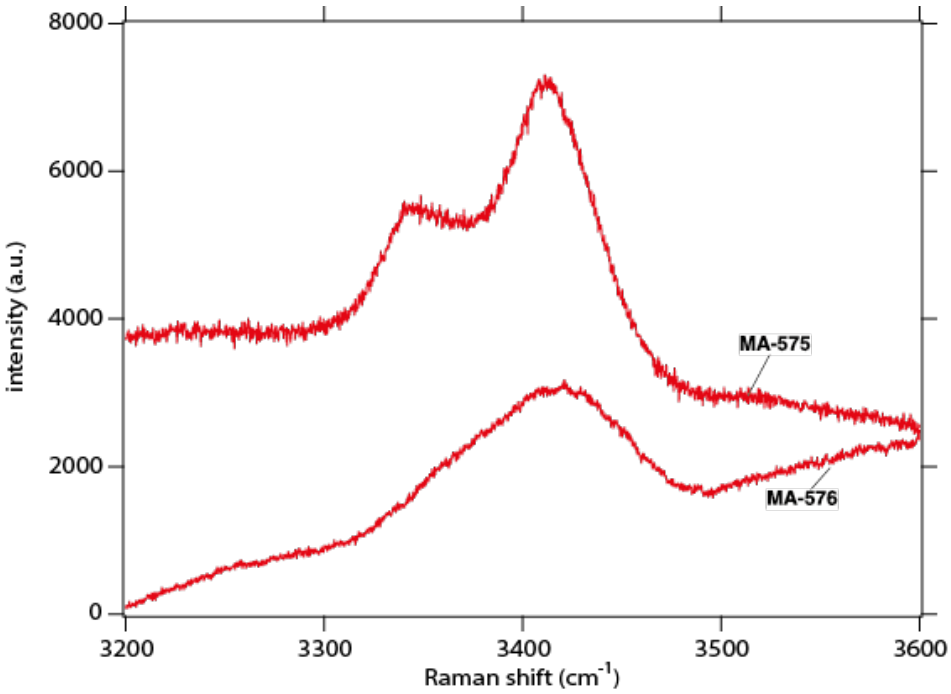

Figure S3. Raman spectra of shy-B with different Al content at the frequency range of 3200-3600 cm^{-1}.

Figure S4

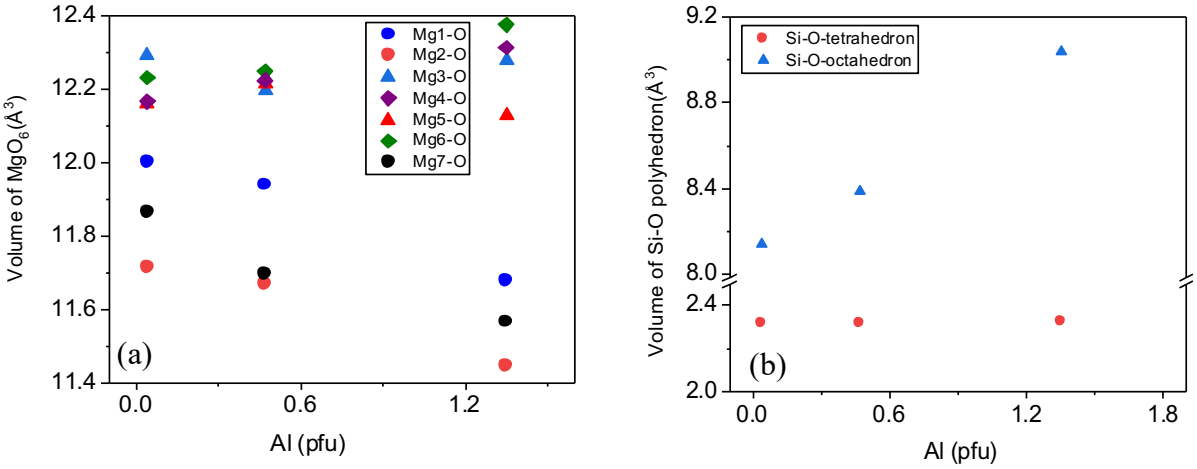

Figure S4. Volume of various Mg- and Si-polyhedra for shy-B with different Al content in *Pnn*2 space group. (a) Volume of MgO_6 octahedra; blue circles, red circles, blue triangles, purple diamonds, red triangles, green diamonds and black circles represent the octahedral volume for the site of Mg1, Mg2, Mg3, Mg4, Mg5, Mg6 and Mg7, respectively. (b) Volume of SiO_4 octahedron and SiO_6 tetrahedron; triangles and circles represent the octahedron and tetrahedron of SiO_6 and SiO_4, respectively. Error bars are smaller than the symbols in both two figures.

Figure S5

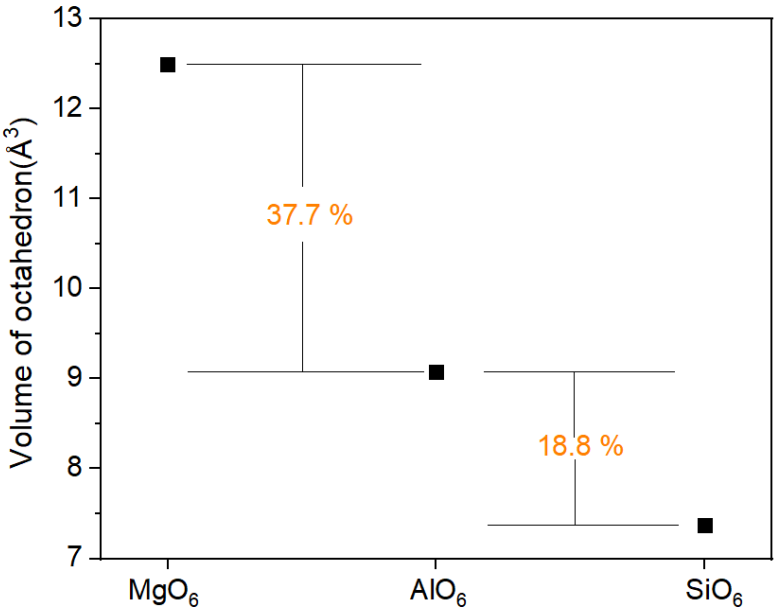

Figure S5. Volume of MgO_6, AlO_6 and SiO_6 octahedra in the structures of periclase (MgO), corundum (Al_2O_3) and stishovite (rutile-structured SiO_2).