Table S1. EPMA analysis on chemical compositions of synthesized Al-bearing stishovite crystals

# of measurements	oxides in wt%		
	SiO_2	Al_2O_3	Total
Al1.3-SiO_2, run# 5K3302			
1	97.36	3.36	100.72
2	96.49	3.40	99.89
3	95.89	3.43	99.33
4	94.63	3.54	98.17
5	94.91	3.41	98.32
average	95.86(101)	3.43(6)	99.28(96)
Al2.1-SiO_2, run# 1K2965			
1	95.34	5.41	100.75
2	94.44	5.32	99.76
3	93.68	5.29	98.97
4	93.96	5.40	99.35
5	94.10	5.35	99.45
6	94.22	5.40	99.62
7	93.73	5.41	99.15
8	94.09	5.36	99.45
average	94.20(49)	5.37(4)	99.56(51)

Note: numbers in parentheses represent ±1σ uncertainties

Table S2. Experimental Raman shifts in Al1.3-SiO_2 at high pressure

Stishovite				Post-stishovite			
P (GPa)	B_{1g} (cm^{-1})	E_g (cm^{-1})	A_{1g} (cm^{-1})	P (GPa)	A_g^* (cm^{-1})	A_g (cm^{-1})	A_g (cm^{-1})
0.0001	225.9(1)	583.0(4)	747.7(6)	24.7(1)	202.2(4)	211.5(4)	806.5(15)
3.2(1)	222.5(2)	589.4(5)	757.2(8)	27.6(1)	198.5(6)	213.1(4)	808.9(14)
4.5(1)	221.4(2)	592.2(5)	760.0(7)	30.6(2)	198.5(4)	214.3(4)	
6.9(4)	219.0(2)	596.3(5)	768.6(8)	33.5(3)	199.8(6)	215.5(5)	
8.7(2)	217.1(2)	600.9(5)	775.1(8)	36.5(5)	202.1(6)	216.6(5)	
10.3(6)	214.8(2)	605.8(6)	780.2(8)	40.9(1)		219.6(5)	
14.1(1)	213.7(2)	607.3(6)	788.6(12)	42.7(1)		220.5(5)	
16.4(4)	211.1(2)	612.2(6)	794.6(12)	44.3(1)		222.2(5)	
20.3(1)	207.3(4)		802.3(13)	47.8(1)		224.8(6)	
				51.3(6)		227.3(6)	
				54.5(1)		230.9(6)	
				58.3(3)		230.1(6)	

Note: numbers in parentheses represent ±1σ uncertainties

Table S3. Experimental Raman shifts in Al2.1-SiO_2 at high pressure

Stishovite				Post-stishovite		
P (GPa)	B_{1g} (cm^{-1})	E_g (cm^{-1})	A_{1g} (cm^{-1})	P (cm^{-1})	A_g (cm^{-1})	A_g (cm^{-1})
0.0001	224.1(1)	579.3(3)	744.2(8)	20.3(1)	220.3(3)	818.3(12)
3.2(1)	221.6(1)	587.5(4)	756.3(12)	24.7(1)	228.9(3)	832.2(13)
4.5(1)	220.5(1)	590.7(4)	757.3(12)	27.6(1)	234.4(4)	840.2(15)
6.9(4)	218.4(1)	594.5(4)	765.5(18)	30.6(2)	231.8(4)	848.9(24)
8.7(2)	217.3(2)		774.5(16)	33.5(3)	244.5(7)	861.1(20)
10.3(6)	215.9(2)			36.5(5)	243.0(13)	866.0(18)
14.1(1)	214.1(2)	611.7(11)	790.5(13)	40.9(1)	256.2(12)	875.9(21)
16.4(4)	212.4(2)		804.1(13)	42.7(1)	254.2(12)	877.4(18)
				44.3(1)	261.2(12)	879.6(19)
				47.8(1)	269.3(12)	885.6(19)
				51.3(6)	279.5(12)	890.1(19)
				54.5(1)	272.6(12)	894.6(19)
				58.3(3)	275.2(12)	901.1(22)

Note: numbers in parentheses represent ±1σ uncertainties

Table S4. Experimental Raman shifts of major optic modes in stishovite with different Al and H contents at ambient conditions

References	Compositions	B_{1g} (cm^{-1})	E_g (cm^{-1})	A_{1g} (cm^{-1})	B_{2g} (cm^{-1})
This study	Al1.3-SiO_2, 0.7 mol% H^+	225.9(2)	583.0(5)	747.7(7)	959.8(11)
This study	Al2.1-SiO_2, 0.8 mol% H^+	224.1(1)	579.3(4)	744.2(8)	957.2(12)
Zhang et al. (2021)	SiO_2, 0.004 mol% H^+	230.9(1)	588.8(6)	753.9(7)	
Kingma et al. (1995)	SiO_2	231.6(3)	589.0(10)	754.1(3)	966.2(5)
Lakshtanov et al. (2007)	Al1.7-SiO_2, 0.6 mol% H^+	222.7	578.7	740.8	954.3
Lakshtanov et al. (2007)	Al2.4-SiO_2, 0.5 mol% H^+	221.6	574.2	736.1	949.6
Nisr et al. (2017b)	SiO_2, 6.6 mol% H^+	235	592	754	968

Note: numbers in parentheses represent ±1σ uncertainties

Table S5. Unit-cell parameters of Al1.3-SiO_2 at high pressure and 300 K

P (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å)
0.0001	4.1963(8)		2.6723(4)	47.06(2)
4.3(1)	4.1744(7)		2.6648(4)	46.43(1)
5.9(1)	4.1668(7)		2.6619(4)	46.22(1)
7.4(1)	4.1573(7)		2.6593(4)	45.96(1)
9.0(1)	4.1488(7)		2.6572(4)	45.74(1)
10.4(1)	4.1422(7)		2.6548(4)	45.55(1)
12.8(1)	4.1315(7)		2.6507(4)	45.24(1)
14.8(1)	4.1228(6)		2.6477(4)	45.00(1)
16.1(1)	4.1161(6)		2.6457(4)	44.82(1)
17.1(1)	4.1116(6)		2.6442(4)	44.70(1)
18.3(1)	4.1062(6)		2.6423(4)	44.55(1)
19.6(1)	4.1000(12)		2.6399(4)	44.38(8)
19.8(1)	4.0992(12)		2.6397(4)	44.35(8)
21.9(1)	4.1130(12)	4.0705(79)	2.6363(4)	44.14(8)
22.9(2)	4.1141(12)	4.0600(79)	2.6340(4)	44.00(7)
25.3(1)	4.1114(12)	4.0400(78)	2.6306(4)	43.69(7)
26.8(1)	4.1097(12)	4.0300(78)	2.6274(4)	43.52(7)
27.6(2)	4.1070(12)	4.0240(78)	2.6251(4)	43.38(7)
29.2(2)	4.1056(9)	4.0169(27)	2.6222(4)	43.24(3)
30.8(2)	4.1031(9)	4.0117(27)	2.6188(4)	43.11(3)
32.1(2)	4.1001(9)	4.0053(27)	2.6165(4)	42.97(3)
33.8(2)	4.0965(9)	3.9945(27)	2.6125(4)	42.75(3)
35.2(2)	4.0942(9)	3.9863(27)	2.6100(4)	42.60(3)
37.3(2)	4.0921(9)	3.9764(27)	2.6056(4)	42.40(3)
38.6(2)	4.0897(9)	3.9706(27)	2.6042(4)	42.29(3)
40.3(2)	4.0846(9)	3.9630(27)	2.6018(4)	42.12(3)
42.4(2)	4.0773(9)	3.9532(26)	2.5990(4)	41.89(2)
43.9(2)	4.0745(9)	3.9457(26)	2.5966(4)	41.75(2)
45.2(2)	4.0736(9)	3.9394(26)	2.5938(4)	41.62(2)
47.6(2)	4.0731(9)	3.9272(26)	2.5889(4)	41.41(2)
49.4(2)	4.0715(9)	3.9185(26)	2.5858(4)	41.26(2)
50.8(2)	4.0675(9)	3.9136(26)	2.5836(4)	41.13(2)
52.7(2)	4.0659(9)	3.9035(26)	2.5805(4)	40.96(2)
54.8(2)	4.0643(9)	3.8975(26)	2.5774(4)	40.83(2)
56.9(2)	4.0624(9)	3.8916(25)	2.5748(4)	40.71(2)
58.4(2)	4.0607(9)	3.8841(25)	2.5730(4)	40.58(2)
59.9(2)	4.0600(9)	3.8785(25)	2.5708(4)	40.48(2)
61.5(2)	4.0536(9)	3.8722(10)	2.5679(4)	40.31(1)

63.1(3)	4.0512(9)	3.8661(10)	2.5653(4)	40.18(1)
65.7(3)	4.0477(9)	3.8569(10)	2.5617(4)	39.99(1)
67.0(3)	4.0458(9)	3.8522(10)	2.5598(4)	39.90(1)
68.9(3)	4.0432(9)	3.8456(10)	2.5571(4)	39.76(1)
71.1(3)	4.0402(9)	3.8380(10)	2.5541(4)	39.60(1)
72.6(3)	4.0381(9)	3.8328(10)	2.5519(4)	39.50(1)

Note: numbers in parentheses represent ±1σ uncertainties

Table S6. Unit-cell parameters of Al2.1-SiO_2 at high pressure and 300 K

P (GPa)	*a* (Å)	*b* (Å)	*c* (Å)	*V* (Å)
0.0001	4.2025(9)		2.6788(16)	47.31(2)
4.3(1)	4.1781(5)		2.6715(16)	46.63(2)
5.9(1)	4.1704(5)		2.6685(16)	46.41(2)
7.4(1)	4.1612(4)		2.6672(16)	46.19(2)
9.0(1)	4.1534(4)		2.6633(10)	45.94(2)
10.4(1)	4.1467(4)		2.6611(10)	45.76(2)
12.8(1)	4.1353(4)		2.6576(10)	45.45(2)
14.8(1)	4.1259(4)		2.6544(10)	45.19(2)
16.1(1)	4.1295(6)	4.1119(8)	2.6519(7)	45.03(3)
17.1(1)	4.1322(6)	4.1003(8)	2.6500(7)	44.90(3)
18.3(1)	4.1328(6)	4.0897(8)	2.6476(7)	44.75(3)
19.6(1)	4.1313(6)	4.0798(8)	2.6449(7)	44.58(3)
19.8(1)	4.1338(6)	4.0760(8)	2.6446(7)	44.56(3)
21.9(1)	4.1284(5)	4.0638(8)	2.6405(7)	44.30(3)
22.9(2)	4.1261(5)	4.0631(5)	2.6386(7)	44.23(1)
25.3(1)	4.1194(5)	4.0489(5)	2.6341(7)	43.93(1)
26.8(1)	4.1169(5)	4.0414(5)	2.6313(6)	43.78(1)
27.6(2)	4.1152(5)	4.0365(5)	2.6302(5)	43.69(1)
29.2(2)	4.1120(5)	4.0286(5)	2.6264(5)	43.51(1)
30.8(2)	4.1083(5)	4.0215(5)	2.6231(5)	43.34(1)
32.1(2)	4.1062(5)	4.0157(5)	2.6222(5)	43.24(1)
33.8(2)	4.1022(5)	4.0055(5)	2.6159(5)	42.98(1)
35.2(2)	4.0994(5)	3.9985(4)	2.6141(5)	42.85(1)
37.3(2)	4.0951(5)	3.9879(4)	2.6097(5)	42.62(1)
38.6(2)	4.0931(5)	3.9824(4)	2.6081(5)	42.51(1)
40.3(2)	4.0895(5)	3.9753(4)	2.6056(5)	42.36(1)
42.4(2)	4.0851(5)	3.9660(4)	2.6030(5)	42.17(1)
43.9(2)	4.0830(5)	3.9562(4)	2.6015(5)	42.02(1)
45.2(2)	4.0804(5)	3.9508(4)	2.5995(5)	41.91(1)
47.6(2)	4.0755(5)	3.9386(4)	2.5943(5)	41.64(1)
49.4(2)	4.0718(5)	3.9301(4)	2.5919(5)	41.48(1)
50.8(2)	4.0684(5)	3.9244(4)	2.5892(5)	41.34(1)
52.7(2)	4.0649(5)	3.9165(4)	2.5847(5)	41.15(1)
54.8(2)	4.0613(5)	3.9093(4)	2.5810(5)	40.98(1)
56.9(2)	4.0586(5)	3.9033(4)	2.5777(5)	40.84(1)
58.4(2)	4.0564(5)	3.8991(4)	2.5763(5)	40.75(1)
59.9(2)	4.0549(5)	3.8928(5)	2.5749(5)	40.64(1)
61.5(2)	4.0517(5)	3.8874(5)	2.5724(5)	40.52(1)

63.1(3)	4.0500(5)	3.8823(5)	2.5684(5)	40.39(1)
65.7(3)	4.0470(5)	3.8761(4)	2.5663(5)	40.26(1)
67.0(3)	4.0449(5)	3.8718(4)	2.5646(5)	40.16(1)
68.9(3)	4.0415(5)	3.8663(4)	2.5614(5)	40.02(1)
71.1(3)	4.0388(5)	3.8606(4)	2.5588(5)	39.90(1)
72.6(3)	4.0359(5)	3.8546(4)	2.5553(5)	39.75(1)

Note: numbers in parentheses represent ±1σ uncertainties

Table S7. EOS parameters of stishovite and post-stishovite with different Al and H contents at ambient conditions

References	Compositions	Samples	Stishovite			Post-stishovite		
			V_0	K_{T0}	K_T'	V_0	K_{T0}	K_T'
This study	Al1.3-SiO_2, 0.7 mol% H^+	Single crystal	47.06(2)	302.1(31)	4[a]	47.41(13)	253.2(14)	4.9(1)
This study	Al2.1-SiO_2, 0.8 mol% H^+	Single crystal	47.31(2)	292.5(50)	4[a]	47.40(11)	279.7(26)	4.3(1)
Zhang et al. (2021)	SiO_2, 0.004 mol% H^+	Single crystal	46.57(3)	317.2(26)	4.8(2)	47.92(42)	254.8(51)	4[a]
Andrault et al. (2003)	SiO_2	Poly-crystal	46.513(6)	309.9(11)	4.59(23)	46.31(15)	334(7)	4[a]
Buchen et al. (2018)	SiO_2	Poly-crystal	46.43(10)	344(25)	6.0(11)	48.22(44)	241(18)	4.72(4)
Ono et al. (2002)	Al0.8-SiO_2	Poly-crystal	46.850(8)	297(5)	3.0(3)			
Lakshtanov et al. (2005)	Al0.7-SiO_2, 0.1 mol% H^+	Poly-crystal	46.782(7)	298(7)	4.3(5)			
Bolfan-Casanova et al. (2009)	Al0.9-SiO_2	Poly-crystal	46.866(25)	284(4)	4[a]			
Bolfan-Casanova et al. (2009)	Al0.9-SiO_2	Poly-crystal	46.871(20)	291(5)	4[a]			
Bolfan-Casanova et al. (2009)	Al1.4-SiO_2	Poly-crystal				47.881(49)	259(3)	4[a]
Bolfan-Casanova et al. (2009)	Al1.4-SiO_2	Poly-crystal				47.076(49)	300(4)	4[a]
Nisr et al. (2017a)	SiO_2, 6.6 mol% H^+	Poly-crystal	47.191	257(9)	4.59[a]	47.23(36)	286(18)	4[a]

Note: numbers in parentheses represent ±1σ uncertainties

[a] fixed value

Table S8. Modeled elastic moduli (C_{ij}) of Al1.3-SiO_2 at high pressure and 300 K.

P (GPa)	Phase	C_{11} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{22} (GPa)	C_{23} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{55} (GPa)	C_{66} (GPa)
0	St	434.7	189.0	190.6			743.5	246.7		295.2
2	St	436.9	209.5	193.9			751.5	250.3		301.6
4	St	438.7	230.5	197.2			759.3	253.8		308.0
6	St	439.9	252.0	200.4			766.9	257.4		314.3
8	St	440.6	274.0	203.6			774.4	260.8		320.5
10	St	440.7	296.5	206.8			781.7	264.2		326.7
12	St	440.2	319.5	209.9			788.8	267.6		332.9
14	St	439.2	343.1	213.0			795.7	270.9		339.0
16	St	437.6	367.3	216.0			802.5	274.2		345.2
18	St	435.4	392.0	219.0			809.2	277.4		351.2
20	St	432.5	417.3	222.0			815.7	280.6		357.3
22	Pst	463.2	424.1	205.7	432.8	244.7	821.5	286.4	281.0	363.4
24	Pst	508.2	411.7	195.5	456.7	261.7	826.6	291.5	282.1	369.7
26	Pst	547.0	401.3	190.6	482.8	273.1	831.7	296.0	283.8	376.0
28	Pst	582.1	392.9	188.0	508.8	282.3	836.7	300.2	285.7	382.2
30	Pst	614.4	386.1	186.7	534.2	290.0	841.6	304.1	287.7	388.4
32	Pst	644.6	380.8	186.3	558.7	296.7	846.5	308.0	289.8	394.6
34	Pst	672.8	376.9	186.5	582.5	302.7	851.4	311.7	292.0	400.8
36	Pst	699.4	374.2	187.2	605.4	308.1	856.1	315.3	294.2	406.9
38	Pst	724.5	372.7	188.3	627.4	313.1	860.9	318.9	296.3	413.0
40	Pst	748.3	372.2	189.7	648.7	317.7	865.5	322.4	298.5	419.1
42	Pst	771.0	372.7	191.2	669.2	322.0	870.1	325.8	300.8	425.1
44	Pst	792.5	374.1	193.0	689.0	326.1	874.6	329.1	303.0	431.2
46	Pst	813.2	376.3	194.9	708.1	329.9	879.0	332.4	305.2	437.2
48	Pst	832.9	379.2	196.9	726.6	333.6	883.4	335.7	307.4	443.2
50	Pst	851.8	382.9	199.1	744.5	337.1	887.7	338.9	309.5	449.2
52	Pst	870.0	387.2	201.3	761.7	340.5	892.0	342.1	311.7	455.1
54	Pst	887.5	392.2	203.6	778.5	343.7	896.1	345.2	313.9	461.1
56	Pst	904.3	397.7	205.9	794.7	346.8	900.2	348.3	316.1	467.0
58	Pst	920.5	403.8	208.3	810.5	349.8	904.3	351.4	318.2	472.9
60	Pst	936.2	410.3	210.8	825.7	352.8	908.3	354.4	320.4	478.8
62	Pst	951.3	417.4	213.2	840.6	355.6	912.2	357.4	322.5	484.7
64	Pst	965.9	424.9	215.7	855.0	358.4	916.0	360.3	324.6	490.5
66	Pst	980.1	432.8	218.2	869.0	361.1	919.8	363.2	326.7	496.4
68	Pst	993.9	441.2	220.8	882.7	363.8	923.5	366.1	328.8	502.2
70	Pst	1007.2	449.9	223.3	895.9	366.4	927.1	369.0	330.9	508.0

Note: St: stishovite, Pst: post-stishovite; stishovite phase has six independent C_{ij} while post-stishovite phase has nine independent C_{ij}; estimated standard deviation is 7.5% for all C_{ij}'s (please refer to Text S1 for details).

Table S9. Modeled C_{ij} of Al2.1-SiO_2 at high pressure and 300 K.

P (GPa)	Phase	C_{11} (GPa)	C_{12} (GPa)	C_{13} (GPa)	C_{22} (GPa)	C_{23} (GPa)	C_{33} (GPa)	C_{44} (GPa)	C_{55} (GPa)	C_{66} (GPa)
0	St	423.6	185.0	189.2			734.1	238.2		281.4
2	St	422.7	209.1	192.6			742.2	241.9		287.9
4	St	421.0	233.9	195.9			750.1	245.5		294.4
6	St	418.7	259.2	199.2			757.8	249.1		300.8
8	St	415.7	285.2	202.4			765.4	252.6		307.1
10	St	412.0	311.9	205.6			772.7	256.1		313.4
12	St	407.6	339.2	208.8			779.9	259.5		319.7
14	St	402.6	367.1	211.9			787.0	262.8		325.9
16	St	396.8	395.7	215.0			793.8	266.1		332.2
18	Pst	460.1	380.7	189.9	408.7	246.9	799.7	273.1	265.8	338.6
20	Pst	506.7	366.3	182.5	435.7	261.2	805.4	277.8	267.5	345.0
22	Pst	548.3	354.0	178.3	463.8	272.0	811.1	282.2	269.5	351.5
24	Pst	586.5	343.4	175.8	491.6	281.1	816.6	286.4	271.6	357.8
26	Pst	621.9	334.6	174.5	518.7	288.9	822.1	290.4	273.9	364.2
28	Pst	655.1	327.3	173.9	545.0	295.9	827.4	294.2	276.2	370.5
30	Pst	686.2	321.5	173.9	570.5	302.2	832.7	298.0	278.5	376.8
32	Pst	715.6	316.9	174.3	595.0	308.0	837.9	301.7	280.9	383.0
34	Pst	743.4	313.6	175.1	618.7	313.4	843.0	305.3	283.2	389.3
36	Pst	769.7	311.5	176.1	641.5	318.4	848.0	308.8	285.6	395.5
38	Pst	794.7	310.4	177.4	663.4	323.1	852.9	312.3	287.9	401.7
40	Pst	818.6	310.4	178.9	684.6	327.5	857.7	315.7	290.3	407.9
42	Pst	841.2	311.3	180.6	705.0	331.7	862.5	319.1	292.6	414.0
44	Pst	862.9	313.0	182.4	724.6	335.7	867.1	322.4	294.9	420.1
46	Pst	883.6	315.6	184.2	743.5	339.6	871.7	325.7	297.3	426.2
48	Pst	903.4	319.0	186.2	761.8	343.3	876.2	328.9	299.6	432.3
50	Pst	922.3	323.2	188.3	779.3	346.8	880.6	332.1	301.9	438.4
52	Pst	940.4	328.0	190.5	796.3	350.3	884.9	335.3	304.2	444.4
54	Pst	957.8	333.5	192.6	812.7	353.6	889.2	338.4	306.4	450.5
56	Pst	974.5	339.7	194.9	828.5	356.8	893.3	341.5	308.7	456.5
58	Pst	990.5	346.4	197.2	843.8	359.9	897.4	344.5	310.9	462.5
60	Pst	1005.9	353.7	199.5	858.5	363.0	901.5	347.5	313.2	468.5
62	Pst	1020.7	361.6	201.9	872.8	365.9	905.4	350.5	315.4	474.4
64	Pst	1034.9	370.0	204.3	886.5	368.8	909.3	353.5	317.6	480.4
66	Pst	1048.6	378.9	206.7	899.8	371.7	913.1	356.4	319.8	486.3
68	Pst	1061.8	388.3	209.1	912.7	374.4	916.8	359.3	322.0	492.2
70	Pst	1074.4	398.1	211.5	925.1	377.2	920.4	362.1	324.1	498.2

Note: St: stishovite, Pst: post-stishovite; stishovite phase has six independent C_{ij} while post-stishovite phase has nine independent C_{ij}; estimated standard deviation is 7.5% for all C_{ij}'s (please refer to Text S1 for details).

Table S10. Thermoelastic parameters of subducted MORB components in the model

MORB components	V_0 (cm^3/mol)	K_0 (GPa)	K'_0	μ_0 (GPa)	μ'_0	θ_0	γ_0	q_0	η_{S0}
Al1.3-SiO_2[a]	14.17	298	3.9	238	1.9	1055	1.35	2.9	4.6
Al2.1-SiO_2[a]	14.24	293	3.9	241	2.0	1055	1.35	2.9	4.6
SiO_2[a]	14.02	307	3.7	236	1.8	1055	1.35	2.9	4.6
$(Mg_{0.85}Fe_{0.15})SiO_3$ bridgmanite[b]	24.59	254	4.1	169	1.7	881	1.44	1.4	2.5
Ca-perovskite[c]	27.33	248	4.0	126	1.6	1000	1.42	2.65	1.54
$CaFe_2O_4$-type phase[d]	36.18	211	4.1	130	1.8	863	1.31	1.0	2.1

[a]Values of V_0, K_0, K'_0, μ_0, and μ'_0 for Al1.3-SiO_2 and Al2.1-SiO_2 are taken from this study, while those of pure SiO_2 are taken from Zhang et al. (2021). The θ_0, γ_0, q_0, and η_{S0} are taken from Xu et al. (2008) that have derived these thermoelastic parameters using literature elastic data (Liu et al., 1999; Murakami et al., 2003).

[b]A typical bridgmanite composition in subducted MORB is suggested by Tsuchiya (2011). Thermoelastic parameters have been constrained by Xu et al. (2008) using literature results (Fei & Ahrens, 1995; Fiquet et al., 2000; Kiefer et al., 2002; Shim & Duffy, 2000; Sinogeikin et al., 2004; Smyth & McCormick, 1995; Wentzcovitch et al., 2004).

[c]Thermoelastic parameters are refitted using elasticity data from Gréaux et al. (2019) and Sun et al. (2016).

[d]Thermoelastic parameters are taken from Xu et al. (2008) using literature results (Akaogi et al., 1999; Funamori et al., 1998).