

Supplemental Information for
Hydrous wadsleyite crystal structure up to 32 GPa

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Introduction

This supporting information provides seven supplementary figures and twenty-four supplementary tables which are not included in the main text.

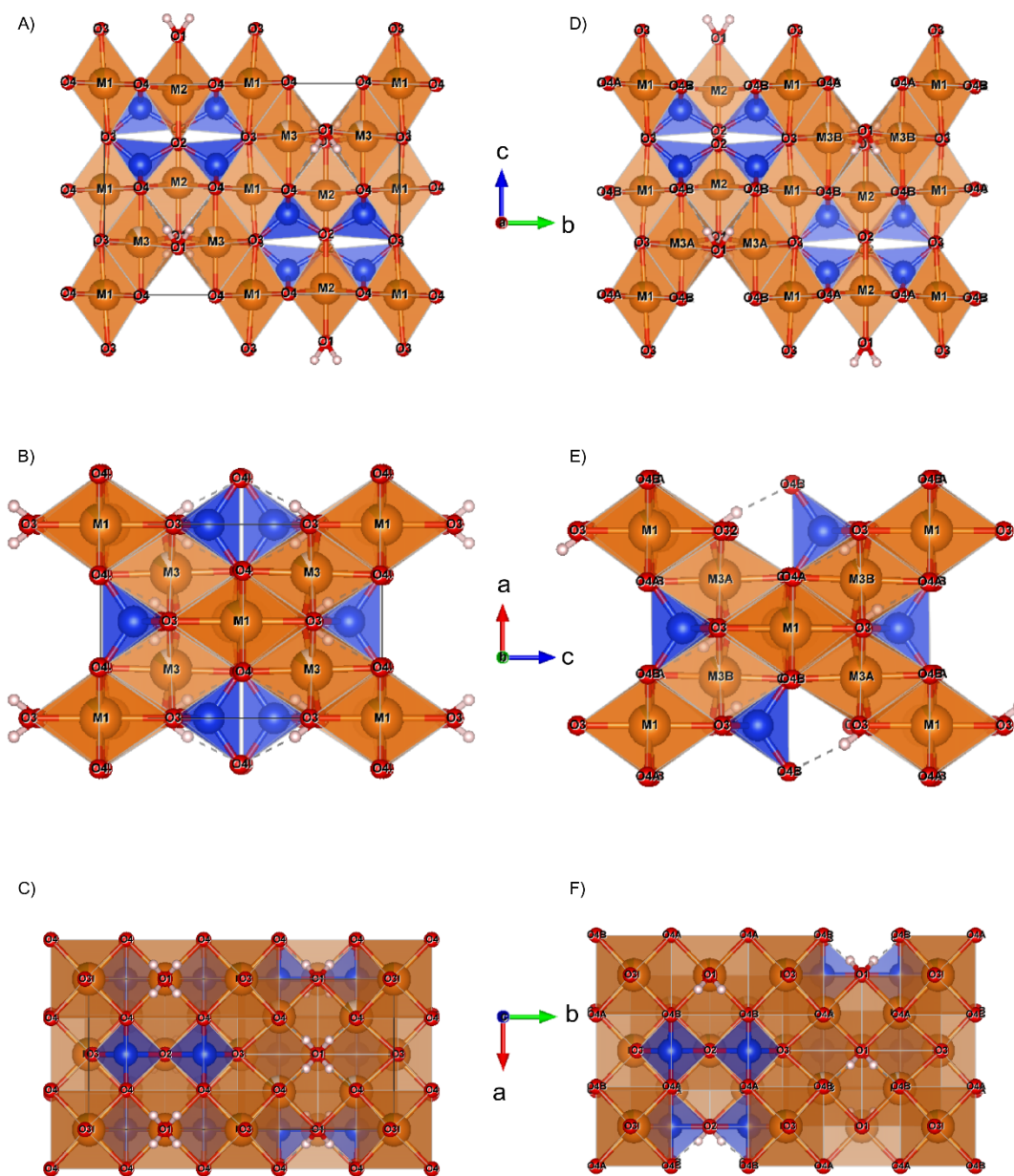


Figure S1. Crystal structure of wadsleyite, including orthorhombic ($Imma$) symmetry (A, B, C) and monoclinic ($I2/m$) symmetry (D, E, and F). Oxygen atoms are denoted by red spheres, magnesium and iron by orange spheres, silicon by blue spheres, and hydrogen by white spheres. Hydrogen positions are from Purevjav et al. (2016). Figures were made using VESTA (Momma and Izumi 2011).

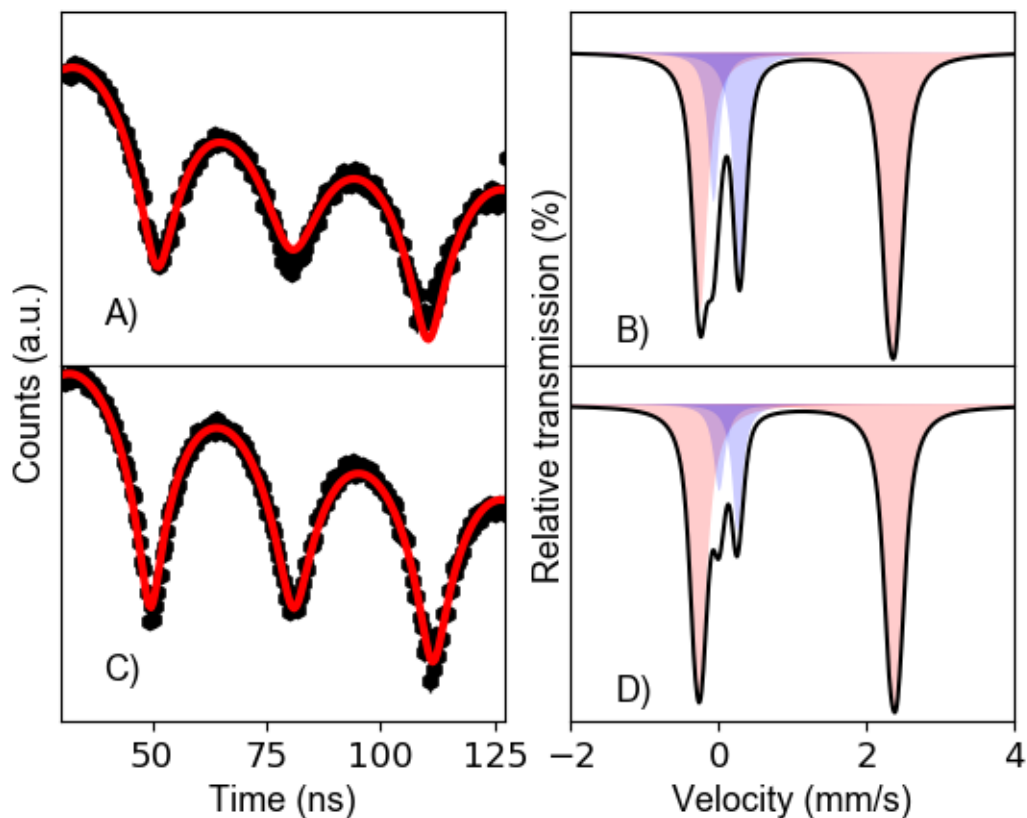


Figure S2. Time-domain synchrotron Mössbauer spectrum for Z0570 (A) and the energy domain spectrum of the best-fit hyperfine model parameters (B). The blue- and pink-shaded doublets correspond to Fe³⁺ and Fe²⁺ sites, respectively. The fit ratio of these doublets provides the $\text{Fe}^{3+}/\square\text{Fe} = 0.247(11)$ for this sample. Time-domain synchrotron Mössbauer spectrum for Z0902 (C) and energy domain spectrum of the best-fit hyperfine model parameters (D). The blue- and pink-shaded doublets correspond to Fe³⁺ and Fe²⁺ sites, respectively, providing a value of $\text{Fe}^{3+}/\square\text{Fe} = 0.128(10)$.

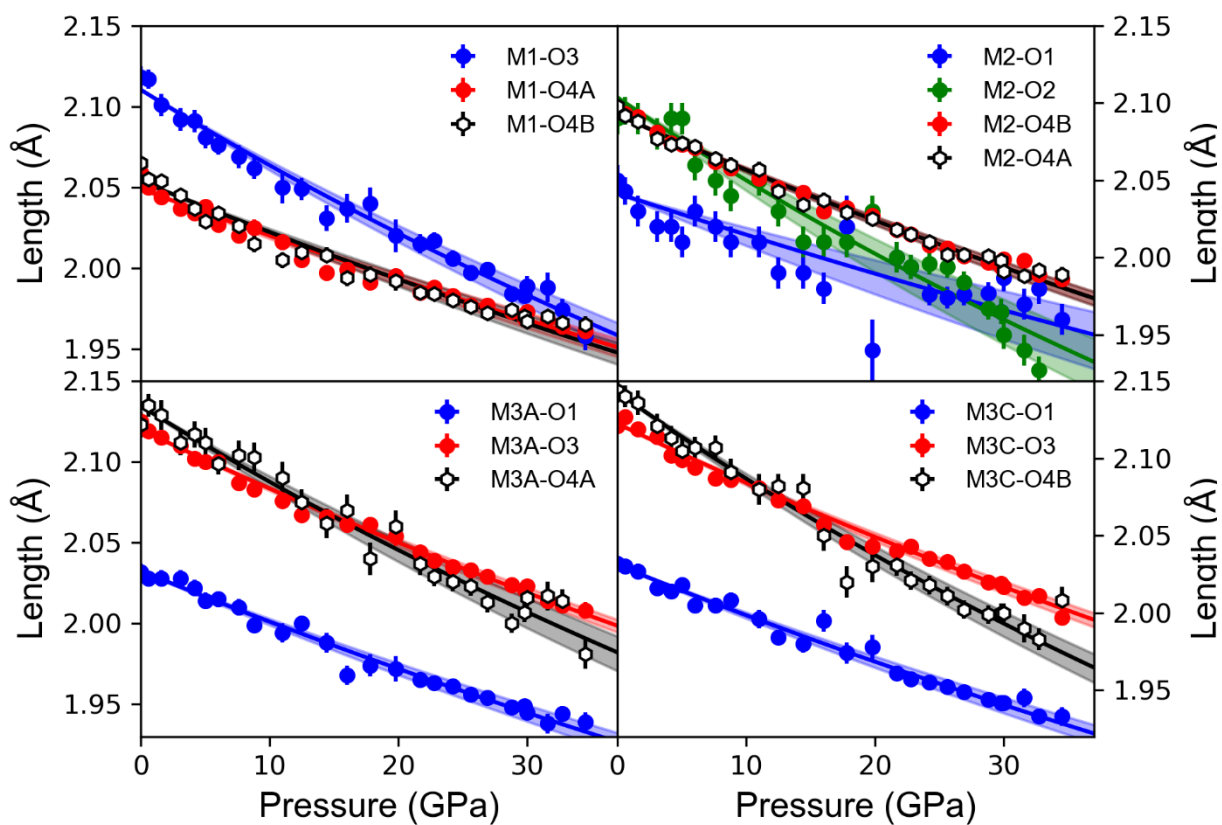


Figure S3. Bond length versus pressure in slightly hydrous wadsleyite (Z0902). The lines show the second-order BM-EOS fit.

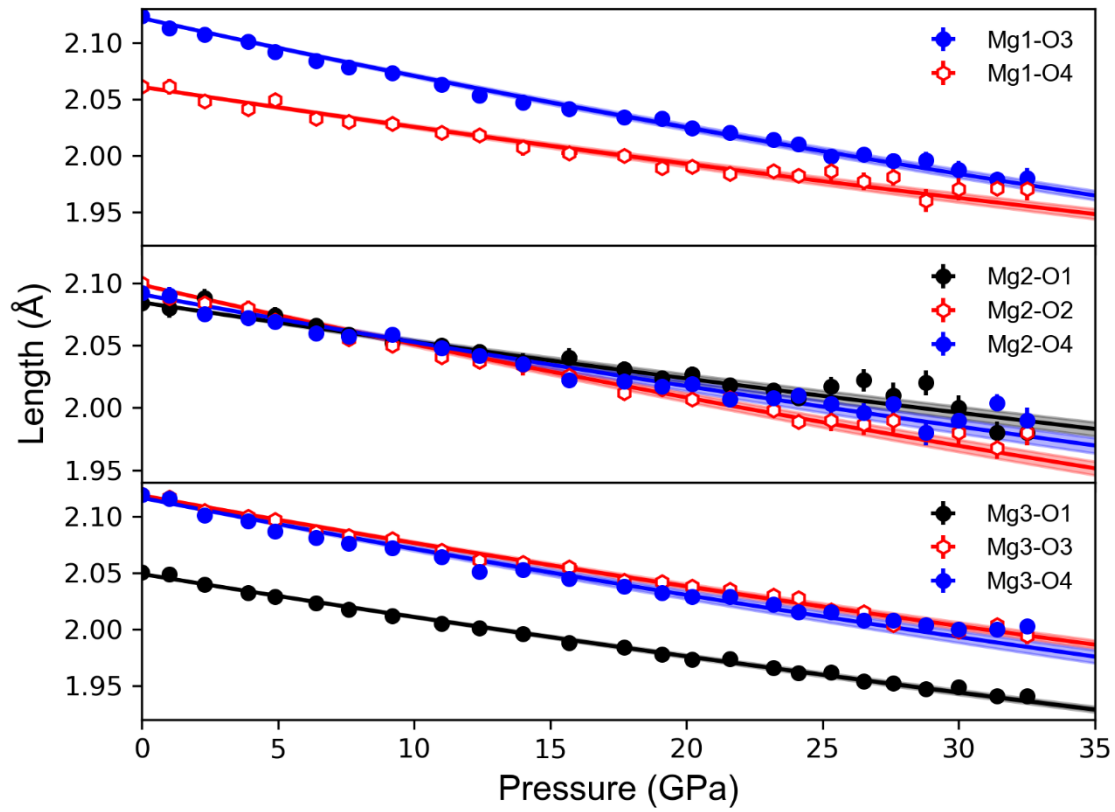


Figure S4. Bond length versus pressure in very hydrous wadsleyite (Z0570). The lines show second-order BM EOS fit to each M–O bond length and the shaded regions show the 95% prediction band .

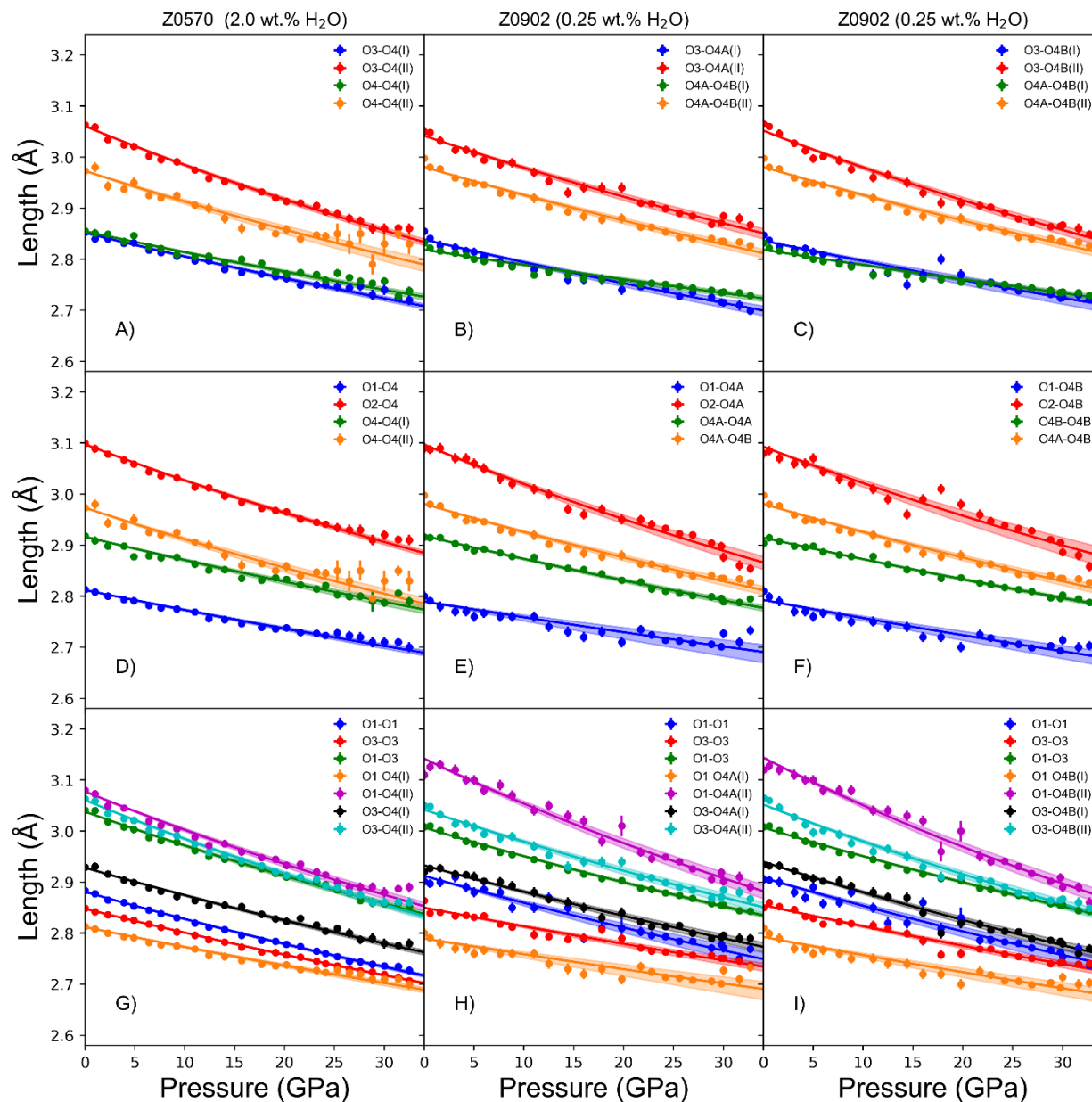


Figure S5. O–O distance versus pressure in very hydrous wadsleyite around the M1 site (A), M2 site (D) and M3 site (G) and slightly hydrous wadsleyite around the M1 site with O4A oxygen site (B), M1 site with O4B oxygen site (C), M2 site with O4A oxygen site (E), M2 site with O4B oxygen site (F), M3A site (H) and M3C site (I). The lines show second-order BM-EOS fit and the shaded regions show the 95% prediction band.

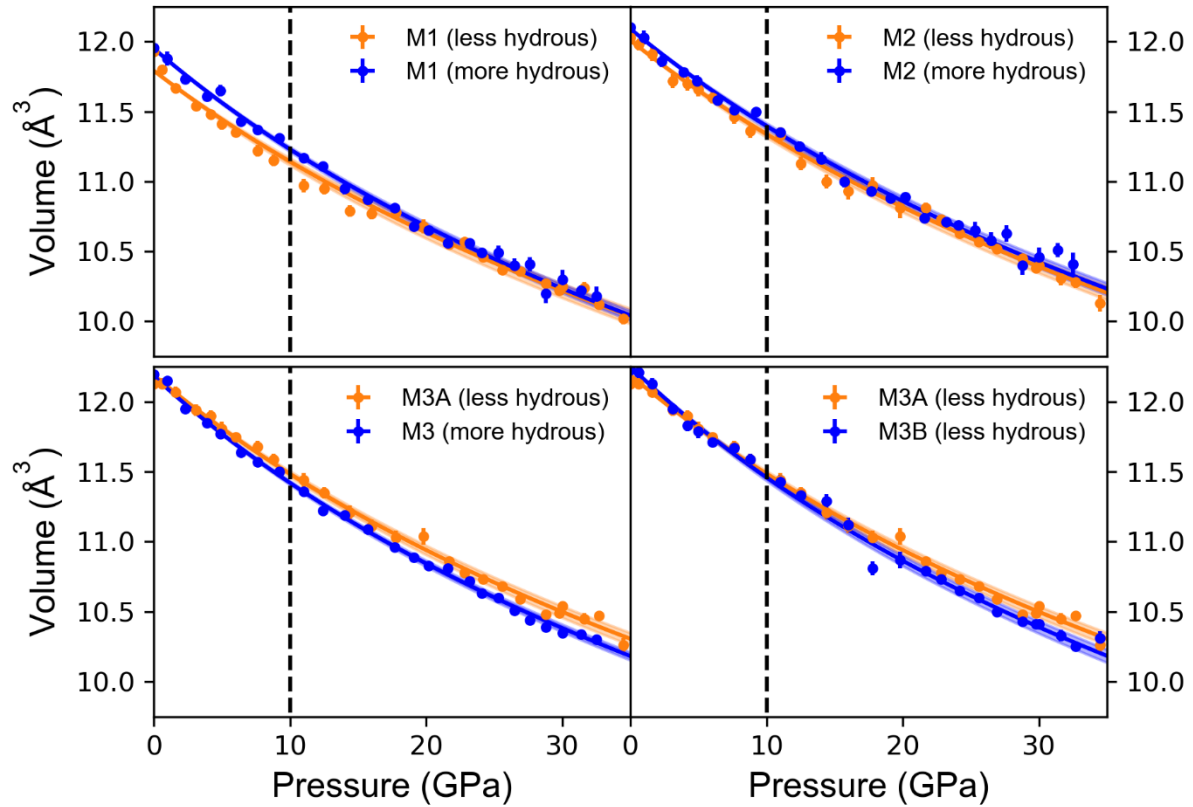


Figure S6. Octahedral volume versus pressure of the M1, M2 and M3 sites of very hydrous wadsleyite and M1, M2, M3A and M3B sites of slightly hydrous wadsleyite. The lines show the fit second-order BM-EOS and the shaded regions show the 95% prediction band.

Table S1. Crystal structure refinement data for wadsleyite (Z0902).

Pressure (GPa)	Measured reflections	R ₁	wR ₂	GoF (F2)	Theta full	h index	k index	l index	R _I [I > 2σ (I)]	R _I (all)
0.0001	922	0.0544	0.2084	1.085	15.094	-6<h<10	-13<k<15	-9<l<5	0.0543	0.0706
0.6(1)	922	0.0515	0.1557	1.075	15.094	-5<h<6	-19<k<10	-4<l<7	0.0514	0.0655
1.6(1)	911	0.0687	0.2004	1.095	15.094	-5<h<6	-19<k<10	-4<l<7	0.0686	0.0808
3.1(1)	905	0.0738	0.1906	1.055	15.094	-5<h<6	-19<k<10	-4<l<7	0.0737	0.0902
4.2(1)	901	0.0711	0.2035	1.044	15.094	-6<h<5	-19<k<10	-7<l<4	0.0710	0.0828
5.0(1)	890	0.097	0.2402	1.082	15.094	-6<h<5	-10<k<19	-4<l<7	0.0970	0.1095
6.0(1)	887	0.0598	0.1659	1.1	15.094	-5<h<6	-19<k<10	-4<l<6	0.0597	0.0770
7.6(1)	870	0.069	0.2094	1.116	15.094	-5<h<6	-19<k<9	-4<l<6	0.0690	0.0821
8.8(1)	843	0.0739	0.2096	1.101	15.094	-5<h<6	-10<k<18	-6<l<4	0.0739	0.0865
11.0(1)	837	0.0685	0.2132	1.041	15.094	-5<h<6	-10<k<18	-6<l<4	0.0684	0.0814
12.5(1)	826	0.0628	0.1847	1.019	15.094	-5<h<5	-18<k<10	-6<l<4	0.0627	0.0808
14.4(1)	796	0.0708	0.2061	1.052	15.094	-5<h<5	-18<k<10	-4<l<6	0.0708	0.0882
16.0(1)	782	0.0589	0.1992	1.019	15.094	-5<h<5	-10<k<18	-6<l<4	0.0588	0.0836
17.8(2)	744	0.0903	0.2385	0.977	15.094	-5<h<5	-10<k<18	-4<l<6	0.0902	0.1181
19.8(2)	724	0.0877	0.2414	0.965	15.094	-5<h<5	-10<k<18	-4<l<6	0.0877	0.1136
21.7(1)	816	0.04	0.1108	0.797	15.094	-5<h<5	-10<k<18	-4<l<6	0.0400	0.0508
22.8(1)	807	0.0393	0.1141	0.966	15.094	-5<h<5	-18<k<10	-6<l<4	0.0392	0.0518
24.2(2)	808	0.0421	0.1181	1.021	15.094	-5<h<5	-18<k<10	-4<l<6	0.0421	0.0527
25.6(1)	804	0.0434	0.1183	0.986	15.094	-5<h<5	-18<k<10	-4<l<6	0.0434	0.0542
26.9(2)	800	0.0403	0.1118	1.031	15.094	-5<h<5	-18<k<10	-6<l<4	0.0403	0.0493
28.8(2)	799	0.0392	0.1177	1.067	15.094	-5<h<5	-18<k<10	-6<l<4	0.0391	0.0503
29.8(1)	786	0.0437	0.1199	1.073	15.094	-5<h<5	-18<k<10	-4<l<6	0.0437	0.0564
30.0(1)	819	0.0345	0.1171	1.126	15.094	-6<h<9	-18<k<12	-8<l<5	0.0344	0.0587
31.6(1)	817	0.0524	0.1913	1.144	15.094	-6<h<9	-18<k<12	-8<l<5	0.0524	0.0771
32.7(1)	812	0.0526	0.1753	1.094	15.094	-9<h<6	-18<k<12	-5<l<8	0.0526	0.0813
34.5(1)	810	0.0771	0.289	1.348	15.094	-9<h<6	-18<k<12	-5<l<8	0.0770	0.1092

Table S2. Crystal structure refinement data for wadsleyite (Z0570).

Pressure (GPa)	Measured reflections	R1	wR2	GoF (F2)	Theta full	h index	k index	l index	R ₁ [I > 2σ(I)]	R ₁ (all)
0.0001	5399	0.0295	0.0822	1.146	15.094	-10<h<9	-20<k<20	-14<l<14	0.0295	0.0306
1.0(1)	374	0.0543	0.115	1.205	15.094	-5<h<3	-12<k<13	-10<l<9	0.0543	0.0705
2.3(1)	898	0.0586	0.1757	1.179	15.094	-3<h<5	-13<k<19	-14<l<10	0.0585	0.0907
3.9(2)	898	0.0549	0.1718	1.124	15.094	-5<h<3	-19<k<13	-14<l<10	0.0549	0.0868
4.9(1)	897	0.0659	0.229	1.134	15.094	-3<h<5	-13<k<19	-14<l<9	0.0658	0.1068
6.4(1)	885	0.0484	0.1557	1.048	15.094	-3<h<5	-12<k<19	-14<l<9	0.0483	0.0826
7.6(2)	882	0.0484	0.1513	1.138	15.094	-5<h<3	-12<k<19	-9<l<14	0.0484	0.0780
9.2(2)	873	0.0496	0.1395	1.211	15.094	-5<h<3	-12<k<19	-9<l<14	0.0495	0.0893
11.0(1)	858	0.0578	0.126	1.118	15.094	-5<h<3	-12<k<19	-10<l<13	0.0578	0.1048
12.4(1)	349	0.0456	0.1175	1.048	15.094	-4<h<3	-12<k<13	-10<l<9	0.0456	0.0537
14.0(2)	348	0.0547	0.1521	1.122	15.094	-3<h<4	-12<k<13	-9<l<10	0.0546	0.0650
15.7(3)	341	0.0593	0.1536	1.049	15.094	-4<h<3	-12<k<13	-9<l<9	0.0592	0.0649
17.7(2)	828	0.0647	0.1851	1.144	15.094	-3<h<5	-12<k<19	-13<l<9	0.0646	0.1132
19.1(2)	830	0.0614	0.1607	1.009	15.094	-5<h<3	-12<k<19	-9<l<13	0.0613	0.1318
20.2(2)	824	0.0782	0.1886	1.133	15.094	-3<h<5	-19<k<12	-9<l<13	0.0781	0.1347
21.6(2)	337	0.0377	0.1017	1.118	15.094	-4<h<3	-13<k<12	-9<l<9	0.0376	0.0480
23.2(1)	802	0.0532	0.1153	0.983	15.094	-3<h<5	-18<k<12	-9<l<13	0.0532	0.1035
24.1(1)	806	0.0637	0.1716	1.173	15.094	-5<h<3	-18<k<12	-13<l<9	0.0637	0.1131
25.3(2)	327	0.0492	0.1328	1.037	15.094	-4<h<3	-12<k<13	-9<l<9	0.0491	0.0626
26.5(2)	326	0.0639	0.1735	1.057	15.094	-4<h<3	-12<k<13	-9<l<9	0.0639	0.0811
27.6(2)	314	0.0871	0.1984	1.016	15.094	-4<h<3	-12<k<12	-9<l<9	0.0871	0.0984
28.8(2)	315	0.0761	0.1888	1.04	15.094	-4<h<3	-12<k<12	-9<l<9	0.0761	0.0893
30.0(2)	310	0.0741	0.1732	1.008	15.094	-3<h<4	-12<k<12	-9<l<9	0.0741	0.0936
31.4(1)	750	0.0904	0.2725	0.993	15.094	-5<h<3	-12<k<18	-9<l<13	0.0903	0.1677
32.5(1)	289	0.0841	0.2132	1.039	15.094	-4<h<3	-12<k<12	-9<l<9	0.0841	0.1056

Table S3. Lattice parameters of monoclinic wadsleyite (Z5070) as a function of pressure. Values in parentheses are uncertainties on the last digit.

Pressure (GPa)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β angle (°)	<i>V</i> (Å ³)
Monoclinic symmetry					
0.0001	5.6965(2)	11.5431(4)	8.269(3)	90.01(3)	543.7(2)
1.0(1)	5.681(1)	11.5167(7)	8.2495(4)	90.006(7)	539.8(1)
2.3(1)	5.6687(9)	11.4917(7)	8.2246(4)	90.004(6)	535.78(9)
3.9(2)	5.655(1)	11.4625(7)	8.1950(5)	90.003(8)	531.2(1)
4.9(1)	5.645(1)	11.4417(8)	8.1750(5)	90.005(8)	528.0(1)
6.4(1)	5.633(3)	11.405(2)	8.1473(1)	90.00(2)	523.4(3)
7.6(2)	5.620(1)	11.3894(8)	8.1278(5)	90.009(8)	520.2(1)
9.2(2)	5.608(1)	11.3630(8)	8.1026(5)	90.002(9)	516.3(1)
11.0(1)	5.589(1)	11.3337(9)	8.0762(6)	90.03(1)	511.6(1)
12.4(1)	5.573(2)	11.312(2)	8.0600(9)	90.08(1)	508.1(2)
14.0(2)	5.565(1)	11.2901(9)	8.0398(5)	90.050(9)	505.1(1)
15.7(3)	5.552(2)	11.264(1)	8.0187(6)	90.05(1)	501.4(2)
17.7(2)	5.533(1)	11.2377(9)	7.9962(6)	90.076(9)	497.2(1)
19.1(2)	5.524(1)	11.2206(9)	7.981(5)	90.075(9)	494.7(3)
20.2(2)	5.518(2)	11.207(1)	7.9665(6)	90.06(1)	492.6(1)
21.6(2)	5.504(1)	11.188(1)	7.9521(7)	90.07(1)	489.6(1)
23.2(1)	5.488(3)	11.165(2)	7.936(1)	90.11(2)	486.2(3)
24.1(1)	5.486(3)	11.150(2)	7.921(1)	90.12(2)	484.5(3)
25.3(2)	5.465(3)	11.146(2)	7.912(1)	90.13(2)	482.0(3)
26.5(2)	5.457(3)	11.123(2)	7.905(1)	90.13(2)	479.8(3)
27.6(2)	5.446(5)	11.118(3)	7.888(2)	90.13(3)	477.6(5)
28.8(2)	5.447(3)	11.101(2)	7.874(1)	90.15(2)	476.1(3)
30.0(2)	5.436(4)	11.083(2)	7.867(1)	90.11(2)	474.0(4)
31.4(1)	5.426(5)	11.069(4)	7.849(2)	90.14(3)	471.4(5)
32.5(1)	5.418(4)	11.063(3)	7.836(1)	90.09(2)	469.7(4)

Table S4. Lattice parameters of orthorhombic wadsleyite (Z5070) as a function of pressure. The β angles in this table have been fixed at 90° and therefore this table does not reflect the best-fit structure refinement parameters from this study. Values in parentheses are uncertainties on the last digit.

Pressure (GPa)	a (Å)	b (Å)	c (Å)	β angle (°)	V (Å ³)
Orthorhombic symmetry					
0.0001	5.6938(6)	11.543(1)	8.2681(8)	90	543.39(9)
1.0(1)	5.681(1)	11.5168(6)	8.2494(4)	90	539.8(1)
2.3(1)	5.6686(9)	11.4917(7)	8.2245(4)	90	535.76(9)
3.9(2)	5.656(1)	11.462(1)	8.1946(5)	90	531.3(1)
4.9(1)	5.648(1)	11.444(1)	8.1737(6)	90	528.3(1)
6.4(1)	5.633(2)	11.405(2)	8.147(1)	90	523.4(2)
7.6(2)	5.620(1)	11.3893(8)	8.1276(5)	90	520.2(1)
9.2(2)	5.602(6)	11.366(4)	8.108(3)	90	516.3(6)
11.0(1)	5.589(3)	11.334(2)	8.078(1)	90	511.7(3)
12.4(1)	5.573(2)	11.313(2)	8.0591(9)	90	508.1(2)
14.0(2)	5.563(1)	11.290(1)	8.0397(6)	90	505.0(1)
15.7(3)	5.545(3)	11.267(2)	8.019(1)	90	501.0(3)
17.7(2)	5.525(3)	11.243(2)	7.994(1)	90	496.6(3)
19.1(2)	5.522(1)	11.220(1)	7.9799(6)	90	494.4(1)
20.2(2)	5.513(2)	11.205(1)	7.9679(6)	90	492.2(1)
21.6(2)	5.505(1)	11.188(1)	7.9513(7)	90	489.7(1)
23.2(1)	5.488(3)	11.165(2)	7.934(1)	90	486.2(3)
24.1(1)	5.478(3)	11.159(2)	7.923(1)	90	484.3(3)
25.3(2)	5.472(5)	11.149(3)	7.912(2)	90	482.7(5)
26.5(2)	5.459(2)	11.124(1)	7.8996(9)	90	479.7(2)
27.6(2)	5.452(2)	11.112(1)	7.8889(9)	90	477.9(2)
28.8(2)	5.448(3)	11.097(2)	7.876(1)	90	476.2(3)
30.0(2)	5.437(2)	11.085(2)	7.8614(9)	90	473.8(2)
31.4(1)	5.428(2)	11.066(1)	7.8492(8)	90	471.4(2)
32.5(1)	5.413(5)	11.054(4)	7.840(2)	90	469.1(5)

Table S5. Lattice parameters of monoclinic wadsleyite (Z0902) as a function of pressure. Values in parentheses are uncertainties on the last digit.

Pressure (GPa)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β angle (°)	<i>V</i> (Å ³)
Monoclinic symmetry					
0.0001	5.7119(5)	11.4785(5)	8.282(2)	90.03(2)	543.0(1)
0.6(1)	5.696(2)	11.469(1)	8.281(6)	90.11(4)	541.0(4)
1.6(1)	5.692(1)	11.449(1)	8.256(5)	90.05(4)	538.0(4)
3.1(1)	5.6786(6)	11.4197(6)	8.228(3)	90.04(2)	533.6(2)
4.2(1)	5.666(1)	11.400(1)	8.219(4)	90.05(3)	530.9(3)
5.0(1)	5.6597(8)	11.3842(8)	8.210(3)	90.03(2)	529.0(2)
6.0(1)	5.6506(8)	11.3676(7)	8.184(3)	90.04(2)	525.7(2)
7.6(1)	5.639(1)	11.342(1)	8.166(6)	90.02(4)	522.2(4)
8.8(1)	5.6302(6)	11.3201(6)	8.132(3)	90.01(2)	518.3(2)
11.0(1)	5.6108(6)	11.2867(6)	8.090(2)	90.08(2)	512.3(1)
12.5(1)	5.6006(6)	11.2661(6)	8.070(3)	90.07(2)	509.2(2)
14.4(1)	5.5863(6)	11.2390(6)	8.038(3)	90.09(2)	504.7(2)
16.0(1)	5.5749(6)	11.2186(6)	8.018(3)	90.11(2)	501.5(2)
17.8(2)	5.5627(6)	11.1974(6)	7.991(3)	90.14(2)	497.7(2)
19.8(2)	5.5504(5)	11.1730(5)	7.966(2)	90.16(2)	494.0(1)
21.7(1)	5.5380(6)	11.1524(6)	7.936(3)	90.22(2)	490.1(2)
22.8(1)	5.5318(6)	11.1396(5)	7.921(3)	90.24(2)	488.1(2)
24.2(2)	5.5207(5)	11.1252(4)	7.900(2)	90.30(2)	485.2(1)
25.6(1)	5.5135(5)	11.1098(4)	7.885(2)	90.28(1)	483.0(1)
26.9(2)	5.5065(6)	11.0959(5)	7.868(3)	90.30(2)	480.7(2)
28.8(2)	5.4955(5)	11.0720(5)	7.836(2)	90.39(1)	476.8(1)
29.8(1)	5.4923(5)	11.0585(6)	7.821(2)	90.38(2)	475.0(1)
30.0(1)	5.4912(5)	11.0585(8)	7.821(2)	90.38(2)	474.9(1)
31.6(1)	5.4822(6)	11.0472(7)	7.796(3)	90.48(2)	472.1(2)
32.7(1)	5.4761(6)	11.0381(8)	7.790(3)	90.48(2)	470.9(2)
34.5(1)	5.4665(6)	11.0228(8)	7.764(3)	90.53(2)	467.8(2)

Table S6. Lattice parameters of orthorhombic wadsleyite (Z0902) as a function of pressure. The β angles in this table have been fixed at 90° and therefore this table does not reflect the best-fit structure refinement parameters from this study. Values in parentheses are uncertainties on the last digit.

Pressure (GPa)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β angle (°)	<i>V</i> (Å ³)
Orthorhombic symmetry					
0.0001	5.7106(6)	11.4766(7)	8.280(2)	90	542.6(1)
0.6(1)	5.7000(6)	11.4652(8)	8.294(2)	90	542.0(1)
1.6(1)	5.6933(7)	11.447(1)	8.262(3)	90	538.5(2)
3.1(1)	5.677(1)	11.424(1)	8.250(4)	90	535.0(3)
4.2(1)	5.6675(6)	11.3995(9)	8.225(2)	90	531.4(1)
5.0(1)	5.6605(6)	11.385(1)	8.217(3)	90	529.5(2)
6.0(1)	5.654(1)	11.367(2)	8.194(5)	90	526.6(4)
7.6(1)	5.6381(8)	11.342(1)	8.164(3)	90	522.1(2)
8.8(1)	5.635(1)	11.321(2)	8.139(5)	90	519.2(4)
11.0(1)	5.6124(4)	11.2860(7)	8.097(2)	90	512.8(1)
12.5(1)	5.6023(4)	11.2650(5)	8.078(2)	90	509.8(1)
14.4(1)	5.5885(3)	11.2380(5)	8.049(2)	90	505.5(1)
16.0(1)	5.576(1)	11.219(2)	8.036(5)	90	502.7(3)
17.8(2)	5.5656(4)	11.1957(6)	8.014(2)	90	499.4(1)
19.8(2)	5.5546(4)	11.1699(7)	7.987(2)	90	495.5(1)
21.7(1)	5.5436(4)	11.1497(5)	7.961(2)	90	492.1(1)
22.8(1)	5.5379(4)	11.1367(5)	7.949(2)	90	490.2(1)
24.2(2)	5.5290(4)	11.1213(5)	7.932(2)	90	487.8(1)
25.6(1)	5.520(1)	11.107(1)	7.918(5)	90	485.5(3)
26.9(2)	5.513(1)	11.090(1)	7.906(5)	90	483.4(3)
28.8(2)	5.507(1)	11.060(2)	7.885(5)	90	480.2(3)
29.8(1)	5.499(1)	11.062(2)	7.873(5)	90	478.9(3)
30.0(1)	5.4991(5)	11.0564(8)	7.864(2)	90	478.1(1)
31.6(1)	5.4918(5)	11.0455(8)	7.848(2)	90	476.1(1)
32.7(1)	5.4850(6)	11.0359(9)	7.843(2)	90	474.8(1)
34.5(1)	5.478(1)	11.019(2)	7.812(4)	90	471.6(3)

Table S7. EOS parameters for both compositions in both settings.

Sample	symmetry	$V_0(\text{\AA}^3)$	$K_{T0}(\text{GPa})$	K_{T0}'
Z0570	orthorhombic	543.19(23)	164.0(2.7)	4.26(23)
Z0902	monoclinic	543.09(22)	172.3(2.3)	3.91(15)
Z0570	monoclinic	543.27(22)	162.0(2.4)	4.49(18)
Z0902	orthorhombic	543.75(29)	164.7(3.3)	5.51(27)

Table S8. Linear moduli in GPa of wadsleyite with 2.0 wt% water (Z0570) and with 0.2 wt% water (Z0902).

Sample	Linear moduli (GPa)			Axial compressibility (GPa^{-1})		
	a -axis	b -axis	c -axis	β_a	β_b	β_c
Z0570	494(6)	559(4)	446(11)	$2.02(1) \times 10^{-3}$	$1.78(1) \times 10^{-3}$	$2.24(1) \times 10^{-3}$
Z0902	619(5)	667(7)	356(6)	$1.61(1) \times 10^{-3}$	$1.49(2) \times 10^{-3}$	$2.80(4) \times 10^{-3}$

Table S9. Compressibilities (GPa^{-1}) of M–O bonds in Fe-bearing wadsleyite with 2.0 wt% water (Z0570) and with 0.25 wt% water (Z0902).

	Z0570	Z0902
M1 octahedron		
M1–O3	0.002233(44)	0.00314(12)
M1–O4A	0.001627(37)	0.00175(5)
M1–O4B		0.00193(7)
M2 octahedron		
M2–O1	0.001404(39)	0.00165(21)
M2–O2	0.002095(54)	0.0040(4)
M2–O4A	0.001749(45)	0.00221(7)
M2–O4B		0.00220(6)
M3A octahedron		
M3–O1	0.001793(29)	0.00196(7)
M3–O3	0.001891(34)	0.00224(5)
M3–O4A(B)	0.001980(55)	0.00313(15)
M3C octahedron		
M3–O1		0.00203(7)
M3–O3		0.00239(6)
M3–O4A(B)		0.00383(17)

Table S10. Volume and selected bond distances in M1O₆ octahedra versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0902)

Pressure (GPa)	M1 Poly. Vol. (Å ³)	M1–O3 (Å)	M1–O4A (Å)	M1–O4B (Å)
0.0001	11.93(4)	2.118(7)	2.059(4)	2.065(4)
0.6(1)	11.80(3)	2.117(6)	2.050(3)	2.055(3)
1.6(1)	11.67(3)	2.101(7)	2.044(4)	2.054(4)
3.1(1)	11.54(3)	2.092(7)	2.037(4)	2.045(4)
4.2(1)	11.48(3)	2.091(7)	2.034(4)	2.037(4)
5.0(1)	11.41(4)	2.081(7)	2.038(4)	2.029(4)
6.0(1)	11.35(3)	2.076(6)	2.027(4)	2.034(3)
7.6(1)	11.22(4)	2.069(7)	2.020(4)	2.026(4)
8.8(1)	11.15(4)	2.062(7)	2.025(5)	2.015(5)
11.0(1)	10.97(5)	2.05(1)	2.016(5)	2.005(5)
12.5(1)	10.95(4)	2.049(7)	2.005(4)	2.010(4)
14.4(1)	10.79(4)	2.031(8)	1.997(5)	2.008(5)
16.0(1)	10.77(4)	2.037(9)	1.999(5)	1.994(5)
17.8(2)	10.78(5)	2.04(1)	1.991(5)	1.996(5)
19.8(2)	10.68(5)	2.02(1)	1.995(5)	1.992(6)
21.7(1)	10.55(3)	2.015(6)	1.985(4)	1.985(4)
22.8(1)	10.57(2)	2.017(5)	1.988(3)	1.984(3)
24.2(2)	10.46(2)	2.006(5)	1.983(3)	1.980(2)
25.6(1)	10.37(2)	1.997(5)	1.977(3)	1.976(2)
26.9(2)	10.36(2)	1.999(5)	1.977(3)	1.972(3)
28.8(2)	10.27(2)	1.984(5)	1.973(3)	1.974(2)
29.8(1)	10.22(2)	1.983(5)	1.969(3)	1.970(3)
30.0(1)	10.25(3)	1.989(6)	1.973(3)	1.967(3)
31.6(1)	10.24(4)	1.988(9)	1.968(4)	1.970(4)
32.7(1)	10.12(3)	1.974(7)	1.964(4)	1.966(4)
34.5(1)	10.02(4)	1.958(9)	1.961(5)	1.965(5)

Table S11. Volume and selected bond distances in M₂O₆ octahedra versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0902)

Pressure (GPa)	M2 Poly. Vol. (Å ³)	M2–O1 (Å)	M2–O2 (Å)	M2–O4A (Å)	M2–O4B (Å)
0.0001	12.03(5)	2.05(1)	2.09(1)	2.098(4)	2.095(4)
0.6(1)	11.98(4)	2.043(9)	2.095(9)	2.092(3)	2.093(3)
1.6(1)	11.91(5)	2.03(1)	2.09(1)	2.088(4)	2.091(4)
3.1(1)	11.72(5)	2.02(1)	2.08(1)	2.077(4)	2.081(4)
4.2(1)	11.70(5)	2.02(1)	2.09(1)	2.073(4)	2.074(4)
5.0(1)	11.66(5)	2.01(1)	2.09(1)	2.074(4)	2.073(4)
6.0(1)	11.60(4)	2.03(1)	2.06(1)	2.072(4)	2.071(3)
7.6(1)	11.46(5)	2.02(1)	2.05(1)	2.064(4)	2.062(4)
8.8(1)	11.36(5)	2.01(1)	2.04(1)	2.060(5)	2.058(5)
11.0(1)	11.33(6)	2.01(1)	2.05(1)	2.057(5)	2.051(5)
12.5(1)	11.13(5)	1.99(1)	2.03(1)	2.043(4)	2.045(4)
14.4(1)	11.00(5)	1.99(1)	2.01(1)	2.034(5)	2.042(5)
16.0(1)	10.93(6)	1.98(1)	2.01(1)	2.037(5)	2.030(5)
17.8(2)	10.97(6)	2.02(2)	2.01(1)	2.029(5)	2.032(5)
19.8(2)	10.81(7)	1.94(2)	2.03(1)	2.025(5)	2.027(6)
21.7(1)	10.81(4)	2.00(1)	2.00(1)	2.018(4)	2.018(4)
22.8(1)	10.73(3)	1.994(8)	1.994(8)	2.015(3)	2.015(3)
24.2(2)	10.63(3)	1.976(7)	1.996(7)	2.010(3)	2.008(2)
25.6(1)	10.57(3)	1.974(7)	1.994(7)	2.002(3)	2.006(2)
26.9(2)	10.52(3)	1.976(7)	1.984(7)	2.002(3)	2.001(3)
28.8(2)	10.45(3)	1.977(7)	1.967(7)	2.001(3)	1.997(2)
29.8(1)	10.38(3)	1.965(8)	1.965(8)	1.998(3)	1.994(3)
30.0(1)	10.40(4)	1.987(9)	1.950(9)	1.991(3)	1.999(3)
31.6(1)	10.31(5)	1.97(1)	1.94(1)	1.988(4)	1.998(4)
32.7(1)	10.28(4)	1.98(1)	1.927(9)	1.992(4)	1.989(4)
34.5(1)	10.13(6)	1.96(1)	1.90(1)	1.989(5)	2.986(5)

Table S12. Volume and selected bond distances in M3AO₆ octahedra versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0902)

Pressure (GPa)	M3A Poly. Vol. (Å ³)	M3A–O1 (Å)	M3A–O3 (Å)	M3A–O4A (Å)
0.0001	12.13(4)	2.032(5)	2.125(4)	2.123(8)
0.6(1)	12.13(4)	2.028(4)	2.119(3)	2.135(7)
1.6(1)	12.07(4)	2.028(5)	2.115(3)	2.129(9)
3.1(1)	11.94(4)	2.028(5)	2.110(3)	2.112(8)
4.2(1)	11.90(4)	2.022(5)	2.102(4)	2.117(8)
5.0(1)	11.81(5)	2.014(5)	2.100(4)	2.112(9)
6.0(1)	11.75(3)	2.015(5)	2.100(3)	2.099(7)
7.6(1)	11.68(4)	2.010(5)	2.087(4)	2.104(9)
8.8(1)	11.59(4)	1.999(5)	2.083(4)	2.103(9)
11.0(1)	11.44(5)	1.994(6)	2.076(5)	2.09(1)
12.5(1)	11.35(4)	2.000(5)	2.067(4)	2.075(8)
14.4(1)	11.21(5)	1.988(6)	2.066(5)	2.062(9)
16.0(1)	11.11(5)	1.968(6)	2.061(5)	2.07(1)
17.8(2)	11.03(5)	1.974(7)	2.061(5)	2.04(1)
19.8(2)	11.04(6)	1.972(8)	2.054(6)	2.06(1)
21.7(1)	10.86(3)	1.965(5)	2.044(3)	2.037(7)
22.8(1)	10.78(3)	1.963(4)	2.039(2)	2.029(6)
24.2(2)	10.73(3)	1.961(4)	2.035(2)	2.026(6)
25.6(1)	10.68(3)	1.956(4)	2.033(2)	2.023(6)
26.9(2)	10.59(3)	1.954(4)	2.029(2)	2.013(6)
28.8(2)	10.48(3)	1.948(3)	2.024(2)	2.000(6)
29.8(1)	10.49(3)	1.949(4)	2.021(2)	2.007(6)
30.0(1)	10.54(3)	1.945(4)	2.023(3)	2.016(6)
31.6(1)	10.45(4)	1.938(6)	2.014(4)	2.017(9)
32.7(1)	10.47(3)	1.944(5)	2.011(4)	2.014(7)
34.5(1)	10.26(5)	1.939(6)	2.008(5)	1.981(9)

Table S13. Volume and selected bond distances in M3CO₆ octahedra versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0902)

Pressure (GPa)	M3B Poly. Vol. (Å ³)	M3B–O1 (Å)	M3B–O3 (Å)	M3B–O4B (Å)
0.0001	12.23(4)	2.032(5)	2.121(4)	2.144(8)
0.6(1)	12.21(4)	2.030(4)	2.127(3)	2.140(7)
1.6(1)	12.13(4)	2.027(5)	2.119(4)	2.136(8)
3.1(1)	11.95(4)	2.016(5)	2.114(3)	2.121(8)
4.2(1)	11.83(4)	2.014(5)	2.102(4)	2.113(8)
5.0(1)	11.79(5)	2.018(5)	2.099(4)	2.105(9)
6.0(1)	11.71(3)	2.005(5)	2.094(3)	2.107(7)
7.6(1)	11.67(4)	2.005(5)	2.087(4)	2.107(8)
8.8(1)	11.59(4)	2.008(5)	2.086(4)	2.091(9)
11.0(1)	11.43(5)	1.996(6)	2.081(5)	2.08(1)
12.5(1)	11.33(4)	1.984(5)	2.073(4)	2.082(8)
14.4(1)	11.29(5)	1.980(6)	2.069(5)	2.081(9)
16.0(1)	11.12(5)	1.995(7)	2.057(5)	2.05(1)
17.8(2)	10.81(5)	1.974(7)	2.046(5)	2.02(1)
19.8(2)	10.87(6)	1.978(8)	2.043(6)	2.03(1)
21.7(1)	10.79(3)	1.961(5)	2.040(3)	2.031(7)
22.8(1)	10.73(3)	1.957(4)	2.043(2)	2.021(6)
24.2(2)	10.65(3)	1.955(4)	2.035(2)	2.018(6)
25.6(1)	10.60(3)	1.952(4)	2.033(2)	2.011(6)
26.9(2)	10.50(3)	1.949(4)	2.027(2)	2.002(6)
28.8(2)	10.43(3)	1.944(3)	2.020(2)	1.999(6)
29.8(1)	10.41(3)	1.942(4)	2.019(2)	2.000(6)
30.0(1)	10.41(3)	1.942(4)	2.017(3)	2.000(6)
31.6(1)	10.33(4)	1.945(6)	2.010(4)	1.990(9)
32.7(1)	10.25(3)	1.933(5)	2.011(4)	1.983(7)
34.5(1)	10.31(5)	1.933(6)	1.997(5)	2.008(9)

Table S14. Volume and selected bond distances in TO₄ tetrahedra versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0902)

Pressure (GPa)	T Poly. Vol. (Å ³)	Si–O2 (Å)	Si–O3 (Å)	Si–O4A (Å)	Si–O4B (Å)
0.0001	2.32(1)	1.713(6)	1.644(5)	1.640(6)	1.624(6)
0.6(1)	2.30(1)	1.709(5)	1.646(5)	1.632(5)	1.619(5)
1.6(1)	2.30(1)	1.703(5)	1.649(5)	1.632(6)	1.617(6)
3.1(1)	2.30(1)	1.703(5)	1.646(5)	1.639(6)	1.622(6)
4.2(1)	2.29(1)	1.695(5)	1.645(5)	1.632(6)	1.628(6)
5.0(1)	2.29(1)	1.696(6)	1.650(6)	1.620(7)	1.634(7)
6.0(1)	2.28(1)	1.699(5)	1.646(4)	1.631(5)	1.612(5)
7.6(1)	2.28(1)	1.696(7)	1.648(6)	1.628(7)	1.610(7)
8.8(1)	2.26(1)	1.692(6)	1.641(6)	1.601(7)	1.631(7)
11.0(1)	2.24(2)	1.682(6)	1.636(7)	1.600(8)	1.624(8)
12.5(1)	2.23(1)	1.684(5)	1.630(5)	1.623(6)	1.605(6)
14.4(1)	2.23(1)	1.690(6)	1.629(6)	1.624(7)	1.596(7)
16.0(1)	2.22(1)	1.682(7)	1.625(6)	1.596(7)	1.627(8)
17.8(2)	2.22(2)	1.666(7)	1.608(7)	1.620(8)	1.627(8)
19.8(2)	2.17(2)	1.664(7)	1.616(7)	1.596(8)	1.605(9)
21.7(1)	2.18(1)	1.668(5)	1.615(4)	1.597(5)	1.606(5)
22.8(1)	2.174(8)	1.669(4)	1.605(3)	1.602(4)	1.605(4)
24.2(2)	2.166(8)	1.667(4)	1.610(3)	1.599(4)	1.599(4)
25.6(1)	2.168(8)	1.666(4)	1.610(3)	1.600(4)	1.600(4)
26.9(2)	2.164(8)	1.664(4)	1.604(3)	1.600(4)	1.604(4)
28.8(2)	2.153(8)	1.665(4)	1.609(3)	1.595(4)	1.591(4)
29.8(1)	2.135(8)	1.658(4)	1.602(3)	1.591(4)	1.592(4)
30.0(1)	2.14(1)	1.668(5)	1.596(4)	1.583(5)	1.597(5)
31.6(1)	2.12(1)	1.667(6)	1.597(6)	1.576(6)	1.591(6)
32.7(1)	2.14(1)	1.675(5)	1.598(5)	1.579(5)	1.597(5)
34.5(1)	2.15(1)	1.695(7)	1.609(6)	1.590(8)	1.566(7)

Table S15. Volume and selected bond distances in M1O₆ octahedra versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0570)

Pressure (GPa)	M1 Poly. Vol. (Å ³)	M1–O3 (Å)	M1–O4A (Å)	M1–O4B (Å)
0.0001	11.957(5)	2.1239(9)	2.0611(5)	4.248(1)
1.0(1)	11.88(5)	2.113(6)	2.061(7)	4.226(8)
2.3(1)	11.73(3)	2.107(4)	2.048(5)	4.215(6)
3.9(2)	11.61(3)	2.101(3)	2.041(4)	4.202(5)
4.9(1)	11.65(4)	2.092(5)	2.049(5)	4.183(7)
6.4(1)	11.43(2)	2.084(2)	2.033(3)	4.168(3)
7.6(2)	11.37(2)	2.078(2)	2.030(3)	4.156(3)
9.2(2)	11.31(2)	2.073(3)	2.028(3)	4.146(4)
11.0(1)	11.17(2)	2.063(2)	2.020(3)	4.127(3)
12.4(1)	11.11(3)	2.053(4)	2.018(5)	4.105(6)
14.0(2)	10.95(4)	2.047(5)	2.007(7)	4.094(7)
15.7(3)	10.87(4)	2.041(5)	2.002(6)	4.081(7)
17.7(2)	10.81(3)	2.034(3)	2.000(5)	4.068(5)
19.1(2)	10.68(2)	2.033(3)	1.989(4)	4.066(5)
20.2(2)	10.65(3)	2.024(3)	1.990(5)	4.048(5)
21.6(2)	10.56(3)	2.020(4)	1.984(6)	4.040(6)
23.2(1)	10.56(2)	2.014(2)	1.986(4)	4.028(3)
24.1(1)	10.49(3)	2.010(3)	1.982(4)	4.020(5)
25.3(2)	10.49(5)	1.999(6)	1.986(9)	3.998(9)
26.5(2)	10.40(5)	2.001(6)	1.977(8)	4.001(9)
27.6(2)	10.41(5)	1.995(7)	1.981(8)	3.99(1)
28.8(2)	10.20(7)	1.996(7)	1.96(1)	3.99(1)
30.0(2)	10.30(7)	1.987(8)	1.97(1)	3.97(1)
31.4(1)	10.22(4)	1.979(6)	1.971(7)	3.958(8)
32.5(1)	10.18(7)	1.980(9)	1.97(1)	3.96(1)

Table S16. Volume and selected bond distances in M₂O₆ octahedra versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0570)

Pressure (GPa)	M2 Poly. Vol. (Å ³)	M2–O1 (Å)	M2–O2 (Å)	M2–O4 (Å)
0.0001	12.102(6)	2.084(1)	2.100(1)	2.0920(9)
1.0(1)	12.03(5)	2.080(8)	2.088(7)	2.090(7)
2.3(1)	11.86(4)	2.088(7)	2.084(6)	2.075(5)
3.9(2)	11.78(3)	2.073(6)	2.080(6)	2.072(4)
4.9(1)	11.72(4)	2.074(7)	2.070(7)	2.069(5)
6.4(1)	11.58(2)	2.066(4)	2.060(4)	2.060(3)
7.6(2)	11.51(2)	2.059(4)	2.055(4)	2.057(3)
9.2(2)	11.50(3)	2.052(4)	2.050(4)	2.059(4)
11.0(1)	11.35(2)	2.050(4)	2.041(4)	2.048(3)
12.4(1)	11.25(4)	2.045(6)	2.037(6)	2.042(5)
14.0(2)	11.16(5)	2.036(8)	2.034(8)	2.035(7)
15.7(3)	11.00(4)	2.040(8)	2.026(8)	2.022(6)
17.7(2)	10.93(3)	2.031(6)	2.012(6)	2.021(5)
19.1(2)	10.88(3)	2.024(5)	2.015(5)	2.017(4)
20.2(2)	10.89(3)	2.027(6)	2.007(6)	2.019(5)
21.6(2)	10.74(4)	2.018(6)	2.008(6)	2.007(6)
23.2(1)	10.71(3)	2.014(4)	1.998(4)	2.008(4)
24.1(1)	10.69(3)	2.008(5)	1.989(5)	2.010(4)
25.3(2)	10.65(6)	2.017(8)	1.990(9)	2.003(9)
26.5(2)	10.58(6)	2.022(9)	1.987(9)	1.996(8)
27.6(2)	10.63(6)	2.01(1)	1.99(1)	2.003(8)
28.8(2)	10.40(7)	2.02(1)	1.98(1)	1.98(1)
30.0(2)	10.46(7)	2.00(1)	1.98(1)	1.99(1)
31.4(1)	10.51(5)	1.980(9)	1.968(9)	2.004(7)
32.5(1)	10.41(8)	1.98(1)	1.98(1)	1.99(1)

Table S17. Volume and selected bond distances in M3O₆ octahedra versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0570)

Pressure (GPa)	M3 Poly. Vol. (Å ³)	M3–O1 (Å)	M3–O3 (Å)	M3–O4 (Å)
0.0001	12.195(4)	2.0503(3)	2.1197(6)	2.1192(7)
1.0(1)	12.15(3)	2.049(1)	2.117(5)	2.116(4)
2.3(1)	11.95(2)	2.0394(8)	2.105(3)	2.101(3)
3.9(2)	11.85(1)	2.0323(8)	2.100(3)	2.096(2)
4.9(1)	11.77(2)	2.0291(7)	2.097(3)	2.087(3)
6.4(1)	11.64(1)	2.0230(5)	2.086(2)	2.081(2)
7.6(2)	11.57(1)	2.0175(7)	2.083(2)	2.076(2)
9.2(2)	11.50(2)	2.012(2)	2.080(3)	2.072(2)
11.0(1)	11.36(1)	2.005(1)	2.070(3)	2.064(2)
12.4(1)	11.22(2)	2.001(1)	2.061(3)	2.051(3)
14.0(2)	11.19(2)	1.9959(9)	2.059(4)	2.053(4)
15.7(3)	11.09(2)	1.988(2)	2.055(5)	2.045(4)
17.7(2)	10.96(2)	1.984(1)	2.043(3)	2.038(2)
19.1(2)	10.89(1)	1.9775(5)	2.042(3)	2.032(2)
20.2(2)	10.83(2)	1.9733(7)	2.038(3)	2.029(2)
21.6(2)	10.81(2)	1.9736(9)	2.035(4)	2.029(3)
23.2(1)	10.72(1)	1.966(1)	2.030(2)	2.022(2)
24.1(1)	10.63(1)	1.961(1)	2.028(2)	2.015(2)
25.3(2)	10.60(2)	1.962(2)	2.017(5)	2.015(4)
26.5(2)	10.51(3)	1.954(1)	2.015(5)	2.008(5)
27.6(2)	10.44(3)	1.952(1)	2.004(5)	2.008(6)
28.8(2)	10.39(3)	1.947(2)	2.004(5)	2.004(6)
30.0(2)	10.35(3)	1.949(1)	1.998(6)	2.000(6)
31.4(1)	10.34(2)	1.941(1)	2.004(5)	2.000(4)
32.5(1)	10.30(3)	1.941(2)	1.994(7)	2.003(6)

Table S18. Volume and selected bond distances in TO₄ tetrahedra versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0570)

Pressure (GPa)	T Poly. Vol. (Å ³)	Si–O2 (Å)	Si–O3 (Å)	Si–O4A (Å)
0.0001	2.311(1)	1.7060(7)	1.6375(9)	1.6362(7)
1.0(1)	2.29(1)	1.699(4)	1.635(6)	1.629(7)
2.3(1)	2.31(1)	1.702(3)	1.639(4)	1.639(6)
3.9(2)	3.97(1)	1.697(3)	1.637(3)	1.633(4)
4.9(1)	2.28(1)	1.695(3)	1.635(5)	1.627(6)
6.4(1)	2.277(6)	1.694(2)	1.630(2)	1.630(3)
7.6(2)	2.264(6)	1.692(2)	1.628(2)	1.625(3)
9.2(2)	2.233(7)	1.688(3)	1.622(4)	1.614(4)
11.0(1)	2.233(6)	1.686(2)	1.621(3)	1.617(4)
12.4(1)	2.23(1)	1.679(3)	1.627(4)	1.616(6)
14.0(2)	2.22(1)	1.678(4)	1.623(5)	1.614(7)
15.7(3)	2.22(1)	1.675(4)	1.620(5)	1.615(6)
17.7(2)	2.200(9)	1.678(3)	1.616(4)	1.606(5)
19.1(2)	2.205(8)	1.674(2)	1.613(3)	1.612(4)
20.2(2)	2.192(9)	1.672(3)	1.616(4)	1.605(5)
21.6(2)	2.19(1)	1.668(3)	1.610(4)	1.608(7)
23.2(1)	2.164(7)	1.669(2)	1.608(3)	1.597(4)
24.1(1)	2.167(8)	1.671(2)	1.612(3)	1.595(5)
25.3(2)	2.16(2)	1.667(4)	1.620(6)	1.591(9)
26.5(2)	2.16(2)	1.664(5)	1.612(7)	1.595(9)
27.6(2)	2.14(2)	1.659(6)	1.626(7)	1.58(1)
28.8(2)	2.18(2)	1.660(6)	1.618(7)	1.60(1)
30.0(2)	2.13(2)	1.655(5)	1.614(8)	1.58(1)
31.4(1)	2.11(1)	1.661(4)	1.609(6)	1.570(8)
32.5(1)	2.09(2)	1.657(6)	1.607(9)	1.57(1)

Table S19. Selected O–O distances versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0570, part 1 of 2)

Pressure (GPa)	O3–O4(I) (Å)	O3–O4(II) (Å)	O4–O4(I) (Å)	O4–O4(II) (Å)	O1–O4 (Å)	O2–O4 (Å)	O4–O4(I) (Å)	O4–O4(II) (Å)
0.0001	2.8525(9)	3.0629(9)	2.8552(6)	2.9733(9)	2.813(1)	3.099(1)	2.9180(6)	2.9733(9)
1.0(1)	2.840(8)	3.059(8)	2.851(8)	2.98(1)	2.808(8)	3.089(8)	2.909(8)	2.98(1)
2.3(1)	2.840(6)	3.034(6)	2.849(5)	2.943(9)	2.800(6)	3.078(6)	2.898(5)	2.943(9)
3.9(2)	2.831(4)	3.024(4)	2.835(3)	2.937(7)	2.793(5)	3.067(5)	2.898(3)	2.937(7)
4.9(1)	2.832(6)	3.021(6)	2.846(5)	2.95(1)	2.791(6)	3.059(7)	2.877(5)	2.95(1)
6.4(1)	2.818(3)	3.002(3)	2.825(2)	2.925(6)	2.782(4)	3.044(4)	2.879(2)	2.925(6)
7.6(2)	2.813(3)	2.995(3)	2.821(2)	2.920(5)	2.777(4)	3.036(4)	2.875(2)	2.920(5)
9.2(2)	2.806(4)	2.991(4)	2.809(3)	2.925(6)	2.775(4)	3.032(4)	2.876(3)	2.925(6)
11.0(1)	2.797(3)	2.975(4)	2.805(3)	2.906(6)	2.769(4)	3.014(4)	2.863(3)	2.906(6)
12.4(1)	2.797(6)	2.958(6)	2.806(5)	2.90(1)	2.756(6)	3.012(6)	2.851(5)	2.90(1)
14.0(2)	2.780(7)	2.952(7)	2.794(6)	2.88(1)	2.754(8)	2.996(8)	2.852(6)	2.88(1)
15.7(3)	2.774(7)	2.942(7)	2.800(5)	2.86(1)	2.746(7)	2.984(8)	2.835(5)	2.86(1)
17.7(2)	2.771(5)	2.932(5)	2.792(5)	2.864(8)	2.739(5)	2.972(5)	2.831(5)	2.864(8)
19.1(2)	2.766(4)	2.920(4)	2.774(3)	2.850(7)	2.736(5)	2.968(5)	2.836(3)	2.850(7)
20.2(2)	2.762(5)	2.913(5)	2.771(3)	2.858(9)	2.738(5)	2.965(5)	2.833(3)	2.858(9)
21.6(2)	2.749(6)	2.910(6)	2.774(5)	2.84(1)	2.729(7)	2.951(7)	2.822(5)	2.84(1)
23.2(1)	2.750(4)	2.905(4)	2.770(3)	2.847(7)	2.727(4)	2.945(4)	2.814(3)	2.847(7)
24.1(1)	2.750(4)	2.893(4)	2.759(3)	2.845(8)	2.723(5)	2.941(5)	2.821(3)	2.845(8)
25.3(2)	2.746(9)	2.889(9)	2.773(8)	2.85(2)	2.728(9)	2.934(9)	2.803(8)	2.85(2)
26.5(2)	2.744(9)	2.880(9)	2.764(6)	2.83(2)	2.723(9)	2.93(1)	2.799(6)	2.83(2)
27.6(2)	2.747(9)	2.875(9)	2.757(6)	2.85(2)	2.72(1)	2.93(1)	2.800(6)	2.85(2)
28.8(2)	2.73(1)	2.86(1)	2.753(6)	2.79(2)	2.71(1)	2.91(1)	2.79(2)	2.796(6)
30.0(2)	2.74(1)	2.86(1)	2.757(8)	2.83(2)	2.71(1)	2.92(1)	2.787(8)	2.83(2)
31.4(1)	2.724(7)	2.861(7)	2.728(5)	2.85(1)	2.710(8)	2.911(8)	2.806(5)	2.85(1)
32.5(1)	2.72(1)	2.86(1)	2.738(8)	2.83(2)	2.70(1)	2.91(1)	2.790(8)	2.83(2)

Table S20. Selected O–O distances versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0570, part 2 of 2)

Pressure (GPa)	O1–O1 (Å)	O3–O3 (Å)	O1–O3 (Å)	O1–O4(I) (Å)	O1–O4(II) (Å)	O3–O4(I) (Å)	O3–O4(II) (Å)
0.0001	2.8833(4)	2.8488(3)	3.0406(9)	2.813(1)	3.080(1)	2.9292(9)	3.0629(9)
1.0(1)	2.877(2)	2.8421(6)	3.040(7)	2.808(8)	3.073(8)	2.931(8)	3.059(8)
2.3(1)	2.865(1)	2.8359(5)	3.018(5)	2.800(6)	3.049(6)	2.916(6)	3.034(6)
3.9(2)	2.860(1)	2.8296(7)	3.008(3)	2.793(5)	3.045(5)	2.904(4)	3.024(4)
4.9(1)	2.853(1)	2.8254(7)	3.003(5)	2.791(6)	3.021(7)	2.899(6)	3.021(6)
6.4(1)	2.845(1)	2.818(1)	2.987(2)	2.782(4)	3.019(4)	2.889(3)	3.002(3)
7.6(2)	2.838(1)	2.8112(6)	2.981(2)	2.777(4)	3.011(4)	2.882(3)	2.995(3)
9.2(2)	2.830(3)	2.802(3)	2.978(4)	2.775(4)	3.004(4)	2.872(4)	2.991(4)
11.0(1)	2.820(2)	2.796(2)	2.962(3)	2.769(4)	2.988(4)	2.864(4)	2.975(4)
12.4(1)	2.812(2)	2.787(1)	2.950(5)	2.756(6)	2.972(6)	2.854(6)	2.958(6)
14.0(2)	2.807(2)	2.7824(7)	2.945(6)	2.754(8)	2.975(8)	2.855(7)	2.952(7)
15.7(3)	2.796(2)	2.773(2)	2.937(6)	2.746(7)	2.959(8)	2.852(7)	2.942(7)
17.7(2)	2.786(2)	2.763(2)	2.926(5)	2.739(5)	2.948(5)	2.837(5)	2.932(5)
19.1(2)	2.784(1)	2.7621(7)	2.917(3)	2.736(5)	2.945(5)	2.828(4)	2.920(4)
20.2(2)	2.778(1)	2.7572(8)	2.910(5)	2.738(5)	2.933(5)	2.823(5)	2.913(5)
21.6(2)	2.774(1)	2.7531(7)	2.909(5)	2.729(7)	2.935(7)	2.829(6)	2.910(6)
23.2(1)	2.765(2)	2.745(2)	2.901(3)	2.727(4)	2.920(4)	2.816(4)	2.905(4)
24.1(1)	2.760(2)	2.740(2)	2.895(3)	2.723(5)	2.914(5)	2.804(4)	2.893(4)
25.3(2)	2.754(3)	2.736(3)	2.885(6)	2.728(9)	2.899(9)	2.809(8)	2.889(9)
26.5(2)	2.745(2)	2.730(1)	2.879(7)	2.723(9)	2.89(1)	2.800(9)	2.880(9)
27.6(2)	2.744(2)	2.726(1)	2.864(7)	2.72(1)	2.89(1)	2.787(9)	2.875(9)
28.8(2)	2.739(2)	2.724(2)	2.859(7)	2.71(1)	2.89(1)	2.79(1)	2.86(1)
30.0(2)	2.736(2)	2.719(1)	2.858(8)	2.71(1)	2.88(1)	2.78(1)	2.86(1)
31.4(1)	2.735(2)	2.7139(9)	2.859(7)	2.710(8)	2.887(8)	2.776(7)	2.861(7)
32.5(1)	2.727(3)	2.707(3)	2.852(9)	2.70(1)	2.89(1)	2.78(1)	2.86(1)

Table S21. Selected O–O distances versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0902, part 1 of 4)

Pressure (GPa)	O3–O4A(I) (Å)	O3–O4A(II) (Å)	O4A–O4B(I) (Å)	O4A–O4B(II) (Å)	O3–O4B(I) (Å)	O3–O4B(II) (Å)	O4A–O4B(I) (Å)
0.0001	2.855(8)	3.050(8)	2.832(5)	2.998(6)	2.847(8)	3.065(8)	2.832(5)
0.6(1)	2.841(7)	3.048(7)	2.822(3)	2.980(5)	2.837(7)	3.060(7)	2.822(3)
1.6(1)	2.827(9)	3.032(8)	2.816(3)	2.977(7)	2.825(8)	3.046(8)	2.816(3)
3.1(1)	2.823(8)	3.014(8)	2.812(3)	2.959(6)	2.819(8)	3.027(8)	2.812(3)
4.2(1)	2.816(8)	3.014(8)	2.807(3)	2.948(6)	2.821(8)	3.013(8)	2.807(3)
5.0(1)	2.814(9)	3.008(9)	2.800(4)	2.949(7)	2.814(9)	2.997(9)	2.800(4)
6.0(1)	2.806(7)	2.994(7)	2.796(3)	2.946(6)	2.809(7)	3.001(7)	2.796(3)
7.6(1)	2.794(9)	2.986(9)	2.791(3)	2.930(8)	2.795(9)	2.993(9)	2.791(3)
8.8(1)	2.787(9)	2.989(9)	2.785(5)	2.925(8)	2.787(9)	2.976(9)	2.785(5)
11.0(1)	2.78(1)	2.97(1)	2.769(5)	2.92(1)	2.77(1)	2.96(1)	2.769(5)
12.5(1)	2.777(9)	2.953(9)	2.775(3)	2.902(8)	2.773(9)	2.965(9)	2.775(3)
14.4(1)	2.76(1)	2.93(1)	2.769(5)	2.893(8)	2.75(1)	2.95(1)	2.769(5)
16.0(1)	2.76(1)	2.94(1)	2.762(5)	2.884(9)	2.77(1)	2.93(1)	2.762(5)
17.8(2)	2.76(1)	2.94(1)	2.760(5)	2.877(9)	2.80(1)	2.91(1)	2.760(5)
19.8(2)	2.74(1)	2.94(1)	2.755(5)	2.88(1)	2.77(1)	2.91(1)	2.755(5)
21.7(1)	2.746(7)	2.910(7)	2.751(3)	2.863(6)	2.751(8)	2.905(8)	2.751(3)
22.8(1)	2.753(6)	2.909(6)	2.753(2)	2.863(5)	2.755(6)	2.902(6)	2.753(2)
24.2(2)	2.740(6)	2.899(6)	2.751(2)	2.853(4)	2.745(6)	2.891(6)	2.751(2)
25.6(1)	2.728(6)	2.890(6)	2.747(2)	2.843(4)	2.738(6)	2.879(6)	2.747(2)
26.9(2)	2.735(6)	2.885(6)	2.744(2)	2.840(5)	2.742(6)	2.873(6)	2.744(2)
28.8(2)	2.725(6)	2.868(6)	2.739(2)	2.841(4)	2.731(6)	2.864(6)	2.739(2)
29.8(1)	2.716(6)	2.871(6)	2.735(2)	2.835(5)	2.724(6)	2.865(6)	2.735(2)
30.0(1)	2.715(7)	2.885(7)	2.736(3)	2.835(5)	2.725(7)	2.867(7)	2.736(3)
31.6(1)	2.71(1)	2.88(1)	2.734(5)	2.834(7)	2.73(1)	2.86(1)	2.734(5)
32.7(1)	2.699(8)	2.867(8)	2.729(3)	2.827(6)	2.722(8)	2.849(8)	2.729(3)
34.5(1)	2.70(1)	2.84(1)	2.726(5)	2.825(9)	2.69(1)	2.85(1)	2.726(5)

Table S22. Selected O–O distances versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0902, part 2 of 4)

Pressure (GPa)	O4A–O4B(II) (Å)	O1–O4A (Å)	O2–O4A (Å)	O4A–O4A (Å)	O4A–O4B (Å)	O1–O4B (Å)	O2–O4B (Å)
0.0001	2.998(6)	2.80(1)	3.09(1)	2.916(5)	2.998(6)	2.81(1)	3.08(1)
0.6(1)	2.980(5)	2.791(8)	3.087(9)	2.915(3)	2.980(5)	2.799(8)	3.085(9)
1.6(1)	2.977(7)	2.78(1)	3.09(1)	2.915(3)	2.977(7)	2.79(1)	3.07(1)
3.1(1)	2.959(6)	2.77(1)	3.07(1)	2.903(3)	2.959(6)	2.77(1)	3.06(1)
4.2(1)	2.948(6)	2.77(1)	3.07(1)	2.896(3)	2.948(6)	2.77(1)	3.06(1)
5.0(1)	2.949(7)	2.76(1)	3.06(1)	2.889(5)	2.949(7)	2.76(1)	3.07(1)
6.0(1)	2.946(6)	2.767(9)	3.05(1)	2.892(3)	2.946(6)	2.767(9)	3.044(9)
7.6(1)	2.930(8)	2.76(1)	3.03(1)	2.885(3)	2.930(8)	2.76(1)	3.03(1)
8.8(1)	2.925(8)	2.76(1)	3.02(1)	2.878(5)	2.925(8)	2.75(1)	3.02(1)
11.0(1)	2.92(1)	2.76(1)	3.01(1)	2.876(5)	2.92(1)	2.75(1)	3.01(1)
12.5(1)	2.902(8)	2.74(1)	3.00(1)	2.859(3)	2.902(8)	2.74(1)	2.99(1)
14.4(1)	2.893(8)	2.73(1)	2.97(1)	2.855(5)	2.893(8)	2.74(1)	2.96(1)
16.0(1)	2.884(9)	2.72(1)	2.96(1)	2.852(5)	2.884(9)	2.72(1)	2.99(1)
17.8(2)	2.877(9)	2.73(1)	2.97(1)	2.844(5)	2.877(9)	2.72(1)	3.01(1)
19.8(2)	2.88(1)	2.71(1)	2.95(1)	2.831(5)	2.88(1)	2.70(1)	2.98(1)
21.7(1)	2.863(6)	2.735(9)	2.950(9)	2.828(3)	2.863(6)	2.725(9)	2.96(1)
22.8(1)	2.863(5)	2.724(7)	2.941(8)	2.814(2)	2.863(5)	2.718(7)	2.947(8)
24.2(2)	2.853(4)	2.714(7)	2.933(7)	2.810(2)	2.853(4)	2.707(7)	2.939(7)
25.6(1)	2.843(4)	2.712(7)	2.922(7)	2.806(2)	2.843(4)	2.706(7)	2.933(7)
26.9(2)	2.840(5)	2.708(7)	2.920(7)	2.801(2)	2.840(5)	2.699(7)	2.928(7)
28.8(2)	2.841(4)	2.706(7)	2.904(7)	2.799(2)	2.841(4)	2.703(7)	2.911(7)
29.8(1)	2.835(5)	2.701(7)	2.898(8)	2.796(2)	2.835(5)	2.693(7)	2.905(8)
30.0(1)	2.835(5)	2.727(9)	2.876(9)	2.789(3)	2.835(5)	2.714(9)	2.886(9)
31.6(1)	2.834(7)	2.71(1)	2.86(1)	2.788(5)	2.834(7)	2.70(1)	2.88(1)
32.7(1)	2.827(6)	2.733(9)	2.854(9)	2.795(3)	2.827(6)	2.703(9)	2.858(9)
34.5(1)	2.825(9)	2.71(1)	2.82(1)	2.793(5)	2.825(9)	2.72(1)	2.83(1)

Table S23. Selected O–O distances versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0902, part 3 of 4)

Pressure (GPa)	O4B–O4B (Å)	O4A–O4B (Å)	O1–O1 (Å)	O3–O3 (Å)	O1–O3 (Å)	O1–O4A(I) (Å)	O1–O4A(II) (Å)	O3–O4A(I) (Å)
0.0001	2.904(5)	2.998(6)	2.902(9)	2.864(6)	3.008(4)	2.80(1)	3.11(1)	2.920(8)
0.6(1)	2.915(3)	2.980(5)	2.897(8)	2.839(6)	3.010(3)	2.791(8)	3.126(9)	2.927(7)
1.6(1)	2.908(3)	2.977(7)	2.90(1)	2.841(6)	3.001(3)	2.78(1)	3.13(1)	2.927(8)
3.1(1)	2.898(3)	2.959(6)	2.91(1)	2.834(6)	2.992(3)	2.77(1)	3.12(1)	2.916(8)
4.2(1)	2.896(3)	2.948(6)	2.89(1)	2.835(6)	2.980(3)	2.77(1)	3.10(1)	2.914(8)
5.0(1)	2.898(3)	2.949(7)	2.88(1)	2.831(7)	2.975(4)	2.76(1)	3.10(1)	2.911(9)
6.0(1)	2.887(3)	2.946(6)	2.886(9)	2.834(6)	2.970(3)	2.767(9)	3.08(1)	2.902(7)
7.6(1)	2.881(3)	2.930(8)	2.88(1)	2.818(7)	2.958(4)	2.76(1)	3.09(1)	2.901(9)
8.8(1)	2.878(5)	2.925(8)	2.85(1)	2.812(7)	2.954(4)	2.76(1)	3.07(1)	2.893(9)
11.0(1)	2.878(5)	2.92(1)	2.85(1)	2.797(9)	2.944(4)	2.76(1)	3.04(1)	2.88(1)
12.5(1)	2.862(3)	2.902(8)	2.87(1)	2.793(7)	2.932(4)	2.74(1)	3.05(1)	2.867(9)
14.4(1)	2.852(5)	2.893(8)	2.85(1)	2.788(8)	2.924(4)	2.73(1)	3.03(1)	2.86(1)
16.0(1)	2.847(5)	2.884(9)	2.79(1)	2.791(9)	2.916(4)	2.72(1)	3.02(1)	2.85(1)
17.8(2)	2.835(5)	2.877(9)	2.81(1)	2.807(9)	2.907(4)	2.73(1)	2.98(1)	2.83(1)
19.8(2)	2.836(5)	2.88(1)	2.81(2)	2.79(1)	2.903(5)	2.71(1)	3.01(2)	2.84(1)
21.7(1)	2.826(3)	2.863(6)	2.803(9)	2.771(5)	2.888(2)	2.735(9)	2.958(9)	2.822(7)
22.8(1)	2.823(2)	2.863(5)	2.796(8)	2.765(4)	2.886(2)	2.724(7)	2.946(8)	2.813(6)
24.2(2)	2.817(2)	2.853(4)	2.793(7)	2.763(4)	2.879(2)	2.714(7)	2.949(7)	2.813(6)
25.6(1)	2.813(2)	2.843(4)	2.784(7)	2.760(4)	2.874(2)	2.712(7)	2.940(7)	2.815(6)
26.9(2)	2.809(2)	2.840(5)	2.784(7)	2.757(4)	2.868(2)	2.708(7)	2.926(7)	2.800(6)
28.8(2)	2.797(2)	2.841(4)	2.771(6)	2.756(4)	2.858(2)	2.706(7)	2.905(7)	2.790(6)
29.8(1)	2.796(2)	2.835(5)	2.778(7)	2.751(4)	2.855(2)	2.701(7)	2.919(8)	2.792(6)
30.0(1)	2.802(3)	2.835(5)	2.771(9)	2.751(5)	2.855(2)	2.727(9)	2.902(9)	2.796(7)
31.6(1)	2.795(5)	2.834(7)	2.75(1)	2.745(7)	2.844(3)	2.71(1)	2.91(1)	2.79(1)
32.7(1)	2.788(3)	2.827(6)	2.769(9)	2.737(6)	2.843(3)	2.733(9)	2.89(1)	2.790(8)
34.5(1)	2.782(5)	2.825(9)	2.76(1)	2.751(9)	2.832(3)	2.71(1)	2.87(1)	2.77(1)

Table S24. Selected O–O distances versus pressure. Values in parentheses are uncertainties on the last digit. (Sample Z0902, part 4 of 4)

Pressure (GPa)	O3– O4A(II) (Å)	O1–O1 (Å)	O3–O3 (Å)	O1–O3 (Å)	O1– O4B(I) (Å)	O1– O4B(II) (Å)	O3– O4B(I) (Å)	O3– O4B(II) (Å)
0.0001	3.050(8)	2.905(9)	2.850(6)	3.008(4)	2.81(1)	3.12(1)	2.934(8)	3.065(8)
0.6(1)	3.048(7)	2.904(8)	2.860(6)	3.010(3)	2.799(8)	3.128(9)	2.932(7)	3.060(7)
1.6(1)	3.032(8)	2.90(1)	2.852(6)	3.001(3)	2.79(1)	3.12(1)	2.932(8)	3.046(8)
3.1(1)	3.014(8)	2.88(1)	2.846(6)	2.992(3)	2.77(1)	3.11(1)	2.922(8)	3.027(8)
4.2(1)	3.014(8)	2.87(1)	2.833(6)	2.980(3)	2.77(1)	3.10(1)	2.910(8)	3.013(8)
5.0(1)	3.008(9)	2.89(1)	2.829(7)	2.975(4)	2.76(1)	3.10(1)	2.907(9)	2.997(9)
6.0(1)	2.994(7)	2.858(9)	2.818(6)	2.970(3)	2.767(9)	3.08(1)	2.902(7)	3.001(7)
7.6(1)	2.986(9)	2.86(1)	2.822(7)	2.958(4)	2.76(1)	3.08(1)	2.902(9)	2.993(9)
8.8(1)	2.989(9)	2.88(1)	2.819(7)	2.954(4)	2.75(1)	3.08(1)	2.892(9)	2.976(9)
11.0(1)	2.97(1)	2.85(1)	2.815(9)	2.944(4)	2.75(1)	3.04(1)	2.88(1)	2.96(1)
12.5(1)	2.953(9)	2.82(1)	2.809(7)	2.932(4)	2.74(1)	3.04(1)	2.871(9)	2.965(9)
14.4(1)	2.93(1)	2.82(1)	2.799(8)	2.924(4)	2.74(1)	3.03(1)	2.87(1)	2.95(1)
16.0(1)	2.94(1)	2.86(1)	2.785(9)	2.916(4)	2.72(1)	3.02(1)	2.84(1)	2.93(1)
17.8(2)	2.94(1)	2.81(1)	2.758(9)	2.907(4)	2.72(1)	2.96(2)	2.80(1)	2.91(1)
19.8(2)	2.94(1)	2.83(2)	2.76(1)	2.903(5)	2.70(1)	3.00(2)	2.82(1)	2.91(1)
21.7(1)	2.910(7)	2.786(9)	2.769(5)	2.888(2)	2.725(9)	2.95(1)	2.818(8)	2.905(8)
22.8(1)	2.909(6)	2.787(8)	2.769(4)	2.886(2)	2.718(7)	2.940(8)	2.806(6)	2.902(6)
24.2(2)	2.899(6)	2.783(7)	2.759(4)	2.879(2)	2.707(7)	2.941(7)	2.804(6)	2.891(6)
25.6(1)	2.890(6)	2.780(7)	2.754(4)	2.874(2)	2.706(7)	2.931(7)	2.803(6)	2.879(6)
26.9(2)	2.885(6)	2.771(7)	2.751(4)	2.868(2)	2.699(7)	2.917(7)	2.789(6)	2.873(6)
28.8(2)	2.868(6)	2.767(6)	2.740(4)	2.858(2)	2.703(7)	2.902(7)	2.786(6)	2.864(6)
29.8(1)	2.871(6)	2.763(7)	2.742(4)	2.855(2)	2.693(7)	2.909(8)	2.784(6)	2.865(6)
30.0(1)	2.885(7)	2.754(9)	2.742(5)	2.855(2)	2.714(9)	2.890(9)	2.779(7)	2.867(7)
31.6(1)	2.88(1)	2.77(1)	2.739(7)	2.844(3)	2.70(1)	2.89(1)	2.76(1)	2.86(1)
32.7(1)	2.867(8)	2.737(9)	2.740(6)	2.843(3)	2.703(9)	2.86(1)	2.770(8)	2.849(8)
34.5(1)	2.84(1)	2.716(9)	2.716(9)	2.832(3)	2.72(1)	2.88(1)	2.78(1)	2.85(1)