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Supporting information for article:

Microporous crystal structure of labuntsovite-Fe and high-pressure behavior up to 23 GPa

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SUPPORTING INFORMATION

Table S1 Atomic coordinates (xyz), site occupancy, number of refined and calculated electrons, multiplicity (Q) and equivalent displacement parameters (U_{eq}) for labuntsovite-Fe at ambient conditions

Site	Occupancy	e_{ref}	e_{calc}	x	y	z	Q	$U_{\text{eq}}, \text{\AA}^2$
A	Na _{0.5}	22	21.28	0.4138(2)	0.2625(2)	0.0121(4)	8	0.0275(7)
B	K	38	38.87	0.4196(1)	0	0.7022(1)	4	0.0357(3)
C	Ba _{0.35} (H ₂ O) _{0.65}	49.6	47.48	0.0855(1)	0	0.3437(1)	4	0.0177(1)
D	Fe _{0.5} Ti _{0.1} Mg _{0.05}	15.8	14.83	0	0	0.5	2	0.0210(3)
M1	Ti	44	45.25	0	0.2273(1)	0.5	4	0.0162(1)
M2	Ti _{0.95} Nb _{0.05}	45.9	45.95	0.25	0.25	0.5	4	0.0153(1)
Si1	Si			0.3197(1)	0.1113(1)	0.2500(1)	8	0.0068(1)
Si2	Si			0.2083(1)	0.1099(1)	0.8031(1)	8	0.0063(1)
O1	O			0.0821(1)	0.1155(1)	0.6728(2)	8	0.0112(3)
O2	O			0.2738(1)	0.1833(1)	0.7386(2)	8	0.0097(3)
O3	O			0.2650(1)	0.1255(1)	0.3888(2)	8	0.0098(3)
O4	O			0.3644(1)	0	0.2714(2)	4	0.0105(4)
O5	O			0.2476(1)	0	0.7865(3)	4	0.0118(4)
O6	O			0.4195(1)	0.1804(1)	0.3030(2)	8	0.0123(3)
O7	O			0.2323(1)	0.1280(1)	0.0262(2)	8	0.0117(3)
O _h	O _{0.75} (OH) _{0.25}			0.1002(1)	0.2242(1)	0.3967(2)	8	0.0108(3)
O _{w1}	H ₂ O			0.5	0.1455(4)	0	4	0.130(4)
O _{w2}	H ₂ O			0	0.1123(4)	0	4	0.093(4)

Note: U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2 Anisotropic displacement parameters U_{ij} for labuntsovite-Fe at ambient conditions

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A	0.0212(8)	0.024(1)	0.042(1)	-0.0014(7)	0.0181(8)	-0.0032(8)
B	0.0268(3)	0.0596(6)	0.0199(3)	0	0.0100(2)	0
C	0.0193(2)	0.0166(2)	0.0166(2)	0	0.0076(1)	0
D	0.0180(4)	0.0141(4)	0.0236(4)	0	0.0029(3)	0
M1	0.0142(2)	0.0045(2)	0.0148(2)	0	-0.0066(1)	0
M2	0.0331(2)	0.0065(2)	0.0128(2)	0.0057(2)	0.0161(2)	0.0026(1)
Si1	0.0082(2)	0.0053(2)	0.00656(2)	-0.0007(1)	0.0030(1)	-0.0008(1)
Si2	0.0068(2)	0.0052(2)	0.0061(2)	0.0001(1)	0.0022(1)	0.0006(1)
O1	0.0070(4)	0.0110(5)	0.0115(4)	0.0003(3)	0.0005(3)	0.0032(3)
O2	0.0110(4)	0.0091(5)	0.0097(3)	-0.0020(3)	0.0052(3)	0.0018(3)
O3	0.0124(4)	0.0089(4)	0.0117(4)	-0.0005(3)	0.0087(3)	-0.0012(3)
O4	0.0116(5)	0.0056(6)	0.0155(6)	0	0.0071(5)	0
O5	0.0141(6)	0.0053(6)	0.0174(6)	0	0.0084(5)	0
O6	0.0128(4)	0.0110(5)	0.0145(4)	-0.0058(3)	0.0075(3)	-0.0047(3)
O7	0.0128(4)	0.0146(5)	0.0063(3)	0.0018(3)	0.0030(3)	0.0006(3)
OH	0.0073(4)	0.0144(5)	0.0101(4)	-0.0001(3)	0.0033(3)	0.0001(3)
O _w 1	0.234(10)	0.027(2)	0.026(2)	0	-0.031(3)	0
O _w 2	0.200(8)	0.038(2)	0.025(2)	0	0.037(3)	0

Table S3 Atomic coordinates (x yz) and atomic displacement parameters (U) for labuntsovite-Fe at 3.15 GPa.

Site	x	y	z	$U_{\text{iso/eq}^*}, \text{\AA}^2$
<i>A</i>	0.4156(14)	0.2641(5)	0.0131(11)	0.025(2)*
<i>B</i>	0.4244(6)	0	0.7085(4)	0.024(4)*
<i>C</i>	0.0874(3)	0	0.3422(2)	0.0125(5)
<i>D</i>	0	0	0.5	0.024(1)
<i>M1</i>	0	0.2242(1)	0.5	0.0084(5)*
<i>M2</i>	0.25	0.25	0.5	0.0109(5)*
Si1	0.3213(4)	0.1110(1)	0.2553(2)	0.0053(5)*
Si2	0.2094(3)	0.1096(1)	0.8066(2)	0.0051(5)*
O1	0.0827(9)	0.1121(3)	0.6759(7)	0.009(1)
O2	0.2749(8)	0.1875(3)	0.7462(6)	0.007(1)
O3	0.2715(9)	0.1222(3)	0.4026(6)	0.007(1)
O4	0.3735(14)	0	0.2759(10)	0.010(1)
O5	0.2550(13)	0	0.7915(10)	0.009(1)
O6	0.4174(9)	0.1837(3)	0.2980(7)	0.013(1)
O7	0.2314(9)	0.1262(3)	0.0296(7)	0.011(1)
O _h	0.1010(9)	0.2201(3)	0.3935(7)	0.009(1)
O _{w1}	0.5	0.1457(7)	0	0.097(17)
O _{w2}	0	0.1134(7)	0	0.08(2)

Table S4 Atomic coordinates (x yz) and atomic displacement parameters (U) for labuntsovite-Fe at 5.15 GPa.

Site	x	y	z	$U_{\text{iso/eq}^*}, \text{\AA}^2$
<i>A</i>	0.4181(18)	0.2648(6)	0.0154(14)	0.031(11)*
<i>B</i>	0.4260(7)	0	0.7119(5)	0.032(4)*
<i>C</i>	0.0893(4)	0	0.3418(3)	0.0185(5)
<i>D</i>	0	0	0.5	0.030(1)
<i>M</i> 1	0.25	0.25	0.5	0.028(3)*
<i>M</i> 2	0	0.2227(2)	0.5	0.025(3)*
Si1	0.3235(5)	0.1110(2)	0.2585(3)	0.021(3)*
Si2	0.2104(5)	0.1097(2)	0.8086(3)	0.024(3)*
O1	0.0837(12)	0.1107(4)	0.6763(8)	0.014(3)
O2	0.2743(11)	0.1901(4)	0.7496(8)	0.011(1)
O3	0.2730(12)	0.1204(4)	0.4090(8)	0.013(1)
O4	0.3757(16)	0	0.2758(12)	0.014(2)
O5	0.2565(15)	0	0.7933(11)	0.012(2)
O6	0.4179(12)	0.1844(5)	0.2979(9)	0.022(2)
O7	0.2285(12)	0.1245(4)	0.0338(9)	0.017(1)
O _h	0.1019(12)	0.2185(4)	0.3909(8)	0.012(1)
O _w 1	0.5	0.1469(7)	0	0.05(2)
O _w 2	0	0.1103(7)	0	0.11(2)

Table S5 Atomic coordinates (x yz) and atomic displacement parameters (U) for labuntsovite-Fe at 7.21 GPa.

Site	x	y	z	$U_{\text{iso}}, \text{\AA}^2$
<i>A</i>	0.4175(16)	0.2673(6)	0.0163(12)	0.033(10)
<i>B</i>	0.4272(6)	0	0.7147(4)	0.020(4)
<i>C</i>	0.0900(3)	0	0.3412(2)	0.0127(5)
<i>D</i>	0	0	0.5	0.024(1)
<i>M1</i>	0	0.2213(1)	0.5	0.0101(5)
<i>M2</i>	0.25	0.25	0.5	0.0119(5)
Si1	0.3247(4)	0.1105(1)	0.2605(3)	0.0061(5)
Si2	0.2108(4)	0.1095(1)	0.8108(3)	0.0060(5)
O1	0.0818(10)	0.1099(3)	0.6767(8)	0.009(1)
O2	0.2731(10)	0.1920(4)	0.7542(7)	0.007(1)
O3	0.2741(10)	0.1187(3)	0.4156(8)	0.008(1)
O4	0.3816(16)	0	0.2792(11)	0.012(2)
O5	0.2601(14)	0	0.7934(10)	0.007(1)
O6	0.4198(11)	0.1858(4)	0.2949(8)	0.016(1)
O7	0.2269(11)	0.1225(4)	0.0364(8)	0.010(1)
O _h	0.0990(10)	0.2161(3)	0.3885(7)	0.009(1)
O _{w1}	0.5	0.1445(7)	0	0.037(13)
O _{w2}	0	0.1119(8)	0	0.059(19)

Table S6 Atomic coordinates (x yz) and atomic displacement parameters (U) for labuntsovite-Fe at 10.01 GPa.

Site	x	y	z	U_{iso} , Å 2
<i>A</i>	0.4191(15)	0.2682(5)	0.0155(12)	0.025(9)
<i>B</i>	0.4289(5)	0	0.7197(4)	0.020(4)
<i>C</i>	0.0917(3)	0	0.3401(2)	0.0137(5)
<i>D</i>	0	0	0.5	0.026(1)
<i>M1</i>	0	0.2199(1)	0.5	0.0132(6)
<i>M2</i>	0.25	0.25	0.5	0.0141(5)
Si1	0.3268(4)	0.1103(1)	0.2634(3)	0.0085(5)
Si2	0.2112(4)	0.1091(1)	0.8133(3)	0.0079(5)
O1	0.0815(11)	0.1091(3)	0.6797(8)	0.009(1)
O2	0.2729(10)	0.1943(4)	0.7576(7)	0.009(1)
O3	0.2783(11)	0.1182(3)	0.4237(8)	0.010(1)
O4	0.3827(16)	0	0.2844(11)	0.013(2)
O5	0.2628(15)	0	0.7928(11)	0.012(2)
O6	0.4212(11)	0.1868(4)	0.2938(9)	0.018(1)
O7	0.2253(11)	0.1196(3)	0.0393(8)	0.011(1)
Oh	0.0972(10)	0.2129(4)	0.3873(8)	0.011(1)
O _w 1	0.5	0.1440(7)	0	0.056(13)
O _w 2	0	0.1078(7)	0	0.038(17)

Table S7 Atomic coordinates (x yz) and atomic displacement parameters (U) for labuntsovite-Fe at 12.59 GPa.

Site	x	y	z	U_{iso} , Å 2
<i>A</i>	0.4184(17)	0.2701(6)	0.0103(14)	0.029(11)
<i>B</i>	0.4306(6)	0	0.7244(4)	0.028(4)
<i>C</i>	0.0943(4)	0	0.3384(3)	0.0142(5)
<i>D</i>	0	0	0.5	0.025(1)
<i>M1</i>	0	0.2186(2)	0.5	0.0139(6)
<i>M2</i>	0.25	0.25	0.5	0.0151(6)
Si1	0.3284(5)	0.1098(2)	0.2667(3)	0.0082(6)
Si2	0.2109(4)	0.1090(1)	0.8159(3)	0.0074(6)
O1	0.0799(11)	0.1076(4)	0.6810(9)	0.010(1)
O2	0.2721(11)	0.1962(4)	0.7605(9)	0.011(1)
O3	0.2829(12)	0.1170(4)	0.4316(9)	0.011(1)
O4	0.3859(16)	0	0.2875(12)	0.009(2)
O5	0.2617(16)	0	0.7953(12)	0.009(2)
O6	0.4212(12)	0.1889(5)	0.2901(10)	0.018(2)
O7	0.2246(12)	0.1179(4)	0.0454(9)	0.011(1)
O _h	0.0983(11)	0.2117(4)	0.3840(9)	0.010(1)
O _{w1}	0.5	0.1448(8)	0	0.055(15)
O _{w2}	0	0.1075(7)	0	0.028(3)

Table S8 Atomic coordinates (x yz) and atomic displacement parameters (U) for labuntsovite-Fe at 16.30 GPa.

Site	x	y	z	U_{iso} , Å 2
<i>A</i>	0.418(2)	0.2704(8)	0.0128(17)	0.035(3)
<i>B</i>	0.4358(9)	0	0.7315(7)	0.036(1)
<i>C</i>	0.0963(5)	0	0.3344(4)	0.0179(7)
<i>D</i>	0	0	0.5	0.031(2)
<i>M1</i>	0	0.2177(2)	0.5	0.0181(7)
<i>M2</i>	0.25	0.25	0.5	0.0196(7)
Si1	0.3307(6)	0.10970(19)	0.2709(4)	0.0113(7)
Si2	0.2104(5)	0.10875(18)	0.8196(4)	0.0103(7)
O1	0.0805(14)	0.1047(5)	0.6816(11)	0.015(2)
O2	0.2704(14)	0.1987(5)	0.7670(11)	0.015(2)
O3	0.2876(15)	0.1156(5)	0.4395(11)	0.014(2)
O4	0.3877(19)	0	0.2925(15)	0.013(2)
O5	0.272(2)	0	0.7986(16)	0.016(2)
O6	0.4180(16)	0.1883(7)	0.2876(13)	0.024(2)
O7	0.2200(15)	0.1143(5)	0.0522(11)	0.015(2)
O _h	0.0981(14)	0.2098(5)	0.3825(11)	0.012(2)
O _{w1}	0.5	0.1435(11)	0	0.038(4)
O _{w2}	0	0.1077(9)	0	0.033(3)

Table S9 Atomic coordinates (x yz) and atomic displacement parameters (U) for labuntsovite-Fe at 20.00 GPa.

Site	x	y	z	U_{iso} , Å 2
<i>A</i>	0.420(3)	0.2724(13)	0.012(3)	0.049(5)
<i>B</i>	0.4366(16)	0	0.7391(13)	0.059(2)
<i>C</i>	0.0980(7)	0	0.3342(5)	0.022(1)
<i>D</i>	0	0	0.5	0.040(2)
<i>M</i> 1	0	0.2160(3)	0.5	0.025(1)
<i>M</i> 2	0.25	0.25	0.5	0.027(1)
Si1	0.3319(8)	0.1094(3)	0.2753(6)	0.018(1)
Si2	0.2110(7)	0.1086(3)	0.8213(6)	0.016(1)
O1	0.0777(18)	0.1032(7)	0.6867(15)	0.017(2)
O2	0.268(2)	0.2013(7)	0.7695(16)	0.022(2)
O3	0.295(2)	0.1143(8)	0.4513(17)	0.024(3)
O4	0.394(3)	0	0.294(2)	0.017(3)
O5	0.267(3)	0	0.803(2)	0.018(3)
O6	0.420(2)	0.1899(9)	0.2847(18)	0.030(3)
O7	0.2190(19)	0.1122(6)	0.0565(14)	0.013(2)
O _h	0.0989(19)	0.2082(7)	0.3806(15)	0.016(2)
O _w 1	0.5	0.1468(16)	0	0.047(5)
O _w 2	0	0.1058(13)	0	0.036(5)

Table S10 Atomic coordinates (x yz) and atomic displacement parameters (U) for labuntsovite-Fe at 22.53 GPa.

Site	x	y	z	U_{iso} , Å 2
<i>A</i>	0.414(3)	0.2741(13)	0.018(3)	0.053(5)
<i>B</i>	0.4385(16)	0	0.7443(13)	0.067(3)
<i>C</i>	0.0988(7)	0	0.3345(6)	0.028(1)
<i>D</i>	0	0	0.5	0.050(3)
<i>M</i> 1	0	0.2162(3)	0.5	0.031(1)
<i>M</i> 2	0.25	0.25	0.5	0.037(1)
Si1	0.3318(9)	0.1098(3)	0.2777(6)	0.022(1)
Si2	0.2130(8)	0.1087(3)	0.8217(6)	0.021(1)
O1	0.0758(19)	0.1041(7)	0.6874(16)	0.022(2)
O2	0.270(2)	0.2019(8)	0.7708(16)	0.027(3)
O3	0.299(2)	0.1145(8)	0.4537(16)	0.026(3)
O4	0.389(3)	0	0.298(2)	0.030(4)
O5	0.271(3)	0	0.796(2)	0.025(4)
O6	0.416(2)	0.1904(10)	0.2853(19)	0.040(4)
O7	0.221(2)	0.1117(7)	0.0592(15)	0.021(2)
O _h	0.0988(19)	0.2075(7)	0.3788(14)	0.017(2)
O _w 1	0.5	0.146(2)	0	0.075(8)
O _w 2	0	0.1056(13)	0	0.038(5)

Table S11 Selected interatomic distances (Å) in the structure of labuntsovite-Fe at high pressure

Central atom	Ligand	Pressure (GPa)							
		3.15	5.15	7.21	10.01	12.59	16.3	20.0	22.53
A	O _{w1}	2.030(16)	1.993(19)	2.041(17)	2.025(16)	2.018(17)	2.028(2)	1.984(31)	2.059(35)
	O _{w2}	2.075(16)	2.069(18)	2.019(18)	2.023(16)	1.987(17)	1.975(21)	1.943(31)	1.978(32)
	O2	2.355(93)	2.341(64)	2.321(92)	2.293(76)	2.253(60)	2.218(61)	2.222(78)	2.170(51)
	O7	2.451(24)	2.424(27)	2.376(28)	2.371(25)	2.340(26)	2.289(29)	2.282(41)	2.214(38)
	O6	2.431(13)	2.403(17)	2.350(15)	2.321(14)	2.300(16)	2.255(20)	2.216(30)	2.167(30)
	O1	2.909(13)	2.888(16)	2.832(14)	2.793(13)	2.774(15)	2.739(18)	2.676(27)	2.569(27)
	O _h	2.917(140)	2.863(93)	2.815(135)	2.77(11)	2.768(88)	2.724(88)	2.687(109)	2.678(69)
	O _h	3.025(19)	2.975(19)	2.956(19)	2.907(18)	2.806(18)	2.771(21)	2.699(31)	2.738(30)
	<i>mean</i>	2.524	2.495	2.464	2.438	2.432	2.375	2.339	2.322
A	A	2.474(30)	2.400(37)	2.407(34)	2.334(31)	2.297(34)	2.306(40)	2.230(59)	2.416(59)
B	O5	2.731(36)	2.699(30)	2.634(35)	2.569(31)	2.576(29)	2.447(34)	2.511(50)	2.415(47)
	O _{w1}	2.812(46) x2	2.784(30) x2	2.729(43) x2	2.675(35) x2	2.640(27) x2	2.566(26) x2	2.542(33) x2	2.500(26) x2
	O3	2.889(46) x2	2.843(62) x2	2.800(92) x2	2.748(74) x2	2.694(58) x2	2.658(58) x2	2.577(70) x2	2.565(43) x2
	O4	2.794(23)	2.727(25)	2.630(24)	2.602(24)	2.543(24)	2.469(30)	2.389(47)	2.446(47)
	O4	3.060(43)	3.058(29)	3.044(38)	3.000(32)	2.983(26)	2.936(29)	2.957(35)	2.921(28)
	O2	3.400(14) x2	3.419(14) x2	-	-	-	-	-	-
	O6	3.362(11) x2	3.330(14) x2	3.295(13) x2	3.260(12) x2	3.248(13) x2	3.210(18) x2	3.191(24) x2	3.210(25) x2
	<i>mean</i>	3.046	3.069	2.884	2.837	2.807	2.746	2.720	2.704
M1	O6	1.923(50) x2	1.913(34) x2	1.907(49) x2	1.894(40) x2	1.888(32) x2	1.901(34) x2	1.890(41) x2	1.885(28) x2

	O _h	1.933(35) x2	1.940(27) x2	1.902(35) x2	1.866(30) x2	1.880(26) x2	1.864(28) x2	1.865(37) x2	1.859(29) x2
	O1	2.021(42) x2	2.009(29) x2	1.985(41) x2	1.971(34) x2	1.959(27) x2	1.964(27) x2	1.953(34) x2	1.934(22) x2
<i>mean</i>		1.959	1.945	1.931	1.910	1.909	1.910	1.903	1.893
<i>M2</i>	O _h	1.922(49) x2	1.899(36) x2	1.93(5) x2	1.948(42) x2	1.928(35) x2	1.924(37) x2	1.909(46) x2	1.900(33) x2
	O2	1.952(19) x2	1.943(14) x2	1.952(18) x2	1.941(15) x2	1.933(13) x2	1.940(14) x2	1.930(18) x2	1.915(15) x2
<i>mean</i>	O3	1.968(8) x2	1.959(9) x2	1.952(9) x2	1.936(8) x2	1.938(9) x2	1.941(11) x2	1.952(15) x2	1.957(15) x2
		1.947	1.934	1.945	1.942	1.933	1.935	1.930	1.924
<i>D</i>	O1	2.021(42) x4	1.996(29) x4	1.970(41) x4	1.954(35) x4	1.925(28) x4	1.883(28) x4	1.860(35) x4	1.856(22) x4
	C	2.077(39) x2	2.082(26) x2	2.076(39) x2	2.079(32) x2	2.097(27) x2	2.117(27) x2	2.115(34) x2	2.105(22) x2
<i>mean</i>		2.040	2.025	2.005	1.996	1.982	1.961	1.945	1.939
Si1	O6	1.586(19)	1.567(17)	1.588(17)	1.585(15)	1.593(15)	1.534(19)	1.563(23)	1.521(24)
	O3	1.582(29)	1.593(24)	1.61(3)	1.604(26)	1.586(22)	1.562(29)	1.534(29)	1.485(25)
	O7	1.633(72)	1.634(50)	1.632(75)	1.633(64)	1.620(52)	1.633(53)	1.633(67)	1.608(42)
	O4	1.655(9)	1.645(10)	1.656(11)	1.633(10)	1.628(11)	1.611(12)	1.631(21)	1.597(19)
<i>mean</i>		1.614	1.610.	1.622	1.614	1.607	1.585	1.590	1.553
Si2	O2	1.604(17)	1.591(16)	1.575(17)	1.578(15)	1.580(14)	1.572(16)	1.560(21)	1.554(20)
	O1	1.606(61)	1.595(43)	1.614(61)	1.610(51)	1.618(41)	1.598(43)	1.624(52)	1.658(37)
	O7	1.610(19)	1.623(13)	1.618(15)	1.606(12)	1.612(11)	1.624(13)	1.627(16)	1.631(16)
	O5	1.647(9)	1.639(10)	1.65(1)	1.653(11)	1.637(11)	1.695(16)	1.638(21)	1.660(22)
<i>mean</i>		1.617	1.612	1.614	1.612	1.612	1.622	1.612	1.626
<i>C</i>	O1	2.789(13) x2	2.790(16) x2	2.753(14) x2	2.736(15) x2	2.721(15) x2	2.719(18) x2	2.667(24) x2	2.641(24) x2
	O _w 2	2.804(62) x2	2.756(42) x2	2.744(63) x2	2.683(53) x2	2.650(44) x2	2.600(44) x2	2.561(56) x2	2.548(34) x2
	O3	2.935(25) x2	2.882(22) x2	2.844(30) x2	2.833(28) x2	2.819(27) x2	2.806(31) x2	2.831(42) x2	2.849(32) x2

	O1	3.003(8) x2	2.975(10) x2	2.967(10) x2	2.965(10) x2	2.967(11) x2	2.943(14) x2	2.959(19) x2	2.963(18) x2
	O _h	3.013(4) x2	2.967(5) x2	2.918(4) x2	2.855(5) x2	2.822(5) x2	2.779(7) x2	2.739(9) x2	2.719(9) x2
	O5	3.180(137)	3.164(91)	3.156(137)	3.131(113)	3.113(89)	3.143(92)	3.108(111)	3.064(68)
<i>mean</i>		2.933	2.900	2.874	2.843	2.825	2.803	2.784	2.773