Supporting information for "High pressure behavior of liebenbergite: the most incompressible olivine-structured silicate"

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Data set file: raw data file of Liebenbergite crystal structure and lattice parameters at different pressures in IUCr CIF format.

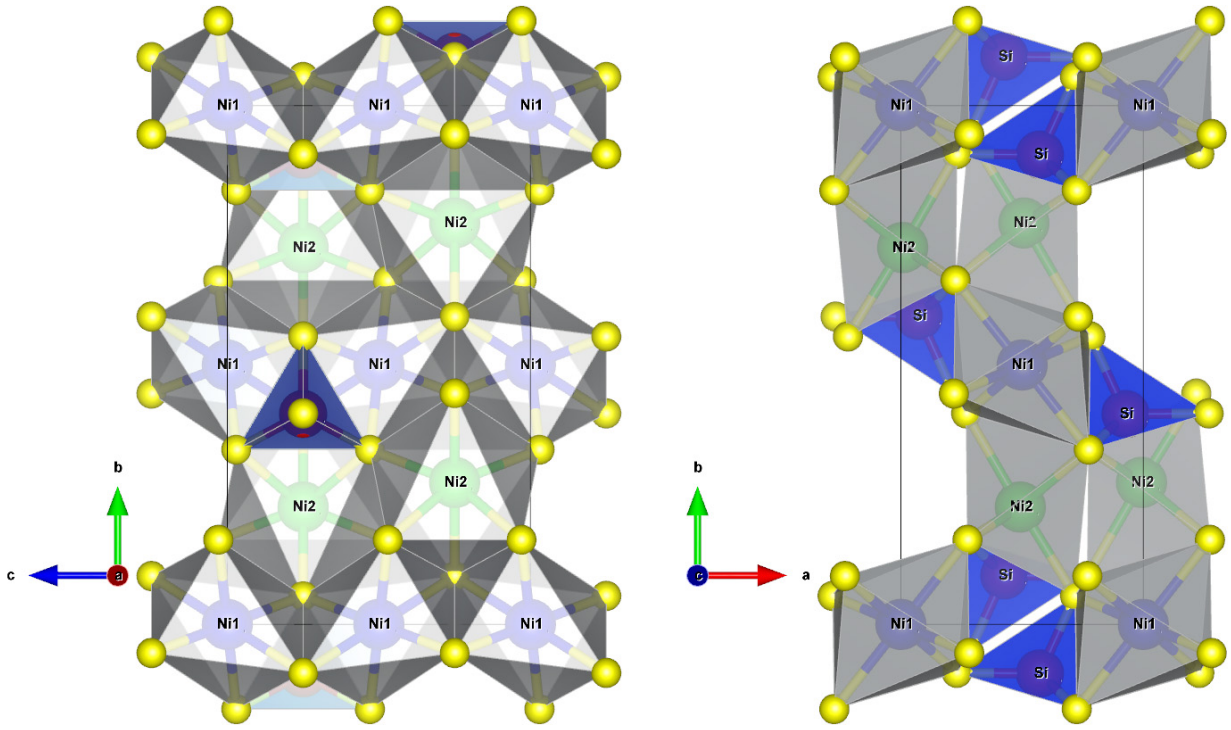

Figure S1: Crystal structure of liebenbergite at ambient condition, viewing down along the **a**-axis (left) and the **c**-axis (right). Ni1, Ni2 and Si polyhedral sites are labeled. Yellow spheres are oxygen atoms.

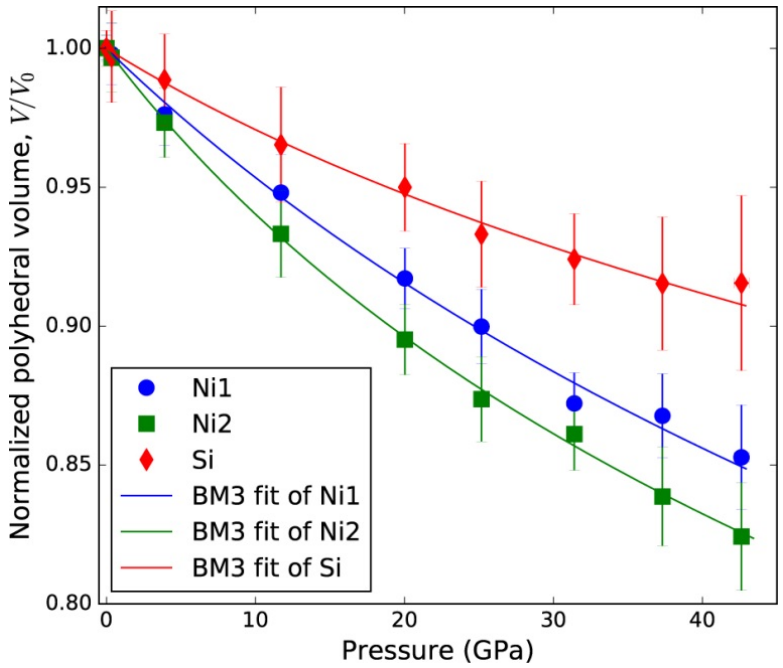

Figure S2: Pressure dependences of polyhedral volumes of liebenbergite. Weighted BM3 fits of the compressional data are plotted in this figure. BM3 fitting is carried out by the EoSFit7c software package (Angel, 2000; Angel et al., 2014).

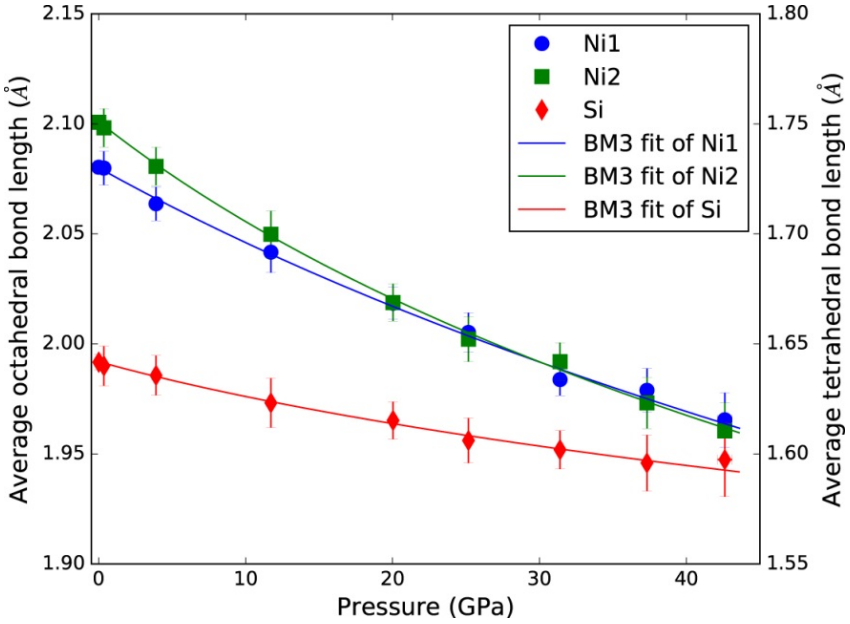

Figure S3: Pressure dependences of the average bond lengths of the three polyhedra. The average bond length is calculated from Table S3, and BM3 fitting is carried out by the EoSFit7c software package (Angel, 2000; Angel et al., 2014).

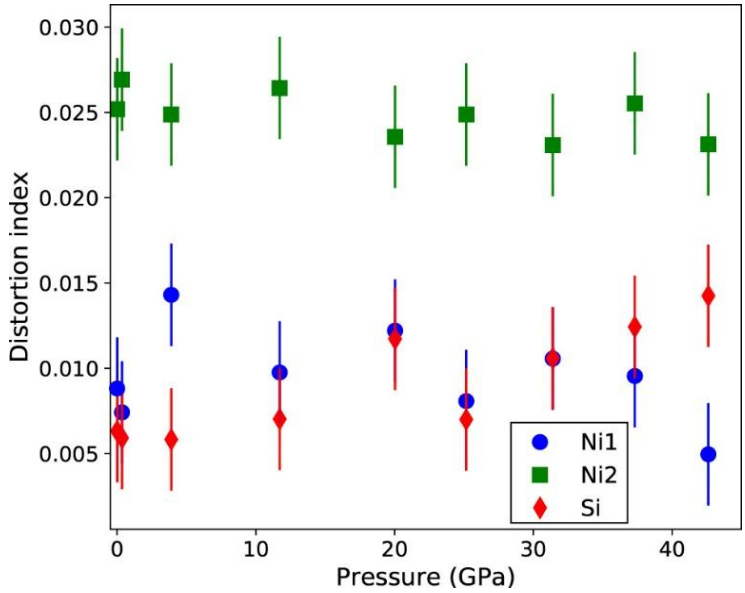

Figure S4: Pressure dependences of distortion indices of different polyhedra. The distortion index is defined by Equation (5) in the main text, and is calculated using the Vesta software (Momma and Izumi, 2008).

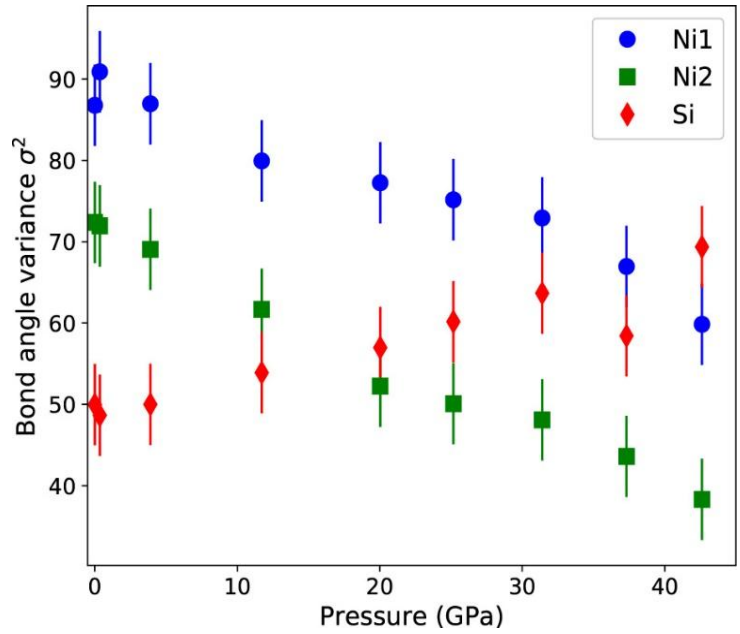

Figure S5: Pressure dependences of bond angle variances in different polyhedra. The bond angle variance is defined by Equation (6) in the main text, and is calculated using the Vesta software (Momma and Izumi, 2008).

Table S1: List of naturally found Ni-containing silicates according to IMA mineral database (Back et al., 2017): They are either an olivine, or highly hydrated minerals that are probably formed from the weathering of olivines.

Mineral Name	IMA Chemistry	Structural Groupname
Brindleyite	$(Ni,Al)_3(Si,Al)_2O_5(OH)_4$	Serpentine
Falcondoite	$Ni_4Si_6O_{15}(OH)_2 \cdot 6H_2O$	Clay
Karpinskite	$(Mg,Ni)_2Si_2O_5(OH)_2$	Corrensite
Liebenbergite	Ni_2SiO_4	Olivine
Népouite	$Ni_3Si_2O_5(OH)_4$	Clay
Nimite	$(Ni,Mg,Al)_6(Si,Al)_4O_{10}(OH)_8$	Clay
Pecoraite	$Ni_3Si_2O_5(OH)_4$	Serpentine
Willemseite	$Ni_3Si_4O_{10}(OH)_2$	Talc

Table S2: Fractional coordinates and displacement parameters of liebenbergite at different pressures.

Pressure (GPa)		0.0001	0.4(2)	3.9(3)	11.7(2)	20.0(1)	25.2(3)	31.4(2)	37.3(2)	42.6(5)
Ni1	x	0	0	0	0	0	0	0	0	0
	y	0	0	0	0	0	0	0	0	0
	z	0	0	0	0	0	0	0	0	0
	Uiso	0.00575(18)	0.0047(4)	0.0049(4)	0.0048(5)	0.0055(4)	0.0047(4)	0.0046(4)	0.0052(6)	0.0053(7)
Ni2	x	0.99257(12)	0.9922(2)	0.9919(2)	0.9914(3)	0.99069(17)	0.9906(2)	0.9901(2)	0.9898(4)	0.9892(4)
	y	0.27367(6)	0.2736(3)	0.2731(3)	0.2729(3)	0.2723(3)	0.2715(3)	0.2713(2)	0.2714(4)	0.2708(4)
	z	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
	Uiso	0.00570(18)	0.0051(4)	0.0050(4)	0.0043(5)	0.0044(4)	0.0044(5)	0.0041(4)	0.0044(5)	0.0050(7)
Si	x	0.4267(3)	0.4272(6)	0.4272(5)	0.4267(7)	0.4260(5)	0.4263(6)	0.4260(5)	0.4236(10)	0.4247(10)
	y	0.09443(14)	0.0933(6)	0.0938(6)	0.0958(8)	0.0959(6)	0.0967(7)	0.0945(6)	0.0954(9)	0.0951(10)
	z	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
	Uiso	0.0049(2)	0.0045(6)	0.0038(6)	0.0041(7)	0.0044(6)	0.0041(7)	0.0034(6)	0.0053(10)	0.0050(12)
O1	x	0.7693(7)	0.7705(13)	0.7716(13)	0.7692(15)	0.7688(12)	0.7692(15)	0.7709(12)	0.767(2)	0.766(3)
	y	0.0933(3)	0.0948(14)	0.0906(14)	0.0916(18)	0.0927(15)	0.0943(18)	0.0899(14)	0.090(2)	0.092(2)
	z	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
	Uiso	0.0063(6)	0.0054(14)	0.0057(13)	0.0044(16)	0.0081(12)	0.0065(15)	0.0063(13)	0.005(2)	0.003(2)
O2	x	0.2185(7)	0.2166(15)	0.2175(15)	0.2166(17)	0.2189(12)	0.2192(15)	0.2190(12)	0.216(2)	0.218(3)
	y	0.4450(3)	0.4461(14)	0.4460(14)	0.4442(18)	0.4460(12)	0.4435(17)	0.4440(15)	0.443(2)	0.441(2)
	z	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
	Uiso	0.0060(6)	0.0081(16)	0.0084(15)	0.0061(17)	0.0050(12)	0.0047(15)	0.0071(13)	0.0035(19)	0.006(2)
O3	x	0.2746(5)	0.2750(9)	0.2743(9)	0.2721(11)	0.2691(10)	0.2696(10)	0.2672(9)	0.2649(13)	0.2610(19)
	y	0.1630(2)	0.1625(10)	0.1653(10)	0.1652(13)	0.1676(10)	0.1661(13)	0.1669(11)	0.1682(15)	0.1670(17)
	z	0.0298(4)	0.0285(8)	0.0292(7)	0.0273(10)	0.0244(7)	0.0248(9)	0.0241(7)	0.0224(11)	0.0208(12)
	Uiso	0.0062(4)	0.0055(11)	0.0047(10)	0.0055(13)	0.0055(10)	0.0041(11)	0.0041(9)	0.0027(14)	0.0044(19)

Table S3: Bond lengths (Å) of liebenbergite at different pressures.

Pressure (GPa)	0.0001	0.4(2)	3.9(3)	11.7(2)	20.0(1)	25.2(3)	31.4(2)	37.3(2)	42.6(5)
Ni1-O1	2.067(2)	2.069(7)	2.032(7)	2.017(9)	1.998(7)	1.991(9)	1.954(7)	1.952(10)	1.952(11)
Ni1-O2	2.067(2)	2.068(6)	2.051(6)	2.036(7)	2.002(4)	1.995(6)	1.982(5)	1.980(8)	1.971(10)
Ni1-O3	2.108(2)	2.103(9)	2.108(8)	2.071(11)	2.055(8)	2.030(10)	2.015(9)	2.005(12)	1.975(14)
Ni2-O1	2.109(3)	2.091(13)	2.104(12)	2.066(16)	2.025(13)	1.987(15)	2.002(12)	1.995(17)	1.966(18)
Ni2-O2	2.037(3)	2.042(13)	2.033(13)	1.990(16)	1.991(10)	1.961(14)	1.954(12)	1.927(18)	1.910(19)
Ni2-O3	2.175(2)	2.183(7)	2.147(6)	2.123(8)	2.087(6)	2.077(7)	2.056(6)	2.037(8)	2.026(10)
Ni2-O3	2.053(2)	2.045(5)	2.027(5)	1.999(6)	1.961(5)	1.955(6)	1.942(5)	1.922(8)	1.917(9)
Si-O1	1.621(3)	1.623(6)	1.621(6)	1.600(8)	1.589(6)	1.584(7)	1.587(5)	1.574(11)	1.560(12)
Si-O2	1.662(4)	1.637(15)	1.631(15)	1.637(18)	1.603(12)	1.618(16)	1.583(14)	1.58(2)	1.59(2)
Si-O3	1.642(2)	1.650(7)	1.645(6)	1.628(8)	1.634(5)	1.611(7)	1.618(6)	1.616(9)	1.620(10)

Table S4: Isothermal bulk moduli and their pressure derivatives of different silicate olivines and spinels at ambient condition.

Olivine	K_{T0} (GPa)	K_{T0}'	Technique	Reference
Ni_2SiO_4	163(3)	4.5(3)	Single crystal X-ray diffraction	**This study**
Mg_2SiO_4	132	4(fixed)	Single-crystal X-ray diffraction	Hazen (1976)
Mg_2SiO_4	123	4.3	Single-crystal X-ray diffraction	Kudoh and Takéuchi (1985)
Mg_2SiO_4	128(8)	4.0(fixed)	Powder X-ray diffraction	Andrault et al. (1995)
Mg_2SiO_4	125(2)	4.0(4)	Single-crystal X-ray diffraction	Downs et al. (1996)
Mg_2SiO_4	124.4	4.9	Single-crystal X-ray diffraction	Poe et al. (2010)
Mg_2SiO_4	127(4)	4.2(8)	Single-crystal X-ray diffraction	Zhang (1998)
Mg_2SiO_4	130.0(9)	4.12(7)	Single-crystal X-ray diffraction	Finkelstein et al. (2014)
Mg_2SiO_4	128(2)	3.8(2)	Single-crystal X-ray diffraction	Zha et al. (1998)
Mg_2SiO_4	136(1)	4.0(1)	Powder X-ray diffraction	Will et al. (1986)
Mg_2SiO_4	125.2(2)	4.75(9)	Single-crystal X-ray diffraction	Kroll et al. (2014)
$Mg_{1.84}Fe_{0.16}SiO_4$	123.4(9)	5.5(3)	Single-crystal X-ray diffraction	Nestola et al. (2011a)
$Mg_{1.66}Fe_{0.34}SiO_4$	134(10)	4(fixed)	Powder X-ray diffraction	Andrault et al. (1995)
$Mg_{0.68}Fe_{1.32}SiO_4$	136(10)	4(fixed)	Powder X-ray diffraction	Andrault et al. (1995)
$Mg_{1.60}Fe_{0.40}SiO_4$	124(1)	5.4(3)	Single-crystal X-ray diffraction	Nestola et al. (2011b)
$Mg_{1.42}Fe_{0.58}SiO_4$	125(1)	5.1(3)	Single-crystal X-ray diffraction	Nestola et al. (2011b)
$Mg_{1.24}Fe_{0.76}SiO_4$	126.8(8)	5.2(2)	Single-crystal X-ray diffraction	Nestola et al. (2011b)
$Fe_{1.89}Mn_{0.11}SiO_4$	132	4(fixed)	Single-crystal X-ray diffraction	Kudoh and Takéuchi (1985)
Fe_2SiO_4	113	4(fixed)	Single-crystal X-ray diffraction	Hazen (1977)
Fe_2SiO_4	136.26(21)	4.88(5)	Brillouin spectroscopy	Speziale et al. (2004)
Fe_2SiO_4	125(6)	4(fixed)	Powder X-ray diffraction	Andrault et al. (1995)

Fe_2SiO_4	136(3)	4.1(7)	Single-crystal diffraction	X-ray	Zhang (1998)
Fe_2SiO_4	133.7(3)	4.84(5)	Single-crystal diffraction	X-ray	Kroll et al. (2014)
Fe_2SiO_4	135	4.0(2)	Single-crystal diffraction	X-ray	Zhang et al. (2016)
Mn_2SiO_4	125.2(4)	4(fixed)	Single-crystal diffraction	X-ray	Zhang (1998)
Co_2SiO_4	144(2)	4.1(5)	Single-crystal diffraction	X-ray	Zhang (1998)
$Mg_{0.91}Ca_{0.99}Fe_{0.09}SiO_4$	113(3)	4	Single-crystal diffraction	X-ray	Sharp et al. (1987)
$LiScSiO_4$	118	4	Single-crystal diffraction	X-ray	Hazen et al. (1996)

Spinel	K_{T0} (GPa)	K_{T0}'	Technique		Reference
Mg_2SiO_4	213(10)	4.0(fixed)	Powder diffraction	X-ray	Mizukami et al. (1975)
Mg_2SiO_4	184(6)	4.8(fixed)	Single-crystal diffraction	X-ray	Hazen (1993)
Mg_2SiO_4	182(3)	4.2(3)	Powder diffraction	X-ray	Meng et al. (1994)
Mg_2SiO_4	187	4.41(1)	Powder diffraction	X-ray	Nishihara 2004
Fe_2SiO_4	212(10)	4.0(fixed)	Powder diffraction	X-ray	Mao et al. (1969)
Fe_2SiO_4	189(12)	4.0(fixed)	Powder diffraction	X-ray	Wilburn and Bassett (1976)
Fe_2SiO_4	197(2)	4.0(fixed)	Powder diffraction	X-ray	Sato (1977)
Fe_2SiO_4	196(6)	4.0(fixed)	Powder diffraction	X-ray	Finger et al. (1979)
Fe_2SiO_4	207(3)	4.8(fixed)	Powder diffraction	X-ray	Hazen et al. (1993)
Fe_2SiO_4	187.3(17)	5.5(4)	Single-crystal diffraction	X-ray	Nestola et al. (2010)
Fe_2SiO_4	202(4)	4.0(fixed)	Powder diffraction	X-ray	Armentrout and Kavner (2011)
Ni_2SiO_4	214(7)	4.0(fixed)	Powder diffraction	X-ray	Mao et al. (1970)
Ni_2SiO_4	223(2)	4.0(fixed)	Powder diffraction	X-ray	Sato (1977)
Ni_2SiO_4	227(4)	4.0(fixed)	Powder diffraction	X-ray	Finger et al. (1979)
Ni_2SiO_4	233(2)	4.8(fixed)	Single-crystal diffraction	X-ray	Hazen (1993)

Co_2SiO_4	210(6)	4.0(6)	Single-crystal diffraction	X-ray	Liu et al. (1974)
Co_2SiO_4	206(2)	4.0(fixed)	Powder diffraction	X-ray	Sato (1977)