

Online Supplementary File

A high-pressure, clinopyroxene-structured polymorph of albite in highly shocked terrestrial and meteoritic rocks

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Table OM1. The starting crystallographic models for the Rietveld refinement the selected portion of albitic jadeite and garnet in ZNL100.**(1) Albitic Jadeite:**Unit cell (a,b,c, α , β , γ): 9.5525 8.6259 5.3000 90.000 108.050 90.000

Na	0.0000	0.3005	0.2500	0.9700	0.0131
Ca	0.0000	0.3005	0.2500	0.0300	0.0131
Al1	0.0000	0.9058	0.2500	0.7000	0.0047
Si1	0.0000	0.9058	0.2500	0.3000	0.0047
Si2	0.2906	0.0933	0.2277	1.0000	0.0044
O1	0.1092	0.0760	0.1285	1.0000	0.0057
O2	0.3611	0.2633	0.2932	1.0000	0.0078
O3	0.3537	0.0072	0.0060	1.0000	0.0070

(2) Garnet:Unit cell (a,b,c, α , β , γ): 11.6425 11.6425 11.6425 90.000 90.000 90.000

MgX	0.1250	0.0000	0.2500	0.23	0.0038
FeX	0.1250	0.0000	0.2500	0.26	0.0038
CaX	0.1250	0.0000	0.2500	0.32	0.0038
NaX	0.1250	0.0000	0.2500	0.10	0.0038
AlY	0.0000	0.0000	0.0000	0.62	0.0051
FeY	0.0000	0.0000	0.0000	0.08	0.0051
SiY	0.0000	0.0000	0.0000	0.30	0.0051
SiT	0.3750	0.0000	0.2500	1.00	0.0063
O	0.0349	0.0543	0.6580	1.00	0.0063

Table OM2. Fractional atom coordinates, site fractional occupancies, and isotropic thermal displacement factors of albitic jadeite and nearby garnet within the melt vein in amphibolite xenolith ZLN100 from Ries. SFO = site fractional occupancy, Wyck. = Wyckoff site. Isotropic displacement parameters are in Å².

Albitic jadeite (space group *C2/c*)

Atom	Wyck.	SFO	x	y	z	U _{iso}
Na M2	4e	0.70(6) ^a	0	0.311(1)	0.25	0.0075(20)
Ca M2	4e	0.03(3)	0	0.311(1)	0.25	0.0075(20)
Al M1	4e	0.70(3)	0	0.90(1)	0.25	0.024(1)
Si M1	4e	0.30(6)	0	0.90(1)	0.25	0.024(1)
Si T	8f	1	0.289(1)	0.092(1)	0.232(1)	0.028(1)
O1	8f	1	0.112(1)	0.082(2)	0.135(3)	0.026(1)
O2	8f	1	0.361(1)	0.256(2)	0.311(1)	0.023(1)
O3	8f	1	0.352(1)	0.013(1)	0.004(2)	0.031(1)

Garnet (space group *Ia-3d*)

Atom	Wyck.	SFO	x	y	z	U
Mg X	24c	0.29(1)	0.125	0	0.25	0.027(1)
Ca X	24c	0.30(3)	0.125	0	0.25	0.027(1)
Na X	24c	0.115(5)	0.125	0	0.25	0.027(1)
Fe X	24c	0.24(1)	0.125	0	0.25	0.027(1)
Al Y	16a	0.70(5)	0	0	0	0.029(1)
Si Y	16a	0.235(1)	0	0	0	0.029(1)
Mg Y	16a	0.06(6)	0	0	0	0.029(1)
Si	24d		0.375	0	0.25	0.020(3)
O	96h		0.0348(1)	0.052(1)	0.655(2)	0.017(2)

^aNumbers in parentheses are uncertainties in terms of the least significant units cited (e.g., 0.70(6) refers to 0.70 ± 0.06).

Table OM3. Interatomic distances for albitic jadeite and ideal jadeite.

Albitic jadeite:			Jadeite:		
M2	O2	2.357(1) ^a	Si	O2	1.594
	O2	2.357		O3	1.629
	O3	2.364(1)		O1	1.636
	O3	2.364		O3	1.639
	O1	2.396(2)	M1	O2	1.852
M1	O1	2.396		O2	1.852
	O2	1.913(1)		O1	1.940
	O2	1.913		O1	1.940
	O1	1.987(1)		O1	1.995
	O1	1.987		O1	1.995
	O1	2.067(1)	M2	O1	2.356
Si1	O1	2.067		O1	2.356
	O2	1.564(1)		O3	2.366
	O1	1.592(1)		O3	2.366
	O3	1.636(1)		O2	2.412
	O3	1.647(1)		O2	2.412

^aNumbers in parentheses are uncertainties in terms of the least significant units cited (e.g., 2.357(1) refers to 2.357 ± 0.001).