Supplementary Figure

Figure S1. Crystal structure of Na-majorite depicting the corner sharing linkages of the SiO_6 units and SiO_4 units as seen in the (***a***) x-y plane and (***b***) z-y plane. In the panel (***a***) and (***b***), the MgO_8 and NaO_8 units are not shown for clarity. Crystal structure of Na-Majorite showing only the arrangements of the NaO_8 units in (***c***) x-y plane and (***d***) z-y plane. The Na cations are arranged around the 4_1 screw axes and along the z-direction the NaO_8 units share edges and act as braces reducing the degree of free rotation for the corner sharing tetrahedral and octahedral units. This is the likely cause for stiffer elastic moduli along the z-axes, i.e., $C_{33} > C_{11}$.

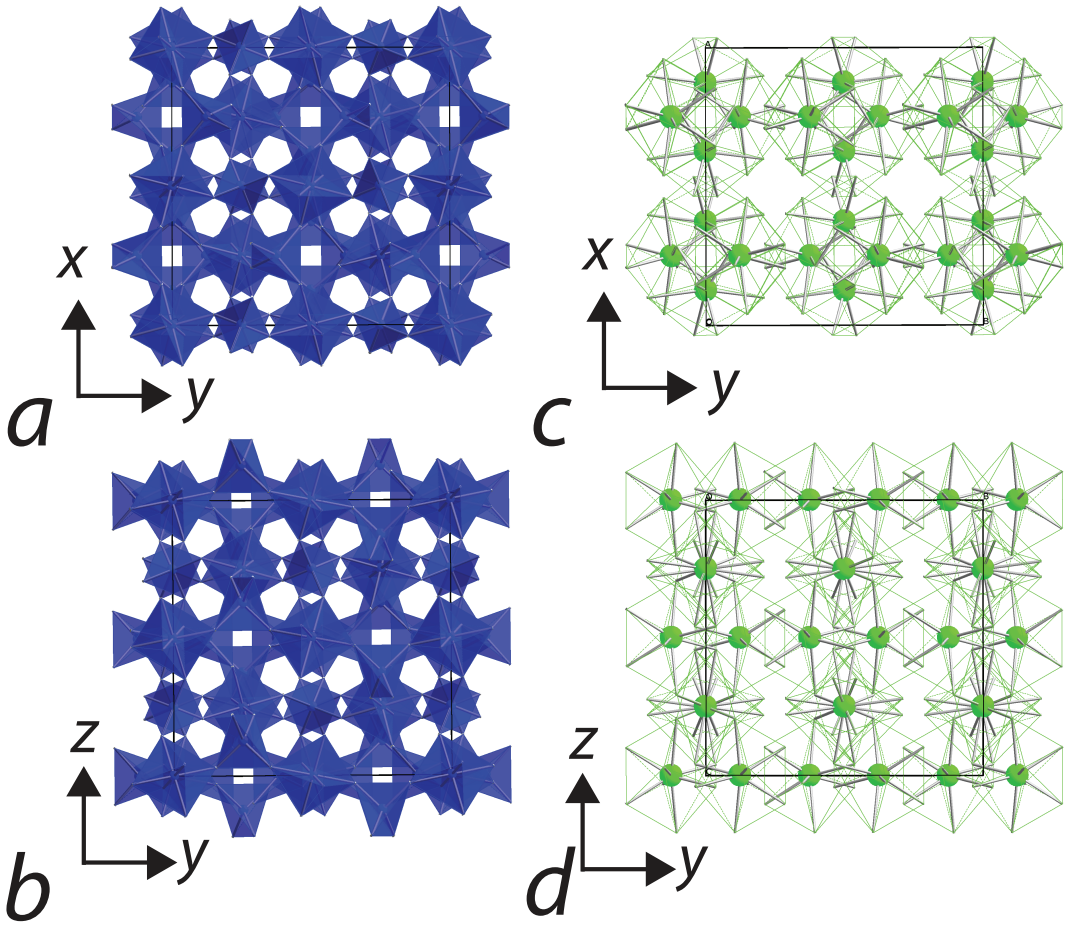

Figure S1

Supplementary Table 1. Unit-cell volume, lattice parameter, polyhedral volume as a function of pressure, based on LDA and GGA methods.

P	V	*a*	*c*	$V^{SiO_4(I)}$	$V^{SiO_4(II)}$	V^{SiO_6}	V^{MgO_8}	V^{NaO_8}
GPa	Å^3	Å				Å^3		
				LDA				
-4.2	1480	11.410	11.368	2.18	2.22	7.66	21.91	20.13
0.5	1440	11.301	11.276	2.15	2.19	7.51	21.08	19.37
5.8	1400	11.190	11.181	2.12	2.15	7.36	20.25	18.63
12.0	1360	11.079	11.080	2.08	2.11	7.21	19.44	17.91
19.1	1320	10.961	10.986	2.04	2.08	7.05	18.65	17.21
27.3	1280	10.845	10.884	2.01	2.04	6.90	17.87	16.52
36.7	1240	10.727	10.776	1.96	1.99	6.74	17.11	15.85
47.5	1200	10.606	10.667	1.92	1.95	6.58	16.36	15.20
				GGA				
-3.4	1560	11.620	11.554	2.27	2.31	8.06	21.45	23.32
0.6	1520	11.513	11.467	2.24	2.28	7.90	20.67	22.48
5.2	1480	11.407	11.374	2.20	2.24	7.73	19.95	21.68
10.4	1440	11.297	11.283	2.16	2.20	7.58	19.24	20.84
16.3	1400	11.187	11.187	2.13	2.17	7.43	18.48	20.04
23.1	1360	11.075	11.088	2.09	2.13	7.27	17.79	19.26
30.9	1320	10.961	10.987	2.05	2.08	7.10	17.13	18.50
39.9	1280	10.845	10.884	2.01	2.04	6.94	16.48	17.73
50.1	1240	10.726	10.778	1.97	2.00	6.78	15.78	17.00
62.0	1200	10.606	10.668	1.93	1.96	6.62	15.15	16.26