

## Supplementary Materials:

**Table S1.** Thermodynamic functions of pseudowollastonite at different pressures and temperatures.

$P$ , GPa	$T$ , K	$V$ , $\text{cm}^3\text{mol}^{-1}$	$\alpha \times 10^6$ , $\text{K}^{-1}$	$S$ , $\text{Jmol}^{-1}\text{K}^{-1}$	$C_P$ , $\text{Jmol}^{-1}\text{K}^{-1}$	$C_V$ , $\text{Jmol}^{-1}\text{K}^{-1}$	$K_T$ , GPa	$K_S$ , GPa	$\Delta G$ , $\text{kJmol}^{-1}$
0.0001	298.15	40.300	24.151	85.384	84.304	83.702	86.00	86.62	-1655.531
0.0001	500	40.529	31.140	135.193	107.011	105.362	83.96	85.27	-1678.027
0.0001	1000	41.245	37.854	215.976	123.959	119.335	78.23	81.26	-1767.659
0.0001	1398	41.900	41.222	258.413	129.296	121.987	73.43	77.83	-1862.474
0.0001	2000	43.019	46.461	305.799	135.683	123.439	65.93	72.47	-2033.038
3	298.15	39.000	20.964	82.710	82.624	82.127	97.21	97.80	-1536.635
3	500	39.193	27.167	131.719	105.663	104.285	95.25	96.51	-1558.500
3	1000	39.796	32.891	211.692	122.818	118.954	89.74	92.66	-1646.164
3	1500	40.490	36.112	262.739	128.818	122.169	83.95	88.52	-1765.531
3	2000	41.259	39.240	300.412	133.233	123.324	77.99	84.25	-1906.717

**Table S2.** Thermodynamic functions of breyite at different pressures and temperatures.

$P$ , GPa	$T$ , K	$V$ , $\text{cm}^3\text{mol}^{-1}$	$\alpha \times 10^6$ , $\text{K}^{-1}$	$S$ , $\text{Jmol}^{-1}\text{K}^{-1}$	$C_P$ , $\text{Jmol}^{-1}\text{K}^{-1}$	$C_V$ , $\text{Jmol}^{-1}\text{K}^{-1}$	$K_T$ , GPa	$K_S$ , GPa	$\Delta G$ , $\text{kJmol}^{-1}$
0.0001	298.15	37.780	21.924	80.428	87.549	87.123	78.60	78.98	-1651.400
0.0001	500	37.974	27.984	131.881	109.814	108.671	76.88	77.69	-1673.080
0.0001	1000	38.573	33.798	214.195	125.775	122.602	72.02	73.88	-1761.511
0.0001	1500	39.269	37.730	266.505	132.257	126.655	66.81	69.77	-1882.459
0.0001	2000	40.058	41.947	305.300	137.710	129.061	61.36	65.47	-2025.810
5	298.15	35.694	17.168	76.876	85.309	85.002	97.99	98.34	-1467.959
5	500	35.838	22.059	127.312	108.157	107.317	96.39	97.15	-1488.806
5	1000	36.282	26.409	208.628	124.338	122.013	91.85	93.60	-1574.668
5	1500	36.788	28.924	260.254	130.204	126.187	87.01	89.78	-1692.660
5	2000	37.346	31.366	298.322	134.583	128.559	81.98	85.82	-1832.708
10	298.15	34.065	14.168	74.161	83.555	83.317	116.44	116.77	-1293.711
10	500	34.179	18.322	123.801	106.873	106.213	114.93	115.64	-1313.919
10	1000	34.529	21.868	204.383	123.365	121.539	110.60	112.26	-1397.812
10	1500	34.926	23.711	255.572	128.944	125.822	105.99	108.62	-1513.570
10	2000	35.357	25.381	293.210	132.793	128.182	101.23	104.87	-1651.170

**Table S3.** Thermodynamic functions of larnite (Ca<sub>2</sub>SiO<sub>4</sub>) at different pressures and temperatures.

$P$ , GPa	$T$ , K	$V$ , cm <sup>3</sup> mol <sup>-1</sup>	$\alpha \times 10^6$ , K <sup>-1</sup>	$S$ , Jmol <sup>-1</sup> K <sup>-1</sup>	$C_P$ , Jmol <sup>-1</sup> K <sup>-1</sup>	$C_V$ , Jmol <sup>-1</sup> K <sup>-1</sup>	$K_T$ , GPa	$K_S$ , GPa	$\Delta G$ , kJmol <sup>-1</sup>
0.0001	298.15	51.880	29.925	124.047	130.523	129.069	105.00	106.18	-2344.025
0.0001	500	52.241	37.715	199.489	158.877	155.155	100.18	102.58	-2377.087
0.0001	1000	53.375	47.644	317.569	180.070	169.560	86.74	92.12	-2509.143
0.0001	1500	54.799	58.296	392.941	192.642	172.477	72.19	80.63	-2687.831
0.0001	2000	56.636	75.179	450.483	209.603	173.504	56.39	68.12	-2899.176
10	298.15	48.116	18.220	112.517	123.690	122.910	163.72	164.76	-1845.671
10	500	48.320	23.070	184.864	153.685	151.634	159.55	161.71	-1876.052
10	1000	48.945	27.642	299.353	173.924	168.391	147.95	152.81	-1999.822
10	1500	49.665	30.771	371.411	181.457	171.882	135.74	143.30	-2168.601
10	2000	50.477	34.191	424.461	187.653	173.121	123.13	133.46	-2368.130
15	298.15	46.777	15.305	108.561	121.256	120.631	191.06	192.05	-1608.542
15	500	46.944	19.475	179.824	151.946	150.281	187.09	189.16	-1637.999
15	1000	47.454	23.147	293.269	172.417	167.943	175.99	180.68	-1758.951
15	1500	48.034	25.348	364.606	179.269	171.661	164.34	171.63	-1924.508
15	2000	48.673	27.563	416.874	184.257	172.987	152.39	162.32	-2120.444

**Table S4.** Thermodynamic functions of titanite-structured CaSi<sub>2</sub>O<sub>5</sub> at different pressures and temperatures.

$P$ , GPa	$T$ , K	$V$ , cm <sup>3</sup> mol <sup>-1</sup>	$\alpha \times 10^6$ , K <sup>-1</sup>	$S$ , Jmol <sup>-1</sup> K <sup>-1</sup>	$C_P$ , Jmol <sup>-1</sup> K <sup>-1</sup>	$C_V$ , Jmol <sup>-1</sup> K <sup>-1</sup>	$K_T$ , GPa	$K_S$ , GPa	$\Delta G$ , kJmol <sup>-1</sup>
0.0001	298.15	48.190	19.961	101.151	132.729	131.710	178.00	179.38	-2524.000
0.0001	500	48.419	26.185	180.693	171.926	169.036	174.15	177.12	-2552.795
0.0001	1000	49.135	31.552	310.573	199.290	191.290	163.55	170.39	-2678.568
0.0001	1500	49.956	34.667	393.502	209.689	195.956	152.49	163.17	-2855.810
0.0001	2000	50.868	37.778	454.983	218.098	197.610	141.11	155.74	-3068.567
10	298.15	45.805	15.657	92.862	126.612	125.886	216.90	218.15	-2054.525
10	500	45.978	20.924	169.674	167.600	165.453	213.32	216.08	-2081.332
10	1000	46.521	25.217	297.126	196.111	190.095	203.36	209.80	-2200.886
10	1500	47.137	27.309	378.623	205.555	195.378	193.00	203.05	-2371.039
10	2000	47.807	29.174	438.680	212.109	197.265	182.41	196.13	-2576.005
15	298.15	44.803	14.124	89.495	124.016	123.388	235.67	236.87	-1828.049
15	500	44.957	19.038	165.139	165.751	163.859	232.19	234.87	-1854.041
15	1000	45.441	22.984	291.594	194.895	189.555	222.48	228.75	-1971.032
15	1500	45.988	24.785	372.570	204.116	195.117	212.37	222.17	-2138.284
15	2000	46.579	26.315	432.146	210.146	197.111	202.06	215.43	-2340.104

**Table S5.** Thermodynamic functions of cubic CaSiO<sub>3</sub>-perovskite at different pressures and temperatures.

<i>P</i> , GPa	<i>T</i> , K	<i>V</i> , cm <sup>3</sup> mol <sup>-1</sup>	<i>α</i> ×10 <sup>6</sup> , K <sup>-1</sup>	<i>S</i> , Jmol <sup>-1</sup> K <sup>-1</sup>	<i>C<sub>P</sub></i> , Jmol <sup>-1</sup> K <sup>-1</sup>	<i>C<sub>V</sub></i> , Jmol <sup>-1</sup> K <sup>-1</sup>	<i>K<sub>T</sub></i> , GPa	<i>K<sub>S</sub></i> , GPa	Δ <i>G</i> , kJmol <sup>-1</sup>
0.0001	298.15	27.403	24.355	61.810	84.541	83.383	239.00	242.32	-1567.400
0.0001	500	27.562	31.873	112.581	109.904	106.643	232.88	240.00	-1585.221
0.0001	1000	28.057	38.133	195.994	128.876	120.020	217.07	233.09	-1664.223
0.0001	1500	28.623	41.666	250.009	137.735	122.746	201.11	225.67	-1776.486
0.0001	2000	29.250	45.132	290.723	145.739	123.692	185.02	217.99	-1912.060
10	298.15	26.364	20.177	55.857	80.058	79.164	279.40	282.55	-1298.734
10	500	26.493	27.053	104.657	106.812	104.161	273.49	280.45	-1315.125
10	1000	26.898	32.552	186.333	126.587	119.229	258.15	274.08	-1389.659
10	1500	27.359	35.228	239.312	134.737	122.377	242.71	267.23	-1496.826
10	2000	27.862	37.614	278.992	141.394	123.480	227.23	260.19	-1626.798
15	298.15	25.912	18.560	53.329	78.040	77.244	299.01	302.09	-1168.058
15	500	26.030	25.177	101.231	105.402	102.983	293.20	300.08	-1183.835
15	1000	26.401	30.418	182.141	125.637	118.846	278.03	293.91	-1256.429
15	1500	26.823	32.821	234.708	133.586	122.197	262.78	287.28	-1361.394
15	2000	27.281	34.877	274.002	139.804	123.376	247.52	280.48	-1488.968
100	298.15	21.327	7.355	30.312	55.876	55.669	601.09	603.32	810.944
100	500	21.368	11.599	67.679	88.018	87.161	596.15	602.01	801.012
100	1000	21.518	15.350	139.617	116.006	113.054	582.19	597.39	747.918
100	1500	21.691	16.548	188.496	124.478	119.417	568.11	592.19	665.208
100	2000	21.875	17.225	224.967	128.962	121.770	554.10	586.83	561.459