

Supplementary Material

High-pressure Phase Transition of Olivine-type Mg₂GeO₄ to a Metastable Forsterite-III type Structure and their Equation of States.

R. Valli Divya¹, Gulshan Kumar¹, R. E. Cohen², Sally J. Tracy², Yue Meng³, Stella Chariton⁴, Vitali B. Prakapenka⁴, and Rajkrishna Dutta^{1,*}

¹Department of Earth Sciences, IIT Gandhinagar, Gujarat 382355, India.

²Earth and Planets Laboratory, Carnegie Institution for Science, Washington DC 20015, USA.

³HPCAT, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA.

⁴Center for Advanced Radiation Sources, University of Chicago, Chicago, IL 60637, USA.

Table S1. Observed (d_{obs}) and calculated (d_{calc}) d -spacings and their difference for olivine

Mg₂GeO₄ at 14.6 GPa.

h	k	l	d_{obs} (Å)	d_{calc} (Å)	$d_{obs} - d_{calc}$
2	0	0	4.95201	4.95116	0.00085
1	0	1	4.32317	4.32473	-0.00156
2	1	0	3.77228	3.77279	-0.00051
0	1	1	3.70813	3.70804	0.00009
2	1	1	2.96979	2.96796	0.00183
0	2	0	2.91275	2.91302	-0.00027
3	0	1	2.72168	2.72112	0.00055
3	1	1	2.46399	2.46546	-0.00147
1	2	1	2.41537	2.41605	-0.00068
2	2	1	2.22637	2.22548	0.00088

Table S2. Lattice parameters of Mg₂GeO₄ olivine at different pressures.

Pressure (GPa)	a (Å)	b (Å)	c (Å)	Volume (Å ³)
5.2	4.872 (2)	10.140 (4)	5.952 (3)	294.1 (2)
6.2	4.865 (2)	10.113 (6)	5.934 (3)	292.0 (2)
8.8	4.844 (4)	10.032 (6)	5.895 (3)	286.5 (2)
14.6	4.807 (4)	9.902 (6)	5.826 (3)	277.3 (2)
20.2	4.779 (2)	9.776 (6)	5.764 (3)	269.3 (2)
26.1	4.752 (5)	9.656 (6)	5.713 (3)	262.1 (2)
30.4	4.716 (5)	9.578 (6)	5.649 (3)	255.2 (2)
3.5	4.874 (8)	10.215 (17)	5.981 (4)	297.7 (4)
3.2	4.878 (8)	10.212 (17)	5.978 (4)	297.8 (4)
2.9	4.884 (7)	10.188 (11)	5.983 (4)	297.7 (4)
3.9	4.881 (7)	10.181 (12)	5.984 (5)	297.4 (4)
3.1	4.890 (7)	10.179 (11)	5.974 (4)	297.3 (4)
3.6	4.872 (7)	10.179 (14)	5.970 (4)	296.1 (4)
5.4	4.867 (7)	10.161 (14)	5.961 (4)	294.8 (4)
5.1	4.871 (8)	10.154 (17)	5.962 (4)	294.9 (4)
5.4	4.879 (7)	10.130 (14)	5.947 (5)	294.0 (4)
5.5	4.871 (6)	10.095 (10)	5.942 (4)	292.2 (3)
7.8	4.861 (6)	10.003 (10)	5.916 (4)	287.7 (3)
9.6	4.843 (7)	10.006 (13)	5.894 (4)	285.6 (3)
10.1	4.831 (7)	9.975 (10)	5.891 (4)	283.8 (4)
12.1	4.829 (7)	9.938 (12)	5.863 (4)	281.3 (3)
12.5	4.829 (7)	9.916 (12)	5.858 (4)	280.5 (3)
13.6	4.825 (7)	9.881 (12)	5.853 (4)	279.1 (3)
13.8	4.811 (7)	9.888 (17)	5.854 (4)	278.5 (4)
15.4	4.799 (7)	9.868 (11)	5.829 (4)	276.0 (4)
16.8	4.797 (7)	9.858 (11)	5.805 (5)	274.5 (4)
17.9	4.786 (6)	9.819 (9)	5.797 (4)	272.4 (3)
18.7	4.778 (6)	9.806 (9)	5.791 (4)	271.3 (3)
21.2	4.778 (6)	9.768 (13)	5.788 (4)	270.1 (4)
22.1	4.794 (7)	9.725 (10)	5.740 (4)	267.6 (4)
25.1	4.770 (6)	9.655 (9)	5.722 (4)	263.5 (3)
27.1	4.741 (7)	9.643 (12)	5.711 (4)	261.1 (3)
29.5	4.714 (12)	9.605 (9)	5.686 (4)	257.5 (5)
28.7	4.723 (7)	9.589 (9)	5.662 (5)	256.4 (4)
4.8	4.866 (4)	10.148 (6)	5.950 (3)	293.8 (2)
4.6	4.870 (4)	10.150 (7)	5.944 (4)	293.8 (3)
4.6	4.866 (4)	10.149 (6)	5.947 (3)	293.7 (3)
4.7	4.862 (4)	10.151 (7)	5.950 (3)	293.6 (2)
4.7	4.859 (4)	10.157 (7)	5.949 (4)	293.6 (3)
5.4	4.863 (4)	10.136 (7)	5.954 (4)	293.5 (3)

6.6	4.862 (4)	10.099 (7)	5.926 (3)	291.0 (2)
8.1	4.847 (5)	10.074 (7)	5.912 (3)	288.7 (2)
9.0	4.846 (4)	10.036 (8)	5.892 (3)	286.6 (2)
9.2	4.848 (4)	10.020 (7)	5.886 (3)	285.9 (2)
10.6	4.841 (4)	9.967 (7)	5.868 (3)	283.1 (2)
12.9	4.815 (5)	9.932 (7)	5.842 (3)	279.4 (2)
15.3	4.805 (5)	9.844 (7)	5.808 (3)	274.8 (2)
18.2	4.801 (5)	9.784 (9)	5.778 (3)	271.4 (2)
21.5	4.772 (5)	9.729 (7)	5.749 (3)	266.9 (2)
22.4	4.762 (5)	9.701 (8)	5.733 (3)	264.9 (2)
24.8	4.765 (5)	9.640 (7)	5.705 (3)	262.1 (2)
27.2	4.741 (5)	9.632 (7)	5.684 (3)	259.6 (2)

Table S3. Observed (d_{obs}) and calculated (d_{calc}) d -spacings and their difference for Fo-III type Mg₂GeO₄ at 68.0 GPa.

h	k	l	d_{obs} (Å)	d_{calc} (Å)	$d_{obs} - d_{calc}$
0	0	2	4.4664	4.45989	0.00651
0	2	1	3.94582	3.94249	0.00332
1	1	0	2.53975	2.53962	0.00014
0	2	3	2.46088	2.46268	-0.0018
1	3	1	1.92031	1.92041	-0.0001

Table S4. Lattice parameters of Fo-III type Mg₂GeO₄ at different pressures.

Pressure (GPa)	a (Å)	b (Å)	c (Å)	Volume (Å ³)
40.4	2.717 (2)	9.020 (8)	9.135 (6)	223.9 (2)
45.5	2.703 (2)	8.986 (8)	9.090 (6)	220.8 (2)
49.9	2.695 (2)	8.906 (8)	9.062 (6)	217.5 (2)
54.1	2.682 (2)	8.871 (8)	9.025 (6)	214.7 (2)
58.7	2.670 (1)	8.849 (7)	8.990 (6)	212.4 (2)
61.6	2.664 (1)	8.831 (7)	8.966 (6)	211.0 (2)
64.9	2.658 (1)	8.811 (7)	8.942 (6)	209.4 (2)
68.0	2.653 (1)	8.790 (7)	8.920 (6)	208.0 (2)
71.0	2.649 (1)	8.772 (7)	8.898 (6)	206.7 (2)
73.8	2.639 (1)	8.773 (7)	8.887 (6)	205.7 (2)