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Order-disorder and the high-pressure P1-I1 transition in anorthite

R. J. Angel

For deposit: Table 2

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Order–disorder and the $P\bar{1}$–$I\bar{1}$ transition in anorthite

Material for deposit.

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Table 2a: Unit cell data for Val Pasmeda.

	P:GPa	ΔP*	a	b	c	α	β	γ	V
1.1	0.001	–	8.171(3)	12.870(2)	14.170(4)	93.12(2)	115.89(2)	91.28(2)	1336.8(6)
2.1	0.13	↑	8.176(2)	12.869(3)	14.175(3)	93.11(3)	115.90(2)	91.29(2)	1337.9(6)
1.2	0.65	↓	8.152(1)	12.849(1)	14.144(2)	93.03(2)	115.87(1)	91.39(1)	1329.4(3)
1.3	1.40	↑	8.120(2)	12.815(2)	14.096(4)	92.88(2)	115.82(2)	91.56(2)	1316.6(6)
2.2	1.61	↑	8.116(3)	12.808(2)	14.087(4)	92.83(2)	115.84(2)	91.58(2)	1314.3(6)
1.4	1.90	↑	8.111(2)	12.805(2)	14.074(9)	92.87(3)	115.80(3)	91.61(2)	1312.5(12)
2.10	2.12	↓	8.097(1)	12.793(1)	14.058(4)	92.75(1)	115.81(2)	91.72(1)	1307.3(4)
2.9	2.38	↓	8.084(1)	12.781(1)	14.041(2)	92.74(1)	115.76(1)	91.78(1)	1302.9(2)
2.4	2.53	↓	8.081(1)	12.772(1)	14.032(3)	92.72(1)	115.75(1)	91.79(1)	1300.6(3)
1.5	2.55	↓	8.080(3)	12.770(1)	14.030(4)	92.70(2)	115.74(2)	91.81(2)	1300.3(5)
2.8	2.59	↓	8.060(1)	12.760(2)	13.997(2)	92.31(2)	115.30(1)	92.55(2)	1297.4(3)
2.5	2.63	↑	8.075(2)	12.766(1)	14.025(2)	92.70(1)	115.74(1)	91.83(1)	1298.7(3)
2.6	2.74	↑	8.055(2)	12.762(3)	13.989(3)	92.24(3)	115.29(2)	92.57(2)	1296.2(5)
2.7	2.77	↑	8.054(2)	12.758(3)	13.986(3)	92.27(3)	115.25(2)	92.58(2)	1295.8(5)
2.3	2.80	↑	8.051(3)	12.758(2)	13.983(7)	92.21(2)	115.29(3)	92.59(2)	1294.7(8)
1.6	2.95	↑	8.051(2)	12.755(2)	13.984(4)	92.27(3)	115.27(2)	92.58(2)	1294.6(5)
1.7	3.55	↓	8.029(2)	12.733(1)	13.942(4)	92.14(2)	115.23(2)	92.71(1)	1285.3(2)
1.8	4.15	↑	8.004(3)	12.711(2)	13.914(4)	92.02(2)	115.20(1)	92.81(1)	1276.8(6)
1.9	4.95	↑	7.987(2)	12.694(2)	13.882(4)	91.97(2)	115.16(2)	92.91(2)	1269.8(5)

Notes: The first column provides an experiment reference number. Uncertainties in pressures are less than ± 0.05 GPa. *Arrows indicate the direction of pressure change in the diamond anvil cell prior to the determination of the unit–cell parameters.

Table 2b: Unit cell data for Val Pasmeda/3.

Expt.	P:GPa	ΔP*	a	b	c	α	β	γ	V
17	0.001	–	8.177(1)	12.867(2)	14.170(2)	93.19(1)	115.83(1)	91.24(1)	1338.1(3)
12	1.50	↑	8.115(3)	12.808(4)	14.078(4)	92.92(3)	115.73(2)	91.57(3)	1314.4(7)
4	2.12	↓	8.099(3)	12.791(4)	14.048(5)	92.76(4)	115.68(2)	91.73(3)	1307.9(7)
3	2.38	↓	8.088(3)	12.779(3)	14.038(6)	92.74(3)	115.65(2)	91.81(3)	1304.2(7)
8	2.44	↓	8.085(3)	12.779(3)	14.034(5)	92.68(4)	115.63(2)	91.82(3)	1303.6(7)
11	2.50	↑	8.080(1)	12.768(3)	14.022(3)	92.57(2)	115.60(1)	92.00(2)	1300.9(5)
5	2.55	↑	8.081(3)	12.777(1)	14.025(2)	92.71(2)	115.61(2)	91.94(3)	1302.0(5)
2	2.58	↓	8.074(1)	12.774(3)	14.012(3)	92.60(2)	115.49(1)	92.08(2)	1300.7(4)
10	2.59	↓	8.071(3)	12.766(4)	14.009(4)	92.54(3)	115.47(2)	92.11(3)	1299.3(6)
9	2.69	↓	8.065(2)	12.769(4)	14.003(2)	92.49(2)	115.41(1)	92.20(3)	1298.7(6)
1	2.77	↑	8.066(2)	12.765(2)	13.999(3)	92.47(2)	115.40(1)	92.23(2)	1298.2(4)
6	2.94	↑	8.059(2)	12.756(2)	13.987(5)	92.45(3)	115.41(2)	92.25(2)	1295.0(6)
16	3.03	↓	8.056(4)	12.754(2)	13.983(4)	92.39(4)	115.37(2)	92.38(4)	1294.2(7)
7	3.28	↑	8.043(1)	12.749(3)	13.961(3)	92.28(2)	115.31(1)	92.50(2)	1290.1(4)
15	3.84	↓	8.023(2)	12.728(3)	13.937(2)	92.22(2)	115.26(1)	92.57(2)	1283.1(4)
14	4.26	↓	8.009(2)	12.706(5)	13.910(2)	92.13(2)	115.20(1)	92.69(3)	1276.7(6)
13	4.92	↑	7.980(2)	12.698(5)	13.866(2)	92.03(2)	115.13(1)	92.86(3)	1268.0(6)

Table 2c: Unit cell data for Val Pasmeda/8.

Expt.	P:GPa	ΔP	a	b	c	α	β	γ	V
12	0.31	↓	8.171(1)	12.866(3)	14.155(2)	93.13(1)	115.79(1)	91.34(1)	1336.0(4)
11	0.93	↓	8.146(2)	12.834(2)	14.118(2)	93.02(2)	115.75(1)	91.45(1)	1325.7(3)
10	1.11	↓	8.139(1)	12.829(2)	14.111(2)	92.97(1)	115.73(1)	91.50(1)	1323.6(3)
1	1.42	↑	8.125(1)	12.814(1)	14.095(2)	92.90(1)	115.69(1)	91.56(1)	1318.7(3)
5	1.82	↓	8.110(2)	12.802(4)	14.069(3)	92.82(2)	115.65(1)	91.70(2)	1313.1(5)
17	2.13	↓	8.099(1)	12.787(1)	14.052(2)	92.79(1)	115.62(1)	91.75(1)	1308.4(2)
4	2.65	↓	8.077(2)	12.767(1)	14.019(2)	92.61(1)	115.51(1)	91.98(2)	1301.0(3)
16	2.86	↓	8.063(1)	12.755(3)	14.003(2)	92.52(2)	115.44(1)	92.17(1)	1296.7(4)
3	3.04	↓	8.056(1)	12.752(2)	13..991(2)	92.46(1)	115.40(1)	92.21(1)	1294.7(3)
2	3.14	↑	8.052(1)	12.745(2)	13.982(2)	92.490(1)	115.37(1)	92.30(2)	1292.7(3)
15	3.48	↓	8.035(1)	12.733(2)	13.955(2)	92.32(2)	115.29(1)	92.39(2)	1287.1(3)
14	3.62	↓	8.034(1)	12.735(1)	13.953(3)	92.31(2)	115.29(1)	92.44(2)	1286.8(3)
13	3.70	↑	8.030(1)	12.736(3)	13.943(3)	92.28(1)	115.26(1)	92.47(1)	1285.6(3)
6	3.86	↑	8.022(1)	12.723(2)	13.935(2)	92.24(1)	115.26(1)	92.51(1)	1282.3(3)
7	4.17	↑	8.010(1)	12.715(2)	13.914(2)	92.16(1)	115.23(1)	92.61(1)	1278.1(3)
8	4.66	↑	7.991(1)	12.698(2)	13.887(2)	92.04(1)	115.16(1)	92.73(1)	1271.5(2)
9	4.94	↑	7.982(2)	12.864(2)	13.872(3)	92.02(2)	115.15(2)	92.74(3)	1267.5(5)

Table 2d: Unit cell data for Val Pasmeda/7.

Expt.	P:GPa	ΔP	a	b	c	α	β	γ	V
1.15	–	↓	8.182(3)	12.869(3)	14.177(2)	93.24(2)	115.79(1)	91.20(2)	1340.2(6)
4.12	–	↓	8.181(2)	12.866(2)	14.171(3)	93.25(1)	115.81(1)	91.20(1)	1339.0(4)
3.9	0.01	↓	8.183(2)	12.868(2)	14.179(5)	93.18(2)	115.79(2)	91.21(2)	1340.5(6)
4.11	0.05	↓	8.182(2)	12.868(3)	14.172(4)	93.27(2)	115.77(2)	91.24(2)	1339.7(5)
2.1	0.10	↑	8.184(1)	12.875(2)	14.174(2)	93.22(1)	115.77(1)	91.25(1)	1341.0(3)
1.1	0.58	↑	8.161(1)	12.850(1)	14.143(2)	93.10(2)	115.75(1)	91.33(1)	1332.1(3)
3.8	0.72	↓	8.157(3)	12.839(3)	14.130(6)	93.09(3)	115.80(2)	91.37(2)	1328.6(7)
1.14	0.84	↓	8.150(1)	12.834(2)	14.125(2)	93.05(1)	115.74(1)	91.39(1)	1327.0(3)
2.2	0.95	↑	8.147(1)	12.837(1)	14.119(5)	92.99(3)	115.70(2)	91.41(1)	1326.8(5)
3.17a	1.04	↓	8.140(2)	12.832(5)	14.117(3)	92.95(2)	115.72(1)	91.46(2)	1324.8(6)
3.17b	1.04	–	8.141(1)	12.826(2)	14.114(2)	93.01(1)	115.71(1)	91.44(1)	1324.2(3)
1.13	1.33	↓	8.124(3)	12.815(2)	14.095(5)	92.98(4)	115.69(3)	91.52(4)	1318.6(7)
1.2	1.40	↑	8.130(1)	12.821(4)	14.097(2)	92.97(2)	115.69(1)	91.53(2)	1320.4(5)
3.7	1.60	↓	8.119(2)	12.807(2)	14.073(5)	92.91(2)	115.67(2)	91.59(1)	1315.1(6)
3.16	1.68	↓	8.123(2)	12.815(3)	14.081(2)	92.89(2)	115.66(1)	91.59(2)	1317.5(4)
1.7	1.91	↓	8.105(1)	12.798(5)	14.062(2)	92.78(2)	115.63(1)	91.70(2)	1311.5(5)
4.10	2.23	↓	8.097(3)	12.783(2)	14.038(4)	92.75(2)	115.60(2)	91.82(2)	1306.6(5)
2.5	2.29	↓	8.093(1)	12.780(1)	14.043(2)	92.71(1)	115.60(1)	91.81(01)	1306.2(3)
3.6	2.29	↓	8.092(1)	12.782(1)	14.042(2)	92.72(1)	115.59(1)	91.81(1)	1306.3(3)
3.15a	2.49	↓	8.084(1)	12.776(2)	14.027(2)	92.67(1)	115.55(1)	91.87(1)	1303.4(3)
3.15b	2.49	–	8.081(1)	12.776(2)	14.027(3)	92.65(2)	115.54(1)	91.88(1)	1303.0(4)
1.3	2.52	↑	8.082(2)	12.769(2)	14.023(4)	92.68(3)	115.54(2)	91.87(3)	1302.1(5)
2.4	2.78	↓	8.074(1)	12.761(1)	14.014(2)	92.62(1)	115.52(1)	91.95(1)	1299.5(3)
1.4	2.83	↑	8.070(1)	12.760(2)	14.006(2)	92.59(1)	115.49(1)	91.99(1)	1298.2(3)
1.12	2.90	↓	8.069(1)	12.761(2)	14.002(2)	92.59(2)	115.49(1)	91.97(2)	1297.7(3)
1.5	3.19	↑	8.056(1)	12.747(5)	13.987(2)	92.51(2)	115.44(1)	92.12(2)	1293.4(6)
2.3	3.26	↑	8.052(1)	12.742(1)	13.981(2)	92.47(1)	115.44(1)	92.13(1)	1291.7(3)
4.1	3.27	↑	8.052(2)	12.741(3)	13.977(3)	92.50(2)	115.42(1)	92.13(5)	1291.4(5)
1.6	3.53	↑	8.044(1)	12.736(2)	13.965(1)	92.43(1)	115.38(1)	92.21(1)	1288.9(2)
3.10	3.64	↑	8.038(1)	12.729(2)	13.954(2)	92.37(1)	115.33(1)	92.27(1)	1286.6(3)
1.8	3.85	↑	8.027(1)	12.723(2)	13.943(2)	92.32(2)	115.33(1)	92.36(2)	1283.3(3)

1.9	3.88	↑	8.022(1)	12.727(3)	13.937(3)	92.29(2)	115.31(1)	92.44(2)	1282.5(4)
3.13	4.04	↓	8.021(2)	12.715(2)	13.934(4)	92.23(2)	115.30(2)	92.46(2)	1281.0(5)
3.11	4.21	↑	8.017(3)	12.715(5)	13.922(4)	92.22(3)	115.28(2)	92.45(3)	1279.5(7)
1.10	4.23	↑	8.013(1)	12.710(5)	13.920(2)	92.20(2)	115.26(1)	92.47(2)	1278.5(5)
3.12a	4.28	↑	8.010(2)	12.708(2)	13.917(3)	92.16(2)	115.27(2)	92.53(2)	1277.3(4)
3.12b	4.28	–	8.013(2)	12.709(2)	13.921(4)	92.16(2)	115.28(2)	92.53(2)	1278.2(5)
3.12c	4.28	–	8.012(3)	12.706(3)	13.920(5)	92.17(3)	115.26(2)	92.53(2)	1277.8(6)
1.11	4.57	↑	8.000(1)	12.697(2)	13.898(2)	92.15(1)	115.23(1)	92.56(1)	1273.2(3)
4.2	4.71	↑	7.992(2)	12.691(3)	13.883(3)	92.11(2)	115.21(1)	92.65(2)	1270.2(5)
4.7	5.11	↓	7.982(3)	12.681(3)	13.859(6)	92.02(3)	115.14(3)	92.76(3)	1265.9(7)
4.6	5.31	↓	7.973(3)	12.678(3)	13.848(4)	91.97(3)	115.14(2)	92.77(3)	1263.3(6)
4.5	5.54	↓	7.964(2)	12.664(6)	13.837(3)	91.93(3)	115.11(2)	92.81(3)	1259.8(7)
4.3	6.12	↑	7.941(1)	12.647(3)	13.795(2)	91.86(2)	115.03(2)	92.94(2)	1251.4(4)
4.4	6.66	↑	7.918(1)	12.630(3)	13.768(2)	91.79(2)	115.02(1)	93.01(2)	1243.8(4)
4.9	6.72	↓	7.914(2)	12.625(3)	13.761(3)	91.77(2)	115.01(1)	93.04(2)	1242.0(4)
4.8	7.52	↑	7.894(2)	12.605(2)	13.725(3)	91.68(2)	114.98(1)	93.12(2)	1234.1(4)

Table 2e: Unit cell data for Val Pasmeda/6.

Expt.	P:GPa	ΔP	a	b	c	α	β	γ	V
3.12	7.74	↑	7.889(3)	12.592(2)	13.722(5)	91.68(3)	114.98(3)	93.04(2)	1231.9(6)
3.11	7.43	↑	7.903(2)	12.602(2)	13.730(9)	91.67(3)	114.97(3)	93.03(2)	1235.8(9)
3.10	6.80	↑	7.923(2)	12.625(2)	13.772(2)	91.80(2)	115.04(1)	92.92(1)	1244.4(3)
3.9	6.17	↑	7.948(2)	12.644(2)	13.818(4)	91.95(2)	115.12(2)	92.77(2)	1253.6(5)
3.8	5.81	↑	7.960(2)	12.654(2)	13.823(6)	91.99(2)	115.14(2)	92.70(1)	1256.8(6)
2.7	5.40	↑	7.976(1)	12.673(3)	13.858(2)	92.06(1)	115.19(1)	92.65(2)	1263.9(4)
3.7	5.30	↑	7.978(2)	12.672(2)	13.863(3)	92.10(2)	115.19(2)	92.55(2)	1264.7(5)
3.6	4.81	↑	7.992(1)	12.684(1)	13.887(3)	92.18(2)	115.25(1)	92.47(2)	1269.6(4)
1.20	4.67	↑	7.998(2)	12.694(7)	13.894(2)	92.18(3)	115.25(1)	92.48(3)	1272.2(8)
2.6	4.44	↑	8.010(1)	12.703(3)	13.915(1)	92.24(1)	115.31(1)	92.40(2)	1276.3(4)
3.5	4.30	↑	8.019(2)	12.705(2)	13.925(4)	92.30(2)	115.36(2)	92.30(2)	1278.3(4)
1.19	4.17	↑	8.016(3)	12.708(7)	13.928(5)	92.23(4)	115.31(3)	92.37(4)	1279.1(9)
1.8	3.99	↑	8.027(2)	12.714(6)	13.941(3)	92.39(3)	115.41(1)	92.21(3)	1281.5(7)
2.3	3.81	↑	8.030(2)	12.724(4)	13.947(2)	92.39(2)	115.37(1)	92.23(2)	1284.0(5)
1.18	3.77	↑	8.031(1)	12.726(5)	13.948(2)	92.38(2)	115.37(1)	92.22(2)	1284.5(6)
1.7	3.66	↑	8.037(2)	12.730(3)	13.958(3)	92.43(2)	115.42(1)	92.16(2)	1286.2(5)
3.4	3.60	↑	8.046(2)	12.729(2)	13.974(8)	92.51(2)	115.49(2)	92.08(2)	1288.2(8)
1.6	3.27	↑	8.053(2)	12.743(5)	13.981(3)	92.52(2)	115.48(1)	92.03(3)	1291.7(7)
1.5	2.97	↑	8.066(2)	12.753(4)	14.002(3)	92.56(2)	115.55(1)	91.95(2)	1296.0(6)
1.2	2.79	↑	8.073(3)	12.761(5)	14.011(3)	92.58(3)	115.56(2)	91.91(4)	1298.5(7)
1.12	2.62	↓	8.080(2)	12.769(6)	14.013(5)	92.66(4)	115.51(2)	91.86(3)	1301.1(8)
1.13	2.67	↓	8.077(2)	12.769(5)	14.011(2)	92.59(2)	115.52(2)	91.90(3)	1300.5(6)
1.14	2.61	↓	8.081(1)	12.768(3)	14.017(2)	92.65(1)	115.56(1)	91.84(2)	1301.2(4)
3.3	2.58	↑	8.082(3)	12.764(3)	14.025(5)	92.67(3)	115.57(3)	91.80(3)	1301.5(6)
1.15	2.58	↓	8.082(2)	12.769(2)	14.019(3)	92.60(2)	115.55(1)	91.88(2)	1301.6(4)
2.2	2.58	↑	8.086(3)	12.766(5)	14.023(3)	92.69(2)	115.56(2)	91.81(3)	1302.4(7)
1.4	2.49	↑	8.084(2)	12.773(3)	14.030(3)	92.70(2)	115.60(1)	91.75(2)	1303.0(5)
1.16	2.47	↓	8.087(2)	12.775(3)	14.024(3)	92.67(2)	115.58(1)	91.78(2)	1303.4(5)
1.11	2.22	↑	8.095(2)	12.785(4)	14.043(3)	92.73(2)	115.62(1)	91.74(2)	1306.9(5)
1.3	2.20	↑	8.098(1)	12.781(4)	14.047(2)	92.76(2)	115.63(1)	91.75(2)	1307.2(5)
2.5	1.97	↑	8.105(2)	12.790(3)	14.059(4)	92.81(3)	115.63(2)	91.67(2)	1310.5(6)