Crystal Structure of Phase A, $Mg_7Si_2H_6O_{14}$ up to 9.4 GPa

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The specimen used in this study was a single crystal of phase A, $Mg_7Si_2H_6O_{14}$ synthesized by Kagi et al. (2000)[1] using a multi-anvil apparatus at conditions of 1000℃ and 10 GPa. Result of electron microprobe analysis yields a chemical composition of $Mg_{6.99}Si_{1.99}H_{6.06}O_{14}$. The difference of the total weight was ascribed to H_2O. Sets of X-ray diffraction intensities up to 9.4 GPa to $\sin\theta / \lambda = 0.72$ Å^{-1} were measured with a single crystal of 60x50x30 μm using synchrotron radiation of wave lengths 0.6965 Å, 0.6993 Å and 0.7026 Å at 4.5 GPa, 9.1 GPa and 9.4 GPa, respectively at the beam line BL-10A, Photon Factory, High Energy Accelerator Reasearch Organization, Tukuba, Japan. The modified Merrill-Bassett type diamond anvil pressure cell [2] was used. The pressure was calibrated using the ruby fluorescence method. The unit cell parameters obtained using 15~24 reflections with 2θ from 10° to 50° are given in Table 1. Out of 2300 reflections in a sphere which were accessible with diamond anvil high pressure cell, a total of 255~300 symmetry independent reflections were obtained by averaging the symmetry equivalent intensities in Laue group 6/m. Intensities were corrected for Lorentz factor and no absorption correction was applied because of the sufficiently small value of μr (<0.04). Final agreement factors applying the weight $1/\sigma_{hkl}^2$ for each reflection with the space froup $P6_3$ (No.173) and final atomic parameters are given in Table 1. Mean bond distances are given in Table 2. Marked compression was observed in Mg1 octahedron.

Table 1. Unit cell parameters, atomic parameters, number of Fo and R values

P(GPa))	0.0*	4.5	9.1	9.4
a (Å)	7.8603(2)	7.756(1)	7.6445(3)	7.644(1)
c (Å)	9.5730(2)	9.469(3)	9.383(7)	9.371(2)
Si1 z	0.1741(4)	0.1785(23)	0.1911(20)	0.1829(22)
B	0.33(1)	0.40(9)	0.6(1)	0.0(1)
Si2 z	0.4018(4)	0.4079(24)	0.4070(24)	0.4092(24)
B	0.36(1)	0.26(8)	0.3(1)	0.6(1)
Mg1 x	0.3722(1)	0.3734(6)	0.3752(6)	0.3757(6)
y	0.4547(1)	0.4584(7)	0.4583(7)	0.4602(6)
z	0.3857(4)	0.3878(21)	0.3946(15)	0.3901(21)
B	0.56(1)	0.47(6)	0.7(1)	0.5(1)
Mg2 x	0.2252(1)	0.2215(6)	0.2192(6)	0.2206(6)
y	0.2438(1)	0.2434(7)	0.2443(6)	0.2450(6)
z	0.1127(4)	0.1179(20)	0.1257(16)	0.1224(20)
B	0.49(1)	0.33(6)	0.2(1)	0.5(1)
Mg3 z	0.1029(4)	0.1101(26)	0.1208(21)	0.1130(25)
B	0.50(2)	0.9(1)	0.0(1)	0.9(1)
O1 x	0.2001(3)	0.2077(11)	0.2011(13)	0.2097(11)
y	0.0274(3)	0.0317(13)	0.0302(14)	0.0330(13)
z	-.0240(4)	-.0230(24)	-.0269(32)	-.0229(24)
B	0.46(2)	0.0(1)	0.9(2)	0.0(1)
O2 x	0.4766(3)	0.4728(15)	0.4748(13)	0.4700(12)
y	0.0988(3)	0.0985(15)	0.1046(13)	0.0985(12)
z	0.4844(4)	0.4848(20)	0.4836(22)	0.4815(20)
B	0.51(2)	0.4(1)	0.0(2)	0.0(1)
O3 x	0.4538(3)	0.4500(11)	0.4475(10)	0.4486(10)
y	0.2947(3)	0.2891(11)	0.2827(10)	0.2873(11)
z	0.2320(4)	0.2421(29)	0.2472(24)	0.2517(30)
B	0.54(2)	0.0(1)	0.0(2)	0.5(1)
O4 x	0.1704(3)	0.1634(10)	0.1539(11)	0.1604(9)
y	0.4367(3)	0.4344(11)	0.4310(11)	0.4370(10)
z	0.2398(5)	0.2443(27)	0.2628(29)	0.2549(25)
B	0.54(2)	0.0(1)	0.0(2)	0.0(1)
O5 B	0.53(3)	0.0(2)	0.9(4)	0.0(2)
O6 z	0.2323(6)	0.2341(32)	0.2405(33)	0.2401(33)
B	0.52(3)	0.0(2)	0.0(2)	0.0(2)
#of Fo	379	300	229	255
R(%)	5.9	9.6	7.4	7.9
Rw(%)		9.1	8.4	7.3

*Data from Horiuchi et al. (1979). z of O5 was fixed to 0.0 as origin.

Table 2. Mean bond distances

P(GPa)	0*	4.5	9.1	9.4
Si1-O	1.647(3)	1.66(2)	1.66(1)	1.67(2)
Si2-O	1.635(4)	1.64(2)	1.56(3)	1.61(2)
Mg1-O	2.140(4)	2.10(2)	2.05(2)	2.04(2)
Mg2-O	2.103(4)	2.09(2)	2,10(2)	2.09(2)
Mg3-O	2.058(3)	2.06(2)	2.09(3)	2.07(2)

*Data from Horiuchi et al. (1979)[3].

References

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