Crystallography

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Effect of pressure on the crystal structure of phase G(D), $Mg_{1.24}Si_{1.76}H_{2.48}O_6$

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The specimen used in this study was a single crystal (47x35x12μm) of phase G(D), $Mg_{1.24}Si_{1.76}H_{2.48}O_6$ synthesized at 1050˚C and 22 GPa which was previously used for the structure determination at room pressure (Kudoh et al., 1997)[1]. X-ray diffraction data at high pressures were measured with the modified Merrill-Bassett type diamond anvil cell [2] using synchrotron radiation (λ=0.6992Å) at 4.1 GPa and MoKα (50kV,40mA) radiation at 5.7 and 6.8 GPa. The fluid pressure medium was a 4:1 mixture of methanol:ethanol. The pressure was calibrated with the ruby fluorescence method. The results of structural analyses at high pressures (*R*w=6.1% for 47 *F*o at 4.1 GPa,, *R*w=8.0% for 23 *F*o at 5.7 GPa and *R*w=7.0% for 18 *F*o at 6.8 GPa) showed that the (Si,Mg)-O distance at the S-site approaches to the Si-O distance of stishovite at corresponding pressures. This fact can be interpreted by the relatively large difference of compressibility between Si and Mg which are located at the same site. The Mg-O distance compresses more than the Si-O and the (Si,Mg)-O distance at the S-site approaches to the distance of Si-O at high pressure.

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References

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Table 1. Final atomic partameters for phase G(D)

Pressure (GPa)	Ambient†	4.1	5.7	6.8
Lattice parameters	*a*=4.790(3)Å,*c*=4.344(3)Å, *V*=86.3(2) Å^3	*a*=4.752(1)Å, *c*=4.299(3)Å, *V*=84.07(9) Å^3	*a*=4.739(1)Å, *c*=4.284(2)Å, *V*=83.32(5) Å^3	*a*=4.725(3)Å, *c*=4.266(5)Å, *V*=82.5(1) Å^3
Radiation	SOR (λ=0.6990 Å)	SOR (λ=0.6992 Å)	MoKα$_1$ (λ=0.7093 Å) 50kVx200mA	MoKα$_1$ (λ=0.7093 Å) 50kVx200mA
Atomic parameters:				
S site (2d)‡	B=0.45(2)	B=1.28(18)	B=0.7(5)	B=0.2(2)
M site (1a) ‡	B=1.10(5)	B=2.07(24)	B=0.9(7)	B=0.0(2)
O site (6k) ‡	*x*=0.6319(5), *z*=0.2686(6), *B*=0.62(5)	*x*=0.627(1), *z*=0.271(4), *B*=1.59(17)	*x*=0.634(3), *z*=0.279(9), *B*=0.4(5)	*x*=0.639(3), *z*=0.276(9), *B*=0.4(3)
S-O distance	1.823(2) Å	1.793(9) Å	1.78(2) Å	1.79(2) Å
M-O distance	2.114(3) Å	2.12(1) Å	2.11(3) Å	2.07(3) Å
2θmax	60°	75°	60°	60°
No. of *F*o(>3σ*F*o)	94	47	23	18
R (%)	3.8	9.3	13.3	8.8
*R*w (%)	3.8	6.1	8.0	7.0

†Kudoh et al. (1997)[1]. ‡Wyckoff letter in space grpou $P\bar{3}1m$ (No.162).