

736 **TABLE 1.** Structure refinement results for stishovite and post-stishovite at high pressure

<i>P</i> , GPa	space group	<i>a</i> , Å	<i>b</i> , Å	<i>c</i> , Å	<i>V</i> , Å <sup>3</sup>	unique refl <sup>1</sup>	<i>R</i> <sub>int</sub> , %	<i>R</i> <sub>1</sub> , %
0	<i>P4<sub>2</sub>/mnm</i>	4.1752(1)		2.6642(1)	46.443(3)	2788	4.63	1.29
2.8(1)	<i>P4<sub>2</sub>/mnm</i>	4.1660(3)		2.6640(3)	46.24(1)	55	0.61	3.48
7.8(1)	<i>P4<sub>2</sub>/mnm</i>	4.1416(5)		2.6564(3)	45.57(1)	48	1.52	5.93
13.0(2)	<i>P4<sub>2</sub>/mnm</i>	4.1200(4)		2.6458(3)	44.91(1)	37	0.78	6.28
16.0(1)	<i>P4<sub>2</sub>/mnm</i>	4.1066(4)		2.6433(4)	44.58(1)	50	5.89	6.14
16.9(3)	<i>P4<sub>2</sub>/mnm</i>	4.1045(4)		2.6393(3)	44.464(8)	48	0.35	6.11
19.7(1)	<i>P4<sub>2</sub>/mnm</i>	4.0891(4)		2.6298(17)	43.97(3)	50	1.65	3.78
21.4(1)	<i>P4<sub>2</sub>/mnm</i>	4.0875(4)		2.6366(3)	44.05(1)	41	12.74	6.00
26.8(2)	<i>P4<sub>2</sub>/mnm</i>	4.0681(5)		2.6259(5)	43.46(1)	43	4.37	7.84
28.5(2)	<i>P4<sub>2</sub>/mnm</i>	4.0520(4)		2.6162(18)	42.95(3)	52	1.70	7.73
33.8(2)	<i>P4<sub>2</sub>/mnm</i>	4.0318(6)		2.6070(8)	42.38(2)	48	5.80	6.17
40.4(2)	<i>P4<sub>2</sub>/mnm</i>	4.0133(7)		2.6000(30)	41.88(5)	34	8.91	5.61
48.7(2)	<i>P4<sub>2</sub>/mnm</i>	3.9875(7)		2.5840(30)	41.09(5)	46	1.06	5.65
49.8(2)	<i>P4<sub>2</sub>/mnm</i>	3.9819(10)		2.5810(60)	40.92(10)	36	1.01	5.35
52.4(2)	<i>Pnmm</i>	3.9440(30)	4.0150(19)	2.5851(13)	40.93(4)	47	1.25	5.66
54.2(2)	<i>Pnmm</i>	3.9320(30)	4.0128(18)	2.5817(12)	40.73(4)	56	0.87	5.38
55.6(2)	<i>Pnmm</i>	3.9300(40)	4.0097(10)	2.5750(5)	40.58(4)	54	4.82	6.22
58.6(3)	<i>Pnmm</i>	3.9140(50)	4.0118(12)	2.5717(6)	40.38(5)	31	14.89	4.97
62.0(3)	<i>Pnmm</i>	3.9010(40)	4.0089(12)	2.5656(8)	40.12(4)	41	2.94	6.88
64.4(3)	<i>Pnmm</i>	3.8880(40)	4.0080(20)	2.5681(14)	40.01(5)	46	4.80	6.66
65.8(3)	<i>Pnmm</i>	3.8820(40)	4.0070(10)	2.5667(8)	39.93(4)	41	12.90	6.62
68.0(3)	<i>Pnmm</i>	3.8710(40)	4.0051(10)	2.5616(7)	39.71(4)	41	1.40	6.85
71.0(3)	<i>Pnmm</i>	3.8580(30)	4.0040(9)	2.5580(7)	39.51(3)	46	1.91	4.57
73.8(3)	<i>Pnmm</i>	3.8500(30)	4.0016(8)	2.5557(6)	39.37(3)	45	2.60	6.05
75.3(3)	<i>Pnmm</i>	3.8380(20)	3.9974(7)	2.5498(5)	39.12(2)	46	0.55	4.42

<sup>1</sup>unique refl: number of unique observed reflections

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745 **TABLE 2.** Oxygen positions, bond lengths, and bond angles of stishovite and post-stishovite at  
 746 high pressure. Please refer to Fig. 2 for the meaning of the atom symbols.

<i>P</i> , GPa	oxygen position		bond length, Å		bond angle, °			
	x	y	Si-O3	Si-O1(2)	∠O1-Si-O3	∠O2-Si-O3	∠O1(2)-Si-O1(2)	∠O1-Si-O2
0	0.3061(1)	0.3061(1)	1.8075(6)	1.7565(4)	90.00(5)	90.00(5)	98.65(5)	81.35(5)
2.8(1)	0.3060(3)	0.3060(3)	1.803(1)	1.755(1)	90.00(7)	90.00(7)	98.74(7)	81.26(7)
7.8(1)	0.3052(5)	0.3052(5)	1.788(3)	1.751(1)	90.00(9)	90.00(9)	98.67(8)	81.33(8)
13.0(2)	0.3046(5)	0.3046(5)	1.775(3)	1.745(1)	90.00(9)	90.00(9)	98.57(8)	81.43(8)
16.0(1)	0.3046(5)	0.3046(5)	1.769(3)	1.742(1)	90.00(9)	90.00(9)	98.70(8)	81.30(8)
16.9(3)	0.3046(3)	0.3046(3)	1.7681(13)	1.7401(9)	90.00(9)	90.00(9)	98.64(8)	81.36(8)
19.7(1)	0.3039(5)	0.3039(5)	1.757(3)	1.736(2)	90.00(9)	90.00(9)	98.45(8)	81.55(8)
21.4(1)	0.3044(6)	0.3044(6)	1.760(3)	1.737(2)	90.00(10)	90.00(10)	98.76(9)	81.24(9)
26.8(2)	0.3048(6)	0.3048(6)	1.754(3)	1.728(2)	90.00(10)	90.00(10)	98.92(9)	81.08(9)
28.5(2)	0.3038(6)	0.3038(6)	1.741(3)	1.725(2)	90.00(10)	90.00(10)	98.64(9)	81.36(9)
33.8(2)	0.3036(4)	0.3036(4)	1.731(2)	1.719(1)	90.00(8)	90.00(8)	98.67(8)	81.33(8)
40.4(2)	0.3036(4)	0.3036(4)	1.7231(17)	1.7125(16)	90.00(10)	90.00(10)	98.78(9)	81.22(9)
48.7(2)	0.3028(5)	0.3028(5)	1.708(3)	1.705(2)	90.00(9)	90.00(9)	98.56(8)	81.44(8)
49.8(2)	0.3023(4)	0.3023(4)	1.702(2)	1.704(3)	90.00(8)	90.00(8)	98.43(8)	81.57(8)
52.4(2)	0.2943(12)	0.3106(5)	1.704(4)	1.705(3)	89.87(15)	90.13(15)	98.59(14)	81.41(14)
54.2(2)	0.2912(12)	0.3121(5)	1.697(4)	1.706(3)	89.92(15)	90.08(15)	98.38(14)	81.62(14)
55.6(2)	0.2927(7)	0.3127(6)	1.702(3)	1.6986(18)	89.91(12)	90.09(12)	98.57(11)	81.43(11)
58.6(3)	0.2877(12)	0.3152(6)	1.693(4)	1.701(3)	89.96(14)	90.04(14)	98.21(13)	81.79(13)
62.0(3)	0.2854(16)	0.3167(8)	1.689(5)	1.699(4)	89.98(16)	90.02(16)	98.06(15)	81.94(15)
64.4(3)	0.2850(14)	0.3175(7)	1.687(5)	1.698(4)	89.91(16)	90.09(16)	98.28(15)	81.72(15)
65.8(3)	0.2841(14)	0.3188(7)	1.688(5)	1.696(3)	89.94(15)	90.06(15)	98.34(15)	81.66(15)
68.0(3)	0.2814(12)	0.3200(6)	1.682(4)	1.696(3)	89.96(14)	90.04(14)	98.09(14)	81.91(14)
71.0(3)	0.2807(9)	0.3211(5)	1.681(3)	1.693(2)	89.90(12)	90.10(12)	98.17(12)	81.83(12)
73.8(3)	0.2794(12)	0.3216(6)	1.677(4)	1.692(3)	89.90(14)	90.10(14)	98.07(14)	81.93(14)
75.3(3)	0.2788(8)	0.3231(4)	1.677(3)	1.687(2)	89.90(11)	90.10(11)	98.17(11)	81.83(11)

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756 **TABLE 3.** Volume ( $V_{oct}$ ), bond length distortion ( $D$ ), angle variance ( $\sigma^2$ ), and rotation angle  
757 about  $c$  axis ( $\Phi$ ) of the  $\text{SiO}_6$  octahedron in the stishovite and post-stishovite phases at high  
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$P$ , GPa	$V_{oct}$ , $\text{\AA}^3$	$D$	$\sigma^2$ , $\text{deg}^2$	$\Phi$ , $^\circ$
0	7.351(2)	0.01278(3)	27.186(7)	0
2.8(1)	7.319(4)	0.01196(7)	27.75(2)	0
7.8(1)	7.224(8)	0.00923(10)	27.35(3)	0
13.0(2)	7.128(8)	0.00745(8)	26.70(3)	0
16.0(1)	7.075(8)	0.00685(8)	27.52(3)	0
16.9(3)	7.057(9)	0.00711(11)	27.16(3)	0
19.7(1)	6.988(8)	0.00537(6)	25.96(3)	0
21.4(1)	6.994(9)	0.00582(7)	27.92(3)	0
26.8(2)	6.895(8)	0.00662(8)	28.91(3)	0
28.5(2)	6.828(9)	0.00412(5)	27.16(3)	0
33.8(2)	6.738(5)	0.00325(3)	27.32(2)	0
40.4(2)	6.659(5)	0.00276(2)	28.01(2)	0
48.7(2)	6.542(8)	0.00075(1)	26.66(3)	0
49.8(2)	6.522(10)	0.00053(1)	25.85(4)	0
52.4(2)	6.530(13)	0.00036(4)	26.85(5)	2.1(2)
54.2(2)	6.511(13)	0.00225(1)	25.52(5)	2.6(2)
55.6(2)	6.473(8)	0.00076(1)	26.71(3)	2.5(1)
58.6(3)	6.466(13)	0.00204(4)	24.52(5)	3.3(2)
62.0(3)	6.435(16)	0.00270(7)	23.63(6)	3.8(2)
64.4(3)	6.418(18)	0.00274(11)	24.92(7)	4.0(2)
65.8(3)	6.405(14)	0.00221(5)	25.31(5)	4.2(2)
68.0(3)	6.386(13)	0.00366(7)	23.79(5)	4.6(2)
71.0(3)	6.356(9)	0.00304(4)	24.26(3)	4.9(1)
73.8(3)	6.341(13)	0.00396(8)	23.68(5)	5.1(2)
75.3(3)	6.300(8)	0.00259(3)	24.29(3)	5.4(1)

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**TABLE 4.** Maximum atomic displacement ( $\Delta$ ) and distortion mode amplitude at high pressure

$P$ , GPa	$\Delta$ , Å	$GM_1^+$ , Å	$GM_2^+$ , Å
0	0.0000	0.0000	-
2.8(1)	0.0006(0)	0.0013(0)	-
7.8(1)	0.0054(1)	0.0107(2)	-
13.0(2)	0.0089(1)	0.0178(3)	-
16.0(1)	0.0089(1)	0.0178(3)	-
16.9(3)	0.0089(1)	0.0178(2)	-
19.7(1)	0.0125(1)	0.0249(2)	-
21.4(1)	0.0101(2)	0.0202(4)	-
26.8(2)	0.0077(2)	0.0155(3)	-
28.5(2)	0.0125(2)	0.0249(4)	-
33.8(2)	0.0148(2)	0.0296(4)	-
40.4(2)	0.0148(2)	0.0296(4)	-
48.7(2)	0.0195(3)	0.0391(6)	-
49.8(2)	0.0225(5)	0.0450(11)	-
52.4(2)	0.0528(18)	0.0432(14)	0.0962(32)
54.2(2)	0.0671(20)	0.0527(16)	0.1234(37)
55.6(2)	0.0624(15)	0.0403(10)	0.1181(28)
58.6(3)	0.0857(36)	0.0550(23)	0.1624(68)
62.0(3)	0.0971(54)	0.0598(34)	0.1848(104)
64.4(3)	0.1001(56)	0.0574(32)	0.1919(108)
65.8(3)	0.1061(52)	0.0550(27)	0.2049(101)
68.0(3)	0.1184(50)	0.0639(27)	0.2279(97)
71.0(3)	0.1232(40)	0.0615(20)	0.2385(76)
73.8(3)	0.1289(55)	0.0663(28)	0.2492(107)
75.3(3)	0.1343(39)	0.0609(17)	0.2616(75)

Note: distortion mode of  $GM_1^+$  occurs in stishovite below ~50 GPa, while both  $GM_1^+$  and  $GM_2^+$  modes are present in post-stishovite above ~52 GPa.

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