AM-90-433

High-pressure crystal chemistry of stishovite

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For deposit: Table 3

American Mineralogist, 75, 7-8, 739-747.

Observed and Calculated Structure Factors, P=0

FACTOR = 10.00

L	OBS	CALC
0 0 L		
0	0	600
2	269	271
0 1 L		
1	114	113
3	84	80
1 1 L		
0	236	236
1	172	165
2	154	153
3	66	64

L	OBS	CALC
0 2 L		
2	56	56
1 2 L		
0	111	109
1	196	196
2	60	59
3	116	115
2 2 L		
0	236	235
1	51	51
2	167	169

L	OBS	CALC
3 2 L		
0	36	33
1	66	64
1 3 L		
0	107	109
1	50	49
2	94	90
3 3 L		
0	186	185
2	146	147

L	OBS	CALC
2 4 L		
0	105	105
1	54	49
2	87	84
3 4 L		
1	106	105
4 4 L		
0	90	89
1	61	58

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC

Observed and Calculated Structure Factors, P=1.7 GPa FACTOR = 10.00

L	OBS	CALC
0 0 L		
0	0	600
2	282	273
0 1 L		
1	122	115
3	82	89
1 1 L		
2	163	158
3	75	59

L	OBS	CALC
0 2 L		
2	61	65
1 2 L		
0	117	108
1	208	199
2	67	57
3	123	122
2 2 L		
0	249	236
1	58	51
2	180	173

L	OBS	CALC
3 2 L		
1	73	73
1 3 L		
0	117	113
1	63	46
2	100	97
3 3 L		
0	194	189
2	156	152

L	OBS	CALC
2 4 L		
0	111	113
1	58	46
2	90	94
3 4 L		
1	114	112
4 4 L		
0	92	97

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC

Observed and Calculated Structure Factors, P=2.5 GPa FACTOR = 10.00

L	OBS	CALC
0 0 L		
0	0	600
2	270	270
3 0 L		
3	137	140
0 1 L		
1	113	112
3	81	73
1 1 L		
0	232	234
1	173	167
2	151	148
3	68	66

L	OBS	CALC
3 1 L		
0	103	105
1	52	51
4 1 L		
1	109	105
2	65	66
0 2 L		
2	49	49
1 2 L		
0	113	109
1	190	193
2	61	60
3	111	109

L	OBS	CALC
2 2 L		
0	231	234
1	53	51
2	169	166
3	30	28
4 2 L		
0	100	97
1	51	49
2	79	76
5 2 L		
1	127	131
1 3 L		
2	89	84
3	28	30

L	OBS	CALC
2 3 L		
0	37	34
1	60	58
2	28	25
3 3 L		
0	177	180
2	137	141
3 4 L		
0	41	36
1	102	100
4 4 L		
0	81	82

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC

Observed and Calculated Structure Factors, P=4.0 GPa FACTOR = 10.00

K	OBS	CALC
0 K 0		
0	0	600
1 K 0		
1	240	235
2	110	107
2 K 0		
2	237	237
3	43	33
3 K 0		
1	115	112
3	184	185
4	43	34

K	OBS	CALC
4 K 0		
2	110	106
4	92	93
1 K 1		
0	115	116
1	170	164
2	197	196
3	54	50
2 K 1		
2	53	49
4	57	46

K	OBS	CALC
3 K 1		
2	73	68
4	111	109
0 K 2		
0	276	272
2	57	59
1 K 2		
1	157	154
2	61	57
3	97	94
2 K 2		
2	175	172
4	86	87

K	OBS	CALC
3 K 2		
3	147	147
4 K 2		
1	65	61
0 K 3		
1	87	85
3	142	145
1 K 3		
1	66	62
2	113	118

K	OBS	CALC	K	OBS	CALC	K	OBS	CALC

Observed and Calculated Structure Factors, P=4.7 GPa FACTOR = 10.00

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
0 0 L			2 1 L			2 2 L			2 4 L											
0	0	600	0	112	109	2	173	172	0	102	103									
2	268	274							1	58	50									
			0 2 L			1 3 L			2	91	83									
0 1 L																				
			2	57	53	0	112	108	3 4 L											
1	113	114				1	56	51												
3	85	79	1 2 L			2	95	89	1	110	106									
1 1 L			1	191	196	2 3 L														
			2	61	60															
1	177	166	3	116	116	1	67	63												
2	154	153																		
3	71	67	2 2 L			3 3 L														
			0	235	237	2	151	149												
			1	57	51															

Observed and Calculated Structure Factors, P=9.0 GPa FACTOR = 10.00

K	OBS	CALC	K	OBS	CALC	K	OBS	CALC	K	OBS	CALC	K	OBS	CALC	K	OBS	CALC	K	OBS	CALC
0 K 0			4 K 0			3 K 1			1 K 2			1 K 3								
0	0	600	2	109	104	0	246	241	1	153	153	2	115	117						
			4	93	90	2	70	63	3	87	90									
1 K 0																				
			0 K 1			4 K 1			2 K 2											
1	234	235																		
			1	113	114	1	110	111	2	169	173									
2 K 0						3	117	107												
			1 K 1						3 K 2											
1	119	108				5 K 1														
2	239	237	1	172	166				3	143	150									
			3	60	51	2	147	139												
3 K 0									0 K 3											
			2 K 1			0 K 2														
1	110	109							1	90	80									
3	187	187	1	196	196	0	265	274	3	145	149									
			2	59	51															
			4	61	50															

Observed and Calculated Structure Factors, P=11.0 GPa FACTOR = 10.00

H	OBS	CALC
H 0 0		
0	0	600
2	33	32
4	147	139
H 1 0		
2	112	105
3	105	110
4	78	78
5	106	120

H	OBS	CALC
H 0 1		
1	114	115
3	229	234
H 1 1		
1	160	163
2	191	194
3	46	48
4	110	110
H 0 2		
0	278	267
2	73	57

H	OBS	CALC
H 0 2		
4	94	110
H 1 2		
1	148	151
2	59	56
3	100	91
4	55	59
H 0 3		
3	140	139

H	OBS	CALC
H 1 3		
0	82	81
1	64	60
2	114	113

H	OBS	CALC	H	OBS	CALC	H	OBS	CALC

Observed and Calculated Structure Factors, P=15.0 GPa FACTOR = 10.00

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
0	0	L	1	1	L	2	2	L	3	3	L									
0	0	600	1	164	162	0	238	237	0	190	185									
2	268	271	2	154	156	1	55	47	2	148	148									
			3	69	59	2	170	174												
1	0	L							4	3	L									
			2	1	L	3	2	L												
1	119	117							1	110	113									
3	87	90	1	199	197	1	74	73												
			2	60	55				4	4	L									
2	0	L	3	120	121	4	2	L												
									0	108	97									
2	63	64	3	1	L	0	111	109												
						1	66	44												
3	0	L	1	53	48	2	88	91												
			2	102	98															
3	151	147																		