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Structure and elastic properties of quartz at pressure

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Abstract

Unit cells and crystal structures were determined on a single crystal of quartz at seven pressures from 1 atm to 61.4 kbar. Unit-cell parameters are a = 4.916(1) and c = 5.4054(4)Å at 1 atm, and a = 4.7022(3) and c = 5.2561(2)Å at 61.4 kbar. Structural changes observed over this pressure range include a decrease in the Si–O–Si angle from 143.73(7)° to 134.2(1)°, a decrease in the average Si–O bond distance from 1.6092(7) to 1.605(1)Å, and an increase in distortion of the silicate tetrahedron. Several O–O distances show very large changes (11%) that can be related to the unit-cell-edge compression. As pressure is increased, the geometry of the SiO_2 (quartz) structure approaches that of the low-pressure GeO_2 (quartz) structure.

The structural changes that take place with increased temperature are not the inverses of those that occur with increased pressure; changes in the Si–O–Si angle and the tetrahedral tilt angle control thermal expansion, whereas smaller changes in the Si–O–Si angle and tetrahedral distortion control isothermal compression.

By constraining the zero-pressure bulk modulus to be equal to that calculated from acoustic data [K_T = 0.371(2) Mbar], the pressure derivative of the bulk modulus at zero pressure [K'_T = 6.2(1)] has been calculated by fitting the P–V data to a Birch-Murnaghan equation of state. The anomalously low value of Poisson's ratio in quartz can be explained by the low ratio of the off-diagonal shear moduli to the pure-shear moduli. This small ratio reflects the easily expanding or contracting spirals of tetrahedra that behave like coiled springs.

Introduction

The literature on the crystal structure and compressibility of quartz leaves many questions about its changes with pressure. As high-pressure structural refinements have not been as precise as those performed under ambient conditions, these studies report large changes (*e.g.*, the Si–O–Si interbond angle); however, subtle ones have not been previously resolvable. Recent experimental developments in our laboratory offer the potential of providing improved resolution in high-pressure structural data.

The crystal structure of quartz at room temperature and pressure has been refined many times (Young and Post, 1962; Smith and Alexander, 1963; Zachariasen and Plettinger, 1965; Le Page and Donnay, 1976; Jorgensen, 1978; d'Amour *et al.*, 1979), with the Young and Post and the Smith and Alexander papers reporting the first quality refinements of positional parameters and thermal ellipsoids. Zachariasen and Plettinger improved upon these studies by applying a secondary-extinction correction to their refinement. The Le Page and Donnay refinement again improved the R value; however, no corrections for crystal X-ray absorption or extinction were made. Both Jorgensen and d'Amour *et al.* collected intensity data for room-pressure structural refinements with crystals already loaded in high-pressure cells; these refinements are of lower precision than the others.

Static-compressibility studies on quartz were first carried out by Adams and Williamson (1923) and Bridgman (1925; 1928), and then greatly improved by Bridgman (1948a,b; 1949) and others (McWhan, 1967; Vaidya *et al.*, 1973; Olinger and Halleck, 1976; Jorgensen, 1978; d'Amour *et al.*, 1979). McWhan measured the compression of quartz in a modified Bridgman-anvil apparatus with Guinier geometry

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Table A-1: Observed and calculated structure factors for quartz at 1 atm.

H	OBS	CALC
H 0 -6		
-3	8*	12
-2	82	81
-1	78	79
0	122	124
1	7*	4
2	167	168
3	59	59
H 0 -4		
-4	9*	11
-3	58	57
-2	80	80
-1	183	186
1	99	98
2	14	14
3	82	81
4	59	58
H 0 -3		
0	86	92
H 0 -2		
-5	178	179
-4	27	26
-3	197	201
-2	87	87
-1	169	172
2	185	177
3	135	138
4	85	85
5	16	14
H 0 0		
-5	8*	0
-4	117	119
-3	84	82
-2	170	172
-1	154	154
0	0	0
H 1 -7		
-1	94	94
0	7*	6
1	78	78
H 1 -6		
-3	35	33
1	60	60
2	87	87
H 1 -5		
-1	172	176
0	103	103
1	114	115
H 1 -4		
-5	102	100
-4	93	94
-3	142	144
1	168	171
2	30	29
3	56	57
4	28	29
H 1 -3		
-1	136	134
0	16	14
1	115	112
H 1 -2		
-6	28	29
-5	62	61
-4	101	104
-3	107	106
1	232	227
2	187	187
3	161	161
4	78	77
5	61	59
H 1 -1		
-1	340	339
C	242	239
1	95	93
5	13*	17
H 1 0		
1	173	170
2	37	37
3	173	178
4	33	35
5	61	62
H 2 -7		
-1	77	78
H 2 -6		
-1	60	61
H 2 -5		
-4	88	83
-3	120	120
-2	40	39
-1	114	116
0	8*	7
1	41	[illegible]9
H 2 -4		
-5	60	60
-4	83	85
-2	8*	14
-1	168	171
3	147	146
H 2 -3		
-4	134	134
-3	81	80
-2	157	157
-1	114	113
0	289	293
1	160	162
3	9*	12
H 2 -2		
-6	46	46
-5	88	89
-4	16	17
-1	232	227
3	24	25
4	100	98
H 2 -1		
-5	19	15
-4	96	98
-3	178	176
-2	86	82
-1	96	92
1	164	164
H 2 0		
-6	113	113
-5	98	99
-4	176	180
-1	173	169
H 3 -6		
-2	87	87
-1	31	33
H 3 -5		
-4	77	77
-3	22	22
-2	119	120
-1	38	40
0	73	73
1	55	55
H 3 -4		
-2	29	30
-1	143	144
H 3 -3		
-5	15	12
-4	71	70
-3	26	27
-2	81	81
-1	160	162
0	75	74
1	63	63
2	7*	6
3	84	83
H 3 -2		
-2	184	187
-1	107	106
3	19	18
H 3 -1		
-5	148	148
-4	127	129
-3	260	260
-2	177	176
-1	163	163
0	14	14
1	73	75
2	12*	15
3	84	83
H 3 0		
-1	37	36
3	106	107
H 4 -5		
-4	8*	3
-3	79	77
-2	90	88
-1	54	55
0	48	46
H 4 -4		
-3	56	56
-2	84	84
-1	94	93
0	13	11
H 4 -3		
-6	71	70
-5	130	130
-4	110	110
-3	71	70
-2	134	134
-1	62	62
0	148	147
1	42	43
2	63	63
H 4 -2		
-3	161	161
-2	13	17
-1	102	103
H 4 -1		
-6	56	57
-5	50	49
-4	51	51
-3	126	129
-2	95	99
-1	72	74
0	153	159
1	130	132
2	38	37
H 4 0		
-3	173	178
-2	175	181
H 5 -4		
-4	30	28
-3	146	145
-2	62	60
-1	103	100
H 5 -3		
-5	7*	2
-4	132	130
-3	14	12
-2	9*	6
-1	45	43
0	22	22
H 5 -2		
-5	7*	14
-4	76	77
-3	25	25
-2	88	89
-1	61	61
H 5 -1		
-6	17	17
-5	55	56
-4	50	49
-3	146	148
-2	16	15
-1	130	132
0	19	17
1	101	99
H 5 0		
-2	98	99
-1	34	35
H 5 3		
-2	7*	12
H 6 -3		
-4	73	70
-3	85	83
-2	65	63
H 6 -2		
-5	59	59
-4	101	98
-3	20	19
-2	49	46
-1	30	29
H 6 -1		
-5	17	17
-4	58	57
-3	84	83
-2	39	37
-1	101	99
H 6 0		
-5	61	62
-4	112	113
-3	108	107

Table A-1: Observed and calculated structure factors for quartz at 20.7 kbar.

L	OBS	CALC
-4 -4 L		
-4	48	46
-3	25	28
-2	71	71
-1	17*	22
0	31	42
-4 -3 L		
-5	13*	15
-4	74	74
-2	56	58
-1	79	79
[illegible]	62	60
-4 -2 L		
-5	47	49
-4	71	69
-3	53	54
-2	44	44
-1	68	69
5	52	56
-4 -1 L		
-3	42	42
-2	72	72
-1	123	126
0	41	45
1	56	56
2	64	68
3	137	138
4	23	22
-3 -4 L		
-4	10*	13
-3	42	43
-2	66	68
-1	84	83
0	26	26
3	55	54
-3 -3 L		
-7	12*	7
-6	55	55
-3 -3 L		
-5	47	49
-4	60	57
-3	93	91
-2	10*	4
-1	66	68
0	142	142
-3 -2 L		
-7	20	7
-6	11*	10
-5	137	136
-4	66	67
-3	6*	6
-2	85	86
-1	24	20
2	18	14
-3 -1 L		
-7	85	87
-6	61	61
-5	45	47
-4	90	90
7	45	45
-3 0 L		
-5	68	69
-2 -4 L		
-4	60	60
-3	57	56
-2	105	105
-1	68	70
0	110	111
-2 -3 L		
-7	45	46
-6	14*	5
-5	51	54
-4	155	157
-3	17	16
-2	16*	14
-1	150	152
-2 -3 L		
7	11*	7
-2 -2 L		
-9	47	49
-8	43	42
-7	7*	12
-6	91	94
-5	93	91
-4	105	106
7	19	12
-2 -1 L		
-8	57	58
-7	97	96
-6	35	43
-5	30	29
9	9*	16
-2 0 L		
-6	96	95
8	17*	14
-1 -3 L		
-6	53	55
-5	87	87
-4	46	47
-1 -2 L		
-8	61	63
-7	46	42
-6	100	102
-5	121	122
-1 -1 L		
-9	38	37
-8	38	38
7	94	88
-1 0 L		
-7	21	7
-1	211	209
-1 1 L		
-7	86	87
0 -2 L		
-6	167	167
0 -1 L		
-9	30	28
-8	63	64
-6	8*	9
0	150	149
0 0 L		
-9	130	127
-6	97	98
0	0	0
0 1 L		
-9	30	32
-7	10*	7
0 2 L		
-7	71	71
-5	7*	8
1 -1 L		
-8	99	98
-6	68	68
1 0 L		
-1	314	316
1 1 L		
-9	36	38
-8	39	39
1 1 L		
-7	93	88
-6	75	76
1 2 L		
-8	57	58
-7	98	96
-6	42	43
-5	32	28
1 3 L		
-6	61	61
-5	48	47
-4	89	90
4	43	47
2 -1 L		
-6	69	76
2 0 L		
-8	19	14
-7	49	48
-5	74	73
2 1 L		
-9	18*	16
-8	61	63
-7	45	42
-6	100	102
-5	122	122
2 2 L		
-8	45	42
-7	23	11
-6	95	94
-5	90	91
-4	106	106
7	11*	11
9	51	49
2 3 L		
-7	19	7
-6	8*	10
-5	137	136
-4	66	67
-3	11*	6
-2	87	86
-1	23	20
3	14*	17
2 4 L		
-3	55	53
-2	47	44
-1	69	69
3 0 L		
-5	29	27
3 1 L		
-7	42	46
-6	53	56
-5	87	87
7	88	87
3 2 L		
-7	48	46
-6	12*	5
-5	55	54
-4	158	157
-3	20	17
-2	13*	14
-1	152	152
7	5*	7
3 3 L		
-7	13*	7
-6	59	55
-5	47	49
-4	61	57
-3	93	91
-2	10*	4
-1	65	68
0	139	142
3 4 L		
-4	75	74
-3	55	54
-2	60	58
-1	81	79
4 1 L		
-4	24	22
-3	139	138
-2	70	68
-1	58	56
0	44	45
1	122	127
2	72	72
3	46	42
4 2 L		
-5	55	56
-4	62	60
-3	57	56
-2	105	105
-1	71	70
0	112	112
4	67	68
5	50	48
4 3 L		
-5	60	60
-4	10*	14
-3	44	44
-2	66	69
-1	86	83
0	29	26
5	11*	16
4 4 L		
-4	48	46
-3	25	28
-2	72	71
-1	24	22
0	41	42

Table A-1: Observed and calculated structure factors for quartz at 37.6 kbar.

L	OBS	CALC
−4 −4 L		
−3	25	21
−2	[illegible]	68
−1	18*	20
0	33	38
1	21	20
−4 −3 L		
−5	11*	17
−4	76	74
−3	47	46
−2	72	71
−1	68	68
5	64	58
−4 −2 L		
−5	50	49
−4	68	67
−3	37	43
−2	30	39
−1	84	85
4	64	62
5	55	57
−4 −1 L		
−3	44	41
−2	75	75
−1	112	114
0	51	52
1	60	60
2	61	62
3	127	128
4	32	39
−3 −4 L		
−4	25	22
−3	45	42
−2	47	48
−1	83	84
0	19*	20
−3 −3 L		
−7	12*	8
−6	49	50
−5	36	38

L	OBS	CALC
−3 −3 L		
−4	59	56
−3	97	94
−1	47	47
0	152	151
2	8*	16
−3 −2 L		
−7	23	12
−6	14*	11
−5	126	124
−4	68	70
−3	11*	10
−2	85	83
−1	33	31
2	20	7
−3 −1 L		
−7	90	90
−6	59	62
−5	36	44
−4	77	79
−3	104	100
7	49	43
−3 0 L		
−5	62	65
−4	25	24
−2 −4 L		
−3	39	41
−2	105	103
−1	70	70
0	99	98
−2 −3 L		
−7	52	46
−6	7*	5
−5	49	51
−4	151	152
−3	29	36
−1	149	147
0	97	97

L	OBS	CALC
−2 −2 L		
−8	49	52
−7	12*	20
−6	85	89
−5	94	92
−4	112	110
−1	117	118
−2 −1 L		
−8	55	54
−7	98	98
−6	44	47
−5	25	22
−3	175	173
−1	170	169
−2 0 L		
−6	99	97
8	20	10
−1 −3 L		
−6	57	57
−5	91	90
−4	38	42
−3	105	104
−1 −2 L		
−8	57	60
−7	37	25
−6	102	103
−5	121	119
−3	50	49
−1	171	168
0	36	36
−1 −1 L		
−9	40	39
−8	34	36
−7	94	91
−3	129	125
−1 1 L		
−7	82	83

L	OBS	CALC
0 −2 L		
−6	158	158
0 −1 L		
−8	77	76
−6	11*	11
0	144	145
0 0 L		
−6	82	80
0	0	0
9	127	125
0 1 L		
−9	38	38
−7	11*	8
−1	195	192
0 2 L		
−7	76	79
−5	9*	2
1 −1 L		
−8	96	95
−6	59	60
1 0 L		
−9	14*	19
−1	309	309
1 1 L		
−9	36	39
−8	34	37
−7	92	90
−6	87	86
−5	136	134
−4	142	146
−3	129	125
1 2 L		
−8	54	54
−7	100	98

L	OBS	CALC
1 2 L		
−6	45	47
−5	26	22
−3	170	173
−1	166	170
1 3 L		
−6	62	62
−5	39	44
−4	79	80
−3	101	101
4	41	42
6	37	58
2 −1 L		
−6	86	87
−5	131	134
−4	144	146
2 0 L		
−8	9*	10
−7	48	48
−5	93	93
2 1 L		
−8	57	60
−7	31	26
−6	102	103
−5	121	119
−3	48	48
−1	162	168
0	35	37
2 2 L		
−8	52	52
−7	18*	20
−6	88	89
−5	91	92
−4	113	110
−1	116	118
7	22	20

L	OBS	CALC
2 3 L		
−6	16*	11
−5	125	124
−4	67	70
−3	11*	10
−2	83	83
−1	33	31
2 4 L		
−3	43	43
−2	43	39
−1	81	85
3 0 L		
−5	26	31
−4	84	85
3 1 L		
−7	44	43
−5	87	91
−3	106	104
7	92	90
3 2 L		
−7	50	46
−6	16*	5
−5	49	51
−4	153	152
−3	17*	36
−2	12*	7
−1	146	147
0	97	97
7	14*	12
3 3 L		
−7	12*	9
−6	51	50
−5	38	38
−4	61	56
−3	98	94
−2	2*	16
−1	46	47
0	148	151
2	21	16

L	OBS	CALC
3 4 L		
−4	76	74
−3	43	46
−2	69	70
−1	67	68
4	30	23
4 1 L		
−4	41	38
−3	127	128
−2	61	63
−1	59	60
0	50	52
1	110	114
2	78	75
3	43	41
4 2 L		
−5	58	57
−4	64	62
−3	38	41
−2	104	104
−1	70	70
0	100	98
4	68	66
5	50	49
4 3 L		
−5	58	58
−4	15*	23
−3	44	43
−2	45	48
−1	85	84
0	26	20
5	5*	17
4 4 L		
−3	22	21
−2	65	68
−1	24	20
0	33	38

Table A-1: Observed and calculated structure factors for quartz at 48.6 kbar.

L	OBS	CALC
-4 -4 L		
-3	22	23
-1	24	18
0	35	38
2	66	65
-4 -3 L		
-5	17*	20
-4	83	74
-3	40	40
-2	77	77
-1	58	61
5	53	54
-4 -2 L		
-5	50	45
-4	69	66
-2	35	33
-1	95	93
4	59	65
5	52	55
-4 -1 L		
-3	49	41
-2	78	78
-1	108	105
0	53	55
1	65	63
2	56	59
3	115	121
-3 -4 L		
-4	32	29
-3	44	41
-2	34	35
-1	81	83
0	13*	16
-3 -3 L		
-7	20*	10
-6	45	45
-5	33	33
-4	53	52
-3	98	95
-2	21	22
-1	32	34

L	OBS	CALC
-3 -3 L		
0	158	155
-3 -2 L		
-7	15*	16
-6	17*	15
-5	116	115
-4	72	72
-3	11*	11
-2	80	80
-1	37	38
7	41	44
-3 -1 L		
-7	98	90
-6	60	62
-5	40	44
-4	71	70
-3	109	107
7	40	39
-3 0 L		
-5	58	61
-4	20	18
-2 -4 L		
-3	28	32
-2	104	102
-1	72	69
0	90	90
3	37	39
-2 -3 L		
-6	14*	10
-5	51	50
-4	145	147
-3	42	46
-2	14*	8
-1	145	145
0	94	94
-2 -2 L		
-8	54	54
-7	25	27
-6	91	84

L	OBS	CALC
-2 -2 L		
-5	93	92
-4	112	112
-3	116	116
-1	119	121
-2 -1 L		
-8	53	52
-7	98	96
-6	48	50
-5	23	22
-3	173	174
-1	169	169
8	54	57
-2 0 L		
-6	100	95
-2	165	164
-1 -3 L		
-6	61	57
-5	91	92
-4	37	37
-3	110	110
-1 -2 L		
-7	26	16
-6	106	101
-5	114	116
-3	40	41
-1	167	165
0	39	37
-1 -1 L		
-9	37	39
-8	36	36
-7	91	89
-6	92	92
-3	128	127
-1 0 L		
-3	11*	9
0	137	142

L	OBS	CALC
-1 1 L		
-7	78	79
-3	138	138
0 -2 L		
-6	149	149
-2	174	169
0 -1 L		
-8	81	80
-6	12*	13
0 0 L		
-6	71	70
0	0	0
9	109	120
0 1 L		
-9	37	38
-7	11*	8
-3	13	9
-1	184	183
9	17*	15
0 2 L		
-7	86	83
-5	10*	1
1 -1 L		
-8	92	92
-6	52	55
1 0 L		
-9	22	15
-6	17	13
-1	303	301
1 1 L		
-9	37	39
-8	32	36
-7	90	89
-6	90	92
-5	134	133

L	OBS	CALC
1 1 L		
-3	128	127
1 2 L		
-8	54	52
-7	97	96
-6	48	49
-5	21	21
-3	164	174
-1	169	169
7	21	16
1 3 L		
-6	60	62
-5	41	44
-4	71	71
-1	106	108
2 -1 L		
-5	131	133
2 0 L		
-7	45	49
-5	101	101
2 1 L		
-8	55	57
-6	97	101
-5	117	116
-3	42	41
-1	171	165
0	36	38
2 2 L		
-8	56	54
-7	30	27
-6	84	85
-5	92	92
-4	113	112
-3	114	116
-1	118	120

L	OBS	CALC
2 3 L		
-6	10*	15
-5	120	115
-4	71	72
-3	10*	11
-2	82	80
-1	36	38
2	14*	8
2 4 L		
-3	34	38
-2	31	33
-1	92	93
3 0 L		
-5	23	31
-4	86	85
4	14*	18
3 1 L		
-7	45	39
-6	56	58
-5	91	92
-4	36	37
-3	110	109
7	89	90
3 2 L		
-7	46	44
-6	10*	10
-5	51	50
-4	150	147
-3	43	46
-2	16	8
-1	140	145
0	93	94
7	21	16
3 3 L		
-6	48	45
-5	36	33
-4	56	52
-3	97	94
-2	21	22
-1	31	34
0	144	155

L	OBS	CALC
3 3 L		
7	8*	10
3 4 L		
-3	41	40
-2	74	77
-1	57	61
4 1 L		
-3	126	121
-2	58	59
-1	65	63
0	55	55
1	102	105
2	79	78
3	41	41
4 2 L		
-5	58	54
-4	68	65
-3	23	32
-2	100	102
-1	71	70
0	88	90
4	62	66
5	44	45
4 3 L		
-5	59	55
-4	36	29
-3	43	41
-2	37	35
-1	83	84
0	19	16
4	75	74
5	16*	20
4 4 L		
-2	70	65
-1	11*	18
0	37	38
1	21	18
3	25	23

Table A-1: Observed and calculated structure factors for quartz at 55.8 kbar.

L	OBS	CALC
-4 -4 L		
-3	26	24
-2	71	66
-1	19	19
0	29	35
-4 -3 L		
-5	18	23
-4	75	74
-2	82	81
-1	57	59
4	32	32
5	55	54
-4 -2 L		
-5	46	45
-4	68	68
-3	29	35
-2	31	33
-1	97	98
4	63	67
5	55	54
-4 -1 L		
-3	45	41
-2	76	79
-1	104	103
0	55	57
1	62	64
2	56	58
3	121	120
4	49	53
-3 -4 L		
-3	42	42
-2	30	31
-1	84	84
0	10*	15
3	40	38
-3 -3 L		
-7	16*	11
-6	47	46
-5	31	31
-4	52	50
-3	97	96
-3 -3 L		
-2	26	25
0	160	157
1	29	29
-3 -2 L		
-7	18	18
-6	13*	17
-5	110	114
-4	70	73
-3	10*	12
-2	79	80
-1	41	42
7	46	46
-3 -1 L		
-6	64	64
-5	42	44
-4	66	67
-3	113	111
7	40	38
-3 0 L		
-4	15	14
-2 -4 L		
-3	27	29
-2	101	103
-1	72	70
0	89	88
-2 -3 L		
-6	13*	10
-5	50	51
-4	147	148
-3	51	51
-2	7*	10
-1	144	144
0	93	94
-2 -2 L		
-8	54	56
-7	30	31
-6	85	84
-5	92	92
-2 -2 L		
-4	114	114
-3	116	114
0	113	113
-2 -1 L		
-8	49	50
-7	98	97
-6	52	52
-3	174	175
-1	167	171
5	118	117
-2 0 L		
-6	100	98
-2	172	170
-1 -3 L		
-6	59	59
-5	96	96
-4	35	37
-3	114	114
-1 -2 L		
-8	60	58
-7	18	12
-6	100	101
-3	39	39
-1	166	164
0	38	39
5	24	23
-1 -1 L		
-9	37	39
-8	34	37
-7	92	91
-3	130	128
-1 0 L		
-9	37	39
-3	9*	8
-1 1 L		
-7	79	80
-6	15	15
-3	137	137
0 -2 L		
-6	147	148
0 -1 L		
-8	85	84
-6	9*	15
0	140	141
0 0 L		
-9	121	120
-6	69	68
0	0	0
0 1 L		
-7	9*	11
-3	12	8
-1	180	179
0 2 L		
-7	83	85
-5	8*	4
1 -1 L		
-8	93	93
-6	51	54
1 0 L		
-9	11*	15
-1	304	304
1 1 L		
-9	39	40
-8	31	37
-7	93	90
-6	98	97
-5	133	134
-3	129	128
1 2 L		
-8	53	50
-7	100	97
-6	50	52
-5	21	22
-3	172	175
-1	167	171
1 3 L		
-5	43	44
-4	69	67
-3	111	111
2 -1 L		
-6	97	97
-5	132	134
2 0 L		
-8	20	6
-7	49	50
-5	105	104
-2	175	168
2 1 L		
-8	60	58
-7	21	13
-6	102	101
-5	117	117
-3	40	38
-1	166	164
0	37	40
2 2 L		
-8	55	56
-7	31	31
-6	84	84
-5	91	93
-4	115	114
-3	116	115
0	114	112
2 3 L		
-6	16	17
-5	114	114
-4	75	73
2 3 L		
-3	10*	12
-2	81	80
-1	39	41
2 4 L		
-2	34	32
3 0 L		
-5	29	32
-4	89	88
5	62	62
3 1 L		
-7	33	38
-6	60	59
-5	95	96
-4	34	37
-3	116	114
6	63	63
3 2 L		
-7	47	46
-6	6*	10
-5	53	51
-4	150	148
-3	52	51
-2	21	10
-1	144	145
0	93	94
7	22	18
3 3 L		
-6	48	46
-5	31	31
-4	51	50
-3	97	96
-1	27	29
0	144	157
2	27	26
7	19	11
3 4 L		
-3	40	37
-2	82	81
3 4 L		
-1	55	59
4 1 L		
-4	54	53
-3	121	120
-2	60	58
-1	65	64
0	57	57
1	93	103
2	79	79
3	46	41
4 2 L		
-5	55	54
-4	68	67
-3	29	30
-2	104	103
-1	69	70
0	88	88
1	96	98
3	32	35
4	70	68
5	62	45
4 3 L		
-5	57	54
-4	33	32
-3	47	42
-2	34	31
-1	84	84
0	8*	14
4	75	74
5	25	23
4 4 L		
-3	25	24
-2	69	66
-1	20	19
0	35	35

Table A-1: Observed and calculated structure factors for quartz at 61.4 kbar.

L	OBS	CALC
-4 -4 L		
-3	30	27
-2	65	64
-1	16*	20
0	36	37
-4 -3 L		
-5	31	27
-4	74	75
-3	36	35
-2	82	83
-1	56	57
4	32	36
5	57	53
-4 -2 L		
-5	42	43
-4	70	68
-3	23	33
-2	26	30
[illegible]	102	103
[illegible]	73	70
3	22	28
4	69	67
5	54	53
-4 -1 L		
-3	48	42
-2	83	81
-1	103	100
0	63	59
1	70	67
2	57	58
3	117	116
-3 -4 L		
-3	43	39
-2	25	26
-1	86	82
0	11*	14
-3 -3 L		
-6	44	45
-5	33	30
-4	52	49
-3 -3 L		
-3	99	96
-2	26	27
-1	14*	23
0	165	159
-3 -2 L		
-7	14*	20
-6	24	18
-5	111	110
-4	73	73
-3	27	14
-1	45	45
2	21	13
7	47	46
-3 -1 L		
-7	94	90
-6	67	64
-5	41	44
-4	64	64
-3	116	114
7	35	36
-3 0 L		
-5	57	61
-4	11*	12
-2 -4 L		
-2	106	102
0	89	85
-2 -3 L		
-6	12*	12
-5	48	50
-4	148	145
-3	60	57
-1	148	145
0	93	93
2	79	80
3	18*	14
-2 -2 L		
-8	57	55
-7	34	34
-6	84	82
-5	95	92
-4	115	113
-3	114	113
0	110	107
-2 -1 L		
-8	48	48
-7	98	96
-6	54	52
-5	13*	23
-3	177	176
-1	173	173
7	12*	8
-1 -3 L		
-6	63	59
-5	96	96
-4	38	37
-3	119	117
-1 -2 L		
-8	58	56
-7	22	8
-6	97	99
-5	112	115
-3	36	36
-1	168	165
0	40	39
-1 -1 L		
-9	39	38
-8	35	37
-7	90	89
-6	102	99
-3	131	129
-1 0 L		
-9	35	38
-1 1 L		
-7	75	78
-6	20	16
0 -2 L		
-6	145	143
-2	173	168
0 -1 L		
-8	85	85
-6	13*	16
0	141	142
3	14	6
0 0 L		
-9	118	116
-6	67	65
0	0	0
0 1 L		
-7	8*	12
-3	8*	6
-1	177	179
0 2 L		
-7	84	85
-6	100	97
-5	11*	6
-2	176	178
1 -1 L		
-8	90	90
-6	48	51
1 0 L		
-9	14*	13
-3	136	136
-1	319	317
1 1 L		
-9	37	38
-8	34	37
1 1 L		
-7	88	89
-6	96	99
-5	133	133
-3	127	129
1 2 L		
-8	49	48
-7	98	96
-6	49	52
-5	15*	22
-1	166	173
1 3 L		
-5	41	44
-4	64	64
-3	112	115
2 -1 L		
-5	138	133
2 0 L		
-7	46	49
-5	106	106
2 1 L		
-8	59	56
-7	17*	8
-6	92	99
-5	112	116
-3	35	35
-1	164	165
0	38	40
3	169	176
2 2 L		
-7	31	34
-6	81	82
-5	94	92
-4	113	113
-3	112	113
0	106	107
8	53	55
2 3 L		
-6	20*	19
-5	112	110
-4	73	73
-3	15*	13
-2	78	80
-1	43	45
2	10*	13
2 4 L		
-2	23	29
-1	96	102
3 0 L		
-5	27	33
-4	89	89
3 1 L		
-7	40	36
-6	58	60
-5	94	96
-4	36	37
-3	118	117
6	62	63
7	92	90
3 2 L		
-7	51	46
-6	12*	12
-5	48	50
-4	143	145
-3	57	57
-2	19	13
-1	140	145
0	90	93
7	16*	20
3 3 L		
-6	48	45
-5	36	30
-4	46	49
-3	97	96
-2	27	27
-1	11*	23
0	151	159
3 4 L		
-3	32	35
-2	83	83
-1	50	57
4 1 L		
-3	118	116
-2	59	58
-1	65	67
0	60	59
1	96	100
2	79	81
3	48	42
4 2 L		
-5	52	53
-4	69	67
-3	21	28
-2	100	103
-1	67	70
0	83	85
3	29	33
4	69	68
5	40	43
4 3 L		
-5	57	53
-4	37	36
-3	40	40
-2	32	26
-1	80	82
0	12*	13
4	76	75
5	31	27
4 4 L		
-3	27	27
-2	65	64
-1	27	20
0	36	37
1	17*	20