

High-pressure crystal structure and compressibility of coesite

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Abstract

Unit-cell and crystal-structure parameters have been measured on a coesite single crystal at six pressures. Unit-cell parameters of coesite change from $a = 7.1356(3)$, $b = 12.3692(8)$, $c = 7.1736(3)$ Å and $\beta = 120.34(02)^\circ$ at 1 atm to $a = 6.9897(4)$, $b = 12.233(2)$, $c = 7.1112(4)$ Å and $\beta = 120.74(03)^\circ$ at 51.9 kbar. Both silicate tetrahedra compress significantly but do not distort over the 52 kbar pressure range. All unconstrained Si-O-Si angles and Si...Si distances decrease over the pressure range, with smaller angles and distances decreasing more than larger ones. Values for the bulk modulus [$K_T = 0.96(3)$ Mbar] and its pressure derivative [$K_T' = 8.4(1.9)$] have been calculated by fitting the P - V data to a Birch-Murnaghan equation of state. The compressibility of the coesite structure is highly anisotropic with the stiffest direction parallel to the chains of tetrahedra, which run \parallel to c , and the most flexible direction \perp to these chains in the a - c plane. The criss-crossing of silicate tetrahedral chains in the a - b planes, at different levels along c , gives b an intermediate compressibility.

The increasing temperature factor of O(1), the central anion in the 180° Si-O-Si angle, suggests that this angle becomes unstable at high pressures. Because substitution of Ge for Si has a similar effect on the structure as does increased pressure, GeO_2 may not exist in the coesite structure because the 180° Ge-O-Ge angle destabilizes the structure.

Introduction

The high-pressure crystal structure of SiO_2 (coesite) has been studied to help us better understand the structural elements which give rise to its single-crystal elastic moduli and to permit a comparison between coesite and SiO_2 (quartz), the low-pressure polymorph. We felt that investigations of these two silica polymorphs, because of their simple chemistry, would increase our understanding of the changes that silicate tetrahedra undergo at high pressure, and we would thus better understand the behavior of all silicates under pressure. We also hoped to gain some insight into why GeO_2 apparently is not stable in the coesite structure.

Experimental techniques

The coesite crystals were synthesized at 65 kbar and 1100°C [this temperature was reported incorrectly as 110°C in Gibbs *et al.* (1977)]. Observations made under the optical microscope and with pre-

cession and Weissenberg X-ray photographs showed the crystals to be untwinned. Crystal #1 was an elongated hexagonal plate with dimensions $90 \times 60 \mu\text{m}$ and thickness of $30 \mu\text{m}$. Intensity data were collected on this crystal at ambient conditions and two high pressures. Refinements of the high-pressure data gave reasonable R values, but very large errors on positional parameters; in addition, structural parameters did not show regular changes as a function of pressure. The combination of the small size of the crystal, coupled with the increased background caused by the diamond cell, resulted in very low peak-to-background ratios (42% of intensities were $< 2\sigma_I$). A third high-pressure data set, collected with a higher-intensity X-ray beam, gave a refinement with smaller errors on the positional parameters, but the refinement still was not satisfactory. Therefore, we have included the unit-cell data collected on crystal #1 in this report, but not the structural refinements. We next selected a larger crystal ($160 \times 80 \times 60 \mu\text{m}$), and collected data until this crystal was broken in the diamond cell during an unsuccessful remounting attempt. The largest remaining fragment ($120 \times 80 \times$

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-4 12 L		-3 3 L		-3 7 L		-3 13 L		-2 2 L		-2 6 L		-2 12 L	
L	OBS	L	OBS	L	OBS	L	OBS	L	OBS	L	OBS	L	OBS
0	197	1	26	6	45	1	211	4	82	7	97	0	367
1	14*	2	330	7	125	2	361	5	21	8	128	1	548
2	367	3	650	8	111	3	196	6	19*	9	25*	2	310
3	299	4	189	9	127	4	340	7	70			3	154
4	202	5	451		126	5	112	8	120	-2	8	4	30
5	139	6	292	-3	9	6	409	9	24*			5	348
6	143	7	104		L		405		29			6	64
7	129	8	109	1	118		L	-2	4	0	285	7	380
		9	259	2	729		L		L	1	466		381
			245	3	121		L		L	2	124		
				4	679	1	147	0	536	3	518	-2	14
0	479			5	170	2	409	1	516	4	442		L
1	88			6	790	3	470	2	346	5	698	0	408
2	629	1	160	7	39	4	186	3	226	6	205	1	85
3	139	2	81	8	34	5	379	4	619	7	674	2	37
4	105	3	103		43		366	5	351	8	200	3	345
5	135	4	93	-3	11		L	6	122			4	154
		5	316		L		L	7	344	-2	10	5	356
		6	629	1	101	0	725	8	15*				365
		7	307	2	95	2	1294	9	242	0	394	-1	1
		8	22*	3	94	4	1301		L	1	185		L
		9	278	4	586	6	486		L	2	217	1	74
			264	5	22*	8	150	0	881	3	389	2	301
			L	6	185		143	1	806	4	313	3	329
1	409			7	155		L	2	269	5	413	4	225
2	212*	1	119		480		L	3	82	6	156	5	1130
3	156	2	298	4	188	0	571	4	106	7	440	6	109
4	251	3	747	5	151	1	1015	5	12*			7	685
5	351	4	162		621	2	225	6	57			8	198
6	749	5	623			3	344		L			9	313
7	565						285		L				323
8	199								L				
9	529								L				

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
-1	3	L	7	41	53	5	251	253	0	1501	1428	5	599	600	2	130	118	0	364*	312
2	478	461	8	99	88	6	132	129	1	377	381	3	273	277	3	235	231	1	653	641
3	364	318							2	280	315	4	409	491	4	265	259	2	132	136
4	347	337	-1	9	L	-1	15	L	3	485	481	5	235	211	5	235	211	3	547	541
5	758	746							4	107	111	0	10	L				4	704	717
6	181	181	1	37	46	1	201	203	5	312	317	0	525	525	1	1	L	5	409	407
7	274	274	2	1052	1035	2	86	77	6	512	529	1	78	79	0	55	55	6	375	382
8	79	84	3	68	70	3	215	216	7	265	253	2	17*	25	1	886	894	7	139	123
9	16*	12	4	643	643	4	60	73	8	544	533	3	351	355	2	515	472			
			5	74	76				5	194	187	4	135	138	3	920	909			
			6	15*	18	0	0	L	6	96	104	4	208	205	4	425	428			
			7	113	114	0	0	L	7	208	205	5	89	79	5	483	489			
-1	5	L				0	0	L	8	544	533	6	96	104	6	89	79	1	7	L
1	108	102				0	0	L	0	43	40	7	208	205	7	38	47	0	680	675
2	41*	69				0	0	L	1	58	57	8	160	145	8	160	145	1	609	597
3	240	253	-1	11	L	2	1324	1298	2	564	564	0	12	L				2	387	399
4	63	56				4	602	583	3	107	107	0	71	68				3	352	348
5	661	661	1	275	276	6	242	244	4	440	441	1	336	337	7	38	47	4	181	180
6	368	372	2	218	219	8	471	460	5	269	286	2	107	110	8	160	145	5	264	264
7	455	453	3	257	263				6	218	227	0	71	68				6	51	47
8	518	510	4	303	313	0	0	L	7	119	139	1	336	337	1	3	L	7	608	603
			5	252	253	0	217	223	8	109	105	2	107	110	0	716	714			
			6	24	7	1	210	209	0	917	887	3	559	555	1	818	813	1	9	L
			7	16*	1	2	431	415	0	8	L	4	76	87	2	179	195	0	893	907
						3	105	108	0	917	887	5	296	301	3	664	660	1	217	223
						4	233	236	0	8	L	6	179	182	4	443	437	2	850	866
						5	452	450	0	917	887	7	8*	0	5	8*	0	3	45	43
						6	74	80	1	524	515	8	66	57	6	66	57	4	79	74
						7	192	197	2	234	234	0	14	L	7	435	430	5	154	156
						8	21*	4	3	810	818	0	273	292	8	121	122	6	74	73
									4	9*	5	1	15*	7						

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
0	207	207	4	506	501	1	51	47	1	34	42	6	31	34	1	88	82	1	34	42
1	312	323	5	202	199	2	750	770	2	33	12	2	678	688	2	187	186	2	33	12
2	546	556	6	217	213	3	131	131	3	21*	6	8	133	135	3	10*	7	3	21*	6
3	347	357	7	131	133	4	772	790	4	212	206	4	115	106	4	138	142	4	212	206
4	671	681	8	131	133	5	182	176	5	161	158	5	115	106	5	209	214	5	161	158
5	384	384	9	131	133	6	244	248	6	33	29	6	9	9	6	65	62	6	33	29
6	321	322	-6	12	L	7	472	483	-5	9	L	7	9	L	7	255	257	-4	4	L
7	420	426	0	212	211	8	194	198	1	88	82	8	252	250	1	88	82	0	25	11
8	36	29	1	296	291	9	56	50	2	187	186	2	252	250	2	187	186	1	68	68
9	503	510	2	345	342	3	417	410	3	10*	7	3	209	214	3	10*	7	2	582	561
-6	8	L	3	417	410	4	204	207	4	138	142	4	252	250	4	138	142	3	228	230
0	121	119	5	23*	11	5	136	137	5	65	62	5	252	250	5	65	62	4	213	212
1	397	395	6	136	137	6	136	137	6	255	257	6	252	250	6	255	257	6	17*	17
2	159	159	-5	1	L	7	136	137	7	255	257	7	252	250	7	255	257	7	196	192
3	646	648	1	257	256	8	136	137	8	252	250	8	252	250	8	252	250	8	73	73
4	159	160	2	470	480	9	136	137	9	252	250	9	252	250	9	252	250	9	144	137
5	301	300	3	396	406	10	136	137	10	252	250	10	252	250	10	252	250	10	144	137
6	57	56	4	640	665	11	136	137	11	252	250	11	252	250	11	252	250	11	144	137
7	294	300	5	528	534	12	136	137	12	252	250	12	252	250	12	252	250	12	144	137
8	203	195	6	106	111	13	136	137	13	252	250	13	252	250	13	252	250	13	144	137
-6	10	L	7	229	232	14	136	137	14	252	250	14	252	250	14	252	250	14	144	137
0	97	96	8	404	410	15	136	137	15	252	250	15	252	250	15	252	250	15	144	137
1	293	291	9	420	439	16	136	137	16	252	250	16	252	250	16	252	250	16	144	137
2	301	300	10	483	476	17	136	137	17	252	250	17	252	250	17	252	250	17	144	137
3	491	488	11	483	476	18	136	137	18	252	250	18	252	250	18	252	250	18	144	137

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
-1	3	L	-1	7	L	-1	13	L	0	4	L	0	8	L	0	14	L	1	5	L
1	436	433	7	41	46	5	251	250	0	1503	1434	5	600	596	2	130	120	0	364*	315
2	478	461	8	99	97	6	132	132	1	377	381	6	273	275	3	235	230	1	654	642
3	364	322	-1	9	L	-1	15	L	2	280	310	7	489	502	4	266	260	2	132	132
4	347	337	1	37	41	1	201	199	3	485	482	0	10	L	5	236	227	3	548	547
5	759	759	2	1053	1043	2	86	80	4	107	109	0	525	530	1	1	L	4	705	726
6	181	180	3	68	68	3	215	211	5	312	310	0	78	79	0	55	56	5	410	412
7	274	271	4	644	650	4	60	61	6	512	522	1	17*	16	1	888	895	6	376	383
8	79	80	5	74	77	0	0	L	7	265	260	2	351	350	2	515	474	7	140	136
9	16*	21	6	15*	19	0	0	L	8	545	545	3	194	194	3	921	915	1	7	L
-1	5	L	7	113	113	0	0	L	0	6	L	0	43	42	4	426	440	0	681	665
1	108	99	0	0	0	0	0	0	0	43	42	1	78	79	1	88	84	1	610	600
2	41*	68	2	1326	1306	1	58	58	1	58	58	2	351	350	2	484	490	2	388	392
3	240	254	4	603	583	2	565	564	2	565	564	3	135	138	3	89	84	3	353	359
4	63	60	6	242	236	3	107	107	3	107	107	4	208	219	6	38	46	4	181	182
5	662	672	8	472	476	4	441	450	4	441	450	5	194	194	7	160	158	5	264	264
6	369	375	0	0	0	5	269	285	5	269	285	6	97	96	8	160	158	6	51	49
7	455	460	0	2	L	6	219	222	6	219	222	0	71	61	1	3	L	7	609	613
8	518	521	1	210	222	7	119	123	7	119	123	1	336	335	0	717	713	0	894	913
-1	7	L	2	431	416	8	109	106	8	109	106	2	107	115	1	819	813	1	218	218
1	396	383	3	105	107	0	8	L	0	8	L	3	559	555	2	179	196	2	851	865
2	576	560	4	234	243	1	210	210	0	919	888	4	77	81	5	8*	3	3	45	43
3	387	374	5	453	465	2	431	416	1	524	516	5	297	295	6	66	59	4	79	80
4	475	473	6	74	80	4	234	243	1	524	516	6	180	184	7	435	442	5	154	157
5	457	461	7	193	187	5	453	465	2	235	235	0	14	L	8	121	126	6	74	71
6	65	63	8	21*	6	6	74	80	3	811	823	0	273	281	1	15*	4			
							8	21*	4	9*	3	1	15*	4						

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
0	140	143	1	61*	83	1	376	389	0	338	367	0	584	586	2	109	110
1	409	408	2	492	487	2	557	557	1	242	234	1	40	52	3	71	69
2	20*	20	3	195	207	3	333	332	2	610	620	2	406	415			
3	126	133	4	187	193	4	161	159	3	108	112	3	755	750			
4	221	217	5	474	478	5	289	289	4	230	228	4	284	288			
5	273	272	6	69	71	6	83	83	5	128	133	5	535	539			
6	153	151	7	492	489				6	302	305	6	57	57			
1	13	L	2	4	L	2	10	L	3	3	L	3	9	L			
0	435	429	1	310	311	1	192	198	0	738	751	0	342	350			
1	98	90	2	838	826	2	565	563	1	270	270	1	40	39			
2	369	360	3	232	221	3	321	323	2	696	703	2	25	22			
3	259	260	4	262	257	4	154	152	3	523	537	3	147	144			
4	186	187	5	188	184	5	134	137	4	345	343	4	70	69			
5	7*	18	6	297	304	6	2	L	5	305	313	5	216	212			
			7	36	33												
1	15	L	2	6	L	2	12	L	3	5	L	3	11	L			
0	239	231	1	189	209	1	320	324	0	559	562	0	28	22			
1	277	275	2	862	878	2	452	456	1	168	169	1	99	95			
2	301	297	3	12*	9	3	135	133	2	766	786	2	142	135			
3	19*	12	4	364	366	4	161	165	3	146	140	3	669	676			
			5	267	274	5	26*	20	4	396	403	4	52	56			
			6	158	156				2	14	L						
2	0	L				1	135	133	3	277	273						
2	58	51				2	604	600	4	123	119						
4	251	277				3	379	379	5	277	273						
6	73	64							6	123	119						

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
-2	0	L	-1	1	L	0	0	L	1	3	L	2	2	L	3	3	L	3	3	L	4	4	L	4	4	L
-10	77*	112	-9	87	75	-2	1478	1428	-9	44*	5	-10	84	79	-9	257	243	-9	110	114	-9	110	114	-11	72*	62
-8	198	212	-7	32*	41	0	0	0	-7	262	262	-9	42*	31	-8	91	92	-8	239	247	-10	365	346	-10	365	346
-6	101	85	-1	934	937	0	0	0	-7	32*	71	-7	32*	71	-4	239	247	-4	239	247	-8	211	210	-8	211	210
-4	260	258	-1	934	937	0	0	0	0	2	L	2	-4	L	1	-3	L	1	-3	L	4	-4	L	4	-4	L
0	746	773	-1	3	L	-9	385	361	-9	215	214	-9	215	214	-9	385	361	-9	215	214	-9	385	361	-9	215	214
-2	2	L	-7	431	434	-7	123	140	-8	58*	12	-8	58*	12	-7	123	140	-8	58*	12	-7	123	140	-8	58*	12
-7	506	486	-3	637	642	8	74	41	8	74	41	8	74	41	8	74	41	8	74	41	8	74	41	8	74	41
-5	478	473	8	74	41	8	74	41	8	74	41	8	74	41	8	74	41	8	74	41	8	74	41	8	74	41
-3	166	166	0	-4	L	0	169	165	-10	92	94	-10	92	94	0	169	165	-10	92	94	0	169	165	-10	92	94
-2	4	L	-8	513	554	-8	41*	41	-10	61*	79	-10	61*	79	-8	41*	41	-10	61*	79	-8	41*	41	-10	61*	79
-5	177	178	-7	251	261	-4	338	337	-8	143	148	-8	143	148	-4	338	337	-8	143	148	-4	338	337	-8	143	148
8	74	12	-6	534	560	1	-1	L	-7	77	71	-7	77	71	1	-1	L	-7	77	71	-7	77	71	-7	77	71
8	74	12	-4	127	132	-4	127	132	-5	23*	47	-5	23*	47	-4	127	132	-5	23*	47	-4	127	132	-5	23*	47
-1	-3	L	0	-2	L	-10	142	130	-2	195	195	-2	195	195	-10	142	130	-2	195	195	-2	195	195	-2	195	195
-9	146	179	0	-2	L	-8	162	151	-8	162	151	-8	162	151	-8	162	151	-8	162	151	-8	162	151	-8	162	151
-8	110	111	-2	306	310	0	54	53	-2	306	310	0	54	53	-2	306	310	0	54	53	-2	306	310	0	54	53
-6	47*	48	-10	104	98	0	54	53	-10	337	351	-10	337	351	0	54	53	-10	337	351	-10	337	351	-10	337	351
-1	-1	L	-8	46*	22	-4	200	205	-8	46*	22	-8	46*	22	-4	200	205	-8	46*	22	-8	46*	22	-8	46*	22
-1	-1	L	-4	200	205	-2	450	441	-6	82	93	-6	82	93	-4	200	205	-6	82	93	-6	82	93	-6	82	93
-10	165	167	-2	450	441	-11	38*	24	-6	467	462	-6	467	462	-11	38*	24	-6	467	462	-6	467	462	-6	467	462
-8	137	115	0	0	L	-9	308	312	-2	1524	1526	-2	1524	1526	0	0	L	-9	308	312	-2	1524	1526	-2	1524	1526
-6	85	83	-7	716	705	-7	716	705	10	112	112	10	112	112	-7	716	705	10	112	112	-7	716	705	10	112	112
-9	186	183	-10	326	314	-1	62	64	-12	337	351	-12	337	351	-1	62	64	-12	337	351	-12	337	351	-12	337	351
-7	468	486	-8	533	525	7	75	41	-10	530	513	-10	530	513	7	75	41	-10	530	513	-10	530	513	-10	530	513
-5	208	209	-4	551	534	9	70*	75	-6	62	64	-6	62	64	9	70*	75	-6	62	64	-6	62	64	-6	62	64
2	62*	87	-4	551	534	9	70*	75	-6	62	64	-6	62	64	9	70*	75	-6	62	64	-6	62	64	-6	62	64
2	62*	87	-4	551	534	9	70*	75	-6	62	64	-6	62	64	9	70*	75	-6	62	64	-6	62	64	-6	62	64

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC						
-9	41*	26	6	-4	L	7	-3	L	7	3	L	8	2	L	9	-1	L	10	0	L	11	1	L	12	0	L
-8	68	37	-10	100	81	-9	319	335	-11	160	158	0	109	119	-12	399	383	-10	293	266	-10	49*	137	-10	50*	36
-6	125	123	-8	265	260	-7	165	164	-9	220	203	-9	277	274	-9	160	159	-8	102	73	-8	136	168	-8	136	168
			-6	336	340	-5	235	239	-7	83	84	9	1	L	-6	480	466	-7	91	87	-7	53*	30	-6	46*	18
			-4	384	386	-3	110	96	-5	63*	91	-12	85	51	-4	625	631	-6	45*	84	-5	202	214	-4	84	60
			-2	268	273	-1	310	330	-3	104	111	-11	36*	5	-2	162	165	-4	75	72	-3	209	210	-3	75	72
-12	237	237	0	169	174	8	-4	L	-1	226	241	-9	466	445	2	104	105	-2	47*	3	2	43*	31	-1	47*	3
-10	195	203	2	60*	60	8	4	L	-7	604	581	-7	604	494	10	2	L	12	0	L	10	2	L	12	0	L
-8	138	152	7	-1	L	7	343	347	-6	343	320	-5	519	494	10	2	L	12	0	L	10	2	L	12	0	L
			-12	161	167	-10	155	161	-7	240	223	-3	187	189	10	2	L	12	0	L	10	2	L	12	0	L
-12	58*	35	-10	155	161	-9	61*	58	-5	289	305	-2	74	72	-10	49*	137	-9	160	159	-9	160	159	-8	136	168
-10	123	120	-8	314	311	-8	314	311	-3	129	141	-2	114	123	-7	53*	30	-7	160	159	-7	53*	30	-6	46*	18
-8	48*	25	-6	248	246	-6	248	246	-2	515	524	-1	114	123	-5	202	214	-5	202	214	-5	202	214	-4	84	60
-4	34*	7	-2	80	50	-2	80	50	-1	199	212	-1	199	212	-1	199	212	-3	209	210	-3	209	210	-2	37*	17
			0	197	192	0	197	192	9	-3	L	9	277	274	9	-3	L	9	277	274	-1	43*	31	-1	43*	31
			7	1	L	-4	41*	12	-8	49*	87	-8	77	87	9	-3	L	9	277	274	11	-1	L	11	-1	L
-11	281	272	-2	31*	22	-2	31*	22	-6	114	105	-7	328	321	-8	49*	87	-5	188	181	-7	328	321	-10	117	130
-9	663	631	2	97	72	2	97	72	-4	319	311	-3	40*	63	-4	319	311	-3	40*	63	-10	117	130	-8	141	152
-7	549	550	-11	44*	14	8	0	L	-2	272	264	-1	297	292	-7	69*	87	-7	69*	87	-8	141	152	-7	69*	87
-3	569	575	-7	288	293	8	0	L	-1	272	264	9	-1	L	10	-2	L	-6	91	79	-6	91	79	-5	81	84
			-5	625	627	-12	190	199	-10	32*	49	9	-1	L	10	-2	L	-6	91	79	-5	81	84	-4	46*	27
			-1	427	418	-10	497	471	-8	52*	31	-10	107	137	-10	32*	49	-10	107	137	-4	46*	27	-4	46*	27
			-7	288	293	-8	372	347	-8	52*	31	-8	118	116	-8	52*	31	-8	118	116	-2	117	106	-2	117	106
			-5	625	627	-6	330	330	-6	156	165	-6	101	103	-6	156	165	-6	101	103	-2	117	106	-2	117	106
			-1	427	418	-4	543	545	-4	46*	44	-4	49*	47	-4	46*	44	-4	49*	47	-2	117	106	-2	117	106
-7	132	125	-2	847	842	-2	847	842	-2	49*	72	-2	56*	85	-2	49*	72	-2	56*	85	-2	117	106	-2	117	106

Table A-3: Observed and calculated structure factors for coesite at 31.5 kbar.

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC			
-12	0	L	-9	-1	L	-7	-3	L	-6	-2	L	-5	-1	L	-4	0	L	-3	1	L
4	4*	56	11	75	28	-4	132	122	-6	42*	4	-8	90	92	-8	105	86	-7	255	255
-11	-1	L	-9	1	L	-2	89	62	-4	44*	4	-6	165	180	-6	226	226	-5	155	172
0	234	242	-1	329	330	-7	-1	L	-2	62*	99	-4	230	244	0	433	446	-3	38*	38
-11	1	L	-8	-4	L	-6	13*	11	-6	34*	72	-2	237	232	-4	742	744	-3	3	L
3	75	67	0	392	409	-5	229	267	-4	463	450	-5	350	357	-4	2	L	-5	272	266
5	39*	76	-8	-2	L	-2	102	113	-2	496	480	-3	83	95	-5	80	52	-1	334	350
-10	-2	L	-2	203	200	-1	72	79	-6	2	L	-3	83	95	-4	4	L	-2	-4	L
0	65*	58	-4	43*	39	-7	1	L	-5	24*	21	-5	3	L	-3	221	222	-7	44*	15
-10	0	L	-2	82	66	-3	292	300	-3	147	132	-3	167	165	-3	-3	L	-6	287	284
0	80	84	-8	0	L	-1	60*	79	-1	403	404	-4	-4	L	-8	193	212	-5	169	171
-9	-3	L	-4	48*	40	9	80	38	-6	4	L	-5	98	95	-8	52*	26	-2	772	799
-1	407	420	-2	332	321	-1	110	112	-1	181	179	-4	31*	91	-6	162	158	-9	290	292
0	274	279	0	699	679	-6	-4	L	9	65	30	-4	-2	L	-4	333	333	-8	98	106
-9	-1	L	-8	2	L	-6	-4	L	-5	-3	L	-8	97	94	-3	-1	L	-6	45*	61
-3	100	113	-1	75	75	-3	228	236	-6	184	203	-7	106	104	-9	188	211	0	529	521
-2	161	146	5	66	74	-2	140	123	-5	214	209	-6	40*	52	-8	208	223	10	23*	88
0	85	95	0	699	679	0	350	364	-4	168	175	0	398	394	-2	638	647	-2	0	L
									-2	74	75				-8	185	191	-6	109	93
															0	751	769			

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
-2	0	L	-1	3	L	0	2	L	2	-4	L	2	4	L	2	4	L	4	-4	L	4	-4	L	5	-3	L
8	58*	65	-7	432	430	-9	354	336	-9	199	207	-9	300	309	-7	300	309	-4	251	263	-4	251	263	-11	81	59
-2	2	L	-3	615	622	-7	104	116	-8	35*	7	-8	35*	7	-8	35*	7	-4	585	638	-4	585	638	-10	361	343
-7	507	491	8	66	27	1	-3	L	-4	585	638	1	-3	L	1	-3	L	3	-3	L	3	-3	L	3	-3	67
-5	470	471	9	67	9	-10	166	164	2	-2	L	2	-2	L	2	-2	L	2	-2	L	2	-2	L	2	-2	219
7	61	64	0	-4	L	-8	38*	27	-11	108	89	-10	83	88	-8	102	97	-8	234	235	-8	234	235	0	693	707
-1	-3	L	-8	530	553	-4	328	330	-10	83	88	-8	165	161	-4	148	151	-4	23*	2	-4	23*	2	5	-1	L
-9	128	172	-7	245	256	1	-1	L	-2	183	186	-8	165	161	-2	183	186	4	60*	74	4	60*	74	-13	62*	46
-8	109	103	-6	546	567	-11	37*	6	2	0	L	-2	183	186	2	0	L	2	0	L	2	0	L	-12	191	193
-6	42*	52	-4	162	149	-10	150	132	-12	346	361	-10	553	533	-8	178	177	-12	242	252	-10	242	252	-10	471	446
-1	-i	L	0	-2	L	-8	144	134	-10	553	533	-8	79	65	-8	178	177	-10	53*	77	-10	53*	77	5	1	L
-10	130	156	-10	97	104	0	53	52	-6	449	443	-6	449	443	3	1	L	-6	184	178	-6	184	178	-11	160	167
-8	113	104	-8	33*	36	1	1	L	-2	1492	1480	-2	1492	1480	-11	151	162	-11	151	162	-11	151	162	-9	386	379
-7	60*	39	-4	183	189	-9	294	297	-8	79	65	-8	79	65	-9	473	483	-9	473	483	-9	473	483	-3	432	421
-6	86	87	-2	450	446	-7	701	702	2	2	L	2	2	L	-5	384	380	-5	384	380	-5	384	380	5	3	L
-1	1	L	0	0	L	-1	57	58	-9	31*	33	-9	31*	33	3	3	L	-11	368	368	-9	110	85	5	3	L
-9	90	71	-10	314	311	9	69*	71	-9	42*	64	-7	42*	64	3	3	L	-9	110	85	-9	110	85	-9	74	67
-7	69	39	-8	544	539	-1	57	58	-7	42*	64	-7	42*	64	-9	250	244	-9	250	244	-9	250	244	-7	465	476
-1	927	922	-4	520	501	1	3	L	-5	60	58	-5	60	58	4	-4	L	-7	186	183	-7	186	183	-5	223	220
			-2	1461	1382	1	3	L	-1	1053	1092	-1	1053	1092	4	-4	L	-7	186	183	-7	186	183	-1	121	127
			0	0	0	-9	39*	9	-9	39*	9	-9	39*	9	-9	115	107	-9	115	107	-9	115	107	4	66	91
			0	0	0	-7	247	255	-7	247	255	-7	247	255	-8	81	99	-8	81	99	-8	81	99	4	66	91

Table A-3: Observed and calculated structure factors for coesite at 38.7 kbar.

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
-12	0	L	-9	1	L	-6	0	L	-5	1	L	-4	2	L	-3	3	L
4	67*	48	-1	326	343	-6	58*	79	-7	165	176	-7	113	99	-5	265	257
-11	-1	L	2	77	69	-4	457	466	-5	347	350	-6	78	54	-1	371	375
0	255	258	-8	-4	L	-2	491	482	-3	85	83	-5	677	696	-4	53*	75
-11	1	L	0	426	433	12	97	19	-5	3	L	-3	701	710	-2	-4	L
7	93	67	-5	270	283	-6	2	L	-3	170	178	-4	4	L	-7	59*	14
-10	-2	L	-3	326	308	-5	48*	9	9	81	74	-4	4	L	-6	315	295
0	48*	51	-1	77	75	-4	39*	8	-4	-4	L	-3	240	239	-2	807	799
-10	0	L	-7	3	L	-3	154	137	-4	-4	L	-3	-3	L	-2	-2	L
0	41*	77	-1	113	112	-1	393	413	-5	100	95	-7	36*	32	-9	321	311
8	85	60	-6	-4	L	-6	4	L	-4	18*	73	-6	162	168	-8	113	109
-9	-3	L	0	686	693	-1	183	184	-4	-2	L	-4	331	335	-6	43*	65
0	265	278	-3	236	240	-5	-3	L	-6	55*	54	-3	-1	L	-2	0	L
-9	-1	L	-2	140	131	-6	199	215	-4	70	75	-9	176	207	-10	88	78
8	70	53	0	353	365	-5	223	207	0	393	392	-8	234	235	-8	176	184
-9	-1	L	-6	-2	L	-4	178	184	-4	0	L	-6	332	314	-6	131	107
0	45*	88	-6	77	6	-2	81	71	-4	0	L	-2	648	658	0	755	779
8	70	53	-4	75	8	-5	-1	L	-8	110	90	-3	1	L	8	72	57
-3	113	115	-2	89	99	-6	232	253	-6	216	210	-7	260	253	-2	2	L
0	45*	88	-2	89	99	-4	404	389	0	735	737	-5	170	182	-7	515	509
8	70	53	-2	91	66	-2	232	234	10	29*	80	-3	39*	24	-6	81	65
												10	85	51	-5	483	483

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
-3	3	L	-2	2	L	0	0	L	1	-1	L	2	-2	L	3	-3	L	-7	296	284
-5	256	253	-7	526	525	-10	320	324	-11	52*	15	-12	112	117	-7	296	284	-12	33*	12
-1	382	387	-5	490	485	-8	574	573	-10	157	134	-11	123	84	-11	103	59	-11	103	59
10	83*	71	7	97	52	-4	503	484	-8	135	111	-10	74*	95	-9	265	249	-9	265	249
11	58*	59	-1	968	955	-2	1475	1453	-2	315	317	-8	184	177	-8	106	98	-8	106	98
-2	-4	L	-2	4	L	0	0	0	0	51	52	-2	166	168	-4	135	137	-4	135	137
-8	54*	74	8	104	5	0	2	L	9	100	72	2	0	L	3	-1	L	3	-1	L
-7	62*	19	-1	-5	L	-3	625	617	1	1	L	-10	601	584	3	-1	L	3	-1	L
-6	318	290	7	61*	84	-7	75*	84	-9	289	300	-8	47*	42	-10	123	71	-10	123	71
-5	181	182	-7	61*	84	10	117	110	-7	723	719	-6	445	451	-9	265	249	-9	265	249
-2	796	795	-6	401	405	11	119	95	-1	59	58	-2	1586	1569	-8	106	98	-8	106	98
-4	720	733	-4	720	733	-9	34*	68	8	110	82	2	2	L	-4	135	137	-4	135	137
-2	-2	L	-1	-3	L	-8	565	569	1	-5	L	2	2	L	3	-1	L	3	-1	L
-10	139	129	-10	148	156	-7	264	270	-9	234	207	-9	53*	31	-12	69*	28	-12	69*	28
-9	334	320	-9	123	169	-6	579	590	-8	432	418	-7	51*	52	-11	176	173	-11	176	173
-8	90*	107	-9	123	169	-4	153	157	-7	506	501	-7	51*	52	-10	114	52	-10	114	52
-6	52*	67	-8	105	94	0	-2	L	-7	506	501	-5	92	93	-8	170	166	-8	170	166
0	506	508	-7	423	426	0	-2	L	-5	683	710	-1	1117	1132	-6	733	752	-6	733	752
9	90	31	-6	59*	57	-11	63*	95	1	-3	L	8	108	107	3	1	L	3	1	L
-2	0	L	-1	-1	L	-10	63*	110	1	144	154	2	4	L	-10	77*	52	-10	77*	52
-8	172	168	-10	148	147	-9	324	321	-11	144	154	-9	225	217	-9	489	484	-9	489	484
-6	110	110	-8	74*	82	-8	90	45	-10	180	176	-8	74*	5	-5	387	385	-5	387	385
0	796	796	-6	119	98	-4	168	176	-9	55*	2	-7	307	315	3	3	L	3	3	L
			-6	119	98	-2	473	467	-8	40*	3	-4	660	659	-9	249	253	-7	107	114
						-4	334	331	-4	334	331	-8	57*	26	-8	57*	26			

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	
			9	-3	L				10	0	L				11	-1	L				12	-2	L	
-4	337	334	-5	209	196	-10	310	276	-10	310	276	-10	66*	109	-4	40*	29							
-3	53*	69	-3	94	69	-8	70*	57	-8	70*	57	-8	294	282	-9	294	282							
-2	280	284	-1	277	279	-6	408	417	-6	408	417	-8	139	167	-8	139	167				12	0	L	
0	265	273				-4	605	621	-4	605	621	-7	79*	60	-7	79*	60							
			10	-4	L	-2	133	137	-2	133	137	-6	120	94	-6	120	94							
			9	-1	L	-9	240	207	10	2	L	-4	74*	28	-4	74*	28							
-12	60*	60	-8	144	124	-7	276	299	-7	276	299	-1	54*	15	-1	54*	15							
-11	60*	49	-7	276	299	-7	52*	12	-7	52*	12													
-10	51*	35	-6	398	393	-5	158	170	-5	158	170	11	1	L										
-8	54*	61	-5	103	98	-3	187	206	-3	187	206	-7	112	60	-7	112	60							
-6	150	151	-4	490	513	-1	81*	58	-1	81*	58	-5	72*	60	-5	72*	60							
-4	53*	65				0	112	48	0	112	48	-3	59*	66	-3	59*	66							
-2	52*	58	10	-2	L							-2	88*	95	-2	88*	95							
0	60*	78				11	-3	L	11	-3	L	-1	98	15	-1	98	15							
			9	1	L	-12	89*	111																
-9	406	399	-11	70*	5	-10	51*	42	-10	51*	42													
-7	576	581	-10	128	141	-9	229	231	-9	229	231	12	-2	L										
-5	487	481	-9	177	179	-8	59*	6	-8	59*	6													
-3	164	165	-8	129	122	-7	171	146	-7	171	146	-10	89*	115	-10	89*	115							
-1	125	133	-7	105	12	-6	136	91	-6	136	91	-9	149	122	-9	149	122							
0	104	78	-6	76*	102	-5	133	124	-5	133	124	-8	154	131	-8	154	131							
3	106	118	-4	125	71	-4	208	212	-4	208	212	-7	277	272	-7	277	272							
			-2	58*	64							-6	85*	61	-6	85*	61							
												-5	445	452	-5	445	452							

Table A-3: Observed and calculated structure factors for coesite at 51.9 kbar.

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
-12	0	L	-9	1	L	-6	-4	L	-5	-3	L	-4	-2	L	-3	-3	L
8	111*	136	-1	337	341	-2	168	141	-7	39*	33	-8	133	102	-6	174	182
-11	-1	L	8	105	65	0	362	368	-5	230	197	-6	116	54	-4	323	328
0	245	261	11	125	61	-4	94*	107	-4	188	197	-4	42*	71	-3	-1	L
8	113*	168	-9	3	L	-6	-2	L	-2	50*	62	0	389	386	-9	167	190
-10	-2	L	8	105	96	-6	68*	8	-5	-1	L	4	73	47	-8	232	239
-1	98*	120	-2	66*	67	-5	71*	5	-4	0	L	-4	0	L	-6	336	319
0	93*	37	-1	78*	105	-4	103	10	-7	148	163	-6	169	186	-2	649	656
6	162	103	-1	78*	105	-2	115	92	-4	395	388	-4	371	396	-3	1	L
-10	0	L	-5	276	282	-6	0	L	-2	216	226	0	724	711	-7	257	244
0	46*	55	-4	121	101	-6	114	86	-5	1	L	10	127	86	-5	161	184
2	137	125	-2	219	205	-4	444	459	-3	63*	62	-4	2	L	-3	49*	10
8	104*	57	9	101	18	-2	471	472	11	89*	117	-5	687	689	-3	3	L
-9	-3	L	-7	1	L	-6	2	L	-5	322	328	-3	712	720	-5	244	248
-1	403	435	-3	324	304	-4	52*	10	-3	181	190	-6	139	109	-1	395	397
0	261	268	-1	77*	62	-3	141	139	-3	181	190	-5	312	296	10	61*	67
-9	-1	L	-7	3	L	-2	60*	92	-3	181	190	-6	139	109	-2	-4	L
-3	109*	109	-1	108	105	-1	400	413	-4	-4	L	-4	438	458	-8	59*	68
-2	94*	125	-8	0	L	-5	-5	L	-6	69*	15	-3	-3	L	-7	101	16
			-2	294	290	-3	266	276	-5	128	102	-8	229	247	-6	331	297
			0	662	679	-2	188	200	-4	54*	54	-7	66*	37	-5	190	175
			-4	203	203	-3	228	242	-3	257	263	-2	821	793	-2	821	793

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC
-2	-2	L	-1	-3	L	0	0	L	1	-3	L	2	-4	L	2	2	L	2	2	L	3	3	L
-10	104*	127	-7	414	422	-11	117	85	-11	162	152	-10	484	463	10	159	127	-8	51*	96	-8	51*	96
-9	332	310	-6	57*	53	-10	103*	111	-10	265*	170	-9	219	208	-9	159	127	-7	110	117	-7	110	117
-8	97*	108	-9	324	313	-9	57*	2	-8	39*	3	-8	69*	1	3	5	L	3	5	L	4	4	L
-6	55*	63	-1	-1	L	-8	54*	53	-8	39*	3	-7	314	306	-9	237	248	-9	237	248	-9	237	248
0	501	495	-4	162	166	-4	162	166	-4	322	327	-4	667	657	-8	51*	27	-8	51*	27	-11	163	155
-2	0	L	-2	479	467	-2	479	467	1	-1	L	2	-2	L	-7	292	282	-10	70*	2	-10	70*	2
-8	150	164	0	0	L	0	0	L	1	1	L	2	2	L	3	-3	L	-9	105	95	-9	105	95
-6	118	118	-10	298	320	-10	298	320	-11	69*	23	-12	130	120	3	-3	L	-8	96	124	-8	96	124
0	796	796	-8	590	568	-8	590	568	-10	150	138	-11	66*	73	-11	48*	54	-7	176	181	-7	176	181
-2	2	L	-4	491	475	-4	491	475	-8	155	106	-10	63*	99	-11	113	67	-4	263	280	-4	263	280
-7	513	510	-2	1494	1441	-2	1494	1441	-2	318	320	-8	172	184	-10	113	67	-3	192	195	-3	192	195
-5	482	482	0	0	0	0	0	0	0	52	55	-2	157	159	-9	259	249	-9	259	249	-9	259	249
12	66*	120	-7	77*	38	-7	77*	38	1	1	L	2	0	L	-8	97	96	4	-2	L	4	-2	L
-1	-5	L	-6	110	90	-6	110	90	1	1	L	2	0	L	-4	139	132	-12	139	146	-12	139	146
-4	745	739	-1	950	952	-1	950	952	-9	288	290	-10	593	583	3	-1	L	-11	390	383	-11	390	383
-7	110	77	-7	44*	74	-7	44*	74	-7	707	708	-8	33*	33	-12	60*	28	-10	229	250	-10	229	250
-6	400	403	10	115	111	10	115	111	-1	52	55	-6	435	433	-11	167	159	-9	106	72	-9	106	72
-4	745	739	-3	602	612	-3	602	612	7	120	38	-2	1592	1555	-11	167	159	-8	276	265	-8	276	265
-1	-3	L	1	-5	L	1	-5	L	6	93*	118	6	93*	118	-10	121	58	-4	32*	47	-4	32*	47
-9	44*	76	-8	404	414	-8	404	414	1	3	L	2	2	L	-8	172	164	4	0	L	4	0	L
-8	570	563	-7	496	497	-7	496	497	-7	243	243	-9	53*	36	3	1	L	-10	58*	86	-10	58*	86
-7	262	262	-5	694	712	-5	694	712	10	107*	151	-7	50*	57	-10	79*	58	-8	116	110	-8	116	110
-6	597	592	-6	597	592	-6	597	592	-1	1072	1123	-5	98	96	-9	476	471	-6	117	102	-6	117	102
-4	138	160	-4	138	160	-4	138	160	8	113	108	-1	1072	1123	-9	476	471	-4	821	803	-4	821	803
-8	72*	92	8	113	108	8	113	108	8	113	108	8	113	108	-5	393	388	-5	393	388	-5	393	388

