

The equation of state and high-pressure behaviour of magnesite

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MATERIAL FOR DEPOSIT

Table 4A: Observed and calculated structure factors of Magnesite at 0 GPa (in DAC)
(Mult. Factor = 4.00)

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L		
	0	0	L		0	1	L		4	1	L		2	2	L		2	3	L	
0		0	1008	2	23		22	0	113		118	12	78		75	2	123		118	
	1	0	L	8	285		298	3	32		42	15	51		48	11	65		68	
					1	1	L	6	62		59						3	3	L	
4	394		395					9	23*		37		3	2	L					
				0	110		118	12	87		89						3	3	L	
	2	0	L	3	277		272		0	2	L		1	84	84	0	125		125	
				6	242		241					4	74		76	3	12*		31	
2	219		217	9	161		173	4	150		153	10	96		92		0	4	L	
8	124		133					10	147		149	13	60		63					
					2	1	L						4	2	L		14	45	48	
	3	0	L						1	2	L									
				1	136		128						2	65	67					
0	332		344	4	153		156	2	153		161	5	48		41					
6	35		36	10	112		114	5	109		113						0	3	L	
				13	61		69	8	144		137		0	3	L					
	4	0	L					11	80		78									
					3	1	L	14	74		85		6	34	36					
4	270		266									12	222		224					
10	47		50	2	22*		21		2	2	L									
				5	28*		28						1	3	L					
	5	0	L	8	195		193	0	106		103									
				11	15*		22	3	77		79		1	33	31					
8	77		81					6	133		139	10	8*		12					
								9	61		64	13	12*		20					

Table 4B: Observed and calculated structure factors of Magnesite at 2.26 GPa.
(Mult. Factor = 4.00)

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC			
	0	0	L		0	1	L		4	1	L		2	2	L		2	3	L	
0	0	1008	8	290	296	0	120	119	15	48	52	2	124	118						
	1	0	L		1	1	L	3	24*	46										
4	394	392				6	70	63		3	2	L		3	3	L				
	2	0	L	0	116	117	9	27*	40											
2	217	215	3	283	273		0	2	L	1	87	82	0	129	135					
8	130	137	6	249	242	4	155	156	4	81	80	3	7*	29						
	3	0	L	9	168	174	10	145	148	10	93	92		0	4	L				
0	335	351	12	89	91					4	2	L	14	28*	47					
6	7*	39		2	1	L		1	2	L		2	68	65						
	4	0	L	1	133	124	2	152	159	5	49	43								
4	263	266	4	162	161	5	108	109		0	3	L								
10	33*	47	7	97	97	8	146	141												
	5	0	L	10	116	113	11	80	75	6	5*	39								
8	76	83	13	70	67	14	84	83	12	228	230									
				3	1	L		2	2	L		1	3	L						
			2	10*	22	0	109	106		1	18*	32								
			5	13*	29	3	85	84	10	13*	13									
			8	197	196	6	134	140	13	11*	21									
			11	20*	23	9	70	68												
			14	13*	5	12	84	78												

Table 4C: Observed and calculated structure factors of Magnesite at 3.09 GPa
(Mult. Factor = 4.00)

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	I					
	0	0	L		0	1	L		4	1	L		2	2	L		1	3	L				
0	0	1008	2	29	25	0	113	118	9	66	65	16	132	133									
	1	0	L	8	298	295	3	45	44	12	85	76											
					1	1	L	6	63	64	15	46	49		2	3	L						
4	386	392					9	24*	38														
				12	88	89					3	2	L		2	120	120						
	2	0	L	0	107	118		5	1	L		1	78	83		5	76	78					
				3	282	271				4	81	78	11	68	66								
2	226	216	6	238	242	1	85	84	7	77	75												
8	137	135	9	172	172				10	93	94		3	3	L								
				12	99	90		0	2	L	13	67	62		0	134	130						
	3	0	L		2	1	L							3	23*	30							
								4	152	154		4	2	L	6	18*	23						
0	345	346	1	132	125	10	148	149															
6	28	35	4	162	159				2	68	69		0	4	L								
12	223	225	7	101	98		1	2	L	5	33*	42											
				10	117	115							14	42	44								
	4	0	L	13	72	67	2	159	161		0	3	L										
								5	116	110													
4	264	264		3	1	L	8	142	138	6	24*	35		2	4	L							
10	44	45					11	79	76	12	218	225		1	52	43							
				2	18*	24	14	82	86				4	80	80								
	5	0	L	5	28	29					1	3	L										
				8	193	193		2	2	L													
2	72	73	11	17*	22				1	20*	31												
8	81	81	14	22*	8	0	110	104	4	216	219												
							3	81	81	10	19*	16											
							6	141	141	13	19*	21											

Table 4D: Observed and calculated structure factors of Magnesite at P=4.16 GPa
(Mult. Factor = 4.00)

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L		
	0	0	L		0	1	L		4	1	L		3	2	L		2	3	L	
0	0	1008	2	29	27	0	116	116	1	81	82	2	123	120						
	1	0	L		1	1	L	3	46	46	4	79	78	8	70	71				
								6	67	65	7	76	74	11	64	66				
4	408	390	0	110	116	12	84	88	10	88	94									
			3	282	273				13	57	62		3	3	L					
	2	0	L	6	244	243		0	2	L		4	2	L	0	123	134			
				9	164	173								3	22*	28				
2	228	215					4	149	156	2	63	67								
8	133	136		2	1	L	10	141	148	5	44	43		0	4	L				
	3	0	L	1	132	123		1	2	L		0	3	L	8	240	236			
				4	162	160								14	41	44				
0	335	350	7	103	96	2	155	159	6	39	38									
6	35	38	10	110	113	5	111	108	12	232	228		1	4	L					
						8	149	140												
	4	0	L		3	1	L	11	79	75		1	3	L	12	82	88			
4	270	264	2	19*	24		2	2	L	1	32	32		2	4	L				
10	47	45	5	32	29				7	31	27									
			8	200	193	0	111	104	10	12*	15	1	47	45						
	5	0	L	11	14*	23	3	80	85	13	13*	21								
						6	143	141												
8	72	80				9	66	68												
						12	77	76												

Table 4E. Observed and calculated structure factors of Magnesite at 4.77 GPa
(Mult. Factor = 4.00)

L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	L	OBS	CALC	I				
	0	0	L		0	1	L		4	1	L		3	2	L		2	3	L			
0		0	1008	2	29	26	0	110	114	1	76	81	2	119	115							
	1	0	L	8	301	292	3	41	45	4	76	76	11	64	64							
4	388	389		1	1	L	6	62	60	7	73	73		3	3	L						
	2	0	L	0	107	116		0	2	L	10	88	89		0	123	129					
2	213	213	3	274	271	4	145	154		4	2	L	3	18*	28							
8	126	134	6	238	240	10	140	144	2	64	63		0	4	L							
	3	0	L	9	158	171		1	2	L	5	51	42	14	43	47						
0	321	345		2	1	L		1	2	L		0	3	L		2	4	L				
6	41	39	1	124	123	2	148	157	6	43	39											
	4	0	L	4	154	158	5	106	108	12	222	222	1	52	43							
4	252	259	7	96	96	8	141	137		1	3	L										
10	39	47	10	112	109	11	74	74	1	34	31											
	5	0	L		3	1	L		2	2	L	7	17*	27								
8	71	78	2	20*	21	0	110	102	10	14*	12											
			5	19*	29	3	78	83	13	11*	21											
			8	190	190	6	135	137														
			11	20*	23	9	65	66														
						12	80	74														

