

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									
4	394	395						9	23*	37		3	2	L		3	3	L	
				0	110	118		12	87	89									
	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										
	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 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	9	24*	38										
				12	88	89	12	88	89		3	2	L	2	120	120			
	2	0	L	0	107	118								5	76	78			
				3	282	271	5	1	L	1	78	83	11	68	66				
				6	238	242				4	81	78							
2	226	216		9	172	172	1	85	84	7	77	75		3	3	L			
8	137	135		12	99	90				10	93	94							
							0	2	L	13	67	62		0	134	130			
	3	0	L	2	1	L								3	23*	30			
							4	152	154					6	18*	23			
0	345	346		1	132	125	10	148	149		4	2	L						
6	28	35		4	162	159					2	68	69						
12	223	225		7	101	98		1	2	L	5	33*	42		0	4	L		
				10	117	115													
	4	0	L	13	72	67	2	159	161		0	3	L	14	42	44			
							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						
				2	18*	24	14	82	86					1	52	43			
	5	0	L	5	28	29					1	3	L	4	80	80			
				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							

