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Room-Temperature Form of Manganese Hexafluorosilicate Hexahydrate: a New Model with Submicroscopic Twinning

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Table 5. Anisotropic thermal parameters of the form :
 $\exp(-B_{11}h^2 - B_{22}k^2 - B_{33}l^2 - B_{12}hk - B_{13}hl - B_{23}kl)$, with their
 standard deviations in parentheses, multiplied by 10000.

	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
Mn(1)	87(04)	87(04)	34(03)	87(04)	0	0
Mn(2)	57(06)	57(06)	74(07)	57(06)	0	0
Si(1)	51(02)	51(02)	83(03)	51(02)	0	0
Si(2)	51(03)	51(03)	35(04)	51(03)	0	0
O(1)	145(17)	131(15)	100(08)	139(27)	61(21)	13(20)
O(2)	348(28)	114(16)	81(08)	172(35)	-180(27)	-28(20)
O(3)	4(10)	324(25)	72(07)	8(28)	69(16)	78(27)
F(1)	90(10)	125(11)	87(06)	142(19)	2(14)	-48(14)
F(2)	88(10)	136(12)	51(05)	73(19)	57(14)	-16(13)
F(3)	129(12)	125(12)	68(06)	181(22)	-22(14)	19(14)

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Table 6. Observed and calculated structure factors, each multiplied by 10, and unobserved reflections are omitted.

H	FOBS	FCAL	H	FOBS	FCAL	H	FOBS	FCCAL	H	FOBS	FCAL	H	FOBS	FCAL
K= 0,L= 0			2	74	75	4	53	48	1	134	133	1	285	284
3	91	99	3	318	324	5	101	105	2	771	770	2	290	339
5	43	43	4	39	34				3	236	232	3	310	298
6	899	918				K= 5,L= 1			4	68	64	5	171	168
9	343	352	K= 7,L= 0			0	73	86	5	580	567	6	123	121
			1	561	551	1	135	132	6	75	76	7	31	45
K= 1,L= 0			2	91	85	2	183	189						
1	1694	1724	3	60	66	3	104	124	K= 4,L= 2			K= 3,L= 3		
2	25	28				4	51	53	0	1329	1332	0	631	608
3	49	51	K= 8,L= 0						1	145	140	1	397	377
4	616	628	1	45	63	K= 6,L= 1			2	140	144	2	299	323
5	26	31				1	279	287	3	438	441	3	141	138
6	32	30	K= 9,L= 0			2	160	161	4	118	122	4	73	79
7	549	551	0	340	352	3	69	75	5	132	136	5	104	106
8	59	63				4	175	172	6	364	353	6	62	65
			K= 0,L= 1											
K= 2,L= 0			1	153	142	K= 7,L= 1			K= 5,L= 2			K= 4,L= 3		
1	22	28	4	263	267	1	73	82	1	578	572	0	29	13
2	123	157	7	219	221	2	112	113	3	94	102	1	109	120
3	41	45							4	332	340	2	232	215
4	60	61	K= 1,L= 1			K= 8,L= 1			5	145	137	4	100	98
5	743	745	1	159	174	0	77	78				5	87	84
6	70	75	2	141	170				K= 6,L= 2					
7	87	85	3	345	338	K= 0,L= 2			0	39	28	K= 5,L= 3		
			4	222	230	0	35	52	2	365	372	1	82	91
K= 3,L= 0			5	281	270	1	26	37	3	113	110	2	75	77
0	96	99	6	56	53	2	395	404	4	85	91	3	47	54
1	38	51	8	78	83	5	537	543				4	41	56
2	49	45				8	369	370	K= 7,L= 2					
3	763	751	K= 2,L= 1						0	482	479	K= 6,L= 3		
4	36	17	0	320	325	K= 1,L= 2						0	106	99
5	42	51	1	325	323	0	1482	1478	K= 8,L= 2			2	34	41
6	319	324	2	377	384	1	38	32	0	45	16	3	222	221
7	64	66	3	636	632	2	63	64	1	450	441			
			4	206	207	3	103	148				K= 7,L= 3		
K= 4,L= 0			5	96	96	4	199	202	K= 0,L= 3			1	289	280
1	631	628	6	93	100	5	111	117	0	371	370	2	55	51
2	53	61				6	750	762	3	359	357			
4	446	448	K= 3,L= 1			7	31	25	6	342	364	K= 0,L= 4		
5	34	40	1	702	685							0	55	83
			2	194	196	K= 2,L= 2			K= 1,L= 3			1	463	433
K= 5,L= 0			3	100	90	0	55	48	1	386	382	2	32	39
2	754	745	4	343	348	1	1385	1380	2	354	333	3	59	65
3	45	51	6	34	18	2	220	209	3	208	217	4	861	865
4	38	40	7	47	60	3	237	242	4	225	238	6	28	10
5	188	186				4	580	587	5	75	72	7	257	264
			K= 4,L= 1			5	107	96	6	79	88	8	33	34
K= 6,L= 0			1	23	25				7	161	169			
0	927	918	2	309	306	K= 3,L= 2						K= 1,L= 4		
1	34	30	3	104	98	0	32	25	K= 2,L= 3			1	51	52

Table 6. (continued)

H	FOBS	FCAL	H	FOBS	FCAL	H	FOBS	FCCAL	H	FOBS	FCAL	H	FOBS	FCAL
K= 1,L= 4			1	60	67	0	123	124	0	51	49	4	410	403
2	1102	1125	2	643	657	2	73	54	1	50	65			
3	217	199	4	27	24	3	993	1028	2	73	95	K= 3,L= 8		
4	109	117	5	165	147	4	26	50	3	170	167	1	50	51
5	304	303	6	32	23	5	44	29	4	30	46	2	352	349
6	26	33				6	117	125	5	85	85	3	107	97
7	42	50	K= 1,L= 5						6	38	35			
			0	648	635	K= 1,L= 6						K= 4,L= 8		
K= 2,L= 4			1	59	52	1	435	439	K= 2,L= 7			0	255	247
0	780	771	2	46	49	2	54	58	0	99	103	1	58	52
1	171	175	3	180	196	3	87	108	1	202	197	2	50	40
2	168	184	4	92	83	4	640	644	2	129	140			
3	723	720	5	40	60	5	111	102	3	88	111	K= 5,L= 8		
4	130	129	6	228	230	6	42	57	4	38	46	1	307	292
6	385	387							5	29	24			
7	102	99	K= 2,L= 5			K= 2,L= 6						K= 0,L= 9		
			0	39	40	1	44	59	K= 3,L= 7			0	69	82
K= 3,L= 4			1	78	82	2	719	708	1	63	92	2	30	25
0	73	70	2	80	94	3	123	121	2	241	218	3	107	113
1	1134	1132	3	48	63	4	90	88	3	46	66			
2	169	166	4	78	84	5	253	255	4	141	146	K= 1,L= 9		
3	71	80	5	101	96	6	80	67				1	50	61
4	386	377	6	38	48				K= 4,L= 7			4	75	68
5	96	87							1	55	67			
6	76	76	K= 3,L= 5			0	293	293	2	231	228	K= 2,L= 9		
			1	28	17	2	63	78	K= 5,L= 7			1	32	32
K= 4,L= 4			2	213	215	3	584	572	0	235	227	2	143	154
0	47	53	4	34	41	4	93	83	1	53	53	3	44	51
1	58	59	5	81	79									
2	482	464	6	62	47	K= 4,L= 6			K= 6,L= 7			K= 3,L= 9		
3	33	49				0	42	22	1	126	123	0	279	282
4	55	57	K= 4,L= 5			1	432	422				1	65	53
5	492	486	0	253	251	2	61	61	K= 0,L= 8			2	49	48
			1	91	106	3	43	32	0	78	91	K= 4,L= 9		
K= 5,L= 4			2	88	93	4	402	388	1	95	94	0	48	37
0	596	578	3	77	80				2	439	441	1	200	203
2	28	26				K= 5,L= 6			3	28	36			
3	378	374	K= 5,L= 5			1	29	15	4	30	49	K= 0,L= 10		
4	49	52	1	290	288	2	419	409	5	405	400	0	99	111
			2	167	149	3	93	84				1	445	458
K= 6,L= 4			3	53	49				K= 1,L= 8			K= 1,L= 10		
1	310	310	4	60	63	K= 6,L= 6			0	741	731	0	112	82
3	39	16				0	298	300	1	66	64	1	76	69
			K= 6,L= 5			2	46	53	2	53	63	2	210	220
K= 7,L= 4			1	78	80				3	308	327			
1	27	33	2	251	247	K= 0,L= 7			4	146	139	K= 2,L= 10		
2	282	281	3	43	44	0	86	86	5	57	46	0	423	409
						1	525	533						
K= 8,L= 4			K= 7,L= 5			2	24	27	K= 2,L= 8					
0	283	281	0	426	431	4	72	87	1	301	297			
			1	69	83	6	26	35	2	197	181			
K= 0,L= 5									3	91	88			
0	40	67	K= 0,L= 6			K= 1,L= 7								