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A new cation ordering pattern in amesite-$2H_2$

C...THIA S. ANDERSON AND S. W. BAILEY

Department of Geology and Geophysics, University of Wisconsin-Madison
Madison, Wisconsin 53706

Abstract

The crystal structure of amesite-$2H_2$ from the Saranovskoye chromite deposit, North Urals Mountains, USSR, was refined in space group $C1$ to a residual of 5.7% with 1719 independent reflections. The study was undertaken to resolve conflicting interpretations of the optics, twinning, and infrared spectra of amesite from the Urals relative to data reported previously for amesite from Antarctica. There is nearly complete ordering of tetrahedral and octahedral cations in the Urals specimen, but the pattern of ordering differs from that found for the same polytype of amesite from Antarctica. Tetrahedral ordering of Si,Al in the Urals specimen preserves the identity of the ideal space group $P6_3$, but octahedral ordering of Mg,Al lowers the symmetry to $P1$. Tetrahedra lying on the pseudo-6_3 axis are all Si-rich. Octahedral Al is in the B site of each layer, but the degree of octahedral order is slightly different in the two layers. Local charge balance between adjacent layers is achieved by localization of all tetrahedral and octahedral Al in spirals around lines that parallel the Z axis and are spaced at intervals of $(a + b)/2$. We postulate that the presence, pattern, and degree of ordering can account for the observed sector and polysynthetic twinning, for differences in the bonding and geometry at the two interlayer junctions, and for the slightly triclinic shape of the unit cell. The possibility of other ordering patterns is examined. The normal assumption that all crystals of the same mineral or the same polytype have the same ordering pattern, crystallization conditions being similar, is not necessarily valid.

Introduction

This study was undertaken because of conflicting evidence as to the likelihood of cation ordering in amesite-$2H_2$ from the Saranovskoye chromite deposit in the North Urals Mountains, USSR. Hall and Bailey (1979) cite the biaxial optical nature and sector twinning of the Urals amesite as evidence of lower symmetry than the ideal space group of $P6_3$. They attribute this reduction in symmetry to cation ordering by analogy with amesite-$2H_2$ from Antarctica, which they determined by structural refinement to have nearly complete ordering of tetrahedral and octahedral cations. Serna *et al.* (1977), however, concluded that the Urals amesite was disordered on the basis of their study of the infrared patterns of a series of synthetic and natural amesites. Hall and Bailey point out one difference in the two samples that may be significant. The Urals crystals are twinned in more complex patterns than the Antarctic crystals, in that polysynthetic twin lamellae parallel to the (010) prism edges are present in some crystals in addition to the ubiquitous 6-fold sector twins on (001). They suggest that the difference in twinning may result from a difference in ordering patterns in the two samples, rather than from the presence or absence of ordering.

Preliminary examination of 30 crystals from the Urals sample (NMNH #103312) indicates that several polytypes are present. The $2H_2$ polytype is most abundant, but $6R_2$, $6R_1$, and $2H_1$ polytypes also are present (terminology of Bailey, 1969, and of Hall *et al.*, 1976). X-ray photographs reveal that some crystals have a disordered stacking of layers, in that the $k \neq 3n$ reflections appear as coalesced streaks and not as individual spots. All crystals examined with crossed nicols under the petrographic microscope are noticeably biaxial and twinned.

The $2H_2$ polytype has alternating interlayer shifts of $-b/3$ and $+b/3$ and alternating occupancy of the I and II sets of octahedral positions in successive layers (equivalent to 180° rotations). Steinfink and Brunton (1956) studied amesite-$2H_2$ from Saranovskoye. They attributed the biaxial nature to strain, and assumed the ideal hexagonal symmetry of $P6_3$ in their refinement. With this assumption, they determined the cat-

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0	12	728	780
0	14	784	791
0	16	783	778
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5	9	213	207
5	-9	223	213
-5	9	131	122
-5	-9	158	154
5	10	91	86
-5	10	119	115
5	11	183	156
-5	11	117	110
-5	12	86	80
7	0	96	88
-7	0	120	126
7	1	135	138
7	-1	143	145
-7	1	169	170
-7	-1	165	162
7	-2	67	22
-7	2	124	131
-7	-2	152	152
7	3	148	142
7	-3	109	111
-7	3	115	104
-7	-3	148	147
7	4	119	112
7	-4	134	126
-7	4	127	124
-7	-4	133	138
7	5	114	111
7	-5	151	145
-7	5	97	97
-7	-5	91	87
7	6	93	78
-7	6	95	85
-7	7	136	117
-7	-7	151	142
-7	8	69	59
-7	-8	88	72
7	9	82	72
-7	9	131	120
-7	-9	111	109
7	10	90	79
9	0	188	185
9	1	161	155
9	-1	155	143
-9	1	155	141
9	2	299	283
9	-2	301	286
-9	2	441	459
-9	-2	449	470
9	3	257	250
9	-3	259	255
-9	3	194	104
-9	-3	201	194
9	-4	91	73
-9	4	132	146
-9	-4	146	137
9	-5	188	192
-9	5	211	213
-9	-5	226	219
H = 6			
0	0	790	798
0	2	350	347
0	-2	360	364
0	3	96	82
0	-3	105	83
0	4	366	365
0	-4	372	376
0	5	102	101
0	-5	111	88
0	6	290	294
0	-6	307	314
0	7	83	101
0	-7	98	97
0	8	139	138
0	-8	136	134
0	9	115	108
0	-9	104	107
0	10	422	400
0	-10	420	408
0	11	145	113
0	-11	134	122
2	0	143	148
2	1	187	183
2	-1	176	167
-2	1	129	131
-2	-1	148	151
2	2	63	42
2	-2	95	79
-2	-2	91	78
2	3	100	97
2	-3	114	104
-2	3	192	175
-2	-3	176	169
2	4	121	120
2	-4	117	109
-2	4	69	56
-2	-4	95	62
2	5	145	142
2	-5	147	143
-2	5	115	108
-2	-5	108	114
2	6	65	53
2	7	110	108
2	-7	116	109
-2	7	90	68
-2	-7	104	95
2	-8	79	61
-2	8	105	101
-2	-8	74	73
2	9	151	146
2	-9	162	153
2	-10	87	79
-2	-10	116	122
2	-11	83	79
-2	-11	85	51
4	0	81	75
4	1	81	53
-4	1	219	222
-4	-1	229	230
4	2	125	114
4	-2	173	170
-4	2	73	63
4	3	121	110
4	-3	113	100
-4	3	128	135
-4	-3	145	140
4	4	120	115
4	-4	100	97
4	5	66	49
-4	5	151	158
-4	-5	163	160
4	-6	86	80
-4	6	122	132
-4	-6	125	114
4	7	88	68
4	-7	101	94
-4	7	133	119
-4	-7	122	115
-4	9	108	93
-4	-9	139	120
4	-10	80	74
-4	10	113	112
-4	-10	138	144
6	0	553	539
-6	0	623	625
6	1	154	100
6	-1	171	105
-6	-1	135	80
6	2	226	214
6	-2	253	247
-6	-2	275	271
6	-3	95	42
-6	-3	100	80
6	-4	264	259
-6	4	286	283
-6	-4	313	307
6	-5	93	71
6	-6	219	224
-6	6	232	244
-6	-6	246	257
-6	-7	75	50
H = 7			
1	1	92	72
-1	1	120	103
-1	-1	134	122
1	2	94	73
1	-2	131	104
-1	-2	85	75
-1	-5	88	79
3	0	165	152
-3	0	157	148
3	1	197	170
3	-1	190	163
-3	1	178	171
-3	-1	175	164
3	2	377	368
3	-2	379	362
-3	2	355	341
-3	-2	356	344
3	3	141	116
3	-3	154	113
-3	3	163	161
-3	-3	172	160
3	4	98	86
3	-4	120	120
-3	-4	108	94
3	5	246	231
3	-5	249	236
-3	-5	262	259

Atom	Axis	rms (Å) displacement	Angle (°) with respect to X	Y	Z
T(1)	r1	0.110(4)	112(6)	52(12)	46(14)
	r2	0.122(4)	106(8)	50(12)	136(15)
	r3	0.145(3)	28(5)	62(6)	86(6)
T(2)	r1	0.109(4)	115(6)	35(9)	66(8)
	r2	0.128(4)	69(16)	57(9)	139(14)
	r3	0.138(3)	33(12)	80(10)	59(15)
T(11)	r1	0.108(4)	112(4)	28(7)	74(9)
	r2	0.128(4)	87(9)	71(9)	161(9)
	r3	0.144(3)	23(5)	70(5)	81(9)
T(22)	r1	0.112(4)	99(7)	54(29)	38(30)
	r2	0.118(4)	99(8)	39(28)	128(30)
	r3	0.142(4)	13(6)	77(6)	89(6)
M(1)	r1	0.116(4)	117(26)	35(57)	69(52)
	r2	0.119(4)	68(33)	58(60)	140(35)
	r3	0.133(4)	36(12)	78(11)	57(13)
M(2)	r1	0.124(4)	119(8)	33(9)	75(13)
	r2	0.137(4)	92(21)	74(16)	164(15)
	r3	0.143(3)	29(8)	62(10)	84(23)
M(3)	r1	0.105(4)	117(6)	37(9)	67(11)
	r2	0.123(4)	91(15)	65(12)	155(12)
	r3	0.134(4)	27(6)	65(9)	80(15)
M(11)	r1	0.109(4)	108(7)	31(7)	66(9)
	r2	0.130(4)	111(22)	73(13)	153(13)
	r3	0.137(4)	28(18)	65(9)	103(21)
M(22)	r1	0.112(4)	98(6)	9(6)	93(14)
	r2	0.123(4)	76(10)	91(14)	167(11)
	r3	0.138(3)	16(9)	82(6)	77(10)
M(33)	r1	0.110(4)	115(6)	29(7)	76(10)
	r2	0.128(4)	92(13)	76(11)	165(11)
	r3	0.141(4)	25(6)	66(6)	86(13)
O(1)	r1	0.119(9)	89(7)	84(10)	6(9)
	r2	0.150(7)	62(9)	151(9)	85(11)
	r3	0.186(7)	29(9)	62(9)	94(5)
O(2)	r1	0.121(8)	120(17)	36(46)	72(94)
	r2	0.125(9)	97(48)	74(80)	162(93)
	r3	0.153(7)	31(10)	59(10)	88(12)
O(3)	r1	0.119(8)	105(8)	29(12)	66(10)
	r2	0.149(7)	64(19)	61(12)	139(17)
	r3	0.166(7)	31(18)	89(11)	59(18)
O(4)	r1	0.13[illegible](8)	91(8)	33(12)	123(10)
	r2	0.13[illegible]	177(19)	90(12)	87(17)
	r3	0.154(7)	87(22)	57(21)	33(21)

Atom	Axis	rms (Å) displacement	Angle (°) with respect to X	Y	Z
O(5)	r1	0.112(8)	123(11)	33(10)	83(10)
	r2	0.142(8)	135(21)	112(17)	127(29)
	r3	0.153(7)	117(24)	114(14)	37(29)
O(11)	r1	0.119(8)	99(16)	91(25)	9(13)
	r2	0.131(8)	62(13)	152(12)	87(28)
	r3	0.158(7)	30(11)	62(12)	82(9)
O(22)	r1	0.121(9)	99(12)	74(34)	18(32)
	r2	0.132(8)	88(19)	163(34)	73(34)
	r3	0.149(7)	9(13)	86(18)	83(13)
O(33)	r1	0.116(9)	104(13)	40(7)	53(8)
	r2	0.144(8)	164(14)	96(14)	104(15)
	r3	0.164(7)	97(15)	130(7)	40(9)
O(44)	r1	0.113(8)	114(7)	30(11)	107(11)
	r2	0.144(8)	108(13)	115(12)	149(13)
	r3	0.169(7)	150(10)	105(8)	64(13)
O(55)	r1	0.109(9)	126(7)	39(8)	78(9)
	r2	0.146(7)	71(16)	62(12)	145(18)
	r3	0.163(7)	43(11)	65(11)	58(18)
OH(1)	r1	0.116(10)	95(5)	84(5)	8(5)
	r2	0.183(7)	97(74)	171(54)	84(9)
	r3	0.188(7)	9(61)	97(74)	85(9)
OH(2)	r1	0.120(10)	98(9)	83(12)	10(5)
	r2	0.149(8)	127(7)	143(7)	89(14)
	r3	0.200(7)	142(6)	54(6)	100(5)
OH(3)	r1	0.119(10)	87(8)	110(30)	20(31)
	r2	0.133(8)	79(6)	157(27)	110(31)
	r3	0.188(7)	11(6)	79(6)	90(6)
OH(4)	r1	0.114(10)	112(15)	91(6)	22(15)
	r2	0.140(8)	153(13)	73(5)	110(16)
	r3	0.213(7)	74(4)	17(5)	83(4)
OH(11)	r1	0.119(9)	89(8)	98(14)	8(14)
	r2	0.144(8)	68(11)	156(11)	97(15)
	r3	0.174(7)	22(11)	68(11)	88(7)
OH(22)	r1	0.116(10)	102(10)	64(10)	29(10)
	r2	0.153(8)	163(13)	107(24)	94(25)
	r3	0.154(7)	102(11)	32(13)	119(27)
OH(33)	r1	0.120(10)	86(9)	111(25)	22(25)
	r2	0.136(8)	87(13)	158(24)	111(25)
	r3	0.162(7)	5(11)	85(13)	93(10)
OH(44)	r1	0.108(10)	103(6)	58(13)	35(14)
	r2	0.136(8)	104(8)	38(13)	125(14)
	r3	0.179(7)	19(7)	71(7)	88(6)