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The crystal structure of deerite

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Abstract

The crystal structure of deerite [$P2_1/a$, a = 10.786(8), b = 18.88(2), c = 9.564(9)A, β = 107.45(5)°] from Panoche, California, has been investigated using intensity data collected with Mo$K\alpha$ radiation on a Picker FACS 1 diffractometer. The structure of the pseudocell with $c' = c/3$ and space group $P2_1/a$ has been determined and refined to a weighted residual index of 0.07. The pseudocell structure has disordered Si and oxygen positions, and there are only three possible ordered arrangements of these: the preferred full structure of deerite has a weighted residual index of 0.08, but it was not possible to refine it. The ideal structural formula is $Fe^{2+}_6Fe^{3+}_3O_3[Si_6O_{17}](OH)_5$, Z = 4. The structure is formed of two structural units continuous along the c-axis direction: (1) a strip of edge-sharing M-atom octahedra, six octahedra in width, oriented parallel to {110}, and (2) a hybrid single-double $[Si_6O_{17}]$ silicate chain. Apical and lateral oxygens of the silicate chain are shared with M octahedra, but the familiar sandwich of tetrahedral–octahedral–tetrahedral coordination polyhedra is not well developed. The basal tetrahedral oxygens enclose a structural void. Fe^{3+} probably occupies the lateral sites in the octahedral strip.

Similar structural units have been reported recently for howieite, which is associated with deerite in rocks of the Franciscan Formation. The arrangement of the silicate chain in chain-silicate structures is constrained by the close-packed oxygen distances in the octahedral strip. This constraint results in a distinctly different structural topology in deerite and howieite compared to pyroxene and amphibole and imparts a characteristic distortion to the silicate chain. In particular, the sides of the six-membered rings in both deerite and howieite are buckled inward.

Introduction

Deerite (along with howieite and zussmanite) occurs in blocks of riebeckite–stilpnomelane schists within metasediments of the Franciscan Formation, California. The type locality is the Laytonville quarry, Mendocino County (Agrell *et al.*, 1965). Deerite has also been reported in stilpnomelane schists, associated with glaucophane schists, in the French and Italian Alps (for example, Agrell and Gay, 1970).

Deerite is a hydrous ferrous, ferric silicate: the proposed formula for a half unit-cell content with (O,OH) = 50 is $(Mg_{0.08}Mn_{0.86}Fe^{2+}_{10.90})_{11.84}(Fe^{3+}_{5.89}Al_{0.38})_{6.27}Si_{11.86}O_{39.95}(OH)_{10.05}$ (Agrell *et al.*, 1967, footnote by Agrell). Agrell *et al.* (1965) report that it is monoclinic, space group $P2_1/a$, with a = 10.755(2), b = 18.870(6), c = 9.568(2)A, β = 107.12(4)°, density 3.837 gm cm^{-3}. It forms black acicular crystals, elongated parallel to c and lozenge-shaped in cross section, with a good {110} cleavage. The crystals are twinned submicroscopically: the twin axis is [001]. More recently, Wenk (1974) has suggested that deerite is in fact orthorhombic, space group *Pnma*, with a = 18.885, b = 3.182 (needle axis), c = 10.337A.

Characteristic Mössbauer spectra and magnetic susceptibility data for deerite have been reported by several laboratories, and the initial interpretations of these data resulted in a certain amount of controversy. Bancroft *et al.*, (1968) interpreted their room-temperature Mössbauer spectrum in terms of three quadrupole doublets: A,A', assigned to Fe^{2+} in sixfold coordination; B,B', assigned to Fe^{3+} in sixfold coordination; C,C', assigned to Fe^{2+} in a distorted fourfold coordination. The fraction of the total Fe content of deerite accommodated in each of the sites, or group of sites, associated with these doublets is approximately 0.47, 0.37, and 0.16, respectively. In a subsequent Mössbauer study, Frank and Bunbury

Table 4. Observed and Calculated Structure Factors

K	L	F_o	F_c	K	L	F_o	F_c	K	L	F_o	F_c	K	L	F_o	F_c	K	L	F_o	F_c	K	L	F_o	F_c
	H = 0			8	0	254	276		-3	399	386	3	0	551	603		-1	93	121		-6	78	31
1	9	177	224		6	72	13		-9	120	149		1	69	71		-3	185	180	17	-3	145	166
2	6	137	133		-3	67	76	6	0	259	291		5	72	7		-6	99	93	18	4	85	10
3	3	96	104		-4	76	78		3	241	238		6	216	222	1	3	213	211	19	0	206	227
4	3	225	230		-6	232	214		9	85	68		-3	80	44		9	86	43	20	-3	84	81
5	3	387	384	9	0	172	194	7	3	452	444	4	0	236	252		-3	370	382				
	6	118	108		3	301	307		-3	143	139		9	144	172		-6	82	28		H = 5		
6	0	127	151		-6	82	94	8	3	120	107		-7	73	66	2	0	146	159				
	1	85	128		-9	104	135		-2	65	7		-9	374	433		6	290	289	1	0	124	136
	6	213	195	10	3	403	385		-3	73	74	5	0	500	547		9	143	120		3	299	310
	9	95	127		6	147	139		-6	367	339		3	89	54		-3	140	142		-1	64	53
7	3	143	137		-9	186	213	9	0	112	122		9	83	41		-6	140	146		-3	156	146
	9	182	205	11	0	100	114		3	596	571		-3	216	198		-7	71	51	2	0	93	114
8	0	267	307		6	231	222		-3	66	54	6	0	141	148	3	0	201	208		3	345	347
9	9	227	283		-6	75	67	10	0	119	124		3	134	129		3	116	106		6	104	79
10	0	197	200	12	-3	317	310		6	81	76		9	110	117		6	225	217		-3	180	185
	3	114	123	13	6	209	247		-3	143	134		-3	242	243		-9	86	86		-5	69	19
11	2	67	52	14	0	177	180		-6	128	120		-4	74	69	4	0	332	336		-6	162	175
	3	191	181		6	78	19	11	0	181	172		-9	120	120		-3	68	56		-9	76	54
	6	134	134		-3	129	129		6	280	280	7	3	382	372		-9	100	120	3	0	327	318
12	0	120	124		-6	117	144		-2	67	65		9	108	95	5	0	93	104		-3	106	90
	3	258	256	15	0	150	167		-3	177	177	8	-5	68	24		3	121	127		-6	310	315
	6	103	85		3	79	85		-6	72	17		-6	217	208		6	149	158	4	0	82	92
13	3	106	95		-6	119	154	12	0	74	82	9	0	94	105		-6	112	116		3	309	324
	6	193	175	16	0	318	310		-3	258	261		6	95	88		9	128	152		6	91	104
14	6	177	224		-6	179	215		-6	89	88		-3	305	296	6	3	139	147		-4	89	43
16	0	329	323	17	3	121	142		-9	140	145		-6	99	95		6	161	150		-6	146	154
18	0	166	169	18	3	98	112	13	0	253	251		-9	81	15		-3	240	231		-7	71	22
	3	115	141	21	0	91	79		2	76	50	10	0	163	174		-6	218	198	5	-6	422	431
20	0	133	134		3	124	156		3	95	92		6	126	159	7	3	152	161	6	3	210	209
	3	161	213		-2	87	10		6	91	99		-3	403	397		6	87	98		4	80	64
22	3	107	92	22	-3	120	153		-3	115	95	11	0	248	249		-3	449	451		6	115	141
								14	0	325	321	12	6	98	149	8	3	114	120		-3	145	135
	H = 1				H = 2			15	5	73	22		-9	156	179		6	178	219		-6	121	115
								16	0	87	53	13	0	383	390		-3	114	109		-9	96	120
1	0	235	278	0	0	149	129		-6	157	198	14	6	95	86		-6	85	56	7	0	112	98
	5	70	32		3	178	180	17	0	116	104		-6	134	134	9	0	98	94		3	185	172
	-6	237	230		7	79	80		3	142	159	15	0	69	13		-3	578	571		6	91	86
	3	76	108		-6	978	959	18	-3	98	128		3	296	278	10	0	123	144		-3	374	370
	6	178	184	1	3	372	372		-6	101	134		-6	123	156		6	92	113	9	0	135	126
3	6	325	312		9	101	94	20	3	96	92	16	-6	213	215		-3	98	73		3	80	76
4	3	74	70		-9	82	19		-3	183	204	17	1	69	20		-6	85	59		-9	112	139
	6	154	160	2	0	161	192	21	0	95	112		3	132	138		-9	90	72	10	0	204	213
	-1	96	130		1	68	108		4	86	16		-3	132	151	11	0	353	378		3	80	48
	-3	885	903		3	162	163	22	-3	92	101	18	6	156	155		-6	110	137		-6	122	144
5	1	92	101		6	137	138						-3	110	109	12	0	203	218		-9	189	220
	3	215	200		-6	153	138		H = 3			19	-5	84	14		4	79	18	11	3	112	100
	6	438	431	3	3	77	50					20	-3	96	67		-6	89	92		-6	194	217
	-7	78	52		6	177	166	1	3	156	138	21	-3	149	163		-9	128	145	12	0	213	235
6	3	257	246		-3	87	114		6	119	91		-4	88	14	13	0	143	170		3	216	213
	6	105	121	4	0	71	93		9	124	171						3	88	60	13	3	111	123
	-3	319	317		6	109	103		-6	236	235		H = 4				-6	148	168		6	99	83
	-9	105	123		-3	233	235	2	0	308	329					14	3	180	204		-6	238	259
7	0	118	121		-6	71	43		3	200	191	0	1	74	117		-6	196	235	14	0	94	78
	6	79	48		-9	104	112		9	153	193		3	122	110	15	-4	81	26		3	145	150
	9	178	194	5	0	150	171		-3	90	97		6	239	239	16	3	130	174	15	-3	253	277

Table 4. cont.

K	L	F_o	F_c	K	L	F_o	F_c	K	L	F_o	F_c	K	L	F_o	F_c	K	L	F_o	F_c
17	3	94	64		3	92	96		-6	239	230	5	0	170	159				
	-3	141	131	18	0	100	101	1	3	194	175	5	-3	89	75		H = 11		
18	0	180	188		-3	93	99		-3	74	75		-6	117	97				
19	0	113	98	19	-6	161	178	2	0	99	90	6	0	83	47	1	-6	145	111
	3	107	109						3	104	94		2	80	17	2	3	166	181
					H = 7				6	97	34		-6	162	153		-3	170	156
	H = 6								-3	241	227		-9	130	111		-4	78	5
				1	0	102	103		-6	290	285	7	0	280	262		-6	91	89
0	0	404	397		6	118	118	3	3	224	192		2	30	10	3	0	157	136
	3	245	265		-3	312	309		-3	196	185		3	108	79		3	103	102
	-3	113	106		-6	106	111		-6	217	213		-4	87	69		-6	155	133
	-5	79	36		-9	84	77	4	-3	112	84		-6	104	79	4	-3	170	149
	-9	81	85	2	0	165	151	5	0	154	135		-9	110	103		-9	117	86
1	-3	209	203		-3	368	350		3	175	170	8	-3	99	82	5	0	191	166
	-9	225	229	3	-6	231	230		-6	154	156		-6	125	130		-6	164	135
2	0	392	386	4	0	154	139	6	0	89	83	9	0	201	169		-7	90	3
	3	214	220		3	123	145		3	167	174		-3	113	98	6	-6	89	50
	-6	150	144		-2	68	23		6	142	139	10	0	251	213	7	1	78	13
	-9	111	75		-3	337	335		-6	127	134	11	0	156	153		-6	208	193
3	0	294	381	5	0	104	99	7	3	149	148		3	85	47	9	-3	93	52
	3	193	184		6	110	121		-6	105	93	12	-3	212	195		-6	131	121
	-3	116	119	6	0	194	165		-9	96	98	13	-3	127	120	10	-3	91	79
	-6	154	166		-3	209	200	8	0	273	284		-6	85	65		-6	206	193
4	3	85	90		-9	104	87		-6	243	235	14	-6	121	101		-7	88	1
	-4	87	104	7	6	167	191	9	0	203	191	15	-4	84	5	11	0	99	76
	-6	102	105		-3	183	176		3	131	121	16	-3	99	82		-6	145	126
5	0	268	259		-9	195	192	10	-3	157	140			H = 10		12	-3	87	53
	-3	107	116	8	0	166	165		-6	127	117					13	-3	121	102
	-10	82	14		3	83	90	11	3	141	140	0	0	187	193				
6	0	221	232		-3	92	68		-6	120	95		1	94	10		H = 12		
	-3	148	142	9	6	105	131	12	0	89	100		-9	118	123				
	-9	138	125		-6	87	82		-3	202	196	1	3	155	179	0	0	103	67
7	0	104	106	10	6	165	188	13	0	127	117		-3	193	183		-3	113	104
	-3	172	162		-5	74	20		-6	104	73	2	0	87	70		-6	110	121
	-9	195	208		-6	159	162	14	3	183	181		-9	136	126	1	0	116	98
8	0	289	266	11	0	80	34		-6	90	73	3	-3	216	191		-3	210	182
	6	142	194		6	100	123		-7	85	13	5	-3	189	173	2	0	140	133
	-3	127	123		-2	73	44	15	3	154	132		-6	89	81	3	-6	105	57
	-9	88	66		-3	98	98	16	-6	102	82		-7	87	9	5	0	109	73
9	3	101	108	12	3	174	188	18	-3	130	114	6	0	175	153	6	0	208	183
	6	86	119		-3	222	207						-3	187	178		-6	136	138
	-9	273	296		-6	143	153			H = 9			-6	108	76	7	0	114	91
10	0	183	169	13	0	96	113					7	-3	157	151				
	3	149	142		-3	117	123	1	0	142	137	8	-5	80	23		H = 13		
11	0	138	128	14	0	166	154		-9	167	165		-6	208	197				
	-6	247	265		-3	177	154	2	0	162	146	9	0	94	58	2	-3	209	178
12	3	181	188		-6	85	87		3	153	154		3	92	78	3	-3	151	110
	-6	118	108	15	-3	94	85		-3	140	109		-3	137	116		-6	149	117
13	-3	81	71		-7	98	10		-6	84	79		-6	120	116	6	-3	100	98
	-6	84	101	16	0	185	191		-9	199	187	11	0	146	130	6	-4	96	21
14	-3	206	208		3	91	74	3	0	202	190		2	86	12				
15	0	99	100	18	-6	184	152		-8	80	19		-3	108	137				
	-3	108	85					4	3	164	156	12	-6	85	86				
16	0	145	127		H = 8				-3	151	137	13	-6	146	95				
	-3	170	168						-6	93	106	14	-3	206	181				
17	0	117	127	0	-3	265	251		-9	194	183	15	-3	141	123				