

The crystal structure of jagoite

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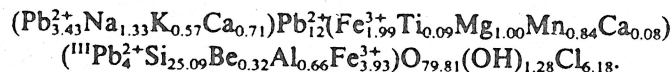
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Abstract

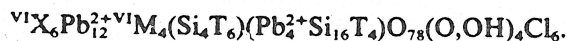
The crystal structure of jagoite ($a = 8.528(8)$, $c = 33.33(3)\text{\AA}$) was solved and refined in space group $P\bar{6}2c$ to $R_1 = 0.057$.

The structure is characterized by the presence of double and single tetrahedral layers connected by a sheet of iron and lead cations. Other lead cations as well as chloride anions are located inside the double layer. The single layer is characterized by an incomplete net of tetrahedra: the absent tetrahedron at the origin is replaced by the Fe(1) octahedron. The double layer is made up of two tetrahedral sheets, each of them built up of six membered rings of tetrahedra and PbO_3 ψ -tetrahedra.

The chemical data give rise to the following crystal chemical formula:



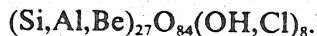
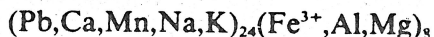
The corresponding idealized crystal chemical formula is



The chemical and structural data suggest ordering of silicon and iron in tetrahedral sites and of iron, magnesium, and manganese in octahedral sites. Possible ordering schemes, in space group $P31c$, are proposed.

Introduction

Jagoite is a rare lead and iron silicate, which was described from Långban, Sweden, by Blix *et al.* (1957). On the basis of its physical properties and chemical composition they suggested that jagoite is a sheet silicate with unit cell content



The absence of adequate data concerning its crystal chemistry and its classification among the silicate minerals led us to undertake a crystal structure analysis.

Experimental

The specimen of jagoite from Långban used in this study (NMNH #113302) was kindly given us by Dr. J. S. White of the Smithsonian Institution.

Whereas Blix *et al.* (1957) reported that jagoite is trigonal with Laue group $\bar{3}$, no systematic ex-

tinctions, and lattice parameters $a = 8.65(3)$ and $c = 33.5(1)\text{\AA}$, the many crystals we examined displayed the Laue symmetry $6/mmm$ and systematic extinctions in hhl for $l = 2n + 1$. This indicated $P6_3/mmc$, $P6_3mc$ and $P\bar{6}2c$ as possible space groups for jagoite. It is worthwhile to recall that Blix *et al.* (1957) reported that the "quality of the photographs was rather poor on account of the easiness with which the plates of jagoite are deformed." Actually, we too observed the easy deformability of jagoite crystals; notwithstanding, we obtained very fine diffraction patterns by carefully picking very tiny crystals.

From the many crystals we examined, a small platelet (nearly $0.17 \times 0.14 \times 0.03 \text{ mm}^3$) was chosen for intensity data collection. The lattice parameters, refined by least squares fitting of 18 medium range θ values, were $a = 8.528(8)$, $c = 33.33(3)\text{\AA}$, measured by a Philips PW1100 single crystal diffractometer, using graphite monochromatized $\text{MoK}\alpha$ radiation ($\lambda = 0.7107\text{\AA}$). A total of 3376 reflections were collected by the same diffractometer and the same radiation

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR JAGDITE

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
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3	7	6	160	169	4	5	7	182	181	1	3	8	168	160	0	7	8	134	134	3	5	9	207	305
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1	3	6	122	116	1	6	7	113	117	2	4	8	272	268	1	8	8	71	87	1	6	9	97	118
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2	4	7	227	224	0	8	7	84	99	3	5	3	130	123	3	4	9	246	246	1	8	9	74	79
1	4	7	126	128	0	8	7	93	99	4	5	3	136	122	2	4	9	116	124	0	8	9	28	65
0	4	7	199	201	1	8	7	77	78	5	5	3	182	202	1	4	9	237	244	0	8	9	61	65
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4	5	7	163	181	1	2	8	257	251	0	6	8	204	200	3	4	9	250	246	1	10	10	214	215
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1	5	7	147	149	1	2	8	257	251	2	6	8	175	176	2	5	9	255	269	0	10	10	112	114

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR JAGGITE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
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3	5	13	74	23	1	4	14	132	142	0	1	15	39	25	2	7	15	110	109	1	5	16	172	190
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OBSERVED AND CALCULATED STRUCTURE FACTORS FOR JAGDITE

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0	7	17	98	92	2	5	18	131	128	0	4	19	314	319	2	2	20	256	251	0	7	20	162	160	0	7	20	162	160
1	7	17	234	265	3	5	18	203	206	1	4	19	182	162	2	3	20	265	279	0	7	20	170	160	0	7	20	170	160

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR JAGOITE

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H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
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0	1	21	284	273	0	7	21	85	108	2	6	22	75	71	1	5	23	252	234	3	4	24	199	197
0	1	21	304	273	0	7	21	73	108	1	6	22	107	89	2	5	23	177	160	4	4	24	216	232
1	2	21	58	70	1	7	21	200	213	0	6	22	55	70	3	5	23	163	163	3	5	24	133	117
0	2	21	111	117	0	0	22	631	569	0	6	22	64	70	2	5	23	159	174	2	5	24	154	163
0	2	21	127	117	0	1	22	89	54	1	6	22	115	89	1	5	23	159	175	1	5	24	115	119
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3	4	21	152	160	2	2	22	146	135	0	1	23	152	146	0	7	23	193	212	1	6	24	110	135
2	4	21	54	66	2	3	22	232	221	0	1	23	167	146	1	7	23	219	224	0	6	24	17	8
1	4	21	193	196	1	3	22	246	235	1	2	23	331	310	0	0	24	813	750	1	0	24	39	9
0	4	21	356	362	0	3	22	212	213	0	2	23	83	75	0	1	24	230	207	1	6	24	143	135
0	4	21	364	362	0	3	22	212	213	0	2	23	83	75	0	1	24	235	207	2	6	24	110	122
1	4	21	204	196	1	3	22	248	235	1	2	23	335	310	1	1	24	46	41	0	7	24	53	49
2	4	21	84	66	2	3	22	225	221	2	3	23	343	351	1	2	24	135	113	0	7	24	51	49
3	4	21	154	160	3	3	22	71	71	1	3	23	119	120	0	2	24	122	111	0	0	25	93	0
4	5	21	78	93	3	4	22	154	162	0	3	23	155	163	0	2	24	112	111	0	1	25	59	41
3	5	21	185	192	2	4	22	116	115	0	3	23	173	163	1	2	24	134	113	0	1	25	60	41
2	5	21	149	161	1	4	22	180	170	1	3	23	128	120	2	2	24	141	136	1	2	25	237	219
1	5	21	124	122	0	4	22	227	243	2	3	23	372	351	2	3	24	133	131	0	2	25	324	297
0	5	21	84	101	0	4	22	234	243	3	4	23	347	349	1	3	24	292	290	0	2	25	332	297
0	5	21	102	101	1	4	22	183	170	2	4	23	125	122	0	3	24	401	386	1	2	25	241	219
1	5	21	132	122	2	4	22	116	115	1	4	23	133	124	0	3	24	413	386	2	3	25	237	233
2	5	21	185	161	3	4	22	157	162	0	4	23	333	336	1	3	24	326	290	1	3	25	120	106
3	5	21	201	192	4	4	22	77	106	0	4	23	346	336	2	3	24	142	131	0	2	25	17	16
4	5	21	93	93	3	5	22	151	162	1	4	23	131	124	3	3	24	115	109	0	3	25	50	16
2	6	21	184	189	2	5	22	128	130	2	4	23	147	122	3	4	24	199	197	1	3	25	117	106
1	6	21	98	89	1	5	22	132	133	3	4	23	349	349	2	4	24	90	104	2	3	25	236	233
0	6	21	50	56	0	5	22	119	126	3	5	23	152	163	1	4	24	205	219	3	4	25	86	77
0	6	21	27	56	0	5	22	129	126	2	5	23	173	160	0	4	24	262	259	2	4	25	178	196
1	6	21	81	89	1	5	22	143	133	1	5	23	218	234	0	4	24	288	259	1	4	25	145	145

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR JAGGITE

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	4	25	116	113	2	4	26	181	198	2	4	27	62	69	0	4	28	126	134	1	5	29	250	252
0	4	25	123	113	1	4	26	117	115	1	4	27	151	113	0	4	28	113	134	0	5	29	47	16
1	4	25	157	145	0	4	26	41	20	0	4	27	75	65	1	4	28	93	73	0	5	29	61	16
2	4	25	191	196	0	4	26	41	20	0	4	27	65	65	2	4	28	156	149	1	5	29	259	252
3	4	25	84	77	1	4	26	121	115	1	4	27	122	113	3	4	28	196	187	2	5	29	140	123
3	5	25	140	150	2	4	26	205	193	2	4	27	75	69	2	5	28	53	46	0	6	29	305	320
2	5	25	159	161	3	4	26	74	95	3	4	27	92	69	1	5	28	135	131	0	6	29	219	320
1	5	25	243	247	4	4	26	89	95	2	5	27	101	98	0	5	28	113	123	0	0	30	72	42
0	5	25	151	166	3	5	26	156	159	1	5	27	147	130	0	5	28	134	123	0	1	30	75	40
0	5	25	162	160	2	5	26	145	154	0	5	27	108	116	1	5	28	145	131	0	1	30	37	40
1	5	25	275	247	1	5	26	112	103	0	5	27	105	116	2	5	28	46	46	1	1	30	323	307
2	5	25	165	161	0	5	26	348	368	1	5	27	143	130	1	6	28	76	77	1	2	30	125	108
3	5	25	169	150	0	5	26	373	368	2	5	27	81	98	0	6	28	143	147	0	2	30	42	50
2	6	25	119	115	1	5	26	135	103	1	6	27	70	86	0	6	28	157	147	0	2	30	78	58
1	6	25	125	119	2	5	26	156	154	0	6	27	48	41	1	5	28	90	77	1	2	30	129	108
0	6	25	38	27	3	5	26	175	159	0	6	27	41	41	0	0	29	79	0	2	2	30	263	225
0	6	25	49	27	1	6	26	134	147	1	6	27	90	86	0	1	29	74	52	2	3	30	146	123
1	6	25	142	119	0	6	26	108	109	0	0	28	851	789	0	1	29	54	52	1	3	30	66	81
2	6	25	118	115	0	6	26	85	109	0	1	28	55	15	1	2	29	350	323	0	3	30	225	199
0	6	26	213	161	1	6	26	154	147	0	1	28	49	15	0	2	29	25	19	0	3	30	226	190
0	1	26	76	47	0	7	26	65	30	1	1	28	284	260	1	2	29	347	323	1	3	30	90	81
0	1	26	54	47	0	7	26	62	30	1	2	28	221	208	2	3	29	283	271	2	3	30	146	123
1	1	26	657	565	0	0	27	54	0	0	2	28	113	106	1	3	29	33	37	3	3	30	320	284
1	2	26	224	216	0	1	27	39	27	0	2	28	125	106	0	3	29	123	106	3	4	30	119	108
0	2	26	371	348	0	1	27	66	27	1	2	28	232	208	0	3	29	119	106	2	4	30	80	83
0	2	26	372	348	1	2	27	191	170	2	2	28	172	139	1	3	29	50	37	1	4	30	171	165
1	2	26	245	216	0	2	27	268	252	2	3	28	87	104	2	3	29	291	271	0	4	30	137	125
2	2	26	227	197	0	2	27	281	252	1	3	28	253	244	3	4	29	214	220	0	4	30	124	125
2	3	26	410	373	1	2	27	174	170	1	3	28	275	269	2	4	29	225	218	1	4	30	182	165
1	3	26	132	134	2	3	27	139	141	0	3	28	303	269	1	4	29	117	106	2	4	30	87	83
0	3	26	141	129	1	3	27	65	79	1	3	28	261	244	0	4	29	131	154	3	4	30	134	108
0	3	26	142	129	0	3	27	18	29	2	3	28	113	104	0	4	29	140	154	1	5	30	103	102
1	3	26	148	134	0	3	27	28	29	3	3	28	21	40	1	4	29	148	106	0	5	30	34	42
2	3	26	417	373	1	3	27	55	79	3	4	28	176	187	2	4	29	239	218	0	5	30	54	42
3	3	26	23	9	2	3	27	160	141	2	4	28	133	149	3	4	29	215	220	1	5	30	114	102
3	4	26	101	95	3	4	27	61	69	1	4	28	58	73	2	5	29	118	123	0	6	30	215	220

