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Schoonerite: its atomic arrangement

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Abstract

Schoonerite, $ZnMn^{2+}Fe_2^{2+}Fe^{3+}(OH)_2(H_2O)_7(PO_4)_3 \cdot 2H_2O$, orthorhombic, *a* 11.119(4), *b* 25.546(11), *c* 6.437(3) A, *Pmab*, $Z = 4$, is one of several structurally-related phosphate minerals having axial repeats approximating 6.4 A. The structure was solved by Patterson and Fourier syntheses, and least-squares refinement converged to $R(hkl) = 0.085$ for 897 nonequivalent reflections.

Edge-sharing Fe^{2+}–O octahedral chains join by sharing corners with Fe^{3+}–O octahedra and $[PO_4]$ tetrahedra forming a sheet parallel to {010}. To this sheet are linked additional $[PO_4]$ tetrahedra, $[MnO_6]$ octahedra and $[ZnO_5]$ polyhedra. The resultant slabs are joined in the *b* direction by a network of hydrogen bonds only. Interlayer water molecules contribute to this hydrogen bond network.

Average interatomic distances are $^6Fe^{2+}(1)$–O 2.12 A, $^6Fe^{2+}(2)$–O 2.15, $^6Fe^{3+}(3)$–O 2.00, $^6Mn^{2+}$–O 2.16, ^5Zn–O 2.09, $^4P(1)$–O 1.54, and $^4P(2)$–O 1.54.

Introduction

In the preceding paper, Moore and Kampf (1977) described the new species, schoonerite, $ZnMn^{2+}Fe_2^{2+}Fe^{3+}(OH)_2(H_2O)_7(PO_4)_3 \cdot 2H_2O$, $Z = 4$, from the Palermo No. 1 pegmatite in North Groton, New Hampshire. Although this species is rather widely distributed at Palermo, it occurs only sparingly as sprays of small, thin, feathery crystals in pockets and on fracture surfaces. A water determination was deemed unfeasible due to the difficulty in obtaining a sufficient quantity of pure material. The determination of the crystal structure of schoonerite was considered the best method for obtaining an accurate measure of its water content and for characterizing its rather complex crystal chemistry.

Besides accomplishing these ends, the crystal structure determination revealed a close similarity between the structures of schoonerite and montgomeryite, and in addition showed that schoonerite possesses octahedral and tetrahedral clusters locally similar to those in elmsteadite and melonjosephite.

Experimental

Good single crystals of schoonerite are exceedingly rare, and such crystals large enough for structure analysis seemed for quite some time nonexistent. The crystal chosen, a thin rectangular tablet measuring 0.32×0.01×0.08 mm along the three crystallographic axes, was mounted with the *a* axis parallel to the ϕ axis on a Picker automated diffractometer. The intensities of 2383 reflections (maximum $2\theta = 45°$) were gathered, utilizing graphite-monochromatized Mo$K\alpha$ radiation. A rather large mosaic spread necessitated wide half-angle scans of 1.0° with a scan rate of 2.0°/minute. Twenty-second background counting times were used on either side of each reflection. The least-squares refinement of 30 reference reflections ($2\theta = 20$–$30°$) yielded cell constants, *a* 11.119(4), *b* 25.546(11), and *c* 6.437(3) A. Systematic extinctions were consistent with either of the space groups *P2ab* or *Pmab*.

The measured intensities were corrected for absorption using the Gaussian integral method described by Burnham (1966). The data were processed by conventional computational procedures. After averaging symmetry-equivalent reflections and rejecting all $I(hkl) < 3\sigma[I(hkl)]$, 897 independent data were available for the ensuing analysis.

Solution and refinement of the structure

The Patterson map, $P(uvw)$, revealed strong vector concentrations at the levels $u = 0, \frac{1}{4}$, and $\frac{1}{2}$, indicating that the twenty heavy atoms (Fe, Mn, Zn) in

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SCHOENEFITE. OBSERVED AND CALCULATED STRUCTURE FACTORS (X10)

(1)

L= 0

K	H	FOBS	FCALC
0	2	416	448
0	4	6180	5505
0	6	2272	2215
0	8	4330	4106
0	10	1602	1591
2	0	3207	2933
2	1	1674	1642
2	2	1414	1378
2	3	567	540
2	4	1209	1245
2	5	504	434
2	6	1855	1789
2	7	1086	1029
2	8	2251	2051
2	9	913	874
2	10	785	589
4	0	521	584
4	1	1843	1836
4	2	1614	1541
4	3	1810	1755
4	4	560	504
4	5	1192	1087
4	6	2145	2052
4	7	1530	1431
4	8	391	442
4	9	545	580
4	10	1221	1119
4	11	1073	1158
6	0	2542	2676
6	2	882	864
6	3	1597	1834
6	6	452	417
6	7	1064	994
6	8	1529	1286
6	10	491	632
6	11	811	806
8	0	2356	2282
8	1	1738	1579
8	2	3078	2920
8	3	326	316
8	4	305	350
8	5	1448	1434
8	6	2192	2152
8	8	966	787
8	9	914	878
8	10	860	998
10	0	282	101
10	2	2795	2749
10	3	1374	1200
10	4	750	759
10	5	468	369
10	6	3075	2895
10	7	608	763
10	8	336	414

K	H	FOBS	FCALC
4	6	346	357
4	7	288	288
5	0	839	868
5	1	1534	1530
5	3	1019	1127
5	5	1626	1682
5	7	1252	1277
5	9	488	416
5	11	1138	1081
6	0	1226	1176
6	1	425	395
6	2	383	410
6	4	278	268
6	5	715	748
6	6	792	714
6	8	403	390
6	9	437	436
6	10	365	300
7	0	609	565
7	1	1554	1541
7	2	2124	2052
7	3	240	156
7	4	455	422
7	5	1314	1342
7	6	746	693
7	7	359	280
7	8	645	651
7	9	645	654
7	10	301	355
7	11	307	266
8	0	1310	1259
8	1	634	632
8	2	773	793
8	4	1294	1294
8	5	584	484
8	6	421	493
8	7	350	355
8	8	382	465
8	9	294	189
8	10	573	549
9	0	911	874
9	1	737	820
9	2	599	633
9	3	1590	1599
9	4	844	835
9	5	1160	693
9	6	860	866
9	7	1153	1088
9	9	287	287
9	10	749	699
9	11	892	790
10	0	1674	1629
10	1	351	340
10	2	513	480
10	3	481	526
10	4	621	658

K	H	FOBS	FCALC
1	2	3766	3836
1	3	541	640
1	4	1642	1773
1	5	557	535
1	6	2176	2369
1	7	1006	1058
1	8	315	331
1	9	289	297
1	10	1065	1185
1	11	528	550
2	0	560	617
2	2	1889	1858
2	3	605	558
2	4	1027	1108
2	6	716	743
2	7	319	39
2	9	555	622
2	10	392	398
3	0	260	388
3	1	823	830
3	2	855	867
3	3	209	152
3	4	1143	1182
3	5	407	464
3	6	505	631
3	7	536	591
3	8	658	616
3	9	314	447
3	10	769	911
3	11	367	298
4	0	518	620
4	1	1514	1468
4	4	1183	1305
4	5	1203	1288
4	6	257	342
4	7	497	569
4	8	652	654
4	9	454	496
4	10	351	234
4	11	460	466
5	0	349	408
5	1	152	291
5	2	369	243
5	3	313	299
5	4	1277	1344
5	5	325	381
5	7	771	827
5	8	677	812
5	9	462	575
5	10	582	566
5	11	337	413
6	0	862	894
6	1	198	128
6	2	1601	1630
6	3	580	580
6	4	305	253

K	H	FOBS	FCALC
19	2	309	244
19	3	327	358
19	6	539	437
20	0	659	654
20	2	548	452
20	4	502	507
20	5	575	458
21	0	280	86
21	1	466	561
21	2	870	910
21	4	413	267
21	5	665	494
21	6	755	737
22	1	470	387
22	3	372	431
22	4	647	678
23	0	1732	1691
23	2	745	698
23	3	409	265
23	4	1609	1587
24	1	265	8
24	2	431	410
25	0	897	939
25	2	339	271
26	1	512	501

L= 3

K	H	FOBS	FCALC
0	4	1018	1081
0	10	541	488
1	0	607	630
1	1	241	106
1	2	657	672
1	4	229	163
1	6	630	713
1	10	311	212
2	0	1002	949
2	1	539	444
2	2	538	526
2	4	686	702
2	5	540	541
2	6	553	655
2	7	838	975
2	8	314	327
2	9	456	479
2	10	331	369
3	0	1533	1487
3	2	970	1008
3	3	237	350
3	4	526	572
3	6	1045	1079
3	7	334	383
3	8	341	547
3	10	427	335
4	1	693	711

K	H	FOBS	FCALC
18	5	282	258
18	6	688	668
18	7	1024	1033
19	0	837	877
19	1	419	440
19	3	285	443
19	4	409	366
19	5	398	414
19	6	302	388
20	0	348	273
20	1	1367	1434
20	2	445	560
20	3	494	614
20	5	1176	1161
21	0	582	573
21	2	350	186
21	4	329	183
22	0	1028	948
22	4	374	387
23	1	509	599
23	3	358	418
24	0	556	599
24	2	287	109

L= 4

K	H	FOBS	FCALC
0	0	1377	1344
0	2	577	617
0	4	1184	1173
0	6	605	769
0	8	908	994
1	0	2410	2419
1	1	959	934
1	2	213	207
1	3	973	1035
1	4	1132	1176
1	5	432	440
1	6	369	339
1	7	811	900
1	8	1515	1631
1	9	455	411
2	0	1710	1709
2	1	1412	1478
2	2	462	457
2	3	671	677
2	4	731	781
2	5	1390	1476
2	7	540	515
2	8	625	584
2	9	1002	1000
3	0	2280	2329
3	1	1289	1315
3	2	893	919
3	3	1086	1162
3	4	1044	1009

K	H	FOBS	FCALC
19	0	434	445
19	2	762	742
20	0	325	365
20	2	322	245
20	3	392	331
20	4	299	258
21	0	878	787
21	2	372	470
22	0	889	859

L= 5

K	H	FOBS	FCALC
0	0	407	276
0	2	318	281
0	4	246	241
0	6	391	402
1	0	272	106
1	1	253	180
1	2	632	667
1	3	461	513
1	4	370	381
1	5	344	279
1	6	361	385
2	0	297	285
2	1	509	536
2	4	278	142
2	5	455	442
2	7	281	145
3	1	242	115
3	2	926	932
3	3	675	657
3	4	534	541
3	5	382	377
3	6	442	586
3	7	445	520
3	9	451	389
5	0	264	165
5	2	284	272
5	3	854	907
5	7	510	466
6	0	341	367
6	1	343	293
6	2	569	608
6	4	234	100
6	6	442	543
6	7	283	127
7	0	236	74
7	2	1430	1452
7	4	387	319
7	6	927	954
8	0	282	354
8	1	272	141
8	2	380	323
8	3	237	155
9	0	863	919

10	9	580	604
10	10	1662	1541
10	11	760	675
12	0	3426	3246
12	1	1259	1290
12	2	1264	1160
12	3	1744	1681
12	4	1346	1320
12	5	1338	1285
12	6	479	380
12	7	909	941
12	8	1203	1150
12	9	824	759
12	10	638	466
14	0	3185	3125
14	1	1345	1292
14	2	1201	1123
14	4	1526	1525
14	5	1768	1742
14	6	875	793
14	7	419	278
14	8	1552	1522
14	9	1269	1151
16	0	1639	1523
16	1	1418	1374
16	2	1510	1484
16	3	833	913
16	4	646	658
16	5	1392	1272
16	6	1663	1566
16	7	704	714
16	8	1130	1036
16	9	553	588
18	0	1613	1603
18	1	545	466
18	2	470	340
18	5	309	228
18	8	584	656
18	9	575	621
20	0	441	406
20	3	507	526
20	4	291	156
20	5	564	519
20	6	535	480
20	8	835	767
22	0	634	438
22	1	802	750
22	2	1838	1826
22	3	734	647
22	4	416	351
22	5	547	523
22	6	1629	1622
22	7	708	646
24	0	1242	1154
24	1	333	304
24	2	1839	1830
24	3	606	472
26	0	1065	944
26	1	1230	1194
26	2	667	659
26	3	1290	1406

L= 1

K	H	FOBS	FCALC
0	0	1623	1715
10	5	812	858
10	6	784	789
10	8	500	444
10	9	658	618
10	10	388	266
11	0	320	459
11	1	843	929
11	2	752	808
11	3	386	395
11	4	364	389
11	5	323	323
11	6	1026	948
11	7	275	245
11	10	340	239
12	0	327	130
12	1	369	400
12	2	251	243
12	4	515	417
12	6	372	255
13	0	311	330
13	1	1084	1036
13	2	703	727
13	3	434	458
13	4	548	509
13	5	1272	1261
13	6	433	428
13	9	654	714
14	0	350	340
14	1	456	414
14	2	483	362
14	3	301	277
14	6	282	221
14	7	1047	639
15	0	551	500
15	1	935	539
15	2	657	647
15	3	681	644
15	4	503	430
15	5	726	655
15	7	616	615
15	8	268	152
15	9	603	508
16	1	585	694
16	2	709	653
16	3	518	557
16	5	688	671
16	6	773	743
16	7	393	271
16	8	341	279
16	9	604	442
17	0	1666	1636
17	1	933	942
17	2	1057	1085
17	4	1273	1168
17	5	957	910
17	6	1059	1009
17	8	1203	1088
17	9	657	688
18	1	1012	1028
18	3	716	671
18	4	303	455
18	5	555	513
18	7	901	919
19	0	393	435
19	1	921	944
19	2	757	665
6	6	942	1035
6	7	274	390
6	8	304	260
6	10	938	896
7	0	265	116
7	1	893	879
7	2	1767	1810
7	3	554	606
7	4	1366	1425
7	5	1024	1023
7	6	1194	1224
7	7	341	401
7	9	605	542
7	10	637	609
7	11	298	394
8	1	948	926
8	4	1353	1378
8	5	550	599
8	7	401	465
8	8	374	480
8	10	250	140
9	0	1038	1060
9	1	1180	1218
9	2	944	978
9	3	1471	1495
9	4	2259	2222
9	6	459	511
9	7	1698	1658
9	8	765	750
9	10	273	338
10	0	1565	1585
10	1	1215	1183
10	3	480	529
10	4	2152	2184
10	5	530	511
10	6	356	318
10	7	782	821
10	8	747	769
10	9	355	339
10	10	380	341
11	0	1593	1631
11	1	899	896
11	3	662	609
11	4	2075	2086
11	5	1385	1362
11	6	1147	1114
11	9	725	635
11	10	310	204
12	0	353	294
12	2	1213	1249
12	3	696	677
12	4	540	472
12	5	239	140
12	6	988	909
12	8	388	205
12	9	310	226
12	10	682	651
13	0	719	686
13	1	512	467
13	2	1459	1449
13	3	1165	1173
13	4	1074	1079
13	5	267	65
13	6	1084	1055
13	7	854	961
13	8	441	484
4	3	1012	1060
4	4	888	531
4	5	362	349
4	6	354	289
4	7	541	645
4	9	439	471
4	10	354	230
5	0	496	434
5	1	446	442
5	2	259	182
5	4	464	368
5	5	774	791
5	6	266	260
5	7	255	236
5	8	278	96
5	9	344	360
6	0	2327	2346
6	1	902	883
6	2	1251	1234
6	3	776	751
6	4	1524	1562
6	5	1241	1266
6	6	779	860
6	8	1137	1186
6	9	830	818
6	10	898	963
7	0	797	915
7	1	504	509
7	2	336	408
7	5	437	451
7	6	756	765
7	7	246	303
7	8	338	117
8	0	1589	1559
8	1	746	739
8	3	1096	1105
8	4	1670	1647
8	5	554	647
8	6	289	219
8	7	513	553
8	8	590	578
8	9	611	617
8	10	565	650
9	0	1528	1515
9	2	356	235
9	4	715	683
9	5	253	116
9	6	869	811
9	8	279	205
9	10	461	434
10	0	468	438
10	1	1309	1241
10	3	1205	1242
10	4	390	320
10	5	1656	1603
10	7	524	584
10	9	921	885
11	0	645	597
11	2	271	403
11	4	276	263
12	0	723	642
12	1	292	235
12	2	380	378
12	3	547	525
12	4	798	750
12	5	412	374
3	5	581	653
3	6	245	352
3	7	1134	1221
3	8	570	1031
3	9	513	524
4	0	347	310
4	1	676	623
4	2	308	200
4	4	449	436
4	5	700	779
4	6	438	355
4	8	278	236
4	9	445	372
5	0	1155	1221
5	2	630	683
5	4	719	750
5	6	838	764
5	7	243	130
5	8	690	765
6	0	445	381
6	2	235	356
6	4	325	327
6	6	545	559
6	7	325	354
6	8	417	399
6	9	428	390
7	0	355	257
7	1	646	667
7	2	690	720
7	3	635	677
7	4	275	252
7	5	900	942
7	6	961	1080
7	8	635	605
7	9	654	587
8	0	1167	1213
8	1	755	788
8	2	785	715
8	3	615	608
8	4	593	611
8	5	606	621
8	6	434	439
8	7	341	323
8	8	458	513
8	9	685	625
9	0	1177	1119
9	2	1378	1426
9	4	388	445
9	6	748	504
9	7	288	222
9	8	363	353
10	0	376	407
10	2	935	1018
10	3	615	606
10	6	536	585
10	7	578	630
11	0	523	633
11	1	284	315
11	2	1906	1856
11	3	776	832
11	5	552	625
11	6	1577	1537
11	8	318	255
12	0	278	275
12	1	571	674
12	3	416	452
9	1	452	511
9	2	283	211
9	3	626	513
9	4	501	562
9	5	416	361
9	6	252	525
9	7	579	554
10	0	267	151
10	1	405	394
10	3	710	565
10	5	603	455
10	7	422	222
11	0	524	534
11	1	411	388
11	2	767	755
11	3	319	307
11	5	435	477
11	6	367	282
12	0	606	635
12	1	317	357
12	3	320	424
12	5	308	457
13	0	581	656
13	1	326	302
13	2	406	277
13	4	510	547
13	6	324	128
14	0	514	575
14	2	425	375
14	4	676	562
15	0	511	507
15	1	441	431
15	3	567	533
15	4	875	850
15	5	310	264
16	0	715	751
16	1	326	226
16	3	259	135
16	4	395	507
17	0	1022	1045
17	1	321	41
17	2	315	357
17	3	391	374
18	0	267	142

L= 2

K	H	FOBS	FCALC
0	0	400	413
0	2	1510	1516
0	4	1022	1070
1	0	347	358
1	2	360	301
1	4	235	20
1	5	302	259
2	1	1169	1152
2	2	1233	1226
2	3	535	450
2	4	331	469
2	5	1030	1106
3	1	266	36
3	2	874	917
3	3	258	345
3	4	454	411
4	0	822	758
4	1	535	466

0	2	454	502	19	3	612	535	14	0	540	608	12	7	336	415	12	5	782	834	4	2	1015	1088
0	4	698	732	19	4	451	408	14	1	855	797	13	0	221	351	12	6	558	683	4	3	603	528
0	6	328	339	19	5	520	449	14	2	847	834	13	2	422	333	12	8	357	293	4	4	799	874
0	10	351	217	19	6	804	721	14	4	633	651	13	3	270	317	13	0	1335	1198	4	5	388	359
1	0	1036	1023	19	7	732	683	14	5	760	756	13	6	323	435	13	2	870	842	5	0	582	528
1	1	1106	1175	19	8	303	267	14	6	332	392	13	7	429	360	13	3	372	287	5	3	604	711
1	2	453	596	20	1	309	457	14	7	356	307	13	8	330	163	13	4	942	959	5	4	494	441
1	3	1627	1791	20	3	258	272	15	0	599	545	14	1	253	325	13	5	272	35	6	0	641	558
1	5	726	796	20	5	379	434	15	1	567	603	14	2	358	380	13	6	846	855	6	3	334	361
1	6	254	147	20	7	338	108	15	2	1903	1890	14	3	856	840	13	7	381	284	6	4	933	547
1	7	1149	1255	21	0	1261	1259	15	3	288	179	14	5	442	473	14	0	1341	1395	7	1	389	350
1	11	801	857	21	2	506	511	15	4	1310	1279	14	7	567	622	14	1	360	330	7	2	656	657
2	0	489	497	21	3	765	677	15	5	750	807	15	0	605	565	14	2	304	189	7	5	307	316
2	1	452	438	21	4	463	471	15	6	1131	1139	15	5	304	183	14	3	385	443	8	1	608	597
2	3	216	229	21	6	781	666	15	9	514	501	15	6	248	26	14	4	900	976	8	3	544	560
2	5	699	719	21	7	828	814	16	1	618	522	16	0	897	945	14	7	562	568	8	4	956	577
2	6	415	388	23	0	356	370	16	4	956	1025	16	1	326	326	15	0	1641	1627	9	0	595	612
2	9	247	280	23	1	428	507	16	5	718	724	16	2	1909	1969	15	2	285	87	9	2	281	46
2	11	275	87	23	2	305	446	16	9	310	257	16	4	854	508	15	4	746	737	9	3	344	377
3	0	990	1188	23	5	501	574	17	0	857	849	16	5	518	550	16	0	1179	1145	10	0	967	983
3	1	263	269	27	0	1260	1288	17	1	250	163	16	6	1400	1467	16	2	626	673	10	1	320	126
3	2	550	548					17	4	1543	1542	16	8	534	581	16	4	490	509	10	3	317	453
3	3	201	180			L=	2	17	5	362	452	17	1	444	440	17	0	625	537	10	4	1394	1480
3	9	413	455					17	7	300	218	17	2	278	319	17	2	558	587	11	1	343	185
3	10	256	330	K	H	FOBS	FCALC	17	8	649	594	17	3	556	549	17	3	295	71	11	2	465	458
3	11	293	348	0	0	950	947	18	0	374	379	17	4	245	47	17	5	258	419	11	3	256	58
4	0	1139	1188	0	2	1023	1123	18	2	499	557	17	7	451	438	17	6	454	519	12	0	1397	1312
4	1	502	458	0	4	622	644	18	4	414	295	18	0	773	712	18	0	627	686	12	1	651	535
4	2	320	341	0	6	1324	1373	18	5	246	120	18	1	890	861	18	2	359	377	12	2	498	669
4	3	200	260	0	10	1152	1213	18	6	688	635	18	2	635	676	18	3	568	570	13	0	446	450
4	4	647	656	1	0	269	284	18	7	333	20	18	3	845	854	18	4	400	454	13	2	271	346
4	5	351	260	1	1	1154	1217	19	0	404	561	18	4	538	491	18	5	273	103				