Supplementary information

(Tables S1 and S2 to be included also in the American Mineralogist Crystal Structure Database)

Table S1. Fractional positions and thermal factors for atoms in the ferricopiapite structure at low temperature. These data were obtained by refinement of the structural model with the low-temperature neutron diffraction pattern.

atom	*x*	*y*	*z*	U*100
Fe*A*	0	0	0	0.0(6)
Fe1	0.7866(6)	0.3142(2)	0.5493(6)	1.5(3)
Fe2	0.5948(5)	0.6691(2)	0.8053(6)	3.7(4)
S1	0.8347(11)	0.7366(4)	0.2177(11)	1.4(9)
S2	0.8216(11)	0.4175(4)	0.2243(12)	5.5(16)
S3	0.6381(11)	0.1936(4)	0.1974(11)	1.7(10)
O1	0.745(2)	0.6687(6)	0.090(2)	8.3(11)
O2	0.692(2)	0.7688(8)	0.296(2)	7.2(9)
O3	0.055(2)	0.2980(7)	0.628(2)	2.6(6)
O4	0.052(2)	0.2046(7)	0.857(2)	4.3(6)
O5	0.629(2)	0.3902(7)	0.109(2)	0.5(5)
O6	0.852(2)	0.4942(6)	0.324(2)	1.5(6)
O7	0.886(2)	0.3601(7)	0.338(2)	0.5(5)
O8	0.939(2)	0.4251(7)	0.087(2)	0.0(4)
O9	0.563(2)	0.1136(6)	0.167(2)	2.1(6)
O10	0.511(2)	0.7610(8)	0.865(2)	0.0(4)
O11	0.783(2)	0.2151(8)	0.089(2)	3.5(6)
O12	0.724(2)	0.2204(7)	0.399(2)	2.0(5)
O13H	0.463(2)	0.6602(8)	0.544(2)	0.0(4)
O14w	0.702(2)	0.2760(8)	0.759(2)	3.6(6)
O15w	0.850(2)	0.4107(7)	0.723(2)	8.8(12)
O16w	0.232(2)	0.9485(8)	0.086(2)	7.7(10)
O17w	0.693(2)	0.5719(8)	0.757(2)	2.6(6)
O18w	0.052(2)	0.9873(8)	0.730(2)	25.5(31)
O19w	0.831(2)	0.7291(7)	0.740(2)	5.5(7)
O20w	0.178(2)	0.0939(7)	0.059(2)	5.2(7)
O21w	0.775(2)	0.9088(7)	0.450(2)	1.7(5)
O22w	0.542(2)	0.5597(8)	0.289(2)	0.6(5)
O23w	0.646(2)	0.0789(7)	0.575(2)	21.1(25)
D1 (O13)	0.499(3)	0.6255(9)	0.466(3)	4.1(6)
D2 (O14)	0.751(2)	0.2566(8)	0.879(2)	3.3(5)
D3 (O14)	0.559(2)	0.2588(9)	0.750(2)	3.2(5)
D4 (O15)	0.896(2)	0.4179(9)	0.864(2)	2.2(5)
D5 (O15)	0.946(2)	0.4384(8)	0.666(2)	1.8(4)
D6 (O16)	0.321(3)	0.9421(16)	0.213(3)	11.1(11)
D7 (O16)	0.299(3)	0.9506(13)	-0.035(3)	8.0(9)
D8 (O17)	0.833(2)	0.5739(10)	0.803(3)	4.5(6)
D9 (O17)	0.638(2)	0.5206(9)	0.737(3)	7.6(8)
D10 (O18)	0.110(3)	1.0292(11)	0.684(3)	9.3(10)
D11 (O18)	-0.078(3)	0.9671(15)	0.643(3)	12.2(11)
D12 (O19)	0.850(2)	0.7130(10)	0.622(2)	3.8(6)
D13 (O19)	0.961(2)	0.7497(12)	0.822(3)	5.5(7)
D14 (O20)	0.301(3)	0.1106(13)	0.044(4)	8.7(8)
D15 (O20)	0.111(5)	0.1332(13)	0.088(6)	18.3(18)
D16 (O21)	0.703(3)	0.9373(12)	0.363(3)	8.6(9)
D17 (O21)	0.754(2)	0.8570(7)	0.390(2)	1.4(4)
D18 (O22)	0.657(3)	0.5356(13)	0.308(3)	9.3(10)
D19 (O22)	0.508(2)	0.5808(8)	0.161(2)	1.2(4)
D20 (O23)	0.499(3)	0.0771(15)	0.583(4)	9.3(9)
D21 (O23)	0.716(3)	0.1255(10)	0.558(4)	9.6(10)

* occupancy 0.626(6); occupancies of other sites are 1.00

Table S2. Fractional positions and thermal factors for atoms in the copiapite structure. These data are the result of GGA *ab-initio* calculations. *A* site is vacant, Fe^{3+} is in high-spin state.

atom	*x*	*y*	*z*
Fe1	0.7809	0.3176	0.5340
Fe2	0.6154	0.6692	0.8207
S1	0.8435	0.7367	0.2451
S2	0.8061	0.4226	0.2092
S3	0.6225	0.1991	0.1646
O1	0.7575	0.6740	0.0839
O2	0.6962	0.7644	0.3151
O3	0.0484	0.2974	0.5998
O4	0.0304	0.2080	0.8124
O5	0.6074	0.3964	0.0959
O6	0.8245	0.4938	0.3237
O7	0.8622	0.3681	0.3327
O8	0.9334	0.4283	0.0827
O9	0.5256	0.1242	0.1246
O10	0.5200	0.7539	0.8921
O11	0.7723	0.2156	0.0678
O12	0.7039	0.2203	0.3761
O13	0.4691	0.6574	0.5605
O14	0.6794	0.2801	0.7495
O15	0.8758	0.4129	0.7106
O16	0.2530	0.9655	0.1435
O17	0.7025	0.5751	0.7468
O18	0.1073	0.9768	0.7305
O19	0.8466	0.7241	0.7492
O20	0.1153	0.1059	0.0376
O21	0.7638	0.9211	0.4652
O22	0.5148	0.5559	0.2812
O23	0.5943	0.0818	0.5416
H1 (O13)	0.4952	0.6200	0.4690
H2 (O14)	0.2647	0.7460	0.1499
H3 (O14)	0.4590	0.7346	0.2744
H4 (O15)	0.1095	0.5858	0.1515
H5 (O15)	0.0146	0.5535	0.3090
H6 (O16)	0.1349	0.9498	0.0446
H7 (O16)	0.3463	0.9852	0.0806
H8 (O17)	0.1653	0.4252	0.1915
H9 (O17)	0.3749	0.4742	0.2580
H10 (O18)	0.8432	0.9845	0.3370
H11 (O18)	0.0246	0.0427	0.3409
H12 (O19)	0.1375	0.2843	0.3797
H13 (O19)	0.0287	0.2532	0.1682
H14 (O20)	0.2491	0.1050	0.0762
H15 (O20)	0.1041	0.1432	0.9553
H16 (O21)	0.6328	0.9232	0.4741
H17 (O21)	0.7567	0.8705	0.4142
H18 (O22)	0.6380	0.5412	0.2982
H19 (O22)	0.4923	0.5756	0.1624
H20 (O23)	0.6671	0.0702	0.6617
H21 (O23)	0.6674	0.1235	0.5074

Table S3. Bond-valence analysis of the structure of ferricopiapite (room-temperature results). The bond-valence values were calculated from data given by Brown (2002).

	Fe*A*	S1	D1	D4	D7	D10	D13	D16	D19	
	Fe1	S2	D2	D5	D8	D11	D14	D17	D20	
	Fe2	S3	D3	D6	D9	D12	D15	D18	D21	
O1	-	1.43	-	-	-	-	-	-	0.10	1.96
	-	-	-	-	-	-	-	-	-	
	0.43	-	-	-	-	-	-	-	-	
O2	-	1.47	-	-	-	-	-	-	-	2.09
	-	-	-	-	-	-	-	0.29	-	
	-	-	0.26	-	-	0.07	-	-	-	
O3	-	1.43	-	-	-	-	-	-	-	2.12
	0.54	-	-	-	-	-	-	-	-	
	-	-	-	-	-	0.15	-	-	-	
O4	-	1.54	-	-	-	-	0.07	-	-	1.97
	-	-	0.07	-	-	-	-	0.05	-	
	-	-	-	-	-	-	0.25	-	-	
O5	-	-	-	-	-	-	-	-	0.13	2.04
	-	1.49	-	-	-	-	-	-	-	
	0.42	-	-	-	-	-	-	-	-	
O6	-	-	-	-	-	-	-	-	-	2.01
	-	1.42	-	0.33	-	-	-	-	-	
	-	-	-	-	-	-	-	0.26	-	
O7	-	-	-	-	-	-	-	-	-	2.21
	0.48	1.59	-	0.05	0.05	-	-	-	-	
	-	-	-	-	-	0.05	-	-	-	
O8	-	-	-	0.34	-	-	-	-	-	2.20
	-	1.53	-	0.05	0.28	-	-	-	-	
	-	-	-	-	-	-	-	-	-	
O9	-	-	-	-	0.16	-	-	-	-	2.01
	-	-	-	-	-	-	0.28	-	-	
	-	1.52	-	-	-	-	-	-	0.05	
O10	-	-	-	-	-	-	-	-	-	2.08
	-	-	-	-	-	-	0.06	-	-	
	0.63	1.39	-	-	-	-	-	-	-	
O11	-	-	-	-	-	-	0.21	-	-	1.97
	-	-	0.25	-	-	-	-	-	-	
	-	1.50	-	-	-	-	-	-	-	
O12	-	-	-	-	-	-	-	-	-	2.18
	0.58	-	-	-	-	-	-	-	-	
	-	1.46	-	-	-	-	-	-	0.14	
O13H	-	-	0.83	-	-	-	-	-	-	2.14
	0.65	-	-	-	-	-	-	-	-	
	0.54	-	0.07	-	-	0.05	-	-	-	
O14w	-	-	-	0.05	-	-	-	-	-	2.19
	0.59	-	0.81	-	-	-	-	-	-	
	-	-	0.74	-	-	-	-	-	-	

Table S3. continued

	Fe1 Fe2 Fe3	S1 S2 S3	D1 D2 D3	D4 D5 D6	D7 D8 D9	D10 D11 D12	D13 D14 D15	D16 D17 D18	D19 D20 D21	
O15w	-	-	0.06	0.76	-	-	-	-	-	2.02
	0.47	-	-	0.73	-	-	-	-	-	
	-	-	-	-	-	-	-	-	-	
O16w	$^{2\times}$0.40	-	-	-	0.71	-	-	-	-	1.82
	-	-	-	-	-	-	0.05	-	-	
	-	-	-	0.66	-	-	-	-	-	
O17w	-	-	0.05	-	-	-	-	-	-	2.00
	-	-	-	-	0.74	-	-	-	-	
	0.44	-	-	-	0.77	-	-	-	-	
O18w	$^{2\times}$0.44	-	-	-	0.07	0.77	-	0.05	-	1.98
	-	-	-	-	-	0.65	-	-	-	
	-	-	-	-	-	-	-	-	-	
O19w	-	-	-	-	-	-	0.84	-	-	2.04
	-	-	-	-	-	-	-	-	-	
	0.44	-	-	-	-	0.76	-	-	-	
O20w	$^{2\times}$0.63	-	-	-	-	0.05	-	-	-	2.22
	-	-	-	-	-	0.06	0.74	-	-	
	-	-	-	-	-	-	0.75	-	-	
O21w	-	-	-	-	-	0.26	-	0.85	-	2.30
	-	-	-	-	-	0.28	-	0.77	0.15	
	-	-	-	-	-	-	-	-	-	
O22w	-	-	0.25	-	-	-	-	-	0.74	2.05
	-	-	-	-	-	-	-	-	-	
	-	-	-	-	0.29	-	-	0.76	-	
O23w	-	-	-	-	-	-	-	0.14	-	2.02
	-	-	-	-	-	-	-	-	0.79	
	-	-	-	0.33	-	-	-	-	0.75	
	2.93	5.87	1.20	1.15	0.94	1.07	1.13	1.05	0.97	
	3.32	6.03	1.12	1.15	1.07	0.98	1.12	1.11	0.94	
	2.90	5.88	1.07	0.99	1.06	1.09	1.00	1.01	0.94	

References

BROWN, I.D. (2002): *The Chemical Bond in Inorganic Chemistry*. IUCr Monograph on Crystallography 12. Oxford Science Publications, 278 pp.