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Cerchiaraite-(Fe) and cerchiaraite-(Al), two new barium cyclosilicate chlorides from Italy and California, USA

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ABSTRACT

The ideal formula for members of the cerchiaraite group is $Ba_4M_4(Si_4O_{12})O_2(OH)_4Cl_2[Si_2O_3(OH)_4]$, where M represents Mn^{3+}, Fe^{3+} or Al in the octahedral site. A suffix-based naming scheme is used in which the original cerchiaraite is renamed cerchiaraite-(Mn) and two new minerals are named cerchiaraite-(Fe) and cerchiaraite-(Al). The type localities for cerchiaraite-(Fe) are the Cerchiara mine, Liguria, Italy and the Esquire No. 7 and No. 8 claims, Big Creek, Fresno County, California, USA. The type localities for cerchiaraite-(Al) are the Esquire No. 1 claim, Rush Creek, Fresno County, California, USA and the Esquire No. 7 and No. 8 claims noted above. At the Cerchiara mine, cerchiaraite-(Fe) occurs in small fractures and veinlets in a Jurassic ophiolitic sequence. It is of secondary hydrothermal origin and occurs as tan to brown thin prisms and matted fibres. Cerchiaraite-(Fe) and cerchiaraite-(Al) from the Esquire No. 1, No. 7 and No. 8 claims occur in parallel-bedded quartz-sanbornite vein assemblages which formed as a result of fluid interaction along the margin of the vein. At the Esquire No. 1, No. 7 and No. 8 claims, both cerchiaraite-(Fe) and cerchiaraite-(Al) occur as subparallel aggregates of blue to bluish green irregular prisms. Both minerals are transparent with a vitreous lustre, Mohs hardness ~4½, brittle tenacity, irregular fracture and no cleavage. The calculated density of cerchiaraite-(Fe) is 3.710 g cm^{-3}; the measured density of cerchiaraite-(Al) is 3.69(3) g cm^{-3} and the calculated density is 3.643 g cm^{-3}. Cerchiaraite-(Fe) is uniaxial (+), with ω = 1.741(2) and ε = 1.768(2); it is weakly pleochroic and O is colourless and E is yellow. Cerchiaraite-(Al) is uniaxial (−), with ω = 1.695(2) and ε = 1.677(2); it is strongly pleochroic and O is colourless and E is blue. Electron-microprobe analyses yielded empirical formulae ranging from $(Ba_{3.82}Na_{0.02}Ca_{0.04})_{\Sigma 3.88}(Fe^{3+}_{3.42}Ti^{4+}_{0.27}Al^{3+}_{0.25}Mn^{3+}_{0.04}Mg_{0.02})_{\Sigma 4.00}Si_{5.62}O_{15.47}(OH)_{9.31}Cl_{2.22}$ (Cerchiara mine) to $Ba_{4.00}(Al^{3+}_{2.40}Fe^{3+}_{1.12}Mg_{0.15}Fe^{2+}_{0.12}Mn^{2+}_{0.06})_{\Sigma 3.85}Si_{5.78}O_{15.34}(OH)_{8.75}Cl_{2.91}$ (Esquire No. 1 claim). Cerchiaraite is tetragonal with Z = 2 and crystallizes in space group $I4/mmm$. The cell parameters for cerchiaraite-(Fe) are a = 14.3554(12), c = 6.0065(5) Å and V = 1237.80(5) Å^3; those for cerchiaraite-(Al) are a = 14.317(4), c = 6.0037(18) Å and V = 1230.6(6) Å^3. In the cerchiaraite-(Fe) structure, SiO_4 tetrahedra share corners forming a four-membered Si_4O_{12} ring. The ring is corner-linked to an edge-sharing chain of $Fe^{3+}O_6$ octahedra running parallel to c. A Cl site alternates along c with the Si_4O_{12} ring. A large channel in the framework contains Ba atoms around its periphery and statistically distributed Si_2O_7 silicate dimers and Cl atoms. The strong blue pleochroic colour is attributed to Fe^{2+}–Fe^{3+} intervalence charge transfer along the octahedral chain.

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Introduction

The sanbornite deposits which are located along Big Creek and Rush Creek (Walstrom and Leising, 2005) in Fresno County and at Trumbull Peak (Dunning and Cooper, 1999) in Mariposa County, California, USA, have yielded a wealth of exotic minerals, including 17 new species. The first of these, sanbornite, was described by Rogers (1932) from Trumbull Peak; fencooperite was described from the same locality by Roberts *et al*. (2001). Seven of the new species, namely fresnoite, krauskopfite, macdonaldite, muirite, traskite, verplanckite and walstromite, were described from Big Creek and Rush Creek by Alfors *et al*. (1965), these were followed by alforsite (Newberry *et al*., 1981), titantaramellite (Alfors and Pabst, 1984), bigcreekite (Basciano *et al*., 2001*a*), kampfite (Basciano *et al*., 2001*b*), devitoite (Kampf *et al*., 2010) and ferroericssonite (Kampf *et al*., 2011). In this paper, we report the two new minerals, cerchiaraite-(Fe) and cerchiaraite-(Al), from Big Creek and Rush Creek.

When they were discovered at the deposits along Big Creek and Rush Creek by one of the authors (REW) in the mid-1960s, the new minerals described herein were thought to be a single phase, which was referred to as 'mineral 10'. Following the description of cerchiaraite from the historic Cerchiara mine in the northern Apennines, Italy, by Basso *et al*. (2000), the similarity of 'mineral 10' to cerchiaraite was recognized by comparing their X-ray powder diffraction data. Subsequent investigations have demonstrated that 'mineral 10' corresponds to two species with identical frameworks, the Fe^{3+}- and Al-analogues of cerchiaraite. The research has also shown that the Fe^{3+}-analogue occurs at the Cerchiara mine.

The cerchiaraite group is therefore made up of three species and in accordance with Mills *et al*. (2009) they have been named using a suffix-based scheme in which cerchiaraite is the root name and the single suffix corresponds to the dominant cation (Mn, Fe or Al) in the octahedral site. The original cerchiaraite described by Basso *et al*. (2000) is renamed cerchiaraite-(Mn) and the two new minerals, described herein, are cerchiaraite-(Fe) and cerchiaraite-(Al). The new minerals (IMA 2012-012 and IMA 2012-011, respectively), their names and the new name for the original cerchiaraite have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association.

The descriptions of the new minerals are based upon five cotype specimens deposited at the Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, California 90007, USA. A specimen from the Esquire No. 1 claim, which contains crystals with compositions that are all in the Al-dominant range, has been assigned catalogue number 63519 and is referred to as 'Esq1'. Specimens from the Esquire No. 7 and No. 8 claims, which contain crystals representing both Fe- and Al-dominant compositions, have been assigned catalogue numbers 63517 and 63518 and are referred to as 'Esq7' and 'Esq8', respectively. Specimens from the Cerchiara mine have been assigned catalogue numbers 63517 and 63518 and are referred to as 'Cer1' and 'Cer2', respectively. Crystals from Cer1 have compositions close to the Fe endmember; crystals from Cer2, are Fe-dominant and exhibit significant substitution of Mn for Fe.

Occurrence and paragenesis

Cerchiaraite-(Fe) occurs at the Cerchiara mine, Borghetto Vara, Vara Valley, La Spezia Province, Liguria, Italy and at the Esquire No. 7 and No. 8 claims, Big Creek, eastern Fresno County, California, USA. The locations of the claims are as follows: Esquire No. 7 is at SE¼ SE¼, Section 27, T11S., R25E., Mount Diablo Meridian, 36º56′40″N, 119º14′28″W; Esquire No. 8 is at SE¼ SW¼, Section 22, T11S., R25E., Mount Diablo Meridian, 36º56′42″N, 119º14′12″W. Cerchiaraite-(Al) occurs at the Esquire No. 1 claim, Rush Creek, eastern Fresno County, California, USA [which is located at NE¼ NW¼, Section 16, T11S., R25E., Mount Diablo Meridian, 37º05′N, 119º16′20″W] and also at the Esquire No. 7 and No. 8 claims, noted above. These are considered to be the type localities.

At the Cerchiara mine, cerchiaraite-(Fe) occurs in small fractures and veinlets within the metacherts of a Jurassic ophiolitic sequence. Associated minerals include aegirine, calcite,

Mn-bearing diopside (variety schefferite), hematite, K-feldspar, norrishite and quartz. The occurrence is very similar to that of cerchiaraite-(Mn), which is described in detail by Basso *et al*. (2000). The new mineral is of secondary hydrothermal origin, related to re-equilibration of the ophiolitic sequences during tectonometamorphic overprinting (~80 Ma) in prehnite-pumpellyite facies conditions (P = 2–3 kbar, T = 250–300ºC) (Lucchetti *et al*., 1988). The occurrence of cerchiaraite-(Fe) in metapelites in the cherts suggests a sedimentary and/or diagenetic barium enrichment, followed by hydrothermal mobilization and concentration processes along fractures (Cabella *et al*., 1993).

The samples of cerchiaraite-(Fe) and cerchiaraite-(Al) from the Esquire No. 1, No. 7 and No. 8 claims were collected during the mid-1960s by one of the authors (REW). The mineral is found in parallel-bedded quartz-sanbornite vein assemblages. At the Esquire No. 1 claim, cerchiaraite-(Al) is associated with bazirite, diopside, goethite, opal, quartz, sanbornite, titantaramellite, traskite and witherite. At the Esquire No. 7 claim, cerchiaraite-(Fe) and cerchiaraite-(Al) are associated with bazirite, diopside, muirite, pyrrhotite, Ba-rich tobermorite, traskite and witherite. At the Esquire No. 8 claim, they are associated with bazirite, calcite, diopside, pyrrhotite, titantaramellite and Ba-rich tobermorite. A description of the mineralogy of the sanbornite deposits located along Big Creek and Rush Creek in eastern Fresno County, California is provided by Walstrom and Leising (2005). The mineral formed on the margins of quartz-sanbornite veins as a result of fluid interactions. The environment in which the cerchiaraite phases occur at the Esquire No. 1, No. 7 and No. 8 claims appears to have been less oxidizing than at Cerchiara mine, based upon the pleochroic blue colour of the Esquire crystals (see below).

The new minerals have also been found at Trumbull Peak, Mariposa County, California, USA (Dunning and Cooper, 1999), the Baumann prospect, Chickencoop Canyon, Tulare County, California, USA (Walstrom and Dunning, 2003) and the Gunn claim, MacMillan Pass, Yukon Territory, Canada (the type locality for pellyite; Montgomery *et al*., 1972). Material from all three localities has compositions between the Fe and Al endmembers, although all of the samples tested thus far from Trumbull Peak fall into the Fe-dominant range. Material from the Gunn claim has been referred to as 'mineral C'.

FIG. 1. Cerchiaraite-(Fe) with hematite (upper right) from the Cerchiara mine (specimen Cer1); field of view is 3 mm.

Physical and optical properties

At the Cerchiara mine, cerchiaraite-(Fe) occurs as tan to brown thin prisms with square cross-sections. Near-endmember cerchiaraite-(Fe) (Cer1) occurs as matted aggregates of very thin tan fibres (Fig. 1); more Mn-rich cerchiaraite-(Fe) (Cer2) occurs as coarser brown crystals reaching 2 mm in length and 0.1 mm across. The streak varies from nearly colourless to tan. At the Esquire No. 1, No. 7 and No. 8 claims, both cerchiaraite-(Fe) and cerchiaraite-(Al) occur as blue, greenish blue and bluish green irregular prisms in subparallel crystal aggregates which are generally less than 1 mm across (Figs 2 and 3). The streak is pale green-blue.

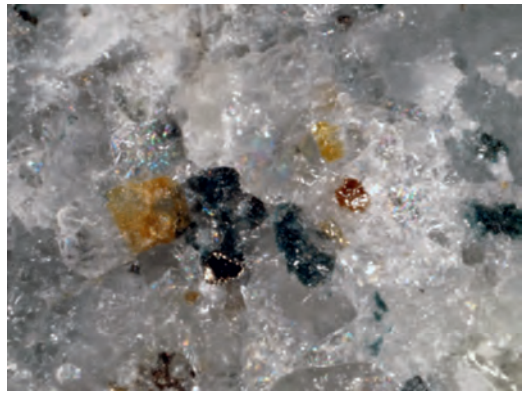

FIG. 2. Cerchiaraite-(Fe)–cerchiaraite-(Al) with pyrrhotite (brown metallic), muirite (yellow), traskite (orange) and diopside (nearly colourless) embedded in witherite from the Esquire No. 7 claim; field of view is 3 mm.

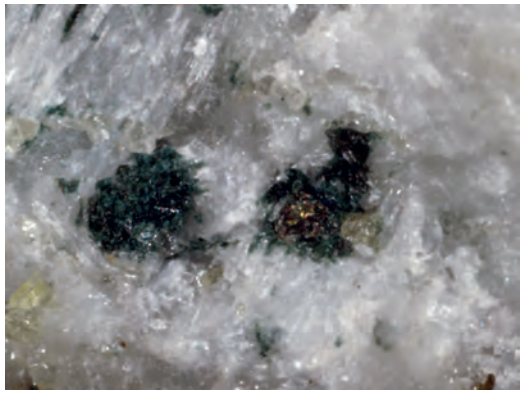

FIG. 3. Cerchiaraite-(Fe)–cerchiaraite-(Al) with pyrrhotite (brown metallic), tobermorite (white silky) and diopside (pale yellow) embedded in calcite from the Esquire No. 8 claim; field of view is 3 mm.

Cerchiaraite-(Fe) and cerchiaraite-(Al) crystals are transparent and have a vitreous lustre. They do not fluoresce in long-wave or short-wave ultraviolet light. Their Mohs hardness is about 4½, their tenacity brittle, their fracture irregular and they exhibit no cleavage. The density of the near-endmember cerchiaraite-(Fe) crystals on Cer1 could not be measured because of difficulty in working with the very thin fibres. The calculated density for these crystals is 3.710 g cm^{-3}, based on the empirical formula and the unit-cell dimensions determined by single-crystal X-ray diffraction. The density of cerchiaraite-(Al) crystals on specimen Esq1 determined by the sink–float technique in an aqueous solution of sodium polytungstate is 3.69(3) g cm^{-3}; the calculated density is 3.643 g cm^{-3}, based on the empirical formula and unit-cell dimensions refined from powder-diffraction data.

The optical properties of cerchiaraite-(Fe) and cerchiaraite-(Al) were measured in white light. Cerchiaraite-(Fe) is uniaxial (+), with ω = 1.741(2) and ε = 1.768(2); it is weakly pleochroic, with O colourless and E yellow. Cerchiaraite-(Al) is uniaxial (–), with ω = 1.695(2) and ε = 1.677(2); it is strongly pleochroic with O colourless and E blue.

Chemical composition

Chemical analyses were carried out on a Cameca SX-50 electron microprobe (EMP) fitted with four wavelength-dispersive spectrometers operating in WDS mode at 15 kV, 10 nA with a 5 μm beam diameter. The acquisition times were 10 s on the peak and 5 s on the low and high background positions. Data were reduced, with a ZAF matrix correction (Armstrong, 1988), using *Probe for Windows* software. A variety of natural and synthetic minerals and metals were used as standards.

Insufficient material was available for a direct determination of H_2O, which was calculated by stoichiometry based upon 27 anions (O + Cl = 27) such that there were no more than four cations in either the large cation sites (Ba + Na + Ca = 4) or the octahedral site (Fe + Al + Mn + Mg + Ti = 4). Analytical data for samples Cer1, Cer2, Esq1, Esq7 and Esq8 and the corresponding empirical formulae are given in Table 1. The presence of a small amount of Fe^{2+} in samples from the Esquire claims is revealed by the strong blue pleochroism of the crystals. On the basis of bond-valence analysis (see below) Fe in the structure was allocated as 90% Fe^{3+} and 10% Fe^{2+}. The presence of Fe^{2+} indicates that all of the Mn must be Mn^{2+} in the Esquire samples. The low analytical total for Cer1 is due to the very limited thickness of the crystals.

The atom percentages of Mn, Fe and Al in the studied specimens, and in cerchiaraite-(Mn) (labelled Cer0; Basso *et al*., 2000), are plotted in Fig. 4. The composition of cerchiaraite from the Cerchiara mine varies between the Mn and Fe endmembers and contains relatively little Al. The compositions from the three Esquire claims are low in Mn and cover a broad range on either side

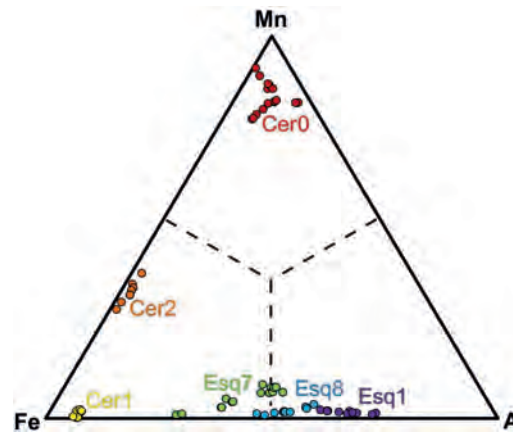

FIG. 4. Ternary plot of cerchiaraite compositions based upon atom% Mn, Fe and Al. The compositions labelled 'Cer0' correspond to those of the original Mn-dominant cerchiaraite of Basso *et al*. (2000).

TABLE 1. Analytical data for cerchiaraite-(Fe) and cerchiaraite-(Al).

	Cer1 [10 analyses (wt.%)]			Cer2 [8 analyses (wt.%)]			Esq1 [11 analyses (wt.%)]			Esq7 [18 analyses (wt.%)]			Esq8 [11 analyses (wt.%)]		
Const.	Mean	Range	SD	Mean	Range	SD	Mean	Range	SD	Mean	Range	SD	Mean	Range	SD
Na_2O	0.05	0.00–0.13	0.05	0.09	0.00–0.21	0.08									
BaO	40.81	39.13–42.08	1.10	41.65	39.81–44.17	1.69	44.82	43.75–46.91	0.95	43.85	41.89–45.75	1.08	44.84	43.21–46.09	0.99
CaO	0.17	0.03–0.42	0.13	0.03	0.00–0.05	0.02									
MgO	0.06	0.00–0.13	0.05	0.02	0.01–0.04	0.01	0.43	0.35–0.59	0.08	0.12	0.06–0.18	0.04	0.21	0.12–0.31	0.06
MnO*							0.30	0.20–0.44	0.07	1.09	0.18–1.69	0.50	0.38	0.16–0.74	0.17
Mn_2O_3	0.22	0.04–0.46	0.18	6.96	5.74–8.03	0.68									
Fe_2O_3	19.03	18.25–20.26	0.59	13.82	12.77–14.46	0.57	(7.27)	5.58–8.25	0.88	(11.44)	9.62–14.99	1.76	(9.90)	8.63–11.49	0.90
FeO*							0.65			1.08			0.89		
Fe_2O_3*							6.55			10.30			8.91		
Al_2O_3	0.87	0.74–0.94	0.66	0.28	0.18–0.34	0.06	8.94	8.12–9.79	0.59	5.74	3.77–6.81	0.92	7.22	6.40–8.14	0.60
TiO_2	1.51	0.52–2.25	0.17	1.02	0.68–1.20	0.17									
SiO_2	23.51	23.26–23.83	0.26	25.16	24.10–25.82	0.62	25.38	25.25–26.22	0.29	24.90	24.29–25.37	0.30	25.15	24.61–26.14	0.50
Cl	5.47	5.13–5.98	1.05	5.07	4.77–5.36	0.18	7.53	7.35–7.94	0.18	6.89	6.50–7.41	0.31	6.73	6.48–6.92	0.18
O=Cl	−1.23			−1.14			−1.70			−1.55			−1.52		
H_2O	5.84			5.07			5.76			5.81			6.24		
Total	96.31			98.03			98.66			98.23			99.05		

* The presence of a small amount of Fe^{2+} in samples from the Esquire claims is indicated by the strong blue pleochroism; based upon the bond-valence analysis Fe has been allocated as 90% Fe^{3+} and 10% Fe^{2+}; furthermore, the presence of Fe^{2+} indicates that all Mn must be present as Mn^{2+}.

Empirical formulae (based on 27 anions):

Cer1: $(Ba_{3.82}Na_{0.02}Ca_{0.04})_{\Sigma 3.88}(Fe^{3+}_{3.42}Ti^{4+}_{0.27}Al^{3+}_{0.25}Mn^{3+}_{0.04}Mg^{+}_{0.02})_{\Sigma 4.00}Si_{5.62}O_{15.47}(OH)_{9.31}Cl_{2.22}$

Cer2: $(Ba_{3.88}Na_{0.04}Ca_{0.01})_{\Sigma 3.93}(Fe^{3+}_{2.47}Mn^{3+}_{1.26}Ti^{4+}_{0.18}Al^{3+}_{0.08}Mg^{+}_{0.01})_{\Sigma 4.00}Si_{5.98}O_{16.92}(OH)_{8.04}Cl_{2.04}$

Esq1: $Ba_{4.00}(Al^{3+}_{2.40}Fe^{3+}_{1.12}Mg_{0.15}Fe^{2+}_{0.12}Mn^{2+}_{0.06})_{\Sigma 3.85}Si_{5.78}O_{15.34}(OH)_{8.75}Cl_{2.91}$

Esq7: $Ba_{4.00}(Fe^{3+}_{1.80}Al^{3+}_{1.57}Fe^{2+}_{0.21}Mn^{2+}_{0.21}Mg_{0.04})_{\Sigma 3.83}Si_{5.80}O_{15.26}(OH)_{9.02}Cl_{2.72}$

Esq8: $Ba_{4.00}(Al^{3+}_{1.94}Fe^{3+}_{1.53}Fe^{2+}_{0.17}Mn^{2+}_{0.07}Mg_{0.07})_{\Sigma 3.78}Si_{5.73}O_{14.92}(OH)_{9.48}Cl_{2.60}$

of the boundary between the Fe and Al endmembers; they do not approach the endmember compositions, extending between Fe:Al ratios of 75:25 and 25:75.

The ideal formula for members of the cerchiaraite group is $Ba_4M_4(Si_4O_{12})O_2(OH)_4Cl_2[Si_2O_3(OH)_4]$, in which *M* represents the cation in the octahedral site, which can be Mn, Fe or Al. The endmember formula for cerchiaraite-(Fe) requires BaO 43.19, Fe_2O_3 22.49, SiO_2 25.38, H_2O 5.07, Cl 4.99, O=Cl −1.13; total 100.00 wt.%. The endmember formula for cerchiaraite-(Al) requires BaO 47.01, Al_2O_3 15.63, SiO_2 27.63, H_2O 5.52, Cl 5.43, O=Cl −1.23; total 100.00 wt.%. Note that Basso *et al*. (2000) reported an ideal formula for cerchiaraite-(Mn) with only one Cl, even though their empirical formula included 1.54 Cl atoms per formula unit (a.p.f.u). All of our empirical formulae for cerchiaraite-(Fe) and cerchiaraite-(Al) (Table 1)

TABLE 2. Powder X-ray data for cerchiaraite-(Fe) (sample Cer1).

I_{obs}	d_{obs} (Å)	d_{calc} (Å)	I_{calc}	*hkl*
25	10.23	10.1366	40	110
17	7.21	7.1677	30	200
21	5.57	5.5466	39	101
7	5.09	5.0683	7	220
5	4.56	4.5332	9	310
26	4.403	4.3866	42	211
9	3.751	3.7415	11	301
19	3.593	3.5838	38	400
		3.3789	7	330
48	3.327	3.3168	73	321
18	3.214	3.2055	38	420
70	3.016	3.0102	100	411
		3.0075	19	002
8	2.887	2.8833	8	112
16	2.788	2.8114	12	510
		2.7733	21	202
100	2.595	2.5881	59	501
		2.5864	76	222
8	2.470	2.5342	38	440
		2.4585	11	530
		2.2666	4	620
29	2.258	2.2465	35	332
		2.1933	5	422
18	2.107	2.0982	33	541
19	2.034	2.0538	9	512
		2.0273	11	550
		2.0137	6	631
		1.9880	4	640
		1.9857	5	103
20	1.907	1.9136	7	213
		1.9035	4	532
26	1.880	1.8823	17	730
		1.8714	34	721
		1.8708	9	602
39	1.8118	1.8101	42	622
		1.7919	15	800
		1.7903	10	323
11	1.7439	1.7384	6	820
		1.7369	11	413
16	1.6818	1.6811	8	552
19	1.6552	1.6584	24	642
		1.6431	18	503
9	1.6016	1.6027	5	840
		1.5956	7	732
		1.5831	5	910
		1.5397	5	901
23	1.5062	1.5054	7	761
		1.5038	13	004
		1.4936	9	543
8	1.4755	1.4733	7	851
		1.4730	4	662
		1.4335	4	860
43	1.4107	1.4147	17	941
		1.4049	14	723
		1.4009	13	912
		1.3924	6	950
		1.3866	5	404
		1.3614	4	424
		1.3159	4	871
29	1.2980	1.3047	4	772
		1.2941	16	10·0·2
		1.2932	11	444
14	1.2609	1.2735	5	10·2·2
		1.2635	8	952
		1.2540	6	11·2·1
		1.2540	9	10·5·1
7	1.2162	1.2171	3	10·4·2
		1.2110	4	853
17	1.1796	1.1784	7	12·2·0
		1.1779	9	943
		1.1749	6	734

Only calculated lines with intensities of 4 or greater are listed, unless they correspond to observed lines. The calculated powder data are based on the structure refinement for Esq8.

have between two and three Cl a.p.f.u. We did not observe any evidence that Cl migration, such as that reported for F and Cl in apatite by Stormer *et al*. (1993), produced higher than actual Cl values in the EMP analyses. In the crystal structure (see below), one Cl a.p.f.u. is located at a fully occupied Cl site (Cl1) at the origin [0;0;0]. The additional Cl is located at a partially occupied channel site (Cl2) 0.8 Å from the partially occupied O5 site of the channel silicate group, leading to the conclusion that both the channel Cl and the silicate group cannot be locally present at the same time. Those samples that provide close to the ideal six Si a.p.f.u., Cer0 and Cer2, have 1.54 and 2.04 Cl a.p.f.u., respectively, leading us to propose two Cl a.p.f.u. (and 27 total anions) for the ideal formula. The other samples, Cer1, Esq1, Esq7 and Esq 8, exhibit significant deficiencies in Si and excesses of Cl.

The Gladstone–Dale compatibility indices, $1 - (K_P/K_C)$, for Cer1 and Esq1 are 0.010 and 0.007, respectively; both of these are in the superior range (Mandarino, 1981).

X-ray crystallography and structure refinement

Powder and single-crystal X-ray studies were carried out using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer, with mono-

TABLE 3. Powder X-ray data for cerchiaraite-(Al) (sample Esq1).

I_{obs}	d_{obs} (Å)	d_{calc} (Å)	I_{calc}	*hkl*
39	10.15	10.1237	41	110
9	7.16	7.1585	9	200
33	5.555	5.5365	39	101
13	5.066	5.0618	18	220
39	4.407	4.5274	9	310
		4.3795	33	211
8	3.736	3.7358	7	301
16	3.584	3.5793	23	400
		3.3746	6	330
77	3.316	3.3119	80	321
24	3.201	3.2014	27	420
100	3.009	3.0058	100	411
		3.0018	24	002
13	2.870	2.8779	8	112
15	2.779	2.8078	11	510
		2.7682	10	202
93	2.580	2.5845	56	501
		2.5819	51	222
11	2.527	2.5309	25	440
16	2.463	2.4553	13	530
3	2.407	2.4309	2	521
2	2.368	2.3862	6	600
9	2.306	2.3000	7	402
38	2.244	2.2637	6	620
		2.2428	36	332
21	2.097	2.0953	33	541
43	2.029	2.0506	9	512
		2.0247	10	550
		2.0110	8	631
		1.9819	5	103
		1.9349	4	442
68	1.880	1.9101	7	213
		1.9005	4	532
		1.8799	20	730
		1.8689	28	721
		1.8679	6	602
		1.8455	3	303
33	1.8004	1.8074	26	622
		1.7896	10	800
		1.7871	8	323
15	1.7395	1.7362	3	820
		1.7339	7	413
10	1.6816	1.6786	8	552
29	1.6473	1.6560	15	642
		1.6403	18	503
17	1.5920	1.5933	7	732
		1.5811	5	910
13	1.4995	1.5377	3	901
		1.5034	4	761
		1.5009	9	004
21	1.4764	1.4912	7	543
		1.4713	4	851
54	1.4031	1.4128	14	941
		1.4027	14	723
		1.3989	11	912
		1.3906	5	950
22	1.3013	1.3142	4	871
		1.3029	5	772
		1.2922	13	10·0·2
		1.2910	8	444
37	1.2570	1.2618	7	952
		1.2524	9	10·5·1
		1.2524	4	11·2·1

Only calculated lines with intensities of 3 or greater are listed, unless they correspond to observed lines. The calculated powder data are based on a whole-pattern-fitting Rietveld structure refinement for Esq1.

chromatic Mo$K\alpha$ radiation. In the powder-diffraction studies, the observed *d*-spacings and intensities were determined by profile fitting using *JADE 2010* software. Powder data are presented for samples Cer1 (Table 2) and Esq1 (Table 3), as these have the closest compositions to endmember cerchiaraite-(Fe) and cerchiaraite-(Al), respectively. Unit-cell parameters refined from the powder data using *JADE 2010* software with whole pattern fitting are as follows: a = 14.3554(12), c = 6.0065(5) Å with V = 1237.80(5) Å^3 for Cer1 and a = 14.317(4), c = 6.0037(18) Å with V = 1230.6(6) Å^3 for Esq1. The unit-cell parameters refined from the powder data should be considered the most definitive as they were obtained from material closest to the endmember compositions.

Single-crystal structure data were obtained from cerchiaraite-(Fe) from specimen Esq8. The Rigaku *CrystalClear* software package was used to process these data, including the application of an empirical absorption correction. The structure was solved by direct methods using *SIR2004* (Burla *et al*., 2005) and refined with *SHELXL-97* (Sheldrick, 2008). Most of the fully occupied sites in the structure were located by direct methods; the remaining sites, including those with partial occupancies, were located in difference-Fourier maps. The occupancy of the octahedral site refined to an Fe:Al ratio of 0.596:0.404, indicating that the crystal used was cerchiaraite-(Fe), rather than cerchiaraite-(Al).

The analysis showed the Ba site on the periphery of the channel to be fully occupied; however, all of the other channel sites are partially occupied. In the structure of cerchiaraite [now cerchiaraite-(Mn)], Basso *et al*. (2000) reported the Si2 tetrahedron to be statistically distributed in the channel and to exhibit a high degree of distortion. We found the same to be true of the Si2 tetrahedron in cerchiaraite-(Fe). For the Si2, O4 and O5 sites of the channel silicate group,

TABLE 4. Data collection and structure refinement details for crystal from Esq8 corresponding to cerchiaraite-(Fe).

Diffractometer	Rigaku R-Axis Rapid II
X-ray radiation; power	Mo$K\alpha$ (λ = 0.71075 Å); 50 kV, 40 mA
Temperature	298(2) K
Structural Formula	$Ba_4Fe^{3+}_{2.38}Al_{1.62}Si_{6.04}Cl_{2.70}O_{25.17}H_{8.88}$
Space group	$I4/mmm$
Unit-cell dimensions	a = 14.3554(12) Å
	c = 6.0065(5) Å
Z	2
V	1237.80(18) Å^3
Density (for above formula)	3.765 g cm^{-3}
Absorption coefficient	8.373 mm^{-1}
F(000)	1295.6
Crystal size	70 × 40 × 40 µm
θ range	3.68 to 25.03°
Index ranges	$-17 \leqslant h \leqslant 17$, $-17 \leqslant k \leqslant 17$, $-7 \leqslant l \leqslant 7$
Reflections collected/unique	10,966/343 [R_{int} = 0.0646]
Reflections with $F_o > 4\sigma F$	329
Completeness to θ = 25.03°	98.0%
Refinement method	Full-matrix least-squares on F^2
Parameters refined	59
GoF	1.134
Final R indices [$F_o > 4\sigma F$]	R_1 = 0.0253, wR_2 = 0.0557
R indices (all data)	R_1 = 0.0269, wR_2 = 0.0566
Largest diff. peak / hole	+0.883 / −0.799 e A^{-3}

$R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})|/\Sigma[F_o^2]$.
GoF = $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n - p)\}^{½}$.
$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$.
$wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{½}$.
$w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where a is 0.0213, b is 17.7504 and P is $[2F_c^2 + \text{Max}(F_o^2,0)]/3$.

Basso *et al*. (2000) assigned occupancies of ¼, ¼ and ½, respectively. Our refined occupancies for these sites are 0.255(11), 0.24(3) and 0.52(7), respectively. In addition, we found a significant residual peak 0.80 Å from the O5 site. This peak is only 1.42 Å from Si2, which is too close for a Si−O bond; however, the peak is at an appropriate distance from the Ba site (3.10 Å) to correspond to a partially occupied Cl site and was assigned as such.

The details of the data collection and structure refinement are provided in Table 4, the final atom coordinates and displacement parameters in Table 5, selected interatomic distances and angles in Table 6 and bond-valence summations in Table 7. Lists of observed and calculated structure factors have been deposited with *Mineralogical Magazine* and can be downloaded from http://www.minersoc.org/pages/e_journals/dep_mat_mm.html.

Description of the structure

The crystal structure of cerchiaraite-(Fe) (Fig. 5) is essentially identical to that reported by Basso *et al*. (2000) for cerchiaraite [now cerchiaraite-(Mn)]. In the structure, SiO_4 tetrahedra share corners to form a four-membered Si_4O_{12} ring about the fourfold axis [0,0,*z*]. The ring is corner-linked to an edge-sharing chain of $Fe^{3+}O_6$ octahedra that runs parallel to **c**. The framework thereby created contains a large channel centred about the 4_2 screw axis [0,½,*z*] with Ba atoms positioned around its periphery. Two silicate dimers, $Si_2O_3(OH)_4$, p.f.u. are statistically distributed within the channel. One fully occupied Cl site is located on the fourfold axis, alternating along **c** with Si_4O_{12} rings. A feature not reported by Basso *et al*. (2000) is an additional partially occupied Cl site (Cl2) in the channel, which accounts for approximately one Cl a.p.f.u. if there are two silicate dimers p.f.u., but which can accommodate more Cl if there are less than two silicate dimers. Note that the very low bond-valence sum of 0.33 vu for Cl2 is likely to be augmented by two hydrogen bonds from the O2 OH groups.

Crystals from the Esquire No. 8 claim (and also from the Esquire No. 1 and No. 7 claims) exhibit a strongly pleochroic blue colour parallel to **c**, which corresponds to the direction of the edge-sharing octahedral chains. The

TABLE 5. Atom coordinates and displacement parameters (Å^2) for cerchiaraite-(Fe).

	x/a	*y/b*	*z/c*	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba	0.21637(5)	0	0	0.0275(2)	0.0349(4)	0.0222(4)	0.0254(4)	0	0	0.000
M	¼	¼	¼	0.0190(6)	0.0207(7)	0.0207(7)	0.0156(9)	0.0001(5)	0.0001(5)	−0.0075(7)
Si1	0.38855(13)	0.38855(13)	0	0.0165(6)	0.0164(8)	0.0164(8)	0.0167(13)	0	0	−0.0010(10)
Si2	0.4183(6)	0.1121(5)	0	0.027(3)	0.041(6)	0.019(5)	0.023(5)	0	0	0.006(4)
Cl1	0	0	0	0.0279(12)	0.0240(16)	0.0240(16)	0.036(3)	0	0	0
Cl2	½	0.1388(15)	0.118(9)	0.082(13)	0.037(10)	0.073(10)	0.14(3)	−0.042(12)	0	0
O1	0.3460(2)	0.3460(2)	0.2268(7)	0.0218(10)	0.0254(15)	0.0254(15)	0.015(2)	0.0018(14)	0.0018(14)	−0.005(2)
O2	0.1766(4)	0.3076(4)	0	0.0293(12)	0.026(3)	0.039(3)	0.024(3)	0	0	−0.009(2)
O3	0.3686(5)	½	0	0.0256(16)	0.037(4)	0.011(3)	0.028(4)	0	0	0
O4	0.394(2)	0	0	0.036(13)	0.04(2)	0.016(18)	0.05(3)	0	0	0
O5	½	0.126(3)	0.247(9)	0.139(18)	0.22(4)	0.10(2)	0.09(3)	−0.074(19)	0	0

* Refined occupancies are *M* (Fe/Al): 0.596/0.404(12); Si2: 0.255(11); Cl2: 0.21(3); O4: 0.24(3); O5: 0.52(7).

TABLE 6. Selected bond distances (Å) and angles (º) in cerchiaraite-(Fe).

Ba–O4	2.55(3)	Si1–O1 (×2)	1.612(5)	Si2–O4	1.646(11)
Ba–O5 (×2)	2.73(2)	Si1–O3 (×2)	1.626(2)	Si2–O2	1.839(10)
Ba–O2 (×2)	2.854(5)	**<Si1–O>**	**1.619**	Si2–O5 (×2)	1.90(4)
Ba–O1 (×4)	2.895(3)			**<Si2–O>**	**1.821**
Ba–Cl2 (×2)	3.10(4)	O1–Si1–O1	115.3(4)		
Ba–Cl1	3.1061(7)	O1–Si1–O3 (×4)	107.80(15)	O2–Si2–O4	108.0(13)
<Ba–φ>*	**2.897**	O3–Si1–O3	110.3(6)	O2–Si2–O5 (×2)	118.8(6)
				O4–Si2–O5 (×2)	103.3(15)
M–O1 (×2)	1.955(5)			O5–Si2–O5	103(2)
M–O2 (×4)	2.012(4)				
<*M*–O>	**1.993**				

* Occupancies for partially occupied O and Cl atoms (O4, O5 and Cl2) have been used for calculating <Ba–φ>.

colour is clearly attributable to Fe^{2+}–Fe^{3+} intervalence charge transfer (IVCT). The <*M*–O> of 1.993 Å is consistent with the site being predominantly occupied by Al and Fe^{3+}. Furthermore, using a bond-valence parameter in accord with the refined site occupancy of Fe^{3+}:Al = 0.595:0.405, the bond-valence sum (BVS) for the site is 2.84 vu, confirming the dominance of trivalent cations. The somewhat low BVS (for a trivalent cation) is consistent with a small

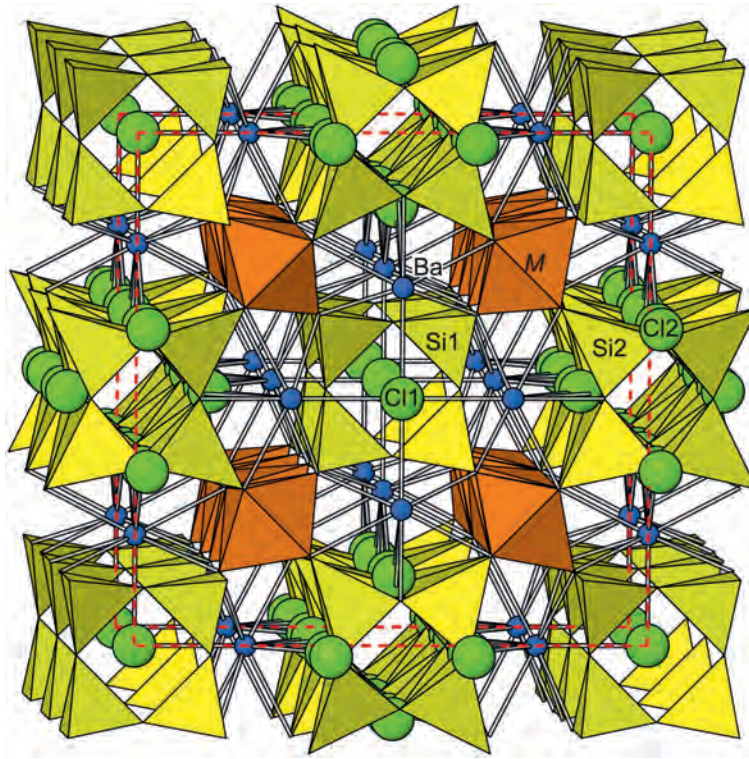

FIG. 5. Structure of cerchiaraite (Esq8) viewed slightly canted down [001].

TABLE 7. Bond-valence analysis for cerchiaraite-(Fe). Values are expressed in valence units.

	O1	O2	O3	O4	O5	Cl1	Cl2	Sum
Ba	$0.19 \times 2\downarrow \times 4\rightarrow$	$0.21 \times 2\rightarrow$		$0.49 \times 0.24\rightarrow$	$0.26 \times 1.04\rightarrow$	$0.32 \times 4\downarrow$	$0.33 \times 0.21\rightarrow$	2.05
M	$0.52 \times 2\rightarrow$	$0.45 \times 2\downarrow \times 4\rightarrow$						2.84
Si1	$1.03 \times 2\rightarrow$		$0.99 \times 2\downarrow\rightarrow$					4.06
Si2		0.14		$0.94 \times 2\downarrow$	$0.47 \times 2\downarrow$			2.45
Sum	1.93	1.25	1.98	2.37	0.94	1.28	0.33	

Multiplicity is indicated by $\times \rightarrow\downarrow$; $Ba^{2+}-O$ and $Fe^{3+}-O$ bond strengths from Brown and Altermatt (1985); $Al^{3+}-O$ and $Si^{4+}-O$ bond strengths from Brese and O'Keefe (1991). The bond strengths for the *M* site are based upon the refined Fe/Al occupancy. Multiplicities for O4, O5 and Cl2 are also based upon occupancies.

proportion of the Fe being Fe^{2+}. For calculation of the empirical formulae for the Esq1, Esq7 and Esq8 samples (Table 1), these considerations led us to an approximate Fe allocation of 90% Fe^{3+} and 10% Fe^{2+}.

Some comments on the highly unusual acid disilicate group, $Si_2O_3(OH)_4$, are warranted. This group was reported in the structure of cerchiaraite by Basso *et al*. (2000) and we noted the same group with a more distorted geometry in our refinement of the cerchiaraite-(Fe) structure. The OH groups were regarded by Basso *et al*. (2000) as being necessary from a bond-valence perspective. They dismissed the possibility of two insular silicate groups, $SiO(OH)_3$, on opposite sides of the channel rather than the disilicate group because that required too high a water content, and too high an occupancy for the O4 site. The statistical occupancy and disorder within the channel leaves some doubt about the nature of the silicate group. The distorted geometry of the Si2 tetrahedron and particularly its very long Si−O bond lengths (which provide a very low bond-valence sum for Si2) are probably an artefact of the positional disorder.

It is worth noting that the disorder within the channel suggests that other constituents, such as H_2O, SO_4 or CO_3, could be accommodated, as in the closely related structures of bobmeyerite, $Pb_4(Al_3Cu)(Si_4O_{12})(S_{0.5}Si_{0.5}O_4)(OH)_7Cl(H_2O)_3$ (Kampf *et al*., 2013) and ashburtonite, $Pb_4Cu_4(Si_4O_{12})(OH)_4Cl(HCO_3)_4$ (Grice *et al*., 1991).

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_exptl_crystal_size_mid           0.04
_exptl_crystal_size_min           0.04
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     3.765
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1296
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_exptl_absorpt_correction_type    multi-scan
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_exptl_special_details
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_diffrn_reflns_limit_l_min        -7
_diffrn_reflns_limit_l_max        7
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_diffrn_reflns_theta_max          25.03
_reflns_number_total              343
_reflns_number_gt                 329
_reflns_threshold_expression      >2sigma(I)

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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and
is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F, and
R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0213P)^2^+17.7504P] where P=(Fo^2^+2Fc^2^)/3'
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Si1 Si 0.38855(13) 0.38855(13) 0.0000 0.0165(6) Uani 1 4 d S . .
Si2 Si 0.4183(6) 0.1121(5) 0.0000 0.027(3) Uani 0.255(11) 2 d SP . .
Cl1 Cl 0.0000 0.0000 0.0000 0.0279(12) Uani 1 16 d S . .
O1 O 0.3460(2) 0.3460(2) 0.2268(7) 0.0218(10) Uani 1 2 d S . .
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Al 0.0207(7) 0.0207(7) 0.0156(9) 0.0001(5) 0.0001(5) -0.0075(7)
Si1 0.0164(8) 0.0164(8) 0.0167(13) 0.000 0.000 -0.0010(10)
Si2 0.041(6) 0.019(5) 0.023(5) 0.000 0.000 0.006(4)
Cl1 0.0240(16) 0.0240(16) 0.036(3) 0.000 0.000 0.000
O1 0.0254(15) 0.0254(15) 0.015(2) 0.0018(14) 0.0018(14) -0.005(2)
O2 0.026(3) 0.039(3) 0.024(3) 0.000 0.000 -0.009(2)
O3 0.037(4) 0.011(3) 0.028(4) 0.000 0.000 0.000
O4 0.04(2) 0.016(18) 0.05(3) 0.000 0.000 0.000
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Cl2 0.037(10) 0.073(10) 0.14(3) -0.042(12) 0.000 0.000

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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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O2 Si2 O5 118.8(6) 6 19 ?
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Ba Cl1 Ba 90.0 2 17 ?
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Ba O3 Ba 82.42(7) 10 26 ?
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Ba O3 Ba 132.81(17) 10_554 26 ?
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Cl2 O5 Ba 110(4) . 26 ?
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Si2 Cl2 Ba 22.3(13) 5_655 17_655 ?
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_diffrn_reflns_theta_full              25.03
_diffrn_measured_fraction_theta_full   0.980
_refine_diff_density_max    0.883
_refine_diff_density_min   -0.799
_refine_diff_density_rms    0.129
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Observed and calculated structure factors for cerchiaraite-(Fe)

h	k	l	10Fo	10Fc	10s
2	2	0	1167	1223	6
1	3	0	889	886	4
3	3	0	1283	1275	7
0	4	0	2699	2760	14
2	4	0	2173	2194	8
4	4	0	3778	3743	25
1	5	0	1526	1555	6
3	5	0	1689	1695	6
5	5	0	2558	2632	16
0	6	0	1618	1547	9
2	6	0	1256	1230	6
4	6	0	719	659	5
6	6	0	1486	1485	11
1	7	0	430	438	7
3	7	0	2834	2843	13
7	7	0	1731	1735	14
0	8	0	3228	3177	22
2	8	0	1435	1428	7
4	8	0	1314	1302	7
6	8	0	1357	1352	8
8	8	0	1392	1390	13
1	9	0	1599	1626	8
3	9	0	374	363	8
5	9	0	1784	1766	10
7	9	0	128	2	22
9	9	0	2216	2149	21
0	10	0	1509	1537	13
2	10	0	461	468	9
6	10	0	527	511	11
10	10	0	1765	1756	19
1	11	0	511	512	10
3	11	0	788	765	9
5	11	0	163	145	19
7	11	0	1339	1345	10
9	11	0	478	479	12
11	11	0	1015	1004	16
0	12	0	1173	1199	15
2	12	0	2348	2349	15
4	12	0	486	440	11
6	12	0	1080	1053	10
8	12	0	48	53	47
10	12	0	820	785	12
12	12	0	405	418	27
1	13	0	479	495	13
3	13	0	281	260	16
5	13	0	1435	1426	12
7	13	0	313	286	16
9	13	0	230	233	21
11	13	0	63	60	63
0	14	0	799	781	19
2	14	0	423	491	13
4	14	0	818	808	12
6	14	0	1160	1181	13
8	14	0	178	136	24
1	15	0	140	133	32
3	15	0	164	167	31
5	15	0	828	835	13
7	15	0	632	645	13
0	16	0	850	829	28
2	16	0	1328	1318	14
4	16	0	441	420	17
6	16	0	931	925	17
1	17	0	116	66	55
0	1	1	1377	1386	5
1	2	1	1190	1207	3
0	3	1	1165	1172	4
2	3	1	2244	2249	5
1	4	1	2800	2769	7
3	4	1	185	129	4

h	k	l	10Fo	10Fc	10s
0	5	1	3745	3743	17
2	5	1	393	386	4
4	5	1	2289	2316	6
1	6	1	104	53	11
3	6	1	1074	1089	4
5	6	1	573	546	4
0	7	1	166	179	12
2	7	1	2517	2486	8
4	7	1	86	59	13
6	7	1	1396	1391	5
1	8	1	503	486	5
3	8	1	548	530	4
5	8	1	1526	1537	5
7	8	1	1252	1254	5
0	9	1	1609	1620	9
2	9	1	156	125	11
4	9	1	2321	2297	8
6	9	1	668	679	7
8	9	1	409	396	6
1	10	1	722	704	5
3	10	1	187	124	10
5	10	1	2043	2068	8
7	10	1	221	215	10
9	10	1	842	815	9
0	11	1	324	310	11
2	11	1	1477	1486	7
4	11	1	438	447	7
6	11	1	724	718	8
8	11	1	704	700	8
10	11	1	87	52	30
1	12	1	125	103	19
3	12	1	930	938	7
5	12	1	150	94	16
7	12	1	1119	1122	7
9	12	1	459	487	10
11	12	1	746	689	16
0	13	1	1414	1419	13
2	13	1	355	349	9
4	13	1	759	757	10
6	13	1	155	82	17
8	13	1	358	374	9
10	13	1	784	774	13
1	14	1	1135	1128	8
3	14	1	76	43	44
5	14	1	883	913	8
7	14	1	154	160	22
9	14	1	1318	1272	12
0	15	1	698	710	12
2	15	1	435	444	10
4	15	1	477	477	10
6	15	1	276	249	14
1	16	1	280	348	13
3	16	1	675	740	10
5	16	1	254	239	18
0	0	2	3958	3874	32
1	1	2	1221	1235	4
0	2	2	1691	1702	5
2	2	2	3726	3722	16
3	3	2	3300	3208	14
0	4	2	1340	1313	5
2	4	2	499	471	5
4	4	2	1177	1165	7
1	5	2	1191	1226	3
3	5	2	1019	1043	4
5	5	2	2090	2103	11
0	6	2	1773	1770	7
2	6	2	2662	2678	8
4	6	2	2247	2258	7
6	6	2	1207	1178	8

h	k	l	10Fo	10Fc	10s
1	7	2	601	595	4
3	7	2	1477	1491	6
5	7	2	191	111	10
7	7	2	1861	1845	12
0	8	2	544	523	9
2	8	2	222	239	6
4	8	2	428	428	6
6	8	2	110	11	18
8	8	2	209	197	20
1	9	2	2029	2056	7
3	9	2	315	335	7
5	9	2	1702	1718	7
7	9	2	400	429	9
9	9	2	1899	1873	18
0	10	2	3550	3482	22
2	10	2	1192	1217	6
4	10	2	1117	1094	7
6	10	2	265	257	10
8	10	2	1198	1116	17
10	10	2	290	303	22
1	11	2	395	398	7
3	11	2	1021	1020	6
5	11	2	119	24	21
7	11	2	997	979	8
9	11	2	139	143	27
11	11	2	882	853	18
0	12	2	385	423	12
2	12	2	762	766	8
4	12	2	329	330	9
6	12	2	178	122	17
8	12	2	1013	1033	9
10	12	2	321	327	14
1	13	2	233	200	12
3	13	2	119	91	19
5	13	2	1311	1295	9
7	13	2	653	692	9
9	13	2	580	598	11
0	14	2	1359	1347	13
2	14	2	397	420	9
4	14	2	1834	1831	11
6	14	2	69	25	69
8	14	2	836	837	11
1	15	2	236	253	15
3	15	2	188	223	18
5	15	2	660	685	10
0	16	2	227	245	23
2	16	2	570	595	11
0	1	3	1378	1368	6
1	2	3	1123	1129	3
0	3	3	777	808	5
2	3	3	1496	1498	4
1	4	3	1637	1649	5
3	4	3	306	292	5
0	5	3	3108	3056	15
2	5	3	235	210	5
4	5	3	1555	1583	5
1	6	3	182	179	7
3	6	3	913	919	5
5	6	3	560	561	6
0	7	3	367	343	8
2	7	3	2180	2210	8
4	7	3	414	423	5
6	7	3	1042	1012	7
1	8	3	351	361	6
3	8	3	298	285	8
5	8	3	1319	1356	8
7	8	3	1045	1029	8
0	9	3	1269	1284	9
2	9	3	172	152	10

h	k	l	10Fo	10Fc	10s
4	9	3	1913	1932	8
6	9	3	500	506	9
8	9	3	367	355	12
1	10	3	310	313	7
3	10	3	294	254	9
5	10	3	1623	1631	9
7	10	3	418	413	10
9	10	3	757	731	12
0	11	3	372	368	11
2	11	3	1134	1144	7
4	11	3	386	394	9
6	11	3	526	551	9
8	11	3	458	490	11
10	11	3	109	71	43
1	12	3	112	105	20
3	12	3	847	859	8
5	12	3	122	87	23
7	12	3	990	953	10
9	12	3	330	340	16
0	13	3	1337	1351	17
2	13	3	379	372	10
4	13	3	440	463	10
6	13	3	166	168	21
8	13	3	341	347	14
1	14	3	973	999	10
3	14	3	118	11	29
5	14	3	817	831	13
0	15	3	551	571	14
2	15	3	392	410	13
0	0	4	5525	5410	93
1	1	4	903	910	6
0	2	4	750	754	6
2	2	4	790	784	7
1	3	4	517	518	5
3	3	4	1182	1167	7
0	4	4	1737	1751	8
2	4	4	1078	1108	4
4	4	4	2748	2696	14
1	5	4	957	967	4
3	5	4	748	745	5
5	5	4	1619	1642	11
0	6	4	339	349	9
2	6	4	700	706	4
4	6	4	219	212	9
6	6	4	771	757	13
1	7	4	179	165	10
3	7	4	1672	1728	6
5	7	4	114	41	17
7	7	4	1124	1079	17
0	8	4	1817	1856	11
2	8	4	1107	1099	6
4	8	4	870	877	7
6	8	4	1080	1049	11
8	8	4	795	806	21
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3	11	4	667	690	8
5	11	4	85	39	37
7	11	4	952	937	10

h	k	l	10Fo	10Fc	10s
0	12	4	687	731	18
2	12	4	1563	1598	10
4	12	4	433	449	10
6	12	4	775	779	11
1	13	4	352	375	13
3	13	4	195	184	19
5	13	4	1031	996	11
0	14	4	367	416	21
2	14	4	292	333	16
0	1	5	634	613	13
1	2	5	571	598	9
0	3	5	858	868	8
2	3	5	1185	1185	7
1	4	5	1307	1290	7
3	4	5	124	126	14
0	5	5	1994	1985	13
2	5	5	157	150	11
4	5	5	1089	1066	7
1	6	5	76	66	28
3	6	5	425	415	7
5	6	5	305	312	8
0	7	5	0	20	1
2	7	5	1329	1339	7
4	7	5	81	57	35
6	7	5	932	894	14
1	8	5	233	267	9
3	8	5	206	211	11
5	8	5	912	906	9
7	8	5	730	727	21
0	9	5	1015	1072	11
2	9	5	78	6	31
4	9	5	1206	1220	13
6	9	5	481	521	14
8	9	5	288	258	20
1	10	5	368	383	9
3	10	5	41	19	40
5	10	5	1203	1182	11
7	10	5	158	123	31
0	11	5	258	265	19
2	11	5	854	876	12
4	11	5	248	208	19
1	12	5	151	118	24
0	0	6	1740	1633	45
1	1	6	504	466	18
0	2	6	807	748	15
2	2	6	1649	1633	22
1	3	6	159	130	23
3	3	6	1069	1062	14
0	4	6	348	362	15
2	4	6	215	240	12
4	4	6	569	601	18
1	5	6	525	559	10
3	5	6	406	447	10
5	5	6	1089	1094	24
0	6	6	825	803	12
2	6	6	1243	1261	9
4	6	6	1018	1000	11
1	7	6	291	284	12
3	7	6	793	791	14
5	7	6	126	62	36
0	8	6	264	279	19
2	8	6	0	102	1
4	8	6	250	244	19
1	9	6	944	928	11
0	1	7	597	538	19
1	2	7	402	417	15
0	3	7	235	196	30