

Supplementary Material

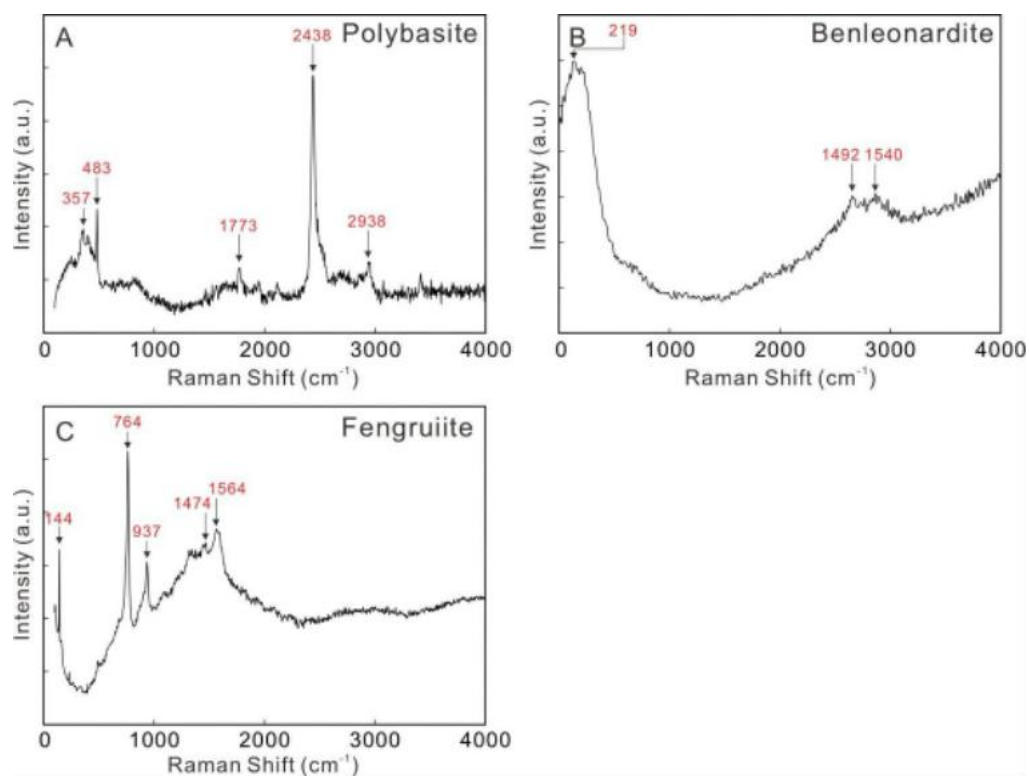


Figure S1. The Raman spectra of fengruite compared to polybasite and benleonardite (<https://rruff.info/polybasite/display=default/> and <https://rruff.info/benleonardite/display=default/>)

Table S1. Reflectance values (%) of fengruite and coexisting cervelleite measured in air under identical analytical conditions

fengruite						cervelleite					
R _{max}	R _{min}	λ (nm)	R _{max}	R _{min}	λ (nm)	R _{max}	R _{min}	λ (nm)	R _{max}	R _{min}	λ (nm)
44.68	36.184	400	34.476	32.97	560	34.461	32.676	400	33.605	31.826	560
33.791	31.044	420	34.582	33.153	580	35.353	34.532	420	33.494	31.611	580
32.358	30.657	440	35.033	33.558	589 (COM)	35.002	34.81	440	33.377	31.516	589 (COM)
33.253	31.519	460	34.966	33.681	600	35.433	34.413	460	33.153	31.224	600
33.787	32.224	470 (COM)	35.046	33.795	620	35.566	34.204	470 (COM)	32.963	31.222	620
34.104	32.481	480	35.029	33.285	640	35.56	33.924	480	32.854	31.058	640
34.296	32.794	500	34.367	32.588	650 (COM)	34.849	33.223	500	32.757	30.913	650 (COM)
34.378	32.883	520	35.09	33.513	660	34.448	32.744	520	32.621	30.886	660
34.579	33.278	540	35.023	33.191	680	33.956	32.215	540	32.485	30.801	680
34.56	33.118	546 (COM)	34.821	32.768	700	33.827	32.099	546 (COM)	32.497	30.981	700

Table S2. Comparison of EPMA data for fengruite obtained using beam diameters of 3–5 and 8 μm

No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Spot size	5μm	5μm	5μm	3μm	3μm	3μm	3μm	3μm	3μm	3μm	3μm	8μm	8μm	8μm	8μm
Sb	9.14	9.67	9.53	9.38	9.24	9.84	9.24	9.74	10.13	9.89	9.89	9.08	8.74	8.95	9.64
Te	7.09	7.56	6.88	7.04	6.45	6.67	6.53	6.34	6.79	6.61	6.87	7.16	6.46	6.37	7.11
Cu	3.41	3.34	3.26	3.28	3.34	3.38	3.37	3.34	3.63	3.63	3.76	3.12	4.06	3.70	2.69
As	0.29	0.03	0.04	0.16	0.03	0.04	0.01	0.08	0.08	0.22	0.08	0.03	0.04	0.05	0.17

Ag	66.56	66.13	66.69	67.05	67.87	67.03	68.63	67.58	66.02	66.60	65.89	67.39	67.25	67.61	68.10
S	13.09	12.94	13.11	12.56	12.80	12.99	12.82	12.78	12.67	12.94	13.03	12.34	13.10	12.59	12.33
Total	99.59	99.67	99.51	99.46	99.73	99.95	100.60	99.86	99.33	99.89	99.53	99.13	99.64	99.28	100.04
Atoms	29	29	29	29	29	29	29	29	29	29	29	29	29	29	29
Sb	1.79	1.91	1.87	1.86	1.82	1.93	1.81	1.92	2.01	1.94	1.94	1.82	1.71	1.77	1.92
Te	1.33	1.42	1.29	1.33	1.21	1.25	1.22	1.19	1.28	1.24	1.29	1.37	1.20	1.21	1.35
Cu	1.28	1.26	1.23	1.25	1.26	1.27	1.27	1.26	1.38	1.37	1.42	1.20	1.52	1.41	1.03
As	0.09	0.01	0.01	0.05	0.01	0.01	0.00	0.03	0.03	0.07	0.02	0.01	0.01	0.02	0.06
Ag	14.75	14.72	14.81	15.03	15.11	14.85	15.17	15.04	14.77	14.75	14.61	15.23	14.83	15.12	15.32
S	9.76	9.68	9.79	9.47	9.59	9.68	9.53	9.56	9.54	9.64	9.72	9.38	9.72	9.48	9.33

Note: Analyses 1–11 were obtained using 3–5 μm beams and were used to calculate the mean and range reported in Table 1. Analyses 12–15 were obtained using an 8 μm defocused beam solely to evaluate possible beam-size-dependent compositional changes and were not included in the mean composition or empirical-formula calculation.

Table S3. X-ray powder diffraction data (d in $\text{\AA}$, intensity is I/I_0) for fengruite

d_{calc}	I_{calc}	I_{obs}	d_{obs}	$h\ k\ l$
5.985	14	18	5.987	0 0 2
5.772	5			1 0 1
3.413	3			1 0 3
3.295	7			2 0 0
3.211	30			1 1 2

3.177	33	37	3.177	2 0 1
3.177	6			0 2 1
2.993	66	81	2.977	0 0 4
2.886	29			0 2 2
2.886	100	100	2.873	2 0 2
2.753	9			1 1 3
2.725	6	5	2.723	0 1 4
2.541	13	23	2.531	2 0 3
2.541	15			0 2 3
2.438	15	13	2.427	2 1 1
2.352	35	21	2.344	1 1 4
2.215	23	10	2.201	0 2 4
2.196	15			3 0 0
2.160	4	8	2.153	0 3 1
2.160	15			3 0 1
2.113	7	20	2.097	1 2 3
2.113	4			2 1 3
2.062	9			0 3 2
2.026	27	16	2.020	1 1 5
1.937	9			2 0 5
1.924	5			0 3 3
1.909	3			1 0 6
1.902	39	21	1.897	2 2 0

1.879	6			2 2 1
1.717	10	11	1.711	2 2 3
1.707	9			2 0 6
1.605	5			2 2 4
1.588	7	5	1.584	0 4 2
1.557	3			2 1 6
1.496	3	4	1.517	0 0 8
1.489	7	5	1.487	2 2 5
1.443	4			4 0 4
1.233	3			4 1 5
1.219	4	4	1.211	4 2 2

Table S4. Selected interatomic distances (Å) for fengruite

Ag1—S2	2.334(15)	Ag2—S3	2.291(18)
Ag1—S3 ⁱ	2.565(10)	Ag2—S3 ⁱ	2.291(18)
Ag1—S3	2.565(10)	Ag2—S2	2.82(4)
Ag3—S3	2.647(12)	Ag4—S4	2.537(6)
Ag3—S4	2.543(12)	Ag4—Te1 ⁱⁱ	2.699(7)
Ag3—Te1	2.621(11)		

Ag5—S3	2.55(2)	Sb—S3 ^{iv}	2.416(3)
Ag5—Te1	2.66(2)	Sb—S3	2.416(3)
		Sb—S3 ^v	2.416(3)
		<Sb—Te S>	2.416
Cu—S4	2.160(5)		
Cu—S4 ⁱⁱⁱ	2.160(5)		
<Cu—S>	2.160		

Symmetry codes: (i) $-y, x-y+1, z$; (ii) $-x-1, -y+1, -z+1$; (iii) $-x, -y+2, -z+1$; (iv) $-x+y-2, -x, z$; (v) $-y, x-y+2, z$.

Note: Ag1 and Ag2 are mutually exclusive split positions, whereas Ag3–Ag5 are partially occupied statistical positions used to approximate extended Ag electron density.

Table S5. Third-order Gram–Charlier coefficients, $C_{ijk}(\text{\AA}^3)$, for the anharmonically refined Ag sites in fengruite.

Site	Ag1'	Ag2'	Ag3'
C_{111}	−0.033(4)	−0.56(6)	−0.86(7)
C_{112}	−0.0167(19)	0.072(14)	−0.28(2)
C_{113}	−0.0021(13)	−0.052(7)	−0.08(3)
C_{122}	−0.0040(16)	0.115(9)	0.28(2)
C_{123}	−0.0010(7)	0.012(3)	−0.08(2)
C_{133}	−0.0025(7)	0.002(2)	−0.0021(8)
C_{222}	0.002(3)	−0.045(8)	0.86(7)
C_{223}	0.0020(8)	0.012(2)	−0.08(3)

C_{233}	$-0.0012(4)$	$0.0005(12)$	$0.0021(8)$
C_{333}	$-0.0041(7)$	$0.0028(10)$	$-0.0035(15)$
