minerals

MDPI

Supplementary Materials

Frankamenite: relationship between the crystal-chemical and vibrational properties

Ekaterina Kaneva [1]*, Roman Shendrik [1], Elizaveta Pankrushina [2], Emilia Dokuchits [3], Tatiana Radomskaya [1], Mikhail Pechurin [2] and Aleksey Ushakov [4]

[1] Vinogradov Institute of Geochemistry, Siberian Branch of the Russian Academy of Sciences, Favorsky str. 1A, Irkutsk 664033, Russia

[2] Zavaritsky Institute of Geology and Geochemistry, Ural Branch of the Russian Academy of Sciences, Ak. Vonsovsky str. 15, Ekaterinburg, 620110, Russia;

[3] State Key Laboratory of Geological Processes and Mineral Resources, Collaborative Innovation Center for Exploration of Strategic Mineral Resources, School of Earth Resources, China University of Geosci-ences, Wuhan 430074, China

[4] Mikheev Institute of Metal Physics, Ural Branch of the Russian Academy of Sciences, S. Kovalevskaya str. 18, Ekaterinburg 620990, Russia

* Correspondence: kev604@mail.ru

Table S1. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of frankamenite sample.

Site	Atom	x/a	y/b	z/c	Occ.	Ueq
K1	K^+	0.0016(4)	0.5001(3)	0.4992(7)	0.9579(9)	0.0477
K2	K^+	0.3128(3)	0.4991(2)	0.1540(4)	0.9675(9)	0.0204
K3	K^+	0.6821(2)	0.5025(3)	0.8382(4)	1.0432(9)	0.0247
M1	Na^+	0.0004(5)	0.0002(3)	–0.0009(6)	0.7927(7)	0.0302
	Ca^{2+}	0.0004(5)	0.0002(3)	–0.0009(6)	0.2073(7)	0.0302
M2	Ca^{2+}	0.0002(4)	0.0003(3)	0.5006(5)	1	0.0156
M3	Ca^{2+}	0.5068(3)	0.0062(4)	0.2531(3)	0.5783(7)	0.0153
	Na^+	0.5068(3)	0.0062(4)	0.2531(3)	0.4217(7)	0.0153
M4	Ca^{2+}	0.3284(3)	0.1578(3)	–0.0836(3)	0.7821(7)	0.0123
	Na^+	0.3284(3)	0.1578(3)	–0.0836(3)	0.2179(7)	0.0123
M5	Ca^{2+}	0.6717(3)	0.8430(4)	0.5855(3)	0.7564(7)	0.0114
	Na^+	0.6717(3)	0.8430(4)	0.5855(3)	0.2436(7)	0.0114
M6	Ca^{2+}	0.4921(3)	–0.0058(3)	0.7459(3)	0.5835(7)	0.0079
	Na^+	0.4921(3)	–0.0058(3)	0.7459(3)	0.4165(7)	0.0079
M7	Ca^{2+}	0.3281(3)	0.1585(4)	0.4099(3)	0.7764(7)	0.0128
	Na^+	0.3281(3)	0.1585(4)	0.4099(3)	0.2236(7)	0.0128
M8	Ca^{2+}	0.6720(3)	0.8423(3)	0.0849(3)	0.7469(7)	0.0117
	Na^+	0.6720(3)	0.8423(3)	0.0849(3)	0.2530(7)	0.0117
Si1	Si^{4+}	0.0366(3)	0.2467(3)	0.8010(4)	1	0.0081
Si2	Si^{4+}	0.2891(3)	0.7515(2)	0.9284(4)	1	0.0044
Si3	Si^{4+}	0.2767(3)	0.3682(2)	0.6375(4)	1	0.0044
Si4	Si^{4+}	0.4085(3)	0.6306(2)	0.7047(4)	1	0.0077
Si5	Si^{4+}	0.0375(3)	0.2469(3)	0.2339(4)	1	0.0098
Si6	Si^{4+}	0.2889(3)	0.7517(3)	0.3575(4)	1	0.0079
Si7	Si^{4+}	0.9623(3)	0.7534(3)	0.1956(4)	1	0.0078
Si8	Si^{4+}	0.7114(3)	0.2480(3)	0.0671(4)	1	0.0103
Si9	Si^{4+}	0.7255(3)	0.6329(3)	0.3622(4)	1	0.0101
Si10	Si^{4+}	0.5917(3)	0.3678(2)	0.2963(4)	1	0.0084

Si11	Si^{4+}	0.9627(3)	0.7532(2)	0.7648(4)	1	0.0067
Si12	Si^{4+}	0.7107(3)	0.2484(3)	0.6405(4)	1	0.0073
O1	O^{2-}	0.0590(6)	0.1336(6)	0.7747(7)	1	0.0155
O2	O^{2-}	0.1588(5)	0.3541(4)	0.7580(6)	1	0.0123
O3	O^{2-}	0.4196(6)	0.2861(5)	0.2119(6)	1	0.0214
O4	O^{2-}	0.3968(5)	0.5003(4)	0.6970(6)	1	0.0038
O5	O^{2-}	0.3132(5)	0.6466(5)	0.8411(6)	1	0.0130
O6	O^{2-}	0.1302(6)	0.7586(6)	0.7829(6)	1	0.0217
O7	O^{2-}	0.5663(6)	0.1342(6)	0.0281(7)	1	0.0129
O8	O^{2-}	0.6387(5)	0.7166(4)	0.3190(6)	1	0.0097
O9	O^{2-}	0.0580(6)	0.2856(6)	0.0304(7)	1	0.0210
O10	O^{2-}	0.2638(5)	0.7086(4)	0.1290(6)	1	0.0077
O11	O^{2-}	0.0582(6)	0.1363(6)	0.2831(7)	1	0.0235
O12	O^{2-}	0.1630(5)	0.3567(5)	0.3968(6)	1	0.0117
O13	O^{2-}	0.3130(5)	0.6460(5)	0.4735(6)	1	0.0146
O14	O^{2-}	0.1283(6)	0.7580(5)	0.3514(6)	1	0.0198
O15	O^{2-}	0.5668(6)	0.1309(5)	0.5385(6)	1	0.0108
O16	O^{2-}	–0.0643(6)	0.8665(5)	0.2231(7)	1	0.0128
O17	O^{2-}	0.8277(5)	0.6414(4)	0.2319(6)	1	0.0092
O18	O^{2-}	0.5809(5)	0.7131(5)	0.7933(6)	1	0.0129
O19	O^{2-}	0.6081(6)	0.5014(6)	0.3040(7)	1	0.0181
O20	O^{2-}	0.6949(5)	0.3594(4)	0.1724(6)	1	0.0131
O21	O^{2-}	0.8725(5)	0.2446(5)	0.2244(6)	1	0.0113
O22	O^{2-}	0.4361(6)	0.8657(5)	0.9747(6)	1	0.0080
O23	O^{2-}	0.3687(5)	0.2861(5)	0.6848(7)	1	0.0175
O24	O^{2-}	–0.0529(5)	0.7146(4)	0.9741(5)	1	0.0043
O25	O^{2-}	0.7356(6)	0.2921(6)	0.8648(7)	1	0.0181
O26	O^{2-}	–0.0636(5)	0.8687(4)	0.7131(6)	1	0.0059
O27	O^{2-}	0.8325(6)	0.6439(4)	0.5933(6)	1	0.0118
O28	O^{2-}	0.6950(5)	0.3591(4)	0.5231(6)	1	0.0133
O29	O^{2-}	0.8704(5)	0.2442(5)	0.6519(6)	1	0.0135
O30	O^{2-}	0.4367(5)	0.8622(4)	0.4597(6)	1	0.0082
(OH)1	O^{2-}	0.2647(7)	0.0311(5)	0.6303(7)	1	0.0154
(OH)2	O^{2-}	0.7404(6)	0.9709(5)	0.3684(6)	1	0.0133
F1	F^{-}	0.2748(6)	0.0356(4)	0.1373(6)	1	0.0203
F2	F^{-}	0.7255(6)	0.9680(5)	0.8626(6)	1	0.0257
Ow	O^{2-}	0.0036(7)	0.5003(5)	–0.0622(7)	0.6442(10)	0.0331

Table S2. Selected bond distances (Å) for tetrahedra and polyhedra of the studied frankamenite sample.

Distance	Å	Distance	Å	Distance	Å
Si1–O1	1.551(10)	Si2–O5	1.602(8)	Si3–O23	1.583(8)
Si1–O2	1.609(6)	Si2–O22	1.603(6)	Si3–O4	1.639(5)
Si1–O29	1.626(6)	Si2–O6	1.605(7)	Si3–O2	1.675(7)
Si1–O9	1.648(7)	Si2–O10	1.624(6)	Si3–O12	1.679(5)
<Si1–O>	**1.608(15)**	**<Si2–O>**	**1.609(14)**	**<Si3–O>**	**1.644(13)**
Si4–O18	1.573(5)	Si5–O11	1.513(9)	Si6–O30	1.582(5)
Si4–O4	1.617(6)	Si5–O9	1.612(7)	Si6–O13	1.625(8)
Si4–O13	1.654(5)	Si5–O12	1.626(6)	Si6–O14	1.635(8)
Si4–O5	1.661(7)	Si5–O21	1.632(7)	Si6–O10	1.644(6)

<Si4–O>	**1.626(12)**	**<Si5–O>**	**1.596(15)**	**<Si6–O>**	**1.621(14)**
Si7–O16	1.576(9)	Si8–O7	1.597(7)	Si9–O8	1.562(7)
Si7–O24	1.614(5)	Si8–O21	1.631(6)	Si9–O27	1.606(5)
Si7–O14	1.630(6)	Si8–O25	1.636(7)	Si9–O17	1.608(7)
Si7–O17	1.690(6)	Si8–O20	1.692(7)	Si9–O19	1.625(7)
<Si7–O>	**1.628(13)**	**<Si8–O>**	**1.639(14)**	**<Si9–O>**	**1.601(13)**
Si10–O3	1.568(6)	Si11–O26	1.599(7)	Si12–O29	1.604(7)
Si10–O28	1.626(5)	Si11–O6	1.625(8)	Si12–O15	1.616(6)
Si10–O20	1.627(7)	Si11–O24	1.635(6)	Si12–O25	1.617(7)
Si10–O19	1.645(9)	Si11–O27	1.662(5)	Si12–O28	1.666(7)
<Si10–O>	**1.616(14)**	**<Si11–O>**	**1.630(13)**	**<Si12–O>**	**1.626(14)**
M1–O26	2.405(7)	M2–(OH)2	2.335(7)	M3–F1	2.349(8)
M1–O1	2.418(8)	M2–O26	2.352(7)	M3–O15	2.362(7)
M1–O16	2.433(8)	M2–O1	2.369(8)	M3–O7	2.382(8)
M1–O11	2.448(8)	M2–(OH)1	2.375(7)	M3–(OH)2	2.403(8)
M1–F1	2.454(8)	M2–O16	2.374(7)	M3–O22	2.417(7)
M1–F2	2.468(8)	M2–O11	2.399(8)	M3–O30	2.436(7)
<M1–O,F>	**2.438(19)**	**< M2–O>**	**2.368(18)**	**< M3>–O,F>**	**2.392(18)**
M4–F1	2.300(6)	M5–O30	2.316(7)	M6–F2	2.342(8)
M4–O7	2.369(8)	M5–F2	2.336(7)	M6–(OH)1	2.356(8)
M4–(OH)1	2.370(7)	M 5–(OH)2	2.363(7)	M6–O15	2.395(7)
M4–O3	2.372(6)	M5–O8	2.362(6)	M6–O22	2.398(7)
M4–O23	2.377(7)	M5–O26	2.392(6)	M6–O7	2.424(7)
M4–O1	2.441(7)	M5–O18	2.400(6)	M6–O30	2.436(6)
< M4–O,F>	**2.372(17)**	**< M5–O,F>**	**2.362(16)**	**< M6–O,F>**	**2.392(18)**
M7–F1	2.297(6)	M8–F2	2.334(7)		
M7–O3	2.332(7)	M8–O22	2.349(8)		
M7–(OH)1	2.362(7)	M8–(OH)2	2.357(7)		
M–O23	2.389(7)	M8–O18	2.357(6)		
M7–O15	2.401(8)	M8–O8	2.358(6)		
M7–O11	2.453(7)	M8–O16	2.388(7)		
< M7–O,F>	**2.373(17)**	**< M8–O,F>**	**2.357(14)**		
K1–O20	3.048(5)	K2–O19	2.771(7)	K3–O4	2.677(5)
K1–O2	3.059(7)	K2–O10	2.863(7)	K3–O25	2.896(9)
K1–O28	3.060(7)	K2–O9	2.879(6)	K3–O24	2.916(5)
K1–O12	3.072(9)	K2–O5	2.937(6)	K3–O17	2.931(5)
K1–O27	3.115(9)	K2–Ow	2.952(8)	K3–O27	2.951(6)
K1–O13	3.120(7)	K2–O12	2.941(6)	K3–O28	2.985(7)
K1–O17	3.126(7)	K2–O13	2.970(7)	K3–O20	3.016(6)
K1–O5	3.137(5)	K2–O2	2.974(5)	K3–Ow	3.071(8)
K1–Ow	3.166(8)	K2–O3	3.216(8)	K3–O18	3.154(8)
<K1–O>	3.100(22)	K2–O8	3.282(5)	K3–O23	3.202(5)
		<K2–O>	2.978(20)	**<K3–O>**	2.980(21)

Table S3. Selected angles (°) for tetrahedra and polyhedra of the studied frankamenite sample.

Angle	°	Angle	°	Angle	°
O1–Si1–O2	113.7(3)	O5–Si2–O6	109.6(3)	O2–Si3–O4	106.9(3)
O1–Si1–O9	113.8(4)	O5–Si2–O10	101.3(3)	O2–Si3–O12	103.2(3)
O1–Si1–O29	113.0(4)	O5–Si2–O22	110.8(3)	O2–Si3–O23	115.4(3)
O2–Si1–O9	103.0(3)	O6–Si2–O10	106.1(3)	O4–Si3–O12	105.3(3)
O2–Si1–O29	105.1(3)	O6–Si2–O22	115.1(3)	O4–Si3–O23	109.6(3)
O9–Si1–O29	107.3(3)	O10–Si2–O22	113.0(3)	O12–Si3–O23	115.7(3)
<O–Si1–O>	**109.3**	**<O–Si2–O>**	**109.3**	**<O–Si3–O>**	**109.4**
O4–Si4–O5	107.3(3)	O9–Si5–O11	114.7(4)	O10–Si6–O13	102.2(3)
O4–Si4–O13	106.2(3)	O9–Si5–O12	101.5(3)	O10–Si6–O14	107.9(3)
O4–Si4–O18	110.1(3)	O9–Si5–O21	108.8(3)	O10–Si6–O30	112.9(3)
O5–Si4–O13	106.7(3)	O11–Si5–O12	114.2(4)	O13–Si6–O14	107.6(3)
O5–Si4–O18	112.4(3)	O11–Si5–O21	111.9(4)	O13–Si6–O30	109.0(3)
O13–Si4–O18	113.7(3)	O12–Si5–O21	104.8(3)	O14–Si6–O30	116.1(3)
<O–Si4–O>	**109.4**	**<O–Si5–O>**	**109.3**	**<O–Si6–O>**	**109.3**
O14–Si7–O16	112.4(4)	O7–Si8– O20	111.7(3)	O8–Si9–O17	114.0(3)
O14–Si7–O17	107.3(3)	O7–Si8–O21	114.7(4)	O8–Si9–O19	111.7(3)
O14–Si7–O24	107.2(3)	O7–Si8–O25	114.7(4)	O8–Si9–O27	114.1(3)
O16–Si7–O17	111.1(3)	O20–Si8–O21	103.4(3)	O17–Si9–O19	103.5(3)
O16–Si7–O24	115.6(3)	O20–Si8–O25	102.7(3)	O17–Si9–O27	107.8(3)
O17–Si7–O24	102.4(4)	O21–Si8–O25	108.5(3)	O19–Si9–O27	104.7(3)
<O–Si7–O>	**109.3**	**<O–Si8–O>**	**109.3**	**<O–Si9–O>**	**109.3**
O3–Si10–O19	111.2(3)	O6–Si11–O24	105.8(3)	O15–Si12–O25	114.2(4)
O3–Si10–O20	117.3(3)	O6–Si11–O26	112.8(3)	O15–Si12–O28	114.1(3)
O3–Si10–O28	116.6(3)	O6–Si11–O27	107.7(3)	O15–Si12–O29	113.8(3)
O19–Si10–O20	103.7(3)	O24–Si11–O26	114.5(3)	O25–Si12–O28	102.0(3)
O19–Si10–O28	104.0(3)	O24–Si11–O27	103.8(3)	O25–Si12–O29	106.6(3)
O20–Si10–O28	102.5(3)	O26–Si11–O27	111.6(3)	O28–Si12–O29	105.0(3)
<O–Si10–O>	**109.2**	**<O–Si11–O>**	**109.4**	**<O–Si12–O>**	**109.3**
F1–M1–O1	85.5(2)	OH(1)–M2–O1	86.3(2)	F1–M3–O7	83.7(2)
F1–M1–O11	85.7(2)	OH(1)–M2–O11	86.0(2)	F1–M3–O15	84.2(2)
F1–M1–O16	95.8(2)	OH(1)–M2–O16	95.0(2)	F1–M3–O22	95.7(2)
F1–M1–O26	96.0(2)	OH(1)– M2–O26	95.7(2)	F1–M3–O30	96.2(2)
F2–M1–O1	94.1(3)	OH(2)–M2–O1	94.2(2)	(OH)2–M3–O7	97.1(2)
F2–M1–O11	93.4(2)	OH(2)–M2–O11	93.2(2)	(OH)2–M3–O15	96.9(2)
F2–M1–O16	84.6(2)	OH(2)–M2–O16	84.6(2)	(OH)2–M3–O22	83.1(2)
F2–M1–O26	84.8(2)	OH(2)– M2–O26	85.1(2)	(OH)2–M3–O30	82.9(2)
O1–M1–O11	98.3(3)	O1–M2–O11	96.4(3)	O7–M3–O22	82.6(2)
O11–M1–O16	81.4(2)	O11– M2–O16	83.6(2)	O22–M3–O30	92.5(2)
O16–M1–O26	99.5(2)	O16– M2–O26	97.1(2)	O15–M3–O30	82.7(2)
O1–M1–O26	80.8(2)	O1– M2–O26	82.9(2)	O7–M3–O15	102.2(2)
<O,F–M1–O>	**90.0**	**<O–M2–O>**	**90.0**	**<O,F–M3–O>**	**90.0**
F1–M4–O1	88.4(2)	F2–M5–O18	78.9(2)	F2–M6–O7	94.2(2)
F1–M4–O3	78.6(2)	F2–M5–26	88.1(2)	F2–M6–O15	93.6(2)
F1–M4–O7	85.1(2)	F2–M5–O30	85.6(2)	F2–M6–O22	83.4(2)

F1–M4–(OH)1	102.1(2)	F2–M5–(OH)2	101.2(2)	F2–M6–O30	82.8(2)
O1–M4–O23	88.0(2)	O8–M5–O18	101.2(2)	(OH)1–M6–O7	83.9(2)
O3–M4–O23	100.8(2)	O8–M5–26	87.1(2)	(OH)1–M6–O15	84.1(2)
O7–M4–O23	98.7(2)	O8–M5–O30	99.3(2)	(OH)1–M6–O22	98.7(2)
O23–M4–(OH)1	78.8(2)	O8–M5–(OH)2	79.1(2)	(OH)1–M6–O30	98.9(2)
O1–M4–O3	101.4(2)	O18–M5–O26	101.2(2)	O7–M6–O15	94.7(2)
O3–M4–O7	89.2(2)	O18–M5–O30	88.9(2)	O15–M6–O30	82.0(2)
O7–M4–(OH)1	84.8(2)	O30–M5–(OH)2	86.4(2)	O22–M6–O30	100.9(2)
O1–M4–(OH)1	84.8(2)	O26–M5–(OH)2	83.6(2)	O7–M6–O22	82.1(2)
< O,F–M4–O>	**90.1**	**< O,F–M5–O>**	**90.1**	**< O,F–M6–O>**	**89.9**
F1–M7–O3	79.5(2)	F2–M8–O16	88.6(2)		
F1–M7–O11	89.1(2)	F2–M8–O18	79.8(2)		
F1–M7–O15	84.4(2)	F2–M8–O22	84.7(2)		
F1–M7–(OH)1	101.4(2)	F2–M8–(OH)2	100.5(2)		
O23–M7–O3	100.8(2)	O8–M8–O16	86.8(2)		
O23–M7–O11	87.6(2)	O8–M8–O18	100.8(2)		
O23–M7–O15	98.9(2)	O8–M8–O22	99.9(2)		
O23–M7–(OH)1	78.8(2)	O8–M8–(OH)2	79.3(2)		
O3–M7–O11	101.5(2)	O18–M8–O22	89.4(2)		
O3–M7–O15	89.8(2)	O16–M8–O18	101.4(2)		
O11–M7–(OH)1	85.1(2)	O16–M8–(OH)2	83.8(2)		
O15–M7–(OH)1	83.8(2)	O22–M8–(OH)2	85.5(2)		
< O,F–M7–O>	**90.1**	**< O,F–M8–O>**	**90.0**		

Table S4. Bond-valence sum (BVS) and coordination number (CN) of the cation and anion structural positions for the studied frankamenite. CN for Si = 4.

Site	BVS	CN	Site	BVS	Site	BVS	CN	Site	BVS	CN
K1	0.64	9	Si1	4.18	O1	1.98	4	O18	1.77	4
K2	1.02	10	Si2	4.16	O2	2.09	4	O19	2.10	3
K3	1.02	10	Si3	3.82	O3	1.83	4	O20	2.00	4
M1*	1.06	6	Si4	3.99	O4	2.18	3	O21	1.96	2
M2	1.95	6	Si5	4.34	O5	2.13	4	O22	1.85	4
M3*	1.48	6	Si6	4.03	O6	2.04	2	O23	1.74	4
M4*	1.67	6	Si7	3.99	O7	1.87	4	O24	2.11	3
M5*	1.72	6	Si8	3.86	O8	1.81	4	O25	2.06	3
M6*	1.47	6	Si9	4.25	O9	2.09	3	O26	1.89	4
M7*	1.69	6	Si10	4.09	O10	2.07	3	O27	2.12	4
M8*	1.69	6	Si11	3.94	O11	2.05	4	O28	2.06	4
			Si12	3.99	O12	2.05	4	O29	2.04	2
					O13	2.08	4	O30	1.91	4
					O14	1.96	2	(OH)1	0.90	3
					O15	1.83	4	(OH)2	1.49	5
					O16	1.92	4	F1	0.89	4
					O17	2.06	4	F2	0.82	4
								Ow**	0.24	3

* BVSs for M1 and M3–M8 sites with mixed occupancy were calculated using the fractional site occupancies (see Table S1);

** Without taking into account the contribution of H atoms

Table S5. Crystallographic coordinates of the simulated structural model of frankamenite.

Site	Atom	x/a	y/b	z/c
K1	K^{+}	0.001150	0.508820	0.530240
K2	K^{+}	0.324368	0.502186	0.155529
K3	K^{+}	0.700773	0.506016	0.845151
M1	Na^{+}	–0.013119	–0.003140	0.993343
M2	Ca^{2+}	–0.007685	–0.000602	0.487532
M3	Ca^{2+}	0.504939	–0.000669	0.247326
M4	Ca^{2+}	0.326218	0.151224	0.908313
M5	Ca^{2+}	0.673142	0.843992	0.592115
M6	Na^{+}	0.512866	–0.005952	0.759894
M7	Ca^{2+}	0.325746	0.151698	0.410118
M8	Na^{+}	0.672066	0.842449	0.074010
Si1	Si^{4+}	0.036441	0.246140	0.798756
Si2	Si^{4+}	0.291952	0.750733	0.930299
Si3	Si^{4+}	0.277444	0.367220	0.634304
Si4	Si^{4+}	0.413581	0.630205	0.703741
Si5	Si^{4+}	0.037712	0.249220	0.230857
Si6	Si^{4+}	0.285579	0.747365	0.355802
Si7	Si^{4+}	0.961941	0.756751	0.196052
Si8	Si^{4+}	0.709203	0.246601	0.069228
Si9	Si^{4+}	0.721178	0.635379	0.358063
Si10	Si^{4+}	0.590440	0.368632	0.290962
Si11	Si^{4+}	0.966190	0.756166	0.761404
Si12	Si^{4+}	0.706412	0.243657	0.633371
O1	O^{2-}	0.070250	0.133303	0.785117
O2	O^{2-}	0.163047	0.357263	0.756050
O3	O^{2-}	0.416204	0.282991	0.203884
O4	O^{2-}	0.403286	0.497301	0.702373
O5	O^{2-}	0.313495	0.641441	0.836162
O6	O^{2-}	0.131797	0.757317	0.770506
O7	O^{2-}	0.565082	0.133054	0.036854
O8	O^{2-}	0.630242	0.718237	0.319618
O9	O^{2-}	0.051210	0.292710	0.020764
O10	O^{2-}	0.252186	0.700001	0.123957
O11	O^{2-}	0.069607	0.135553	0.278554
O12	O^{2-}	0.169854	0.360636	0.396226
O13	O^{2-}	0.305658	0.637468	0.471334
O14	O^{2-}	0.126760	0.755508	0.354087
O15	O^{2-}	0.561454	0.130469	0.523365
O16	O^{2-}	0.937524	0.871940	0.223719
O17	O^{2-}	0.829938	0.644509	0.228261
O18	O^{2-}	0.586121	0.713716	0.782978
O19	O^{2-}	0.602511	0.500946	0.300867
O20	O^{2-}	0.690000	0.358981	0.157359
O21	O^{2-}	0.872517	0.244698	0.225492
O22	O^{2-}	0.434148	0.866673	0.981588
O23	O^{2-}	0.359388	0.277451	0.676237
O24	O^{2-}	0.949608	0.720477	0.971451
O25	O^{2-}	0.730116	0.282457	0.861461
O26	O^{2-}	0.937052	0.870215	0.706634

O27	O^{2-}	0.835895	0.644617	0.594681
O28	O^{2-}	0.690854	0.355465	0.521914
O29	O^{2-}	0.866270	0.233898	0.639241
O30	O^{2-}	0.430979	0.862445	0.449406
(OH)1	O^{2-}	0.256404	0.024167	0.624736
H1	H	0.233731	0.942781	0.612315
(OH)2	O^{2-}	0.744835	0.992634	0.406716
H2	H	0.782451	0.067861	0.483047
F1	F^-	0.274215	0.031184	0.134051
F2	F^-	0.735739	0.969701	0.858630
Ow	O^{2-}	–0.009990	0.500052	0.923521
Hw1	H	0.072287	0.568112	0.011886
Hw2	H	0.003138	0.432378	0.979645

Table S6. Calculated geometrical and distortion parameters for polyhedra in the simulated structure model of frankamenite: ECoN - effective coordination number [1–3], Vp - volume of the coordination polyhedron [4,5], r – average distance from the cation to the ligands, r_v – average distance from the volume center to the ligands [4,5], Δ_V – distance of the central atom to the volume center [4,5], r_s – average distance from the centroid to the ligands [4,5], Δ – distance of the central atom to the centroid [4,5], Vs – volume of the sphere fitted to the positions of ligands [4,5], ECCv – volume eccentricity [4,5], SPHv – volume sphericity [4,5], BLD – bond length distortion [3, 6], A – average ligand–central atom–ligand angle, TAV – tetrahedral angle variance [3,7], TQE – tetrahedral quadratic elongation [3,7], OAV – octahedral angle variance [3,7], OQE – octahedral quadratic elongation [3,7], D% – deviation from the experimental values.

	Si1	**D%**	**Si2**	**D%**	**Si3**	**D%**	**Si4**	**D%**	**Si5**	**D%**	**Si6**	**D%**
ECoN	3.962	1.16	3.944	1.30	3.961	1.41	3.918	0.15	3.962	3.63	3.963	0.08
Vp (Å^3)	2.228	5.14	2.231	5.38	2.239	0.97	2.239	1.77	2.225	7.59	2.235	3.00
r (Å)	1.636	1.74	1.639	1.86	1.638	0.36	1.640	0.86	1.636	2.51	1.638	1.05
r_v (Å)	1.635		1.636		1.636		1.637		1.634		1.636	
Δ_V (Å)	0.042		0.049		0.043		0.059		0.042		0.042	
r_s (Å)	1.633		1.634		1.635		0.1635		1.632		1.634	
Δ (Å)	0.100		0.119		0.093		0.116		0.110		0.105	
Vs (Å^3)	18.291	5.35	18.342	5.27	18.351	1.09	18.374	2.14	18.273	7.86	18.342	2.94
ECCv	0.0750		0.0878		0.0759		0.1037		0.0755		0.0745	
SPHv	1.0000		0.9999		1.0000		1.0000		1.0000		0.9999	
BLD (%)	1.29		1.56		1.28		1.86		1.28		1.26	
A (°)	109.3	0	109.3	0	109.3	0.09	109.3	0.09	109.3	0	109.3	0
TAV	27.724		37.097		21.237		32.840		30.730		27.952	
TQE	1.006		1.008		1.005		1.007		1.007		1.006	
	Si7	**D%**	**Si8**	**D%**	**Si9**	**D%**	**Si10**	**D%**	**Si11**	**D%**	**Si12**	**D%**
ECoN	3.951	1.28	3.970	0.89	3.931	0.91	3.966	0.48	3.967	0.13	3.969	0.03
Vp (Å^3)	2.227	1.37	2.219	0.89	2.245	7.42	2.241	4.87	2.226	0.68	2.222	1.79
r (Å)	1.636	0.49	1.633	0.37	1.641	2.50	1.638	1.36	1.635	0.31	1.633	0.43
r_v (Å)	1.629		1.632		1.639		1.637		1.637		1.632	
Δ_V (Å)	0.050		0.039		0.054		0.040		0.043		0.040	
r_s (Å)	1.627		1.630		1.637		1.635		1.636		1.631	
Δ (Å)	0.107		0.098		0.122		0.093		0.096		0.084	
Vs (Å^3)	18.109	0.71	18.193	0.92	18.431	7.65	18.369	4.39	18.392	1.53	18.199	1.18
ECCv	0.0886		0.0694		0.0961		0.0712		0.0760		0.0710	
SPHv	0.9999		1.0000		0.9999		1.0000		0.9999		1.0000	
BLD (%)	1.43		1.08		1.73		1.22		1.15		1.18	

A (°)	109.3	0	109.3	0	109.3	0	109.3	0.09	109.3	0.09	109.4	0.09
TAV	27.010		23.115		34.789		21.064		21.201		18.320	
TQE	1.006		1.005		1.008		1.005		1.005		1.004	
	M1	**D%**	**M2**	**D%**	**M3**	**D%**	**M4**	**D%**	**M5**	**D%**	**M6**	**D%**
ECoN	5.599	6.42	5.858	2.11	5.961	0.07	5.971	0.71	5.892	1.24	5.316	10.74
Vp (Å^3)	18.092	4.34	17.302	0.80	16.782	5.65	16.727	2.89	16.835	1.10	18.875	6.22
r (Å)	2.409	1.19	2.366	0.08	2.339	2.22	2.347	1.05	2.342	0.85	2.445	2.22
r_v (Å)	2.406		2.364		2.338		2.348		2.341		2.441	
Δ_V (Å)	0.160		0.099		0.046		0.041		0.060		0.179	
r_s (Å)	2.405		2.363		2.337		2.346		2.337		2.441	
Δ (Å)	0.153		0.127		0.092		0.055		0.134		0.176	
Vs (Å^3)	58.342	3.85	55.352	0.46	53.521	6.52	54.251	3.07	53.762	2.69	60.918	6.25
ECCv	0.1862		0.1209		0.0577		0.0510		0.0751		0.2041	
SPHv	0.9835		0.9853		0.9807		0.9761		0.9555		0.9661	
BLD (%)	2.66		2.10		1.16		0.79		1.84		3.25	
A (°)	89.9	0.11	90.0	0	90.0	0	90.1	0	90.0	0.11	89.9	0
OAV	66.013		48.239		38.066		71.563		38.804		70.952	
OQE	1.021		1.014		1.011		1.021		1.012		1.023	
	M7	**D%**	**M8**	**D%**			**K1**	**D%**	**K2**	**D%**	**K3**	**D%**
ECoN	5.968	1.27	5.365	10.43			9.179	2.59	7.987	11.42	8.433	2.52
Vp (Å^3)	16.723	3.04	18.806	10.99			56.245	14.78	49.907	0.36	42.757	15.32
r (Å)	2.347	1.10	2.446	3.78			3.092	0.26	2.974	0.13	2.917	2.11
r_v (Å)	2.348		2.441				3.115		2.970		2.924	
Δ_V (Å)	0.040		0.211				0.202		0.052		0.068	
r_s (Å)	2.346		2.440				3.069		2.953		2.880	
Δ (Å)	0.058		0.204				0.296		0.318		0.398	
Vs (Å^3)	54.255	3.09	60.895	10.94			126.623	1.71	109.774	1.64	104.703	5.53
ECCv	0.0501		0.2374				0.1825		0.0520		0.0683	
SPHv	0.9729		0.8760				0.9239		0.8280		0.8748	
BLD (%)	0.83		4.58				3.64		4.27		3.00	
A (°)	90.1	0	90.0	0			–		–		–	
OAV	71.432		79.023				–		–		–	
OQE	1.021		1.029				–		–		–	

1. Hoppe, R.; Voigt, S.; Glaum, H.; Kissel, J.; Müller, H.P.; Bernet, K. A new route to charge distributions in ionic solids. *J. Less-Common. Met.* **1989**, *156*, 105–122. [https://doi.org/10.1016/0022-5088(89)90411-6]
2. Nespolo, M.; Ferraris, G.; Ohashi, H. Charge distribution as a tool to investigate structural details: meaning and application to pyroxenes. *Acta Crystallogr*. 1999, *B55*, 902–916. [doi.org/10.1107/S0108768199008708]
3. Momma, K.; Izumi, F. VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data. *J. Appl. Crystallogr.* **2011**, *44*, 1272–1276. [https://doi.org/10.1107/S0021889811038970]
4. Balić-Žunić, T.; Makovicky, E. Determination of the centroid or 'the best centre' of a coordination polyhedron. *Acta Crystallogr*. **1996**, *B52*, 78–81. [https://doi.org/10.1107/S0108768195008251]
5. Balić-Žunić, T.; Vicković, I. IVTON – program for the calculation of geometrical aspects of crystal structures and some crystal chemical applications. *J. Appl. Cryst.* **1996**, *29*, 305–306. [https://doi.org/10.1107/S0021889895015081]
6. Renner, B.; Lehmann, G. Correlation of angular and bond length distortions in TO_4 units in crystals. *Z. für Kristallogr*. **1986**, *175*, 43–59 (1986). [https://doi.org/10.1524/zkri.1986.175.1-2.43]
7. Robinson, K.; Gibbs, G.V.; Ribbe, P.H. Quadratic elongation: A quantitative measure of distortion in coordination polyhedra. *Science*. **1971**, *172*, 567–570. [DOI:10.1126/science.172.3983.567]