Supplementary materials

Fedorite from Murun alkaline complex (Russia): Spectroscopy and Crystal Chemical Features

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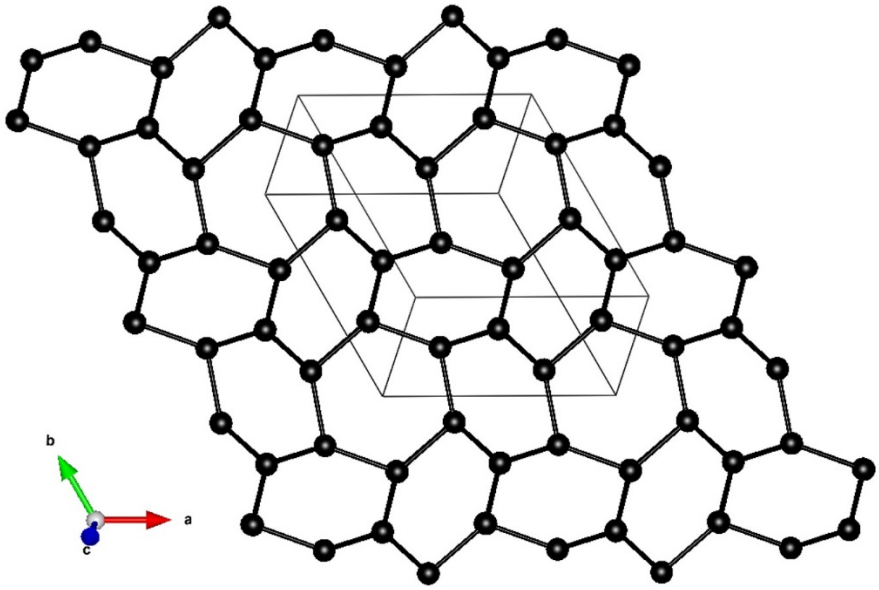

Figure S1. The fedorite 6^3 net with its unit cell.

Table S1. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of fedorite sample Gav-43.

Site	x/a	y/b	z/c	Occ.	Ueq
Na1	0	0	0.5	0.693(8)	0.0145
Ca1	0	0	0.5	0.311(6)	0.0145
Ca2	0.42194(6)	0.28439(6)	0.50974(4)	0.618(5)	0.0115
Na2	0.42194(6)	0.28439(6)	0.50974(4)	0.386(8)	0.0115
Ca3	0.71119(5)	0.14779(5)	0.50051(3)	0.891(5)	0.0105
Na3	0.71119(5)	0.14779(5)	0.50051(3)	0.118(8)	0.0105
Ca4	0.14910(5)	0.43328(5)	0.51551(4)	0.787(5)	0.0104
Na4	0.14910(5)	0.43328(5)	0.51551(4)	0.220(8)	0.0104
Si1	0.28533(6)	0.60327(6)	0.86939(4)	1	0.0070
Si2	0.13894(6)	0.74272(6)	0.72961(4)	1	0.0070
Si3	0.76845(6)	0.49742(6)	0.72718(4)	1	0.0075
Si4	0.26320(6)	0.10886(6)	0.72907(4)	1	0.0080
Si5	0.02045(6)	0.24180(6)	0.73227(4)	1	0.0076
Si6	0.39113(6)	0.73685(6)	0.13713(4)	1	0.0066
Si7	0.65234(6)	-0.00376(6)	0.72906(4)	1	0.0072
Si8	0.52916(6)	0.62822(6)	0.73242(4)	1	0.0079
O1	0.7031(2)	0.3863(2)	0.5991(1)	1	0.0161
O2	0.1295(2)	0.6691(2)	0.6016(1)	1	0.0149
O3	0.2782(2)	0.0830(2)	0.6039(1)	1	0.0176
O4	0.4223(2)	0.5290(2)	0.6066(1)	1	0.0238
O5	0.0148(2)	0.7534(2)	0.3920(1)	1	0.0206
O6	0.5710(2)	0.9558(2)	0.6010(1)	1	0.0151
O7	0.8529(2)	0.1230(2)	0.7662(1)	1	0.0131
O8	0.6762(2)	0.5958(2)	0.7622(1)	1	0.0131
O9	0.1941(2)	0.9385(2)	0.7651(1)	1	0.0125
O10	0.6249(2)	0.8306(2)	0.7593(1)	1	0.0158
O11	0.4379(2)	0.2512(2)	0.8225(1)	1	0.0125
O12	0.5823(2)	0.0800(2)	0.8172(1)	1	0.0122
O13	0.4267(2)	0.5820(2)	0.8268(1)	1	0.0175
O14	0.2674(2)	0.7342(2)	0.8185(1)	1	0.0149
O15	0.0383(2)	0.3526(2)	0.2405(1)	1	0.0149
O16	0.1122(2)	0.4242(2)	0.8285(1)	1	0.0153
O17	0.1322(2)	0.1633(2)	0.7518(2)	1	0.0180
O18	0.7520(2)	0.3929(2)	0.8158(1)	1	0.0137
O19	0.3339(2)	0.6732(2)	0.0028(1)	1	0.0237
F1	0.1597(2)	0.2060(2)	0.4195(1)	1	0.0219
Na5	0.0834(3)	0.1042(3)	0.2138(4)	0.519(7)	0.0247
K1	0.0586(5)	0.0758(6)	0.1523(7)	0.243(5)	0.0512
K2$_1$	0.6575(9)	-0.0185(8)	0.0003(5)	0.128(4)	0.0476
K2$_2$	0.781(5)	0.044(5)	0.003(3)	0.021(3)	0.0476
K3	0.694(1)	0.662(1)	0.0014(4)	0.169(4)	0.0715
K4	0.9908(6)	0.355(1)	0.0047(6)	0.172(5)	0.0413
O20w	0	0	0	0.529(9)	0.1466
O21w	0.225(7)	-0.005(4)	0.002(2)	0.291(9)	0.3223
O22w	-0.032(2)	0.300(2)	0.001(2)	0.207(8)	0.0435
O23w	0.009(5)	0.186(4)	0.001(2)	0.198(8)	0.2297
O24w	0.191(3)	0.199(5)	-0.003(1)	0.320(8)	0.2425

Table S2. Anisotropic atomic displacement parameters (Å^2) of fedorite sample Gav-43.

Site	U11	U22	U33	U23	U13	U12
Na1	0.0129(4)	0.0146(5)	0.0169(5)	0.0057(3)	0.0035(3)	0.0077(3)
Ca1	0.0129(4)	0.0146(5)	0.0169(5)	0.0057(3)	0.0035(3)	0.0077(3)
Ca2	0.0110(2)	0.0111(2)	0.0131(2)	0.0035(2)	0.0029(2)	0.0067(2)
Na2	0.0110(2)	0.0111(2)	0.0131(2)	0.0035(2)	0.0029(2)	0.0067(2)
Ca3	0.0101(2)	0.0105(2)	0.0119(2)	0.0046(1)	0.0034(1)	0.0058(2)
Na3	0.0101(2)	0.0105(2)	0.0119(2)	0.0046(1)	0.0034(1)	0.0058(2)
Ca4	0.0092(2)	0.0104(2)	0.0128(2)	0.0044(2)	0.0032(2)	0.0056(2)
Na4	0.0092(2)	0.0104(2)	0.0128(2)	0.0044(2)	0.0032(2)	0.0056(2)
Si1	0.0076(2)	0.0075(2)	0.0071(2)	0.0027(2)	0.0023(2)	0.0046(2)
Si2	0.0061(2)	0.0073(2)	0.0094(2)	0.0040(2)	0.0029(2)	0.0041(2)
Si3	0.0065(2)	0.0075(2)	0.0110(2)	0.0047(2)	0.0038(2)	0.0045(2)
Si4	0.0066(2)	0.0075(2)	0.0116(2)	0.0038(2)	0.0018(2)	0.0047(2)
Si5	0.0059(2)	0.0074(2)	0.0106(2)	0.0034(2)	0.0020(2)	0.0042(2)
Si6	0.0069(2)	0.0074(2)	0.0062(2)	0.0024(2)	0.0017(2)	0.0042(2)
Si7	0.0072(2)	0.0060(2)	0.0098(2)	0.0031(2)	0.0037(2)	0.0042(2)
Si8	0.0079(2)	0.0075(2)	0.0103(2)	0.0030(2)	0.0031(2)	0.0054(2)
O1	0.0183(7)	0.0165(7)	0.0120(6)	-0.0006(5)	-0.0007(5)	0.0112(6)
O2	0.0223(7)	0.0143(7)	0.0106(6)	0.0051(5)	0.0076(6)	0.0105(6)
O3	0.0242(8)	0.0173(7)	0.0128(6)	0.0053(5)	0.0068(6)	0.0117(6)
O4	0.0222(8)	0.0308(9)	0.0152(7)	-0.0065(6)	-0.0050(6)	0.0191(7)
O5	0.0163(7)	0.0269(8)	0.0149(7)	0.0117(6)	0.0034(6)	0.0073(6)
O6	0.0139(6)	0.0188(7)	0.0098(6)	0.0041(5)	0.0014(5)	0.0074(6)
O7	0.0072(6)	0.0125(6)	0.0177(7)	0.0054(5)	0.0058(5)	0.0033(5)
O8	0.0126(6)	0.0171(7)	0.0191(7)	0.0088(5)	0.0071(5)	0.0128(6)
O9	0.0139(6)	0.0078(6)	0.0157(6)	0.0048(5)	0.0027(5)	0.0055(5)
O10	0.0169(7)	0.0095(6)	0.0265(8)	0.0097(6)	0.0087(6)	0.0088(6)
O11	0.0076(6)	0.0080(6)	0.0196(7)	0.0012(5)	-0.0010(5)	0.0047(5)
O12	0.0125(6)	0.0085(6)	0.0189(7)	0.0050(5)	0.0098(5)	0.0060(5)
O13	0.0182(7)	0.0231(8)	0.0280(8)	0.0187(7)	0.0175(6)	0.0164(6)
O14	0.0104(6)	0.0138(7)	0.0220(7)	0.0098(6)	-0.0004(5)	0.0067(5)
O15	0.0068(6)	0.0147(7)	0.0213(7)	0.0072(6)	0.00552(5)	0.0037(5)
O16	0.0102(6)	0.0086(6)	0.0216(7)	-0.0006(5)	0.0041(5)	0.0033(5)
O17	0.0093(6)	0.0153(7)	0.0330(9)	0.0063(6)	0.0041(6)	0.0099(6)
O18	0.0094(6)	0.0166(7)	0.0231(7)	0.0156(6)	0.0087(5)	0.0081(5)
O19	0.0311(9)	0.0300(9)	0.0075(6)	0.0019(6)	0.0004(6)	0.0171(8)
F1	0.0188(6)	0.0233(7)	0.0234(7)	0.0057(5)	0.0045(5)	0.0120(6)
Na5	0.016(1)	0.019(1)	0.046(2)	0.014(1)	0.011(1)	0.0113(8)
K1	0.033(2)	0.040(2)	0.090(4)	0.029(2)	0.020(2)	0.022(2)
K2$_1$	0.076(4)	0.036(3)	0.016(2)	0.006(2)	0.002(2)	0.022(3)
K2$_2$	0.076(4)	0.036(3)	0.016(2)	0.006(2)	0.002(2)	0.022(3)
K3	0.105(5)	0.106(5)	0.029(2)	0.009(3)	0.004(3)	0.082(4)
K4	0.014(2)	0.061(4)	0.018(2)	0.002(3)	0.000(1)	0.003(2)
O20w	0.177(8)	0.216(8)	0.030(4)	0.014(6)	0.012(5)	0.106(7)
O21w	0.761(9)	0.169(8)	0.036(7)	0.005(7)	0.030(9)	0.273(9)
O22w	0.041(7)	0.030(6)	0.013(4)	-0.005(5)	0.010(4)	-0.010(5)
O23w	0.315(9)	0.132(9)	0.019(6)	0.002(8)	0.025(8)	-0.023(9)
O24w	0.189(8)	0.485(9)	0.035(6)	-0.005(8)	0.009(6)	0.205(8)

Table S3. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of fedorite sample Yak-5.

Site	x/a	y/b	z/c	Occ.	Ueq
Na1	0	0	0.5	0.719(8)	0.0142
Ca1	0	0	0.5	0.287(5)	0.0142
Ca2	0.42225(3)	0.28434(3)	0.51045(2)	0.591(5)	0.0120
Na2	0.42225(3)	0.28434(3)	0.51045(2)	0.415(8)	0.0120
Ca3	0.71122(3)	0.14763(3)	0.50007(2)	0.793(5)	0.0109
Na3	0.71122(3)	0.14763(3)	0.50007(2)	0.213(8)	0.0109
Ca4	0.14918(3)	0.43373(3)	0.51584(2)	0.716(5)	0.0111
Na4	0.14918(3)	0.43373(3)	0.51584(2)	0.293(8)	0.0111
Si1	0.28755(3)	0.60494(3)	0.86905(2)	1	0.0079
Si2	0.13912(3)	0.74266(3)	0.72964(2)	1	0.0078
Si3	0.76875(3)	0.49752(3)	0.72747(2)	1	0.0087
Si4	0.26223(3)	0.10874(3)	0.72946(2)	1	0.0088
Si5	0.02039(3)	0.24261(3)	0.73206(2)	1	0.0085
Si6	0.39291(3)	0.73739(3)	0.13705(2)	1	0.0076
Si7	0.65233(3)	-0.00280(3)	0.72859(2)	1	0.0080
Si8	0.53061(3)	0.62955(3)	0.73227(2)	1	0.0087
O1	0.7034(1)	0.3861(1)	0.59969(7)	1	0.0178
O2	0.1291(1)	0.6693(1)	0.60166(7)	1	0.0160
O3	0.2785(1)	0.0833(1)	0.60454(7)	1	0.0191
O4	0.4234(1)	0.5303(1)	0.60690(8)	1	0.0251
O5	0.0152(1)	0.7534(1)	0.39217(8)	1	0.0212
O6	0.5717(1)	0.9559(1)	0.60054(7)	1	0.0160
O7	0.8529(1)	0.1263(1)	0.76724(7)	1	0.0144
O8	0.6777(1)	0.5974(1)	0.76213(7)	1	0.0146
O9	0.1930(1)	0.9381(1)	0.76559(7)	1	0.0130
O10	0.6258(1)	0.8322(1)	0.75948(8)	1	0.0163
O11	0.4361(1)	0.2511(1)	0.82393(7)	1	0.0133
O12	0.5807(1)	0.0797(1)	0.81585(7)	1	0.0128
O13	0.4294(1)	0.5840(1)	0.82765(8)	1	0.0178
O14	0.2692(1)	0.7355(1)	0.81804(8)	1	0.0158
O15	0.0371(1)	0.3541(1)	0.23907(8)	1	0.0151
O16	0.1138(1)	0.4261(1)	0.82831(8)	1	0.0153
O17	0.1312(1)	0.1632(1)	0.75201(9)	1	0.0189
O18	0.7508(1)	0.3937(1)	0.81702(8)	1	0.0150
O19	0.3336(1)	0.6750(1)	0.00280(7)	1	0.0226
F1	0.1598(1)	0.2059(1)	0.42006(7)	1	0.0233
Na5	0.0827(2)	0.1034(2)	0.2124(2)	0.476(4)	0.0261
K1	0.0540(2)	0.0679(2)	0.1381(3)	0.248(3)	0.0388
$K2_1$	0.6540(8)	0.9809(5)	-0.0007(3)	0.135(3)	0.0594
$K2_2$	0.220(1)	-0.0355(9)	-0.0001(4)	0.136(3)	0.0779
$K3_1$	0.723(2)	0.679(1)	0.0020(4)	0.158(5)	0.1189
$K3_2$	0.250(3)	0.280(3)	-0.001(1)	0.172(7)	0.2471
$K4_1$	0.0098(3)	0.6249(5)	-0.0033(3)	0.208(6)	0.0243
$K4_2$	-0.0170(7)	0.321(2)	0.0029(5)	0.162(6)	0.0532
O20w	0	0	0	0.853(9)	0.4713
O21w	-0.019(4)	0.220(4)	0.002(1)	0.113(6)	0.1253

Table S4. Anisotropic atomic displacement parameters (Å^2) of fedorite sample Yak-5.

Site	U11	U22	U33	U23	U13	U12
Na1	0.0124(3)	0.0136(3)	0.0171(5)	0.0055(2)	0.0037(2)	0.0070(2)
Ca1	0.0124(3)	0.0136(3)	0.0171(5)	0.0055(2)	0.0037(2)	0.0070(2)
Ca2	0.0107(1)	0.0104(1)	0.0143(2)	0.00301(9)	0.00306(9)	0.0057(1)
Na2	0.0107(1)	0.0104(1)	0.0143(2)	0.00301(9)	0.00306(9)	0.0057(1)
Ca3	0.0101(1)	0.0102(1)	0.0128(1)	0.00425(8)	0.00339(8)	0.00532(9)
Na3	0.0101(1)	0.0102(1)	0.0128(1)	0.00425(8)	0.00339(8)	0.00532(9)
Ca4	0.0092(1)	0.0104(1)	0.0136(1)	0.00388(8)	0.00306(8)	0.00519(6)
Na4	0.0092(1)	0.0104(1)	0.0136(1)	0.00388(8)	0.00306(8)	0.00519(6)
Si1	0.0074(1)	0.0073(1)	0.0089(1)	0.00223(9)	0.00184(9)	0.00395(9)
Si2	0.0065(1)	0.0068(1)	0.0104(1)	0.00348(9)	0.00256(9)	0.00333(9)
Si3	0.0065(1)	0.0076(1)	0.0130(1)	0.00412(9)	0.00353(9)	0.00395(9)
Si4	0.0071(1)	0.0073(1)	0.0121(1)	0.00282(9)	0.00142(9)	0.00428(9)
Si5	0.0059(1)	0.0070(1)	0.0122(1)	0.00276(9)	0.00181(9)	0.00343(9)
Si6	0.0072(1)	0.0071(1)	0.0083(1)	0.00225(9)	0.00163(9)	0.00384(9)
Si7	0.0073(1)	0.0062(1)	0.0107(1)	0.00239(9)	0.00316(9)	0.00359(9)
Si8	0.0077(1)	0.0073(1)	0.0120(1)	0.00247(9)	0.00270(9)	0.00480(9)
O1	0.0181(4)	0.0169(4)	0.0151(4)	-0.0013(3)	-0.0010(3)	0.0106(3)
O2	0.0229(4)	0.0138(4)	0.0124(3)	0.0039(3)	0.0076(3)	0.0101(3)
O3	0.0255(4)	0.0173(4)	0.0132(4)	0.0054(3)	0.0065(3)	0.0101(3)
O4	0.0212(4)	0.0297(5)	0.0174(4)	-0.0084(4)	-0.0066(3)	0.0172(4)
O5	0.0172(4)	0.0265(5)	0.0150(4)	0.0110(3)	0.0033(3)	0.0067(4)
O6	0.0145(4)	0.0180(4)	0.0111(3)	0.0038(3)	0.0015(3)	0.0064(3)
O7	0.0072(3)	0.0134(3)	0.0192(4)	0.0051(3)	0.0048(3)	0.0030(3)
O8	0.0141(3)	0.0180(4)	0.0203(4)	0.0088(3)	0.0077(3)	0.0129(3)
O9	0.0148(3)	0.0073(3)	0.0168(4)	0.0046(3)	0.0034(3)	0.0055(3)
O10	0.0171(4)	0.0088(3)	0.0272(4)	0.0092(3)	0.0090(3)	0.0079(3)
O11	0.0079(3)	0.0093(3)	0.0196(4)	0.0004(3)	-0.0010(3)	0.0048(3)
O12	0.0133(3)	0.0080(3)	0.0187(4)	0.0035(3)	0.0091(3)	0.0061(3)
O13	0.0187(4)	0.0222(4)	0.0287(4)	0.0177(4)	0.0174(3)	0.0164(3)
O14	0.0104(3)	0.0135(3)	0.0240(4)	0.0099(3)	0.0002(3)	0.0061(3)
O15	0.0070(3)	0.0130(3)	0.0224(4)	0.0066(3)	0.0055(3)	0.0025(3)
O16	0.0100(3)	0.0072(3)	0.0222(4)	0.0002(3)	0.0038(3)	0.0017(3)
O17	0.0112(3)	0.0142(4)	0.0346(5)	0.0060(3)	0.0045(3)	0.0100(3)
O18	0.0108(3)	0.0153(4)	0.0257(4)	0.0149(3)	0.0084(3)	0.0078(3)
O19	0.0294(5)	0.0265(5)	0.0077(3)	0.0004(3)	-0.0005(3)	0.0151(4)
F1	0.0198(4)	0.0231(4)	0.0260(4)	0.0054(3)	0.0050(3)	0.0118(3)
Na5	0.0161(6)	0.0178(6)	0.048(1)	0.0132(6)	0.0118(6)	0.0096(5)
K1	0.0268(7)	0.0284(7)	0.068(2)	0.0204(9)	0.0178(8)	0.0164(6)
$K2_1$	0.087(4)	0.038(2)	0.025(1)	0.007(1)	0.000(2)	0.019(2)
$K2_2$	0.110(5)	0.090(4)	0.036(2)	0.011(2)	0.009(2)	0.061(4)
$K3_1$	0.256(7)	0.146(4)	0.025(2)	0.011(2)	0.007(3)	0.168(4)
$K3_2$	0.300(7)	0.479(9)	0.078(6)	0.039(7)	0.031(6)	0.311(6)
$K4_1$	0.0124(8)	0.034(1)	0.0172(7)	0.0042(8)	0.0047(5)	0.0077(8)
$K4_2$	0.041(2)	0.073(5)	0.023(1)	0.005(2)	0.007(1)	0.020(2)
O20w	0.657(9)	0.619(9)	0.063(4)	0.033(7)	0.037(7)	0.330(9)
O21w	0.256(9)	0.103(8)	0.017(5)	0.017(6)	0.022(7)	0.099(8)

Table S5. Crystallographic coordinates, occupancies and equivalent/isotropic atomic displacement parameters (Å^2) of fedorite sample Irk-53.

Site	x/a	y/b	z/c	Occ.	Ueq
Na1	0	0	0.5	0.712(8)	0.0128
Ca1	0	0	0.5	0.290(5)	0.0128
Ca2	0.42209(2)	0.28440(2)	0.50942(2)	0.595(5)	0.0103
Na2	0.42209(2)	0.28440(2)	0.50942(2)	0.409(8)	0.0103
Ca3	0.71114(2)	0.14774(2)	0.50055(1)	0.848(5)	0.0093
Na3	0.71114(2)	0.14774(2)	0.50055(1)	0.171(8)	0.0093
Ca4	0.14902(2)	0.43332(2)	0.51551(1)	0.759(5)	0.0095
Na4	0.14902(2)	0.43332(2)	0.51551(1)	0.253(8)	0.0095
Si1	0.28467(2)	0.60287(2)	0.86955(2)	1	0.0064
Si2	0.13886(2)	0.74280(2)	0.72959(2)	1	0.0066
Si3	0.76822(2)	0.49713(2)	0.72704(2)	1	0.0070
Si4	0.26363(2)	0.10917(2)	0.72917(2)	1	0.0073
Si5	0.02028(2)	0.24167(2)	0.73237(2)	1	0.0070
Si6	0.39050(2)	0.73687(2)	0.13709(2)	1	0.0061
Si7	0.65207(2)	-0.00422(2)	0.72916(2)	1	0.0067
Si8	0.52870(2)	0.62750(2)	0.73250(2)	1	0.0072
O1	0.70315(8)	0.38681(8)	0.59879(5)	1	0.0158
O2	0.12945(9)	0.66936(8)	0.60161(5)	1	0.0149
O3	0.27797(9)	0.08305(8)	0.60359(5)	1	0.0174
O4	0.4227(1)	0.5293(1)	0.60656(6)	1	0.0241
O5	0.01497(9)	0.75381(9)	0.39193(5)	1	0.0194
O6	0.57095(8)	0.95535(8)	0.60114(5)	1	0.0152
O7	0.85264(7)	0.12154(7)	0.76602(5)	1	0.0130
O8	0.67605(7)	0.59568(7)	0.76228(5)	1	0.0132
O9	0.19351(7)	0.93828(6)	0.76498(5)	1	0.0121
O10	0.062523(8)	0.83023(7)	0.75946(6)	1	0.0152
O11	0.43832(6)	0.25118(7)	0.82231(5)	1	0.0124
O12	0.58257(7)	0.07971(6)	0.81740(5)	1	0.0116
O13	0.42589(8)	0.58122(8)	0.82694(6)	1	0.0166
O14	0.26684(7)	0.73387(7)	0.81854(5)	1	0.0145
O15	0.03891(7)	0.35181(7)	0.24080(5)	1	0.0137
O16	0.11162(7)	0.42402(6)	0.82859(5)	1	0.0143
O17	0.13230(7)	0.16304(8)	0.75197(6)	1	0.0174
O18	0.75232(7)	0.39220(7)	0.81524(5)	1	0.0138
O19	0.3335(1)	0.6731(1)	0.00312(5)	1	0.0232
F1	0.15977(7)	0.20625(8)	0.41843(5)	1	0.0201
Na5	0.0839(2)	0.1055(2)	0.2155(2)	0.466(7)	0.0197
K1	0.0651(3)	0.0831(4)	0.1678(6)	0.273(5)	0.0567
$K2_1$	0.6590(5)	0.9804(4)	0.0003(2)	0.144(3)	0.0567
$K2_2$	0.232(7)	-0.012(3)	0.0011(9)	0.082(4)	0.2670
$K3_1$	0.6921(5)	0.6600(5)	0.0023(2)	0.171(3)	0.0703
$K3_2$	0.175(3)	0.160(5)	-0.0015(8)	0.152(5)	0.3592
$K4_1$	0.0119(5)	0.0654(1)	-0.0037(4)	0.142(6)	0.0454
$K4_2$	-0.024(2)	0.305(2)	0.003(1)	0.090(6)	0.0611
$K4_3$	0.030(3)	0.174(2)	0.0017(9)	0.105(4)	0.2209
O20w	0	0	0	0.516(8)	0.1513

Table S6. Anisotropic atomic displacement parameters (Å^2) of fedorite sample Irk-53.

Site	U11	U22	U33	U23	U13	U12
Na1	0.0115(2)	0.0116(2)	0.0151(2)	0.0041(1)	0.0029(1)	0.0062(1)
Ca1	0.0115(2)	0.0116(2)	0.0151(2)	0.0041(1)	0.0029(1)	0.0062(1)
Ca2	0.0098(1)	0.0088(1)	0.0121(1)	0.00237(6)	0.00254(5)	0.00508(7)
Na2	0.0098(1)	0.0088(1)	0.0121(1)	0.00237(6)	0.00254(5)	0.00508(7)
Ca3	0.00922(8)	0.00814(8)	0.01068(8)	0.00330(4)	0.00290(4)	0.00464(5)
Na3	0.00922(8)	0.00814(8)	0.01068(8)	0.00330(4)	0.00290(4)	0.00464(5)
Ca4	0.00873(8)	0.00853(8)	0.01119(9)	0.00298(5)	0.00255(5)	0.00464(6)
Na4	0.00873(8)	0.00853(8)	0.01119(9)	0.00298(5)	0.00255(5)	0.00464(6)
Si1	0.00653(7)	0.00581(6)	0.00652(7)	0.00151(5)	0.00151(5)	0.00336(5)
Si2	0.00600(7)	0.00544(6)	0.00855(7)	0.00292(5)	0.00226(5)	0.00294(5)
Si3	0.00592(7)	0.00619(7)	0.00997(7)	0.00339(5)	0.00313(5)	0.00353(5)
Si4	0.00614(7)	0.00551(7)	0.01026(7)	0.00232(5)	0.00113(5)	0.00339(5)
Si5	0.00526(7)	0.00554(7)	0.00969(7)	0.00194(5)	0.00143(5)	0.00276(6)
Si6	0.00635(7)	0.00528(6)	0.00604(7)	0.00128(5)	0.00122(5)	0.00298(5)
Si7	0.00663(7)	0.00457(6)	0.00894(7)	0.00168(5)	0.00286(5)	0.00294(5)
Si8	0.00709(7)	0.00561(6)	0.00971(7)	0.00177(5)	0.00248(5)	0.00409(6)
O1	0.0182(2)	0.0151(2)	0.0121(2)	-0.0009(2)	-0.0004(2)	0.0102(2)
O2	0.0227(3)	0.0134(2)	0.0102(2)	0.0033(2)	0.0069(2)	0.0104(2)
O3	0.0230(3)	0.0164(2)	0.0108(2)	0.0040(2)	0.0050(2)	0.0092(2)
O4	0.0214(3)	0.0284(3)	0.0160(3)	-0.0086(2)	-0.0065(2)	0.0170(3)
O5	0.0167(2)	0.0241(3)	0.0124(2)	0.0094(2)	0.0023(2)	0.0063(2)
O6	0.0148(2)	0.0172(2)	0.0094(2)	0.0030(2)	0.0018(2)	0.0065(2)
O7	0.0071(2)	0.0108(2)	0.0175(2)	0.0042(2)	0.0046(2)	0.0020(2)
O8	0.0138(2)	0.0167(2)	0.0181(2)	0.0077(2)	0.0071(2)	0.0130(2)
O9	0.0141(2)	0.0055(2)	0.0165(2)	0.0042(2)	0.0031(2)	0.0050(2)
O10	0.0171(2)	0.0069(2)	0.0254(3)	0.0080(2)	0.0089(2)	0.0072(2)
O11	0.0069(2)	0.0082(2)	0.0182(2)	-0.0001(2)	-0.0016(2)	0.0040(2)
O12	0.0134(2)	0.0070(2)	0.0167(2)	0.0033(2)	0.0086(2)	0.0063(2)
O13	0.0179(2)	0.0204(3)	0.0272(3)	0.0171(2)	0.0174(2)	0.0151(2)
O14	0.0101(2)	0.0119(2)	0.0217(2)	0.0089(2)	-0.0004(2)	0.0055(2)
O15	0.0063(2)	0.0123(2)	0.0197(2)	0.0067(2)	0.0048(2)	0.0022(2)
O16	0.0095(2)	0.0052(2)	0.0205(2)	-0.0018(2)	0.0032(2)	0.0010(2)
O17	0.0107(2)	0.0136(2)	0.0312(3)	0.0049(2)	0.0040(2)	0.0100(2)
O18	0.0109(2)	0.0144(2)	0.0226(3)	0.0135(2)	0.0078(2)	0.0076(2)
O19	0.0311(3)	0.0268(3)	0.0060(2)	-0.0001(2)	0.0001(2)	0.0143(3)
F1	0.0187(2)	0.0198(2)	0.0201(2)	0.0038(2)	0.0032(2)	0.0104(2)
Na5	0.0133(4)	0.0134(4)	0.0338(8)	0.0082(4)	0.0079(4)	0.0074(3)
K1	0.0361(8)	0.0387(9)	0.106(3)	0.031(1)	0.026(1)	0.0225(7)
$K2_1$	0.097(3)	0.042(1)	0.0205(9)	0.0066(8)	0.003(1)	0.033(2)
$K2_2$	0.60(1)	0.172(7)	0.035(4)	0.000(5)	0.000(8)	0.239(8)
$K3_1$	0.100(3)	0.114(3)	0.0248(9)	0.010(1)	0.008(1)	0.083(2)
$K3_2$	0.328(8)	0.744(9)	0.056(4)	0.026(7)	0.027(6)	0.364(8)
$K4_1$	0.023(1)	0.073(3)	0.016(1)	0.003(1)	0.0041(7)	0.014(1)
$K4_2$	0.065(5)	0.068(6)	0.024(2)	0.005(3)	0.006(2)	0.022(3)
$K4_3$	0.299(9)	0.171(8)	0.060(5)	0.019(6)	0.016(7)	0.048(8)
O20w	0.188(7)	0.170(7)	0.025(2)	0.014(3)	0.010(3)	0.057(6)

Table S7. Selected bond distances (Å) for tetrahedra and polyhedral of the studied fedorite samples.

	Gav-43	Yak-5	Irk-53		Gav-43	Yak-5	Irk-53
			T-sheet				
Si1-O13	1.606(2)	1.602(1)	1.6066(9)	Si5-O5	1.583(2)	1.580(1)	1.5832(7)
Si1-O14	1.607(2)	1.605(1)	1.6082(8)	Si5-O7	1.620(2)	1.6201(9)	1.6219(6)
Si1-O16	1.609(1)	1.6087(7)	1.6090(4)	Si5-O16	1.627(1)	1.6304(8)	1.6275(5)
Si1-O19	1.592(2)	1.5955(9)	1.5934(6)	Si5-O17	1.623(2)	1.622(1)	1.6263(9)
<Si1-O>	1.604(4)	1.603(2)	1.602(1)	<Si5-O>	1.613(4)	1.613(2)	1.615(1)
Si2-O2	1.591(2)	1.5877(9)	1.5901(7)	Si6-O11	1.611(2)	1.608(1)	1.6134(7)
Si2-O9	1.622(2)	1.620(1)	1.6221(6)	Si6-O12	1.612(2)	1.610(1)	1.6131(7)
Si2-O14	1.625(2)	1.623(1)	1.6245(8)	Si6-O18	1.613(2)	1.6110(9)	1.6133(6)
Si2-O15	1.622(2)	1.6229(9)	1.6242(6)	Si6-O19	1.601(2)	1.6010(9)	1.5973(6)
<Si2-O>	1.615(4)	1.613(2)	1.615(1)	<Si6-O>	1.609(4)	1.606(2)	1.609(1)
Si3-O1	1.586(1)	1.5826(8)	1.5865(5)	Si7-O6	1.590(2)	1.5850(9)	1.5888(7)
Si3-O8	1.624(2)	1.623(1)	1.6244(8)	Si7-O7	1.629(1)	1.6290(8)	1.6287(6)
Si3-O15	1.620(1)	1.6187(7)	1.6212(5)	Si7-O10	1.623(2)	1.622(1)	1.6245(8)
Si3-O18	1.630(2)	1.632(1)	1.6298(8)	Si7-O12	1.633(2)	1.630(1)	1.6305(7)
<Si3-O>	1.615(3)	1.614(2)	1.615(1)	<Si7-O>	1.619(4)	1.617(2)	1.618(1)
Si4-O3	1.580(2)	1.579(1)	1.5822(7)	Si8-O4	1.583(2)	1.5775(9)	1.5815(7)
Si4-O9	1.627(2)	1.629(1)	1.6302(6)	Si8- O8	1.621(2)	1.618(1)	1.6201(8)
Si4-O11	1.636(1)	1.6357(7)	1.6349(5)	Si8-O10	1.621(2)	1.6205(9)	1.6246(6)
Si4-O17	1.621(2)	1.620(1)	1.6212(9)	Si8-O13	1.625(2)	1.627(1)	1.6267(8)
<Si4-O>	1.616(4)	1.616(2)	1.617(1)	<Si8-O>	1.613(4)	1.611(2)	1.613(1)
			O-sheet				
	M1 position (Na1Ca1)				M3 position (Ca3Na3)		
M1-F1 (×2)	2.347(2)	2.3407(9)	2.3591(7)	M3-O1	2.411(2)	2.411(1)	2.4147(8)
M1-O3 (×2)	2.490(2)	2.491(1)	2.4872(8)	M3-O2	2.418(2)	2.414(1)	2.4178(7)
M1-O5 (×2)	2.554(2)	2.551(1)	2.5521(9)	M3-O3	2.387(2)	2.384(1)	2.3874(9)
<M1-O,F>	2.464(5)	2.461(2)	2.466(2)	M3-O5	2.426(2)	2.421(1)	2.4264(8)
				M3-O6	2.398(2)	2.394(1)	2.4026(7)
	M2 position (Ca2Na2)			M3-O6′	2.455(2)	2.455(1)	2.4564(7)
M2-F1	2.315(2)	2.315(1)	2.3202(7)	<M2-O >	2.416(5)	2.413(2)	2.418(2)
M2-O1	2.407(2)	2.403(1)	2.4049(7)				
M2-O3	2.403(2)	2.399(1)	2.4044(7)		M4 position (Ca4Na4)		
M2-O4	2.411(2)	2.413(1)	2.413(1)	M4-F1	2.322(2)	2.323(1)	2.3260(8)
M2-O4′	2.564(2)	2.562(1)	2.5575(9)	M4-O1	2.492(2)	2.498(1)	2.4867(7)
M2-O6	2.472(2)	2.465(1)	2.4673(8)	M4-O2	2.409(2)	2.404(1)	2.4107(9)
<M2-O,F>	2.429(5)	2.426(2)	2.428(2)	M4-O2′	2.498(2)	2.494(1)	2.4971(8)
				M4-O4	2.361(2)	2.365(1)	2.3650(9)
				M4-O5	2.361(2)	2.358(1)	2.3642(7)
				<M4-O,F>	2.407(5)	2.407(2)	2.408(2)

Table S8. Selected bond distances (Å) for interlayer atoms of the studied fedorite samples.

Gav-43		Yak-5		Irk-53	
Na5-F1	2.452(5)	Na5-F1	2.473(2)	Na5-F1	2.418(2)
Na5-O7	2.607(4)	Na5-O7	2.633(2)	Na5-O7	2.600(2)
Na5-O8	2.573(3)	Na5-O8	2.558(2)	Na5-O8	2.571(2)
Na5-O9	2.551(4)	Na5-O9	2.538(2)	Na5-O9	2.541(2)
Na5-O10	2.522(4)	Na5-O10	2.519(2)	Na5-O10	2.519(2)
Na5-O15	2.602(4)	Na5-O15	2.624(2)	Na5-O15	2.583(2)
Na5-O17	2.549(4)	Na5-O17	2.543(2)	Na5-O17	2.548(2)
Na5-O20w	2.547(5)	Na5-O20w	2.530(2)	Na5-O20w	2.568(2)
<Na5-O,F>	2.550(9)	<Na5-O,F>	2.552(5)	<Na5-O,F>	2.544(5)
K1-O7	2.786(8)	K1-O7	2.853(3)	K1-O7	2.713(5)
K1-O8	2.754(4)	K1-O8	2.809(2)	K1-O8	2.693(3)
K1-O9	2.706(7)	K1-O9	2.769(3)	K1-O9	2.646(5)
K1-O10	2.730(5)	K1-O10	2.783(2)	K1-O10	2.655(3)
K1-O15	2.775(7)	K1-O15	2.869(3)	K1-O15	2.704(4)
K1-O17	2.762(7)	K1-O17	2.824(3)	K1-O17	2.691(6)
K1-O21w	2.83(6)	K1-O21w	2.73(4)	K1-F1	2.986(7)
K1-O22w	2.86(6)	K1-O21w	2.78(4)		
				$K2_1$-O9	2.895(3)
$K2_1$-O9	2.898(7)	$K2_1$-O9	2.912(4)	$K2_1$-O10	2.976(3)
$K2_1$-O10	2.982(7)	$K2_1$-O10	2.973(4)	$K2_1$-O12	2.842(4)
$K2_1$-O12	2.835(8)	$K2_1$-O12	2.834(5)	$K2_1$-O14	2.881(3)
$K2_1$-O14	2.870(7)	$K2_1$-O14	2.866(5)	$K2_1$-O19	3.072(3)
$K2_1$-O19	3.064(6)	$K2_1$-O19	3.038(5)	$K2_1$-O20w	3.199(5)
$K2_1$-O22w	3.03(2)	$K2_1$-O21w	2.82(3)		
$K2_1$-O23w	2.95(4)			$K2_2$-O9	2.87(1)
$K2_1$-O24w	2.78(5)	$K2_2$-O9	2.883(5)	$K2_2$-O10	2.92(1)
		$K2_2$-O10	2.967(5)	$K2_2$-O12	3.13(5)
$K2_2$-O9	2.87(4)	$K2_2$-O12	3.091(9)	$K2_2$-O14	3.16(4)
$K2_2$-O10	3.02(3)	$K2_2$-O14	3.075(9)		
$K2_2$-O12	3.05(5)			$K3_1$-O8	2.928(3)
$K2_2$-O14	3.00(5)	$K3_1$-O8	2.882(5)	$K3_1$-O11	2.842(4)
		$K3_1$-O11	2.96(1)	$K3_1$-O13	2.857(4)
K3-O8	2.914(6)	$K3_1$-O13	2.98(1)	$K3_1$-O16	3.194(5)
K3-O11	2.854(9)	$K3_1$-O16	3.14(1)	$K3_1$-O17	3.016(2)
K3-O13	2.856(9)	$K3_1$-O17	2.966(5)	$K3_1$-O19	3.084(5)
K3-O17	3.022(5)	$K3_1$-O19	3.16(1)	$K3_1$-O20w	3.152(4)
K3-O19	3.09(1)	$K3_1$-O20w	2.914(9)		
K3-O20w	3.126(7)			$K3_2$-O8	3.06(2)
K3-O21w	3.01(4)	$K3_2$-O8	2.85(1)	$K3_2$-O17	3.10(2)
K3-O22w	3.10(2)	$K3_2$-O11	3.05(2)		
		$K3_2$-O13	3.05(2)	$K4_1$-O7	2.986(6)

K4-O7	3.015(97)	$K3_2$-O17	2.95(1)	$K4_1$-O15	2.962(6)
K4-O15	2.968(8)			$K4_1$-O16	2.695(6)
K4-O16	2.682(8)	$K4_1$-O7	3.043(4)	$K4_1$-O18	2.800(5)
K4-O18	2.755(6)	$K4_1$-O15	3.025(4)	$K4_1$-O19	3.006(8)
K4-O19	2.995(8)	$K4_1$-O16	2.644(4)		
K4-O21w	2.93(3)	$K4_1$-O16′	3.131(4)	$K4_2$-O7	2.88(1)
K4-O24w	2.98(5)	$K4_1$-O18	2.715(3)	$K4_2$-O15	2.89(1)
		$K4_1$-O19	2.898(4)	$K4_2$-O16	2.84(1)
Na5-K1	0.73(1)	$K4_1$-O19	3.126(3)	$K4_2$-O18	2.97(1)
$K2_1$-$K2_2$	1.02(4)			$K4_2$-O19	3.09(2)
$K2_2$-K4	2.65(4)	$K4_2$-O7	2.891(6)	$K4_2$-O20w	3.06(2)
O20w-O21w	2.19(7)	$K4_2$-O15	2.886(7)		
O20w-O23w	1.75(4)	$K4_2$-O16	2.787(8)	$K4_3$-O7	3.07(2)
O20w-O24w	1.90(3)	$K4_2$-O18	2.882(7)	$K4_3$-O15	3.10(2)
O21w-O22w	2.49(4)	$K4_2$-O19	3.07(1)		
O21w-O23w	2.04(6)	$K4_2$-O20w	3.17(2)	Na5-K1	0.569(8)
O21w-O24w	2.16(8)			K1-$K3_2$	2.57(2)
O22w-O23w	1.34(6)	Na5-K1	0.885(4)	K1-$K3_2$	2.58(2)
		$K2_1$-$K2_2$	1.05(1)	K1-$K4_3$	2.49(2)
		$K2_2$-$K4_2$	2.44(1)	K1-$K4_3$	2.57(2)
		$K3_1$-$K3_2$	0.35(2)	$K2_1$-$K2_2$	0.94(7)
		$K4_1$-$K4_2$	0.49(2)	$K2_1$-$K3_2$	2.56(5)
		$K4_1$-$K4_1$	2.340(7)	$K3_1$-$K3_2$	1.57(4)
		O20w-O21w	2.21(4)	$K3_1$-$K4_3$	2.35(2)
				$K4_1$-$K4_2$	0.35(2)
				$K4_1$-$K4_3$	1.88(3)

Table S9. Unit cell parameters of the studied fedorite samples compared with literature data on fedorite [7], lalondeite [39], martinite [40] and ellingsenite [41] (str. sch – structural scheme).

	Gav-43	Yak-5	Irk-53	Fedorite, Murun [7]	Fedorite, Turiy [7]	Lalondeite [39]	Martinite [40]	Ellingsenite [41]
a (Å)	9.6463(5)	9.6355(3)	9.6446(1)	9.6450(7)	9.6300(7)	9.589(2)	9.5437(7)	9.576(11)
b (Å)	9.6485(5)	9.6364(3)	9.6519(1)	9.6498(7)	9.6392(7)	9.613(2)	9.539(6)	9.577(11)
c (Å)	12.6189(5)	12.6153(3)	12.6177(2)	12.6165(9)	12.6118(9)	12.115(2)	14.0268(10)	16.438(19)
α (º)	102.448(4)	102.482(2)	102.459(1)	102.427(1)	102.422(1)	96.62(2)	108.943(1)	85.85(2)
β (º)	96.235(4)	96.237(2)	96.207(1)	96.247(1)	96.227(1)	92.95(2)	74.154(1)	75.23(2)
γ (º)	119.927(5)	119.926(3)	119.900(2)	119.894(1)	119.888(1)	119.81(2)	119.780(1)	60.142(14)
a / *b*	0.9998	0.9999	0.9992	0.9995	0.9990	0.9975	1.0009	0.9999
b / *c*	0.7646	0.7639	0.7650	0.7649	0.7643	0.7935	0.6798	0.5826
c / *a*	1.3082	1.3093	1.3083	1.3081	1.3096	1.2634	1.4697	1.7166
V (Å^3)	960.96(4)	958.20(2)	961.44(1)	961.24	958.54	954.8(1)	1038.1(1)	1262(3)
str. sch.	$OT_2\bar{T}_2O$						$OT_2X\bar{T}_2O$	

Table S10. Calculated geometrical parameters for tetrahedra in the crystal structures of studied fedorite samples, fedorite, lalondeite, martinite and ellingsenite. BVS - bond-valence sum, ECoN - effective coordination number, Vp - volume of the coordination polyhedron, r_v - average distance from the volume center to the ligands, Δ_v - distance of the central atom to the volume center, r_s - average distance from the centroid to the ligands, Vs - volume of the sphere fitted to the positions of ligands, ECCv - volume eccentricity, SPHv – volume sphericity.

	Gav-43	Yak-5	Irk-53	Fedorite, Murun [7]	Fedorite, Turiy [7]	Lalondeite [39]	Martinite [40]	Ellingsenite [41]
T1			**Si1**			**Si3**	**B**	**Si8**
<Si-O> (Å)	1.604(4)	1.603(2)	1.602(1)	1.604(9)	1.609(7)	1.601(12)	1.480(16)	1.60(4)
<O-Si-O> (º)	109.5(2)	109.5(1)	109.48(7)	109.5(5)	109.5(5)	109.5(9)	109.4(5)	109.5(14)
BVS (vu)	4.217	4.222	4.209	4.209	4.160	4.243	2.960	4.309
ECoN	3.9974	3.9988	3.9978	3.9970	3.9983	3.9936	3.9877	3.9902
Vp (Å^3)	2.115	2.112	2.119	2.117	2.137	2.107	1.660	2.080
r_v (Å)	1.603	1.603	1.604	1.604	1.609	1.601	1.479	1.595
Δ_v (Å)	0.005	0.012	0.005	0.005	0.003	0.011	0.036	0.018
r_s (Å)	1.603	1.603	1.604	1.604	1.609	1.602	1.480	1.595
Δ (Å)	0.012	0.009	0.011	0.013	0.010	0.019	0.025	0.024
Vs (Å^3)	17.266	17.249	17.297	17.286	17.447	17.211	13.567	17.003
ECCv	0.0223	0.0158	0.0206	0.0240	0.0181	0.0348	0.0489	0.0439
SPHv	1	0.9998	1	1	1	1	0.9997	0.9993
T2			**Si2**			**Si1**	**Si3**	**Si3**
<Si-O> (Å)	1.615(4)	1.613(2)	1.615(1)	1.614(15)	1.608(23)	1.614(31)	1.614(22)	1.60(4)
<O-Si-O> (º)	109.3(2)	109.3(1)	109.33(7)	109.3(5)	109.3(5)	109.3(9)	109.3(5)	109.3(14)
BVS (vu)	4.096	4.112	4.094	4.101	4.174	4.114	4.104	4.215
ECoN	3.9890	3.9872	3.9880	3.9905	3.9758	3.9547	3.9789	3.9854
Vp (Å^3)	2.147	2.140	2.147	2.144	2.117	2.138	2.144	2.100
r_v (Å)	1.612	1.611	1.612	1.611	1.605	1.610	1.612	1.601
Δ_v (Å)	0.006	0.091	0.089	0.087	0.099	0.112	0.091	0.095
r_s (Å)	1.614	1.612	1.614	1.613	1.607	1.612	1.613	1.603

Δ (Å)	0.023	0.025	0.024	0.022	0.034	0.044	0.033	0.028
Vs (Å^3)	17.613	17.562	17.617	17.587	17.368	17.548	17.581	17.248
ECCv	0.0422	0.0454	0.0443	0.0398	0.0615	0.0803	0.0595	0.0512
SPHv	0.9999	1	0.9998	1	1	1	0.9998	0.9998
T3			**Si3**			**Si4**		**Si5**
<Si-O> (Å)	1.615(3)	1.614(2)	1.615(1)	1.614(20)	1.612(22)	1.613(22)	1.622(25)	1.61(4)
<O-Si-O> (º)	109.3(2)	109.3(1)	109.30(7)	109.3(5)	109.3(5)	109.3(9)	109.3(5)	109.3(14)
BVS (vu)	4.098	4.106	4.092	4.111	4.136	4.125	4.030	4.169
ECoN	3.9836	3.9792	3.9833	3.9824	3.9778	3.9783	3.9712	3.9723
Vp (Å^3)	2.145	2.140	2.147	2.140	2.131	2.131	2.168	2.115
r_v (Å)	1.612	1.611	1.612	1.611	1.608	1.609	1.618	1.605
Δ_V (Å)	0.093	0.097	0.093	0.093	0.097	0.106	0.105	0.102
r_s (Å)	1.614	1.613	1.614	1.612	1.610	1.611	1.620	1.607
Δ (Å)	0.028	0.031	0.028	0.029	0.032	0.032	0.036	0.036
Vs (Å^3)	17.605	17.571	17.621	17.560	17.4900	17.514	17.806	17.395
ECCv	0.0510	0.0569	0.0515	0.0528	0.0586	0.0579	0.0658	0.0661
SPHv	0.9999	0.9999	0.9999	1	1	0.9999	0.9999	0.9998
T4			**Si4**			**Si8**	**Si5**	**Si6**
<Si-O> (Å)	1.616(4)	1.616(2)	1.617(1)	1.616(26)	1.615(27)	1.612(33)	1.617(16)	1.61(4)
<O-Si-O> (º)	109.3(2)	109.3(1)	109.33(7)	109.3(5)	109.3(5)	109.3(9)	109.4(5)	109.3(14)
BVS (vu)	4.089	4.090	4.079	4.093	4.101	4.140	4.075	4.163
ECoN	3.9718	3.9709	3.9745	3.9703	3.9667	3.9470	3.9894	3.9499
Vp (Å^3)	2.152	2.149	2.155	2.151	2.145	2.129	2.157	2.127
r_v (Å)	1.613	1.613	1.614	1.613	1.612	1.608	1.615	1.607
Δ_V (Å)	0.091	0.095	0.091	0.092	0.094	0.112	0.076	0.094
r_s (Å)	1.615	1.614	1.616	1.615	1.613	1.610	1.616	1.608
Δ (Å)	0.036	0.037	0.035	0.037	0.039	0.048	0.023	0.048
Vs (Å^3)	17.636	17.625	17.672	17.629	17.582	17.466	17.682	17.417

ECCv	0.0659	0.0667	0.0630	0.0673	0.0707	0.061	0.0424	0.0871
SPHv	1	1	1	1	1	1	1	0.9998
T5				**Si5**			**Si6**	**Si4**
<Si-O> (Å)	1.613(4)	1.613(2)	1.615(1)	1.615(23)	1.612(24)	1.611(28)	1.617(20)	1.60(4)
<O-Si-O> (º)	109.3(2)	109.3(1)	109.33(7)	109.3(5)	109.3(5)	109.3(9)	109.4(5)	109.4(14)
BVS (vu)	4.114	4.120	4.101	4.102	4.131	4.144	4.074	4.276
ECoN	3.9820	3.9779	3.9803	3.9773	3.9752	3.9641	3.9840	3.9917
Vp (Å^3)	2.140	2.139	2.146	2.146	2.133	2.129	2.157	2.085
r_v (Å)	1.610	1.610	1.612	1.612	1.609	1.608	1.6015	1.596
Δ_V (Å)	0.089	0.092	0.090	0.091	0.094	0.100	0.084	0.068
r_s (Å)	1.612	1.612	1.614	1.613	1.610	1.610	1.616	1.597
Δ (Å)	0.029	0.032	0.031	0.033	0.034	0.041	0.029	0.021
Vs (Å^3)	17.549	17.539	17.595	17.592	17.490	17.466	17.682	17.077
ECCv	0.0535	0.0588	0.0557	0.0594	0.0621	0.0738	0.0530	0.0380
SPHv	0.9999	0.9999	1	1	0.9999	1	0.9999	0.9998
T6				**Si6**			**Si7/B**	**Si1**
<Si-O> (Å)	1.609(4)	1.606(2)	1.609(1)	1.610(7)	1.609(9)	1.611(4)	1.558(37)	1.60(4)
<O-Si-O> (º)	109.5(2)	109.5(1)	109.47(7)	109.5(5)	109.5(5)	109.5(9)	109.5(5)	109.5(14)
BVS (vu)	4.155	4.174	4.158	4.144	4.153	4.141	3.758	4.277
ECoN	3.9989	3.9992	3.9974	3.9981	3.9964	3.9995	3.9300	3.9721
Vp (Å^3)	2.139	2.131	2.138	2.142	2.139	2.143	1.939	2.094
r_v (Å)	1.609	1.607	1.609	1.610	1.609	1.610	1.558	1.598
Δ_V (Å)	0.010	0.016	0.009	0.007	0.010	0.012	0.053	0.025
r_s (Å)	1.609	1.607	1.609	1.610	1.609	1.611	1.558	1.599
Δ (Å)	0.008	0.007	0.012	0.010	0.014	0.006	0.054	0.037
Vs (Å^3)	17.463	17.400	17.459	17.485	17.461	17.499	15.835	17.111
ECCv	0.0150	0.0126	0.0223	0.0190	0.0259	0.0103	0.1009	0.0684
SPHv	1	1	1	1	0.9998	1	0.9999	0.9998

T7			**Si7**			**Si2**	**Si1**	**Si2**
<Si-O> (Å)	1.619(4)	1.617(2)	1.618(1)	1.615(20)	1.610(24)	1.616(19)	1.616(24)	1.60(4)
<O-Si-O> (º)	109.3(2)	109.3(1)	109.30(7)	109.3(5)	109.3(5)	109.3(9)	109.3(5)	109.3(14)
BVS (vu)	4.058	4.083	4.061	4.100	4.158	4.079	4.086	4.241
ECoN	3.9834	3.9803	3.9831	3.9825	3.9738	3.9842	3.9750	3.9543
Vp (Å^3)	2.159	2.150	2.157	2.145	2.124	2.150	2.148	2.098
r_v (Å)	1.615	1.613	1.615	1.612	1.606	1.613	1.613	1.600
Δ_V (Å)	0.092	0.095	0.094	0.091	0.096	0.096	0.101	0.089
r_s (Å)	1.617	1.615	1.617	1.614	1.608	1.615	1.615	1.601
Δ (Å)	0.028	0.031	0.028	0.029	0.035	0.027	0.034	0.047
Vs (Å^3)	17.722	17.647	17.707	17.597	17.419	17.651	17.633	17.184
ECCv	0.0515	0.0557	0.0519	0.0526	0.0632	0.0501	0.0618	0.0854
SPHv	1	0.9999	0.9999	1	1	1	0.9999	0.9996
T8			**Si8**			**Si7**	**Si2**	**Si7**
<Si-O> (Å)	1.613(4)	1.611(2)	1.613(1)	1.610(25)	1.611(24)	1.614(36)	1.622(24)	1.61(4)
<O-Si-O> (º)	109.3(2)	109.3(1)	109.30(7)	109.3(5)	109.3(5)	109.3(9)	109.3(5)	109.3(14)
BVS (vu)	4.124	4.141	4.114	4.150	4.145	4.120	4.024	4.151
ECoN	3.9827	3.9775	3.9800	3.9727	3.9737	3.9390	3.9740	3.9947
Vp (Å^3)	2.137	2.128	2.139	2.129	2.129	2.136	2.171	2.080
r_v (Å)	1.610	1.608	1.610	1.608	1.608	1.610	1.618	1.607
Δ_V (Å)	0.090	0.095	0.092	0.092	0.095	0.109	0.102	0.084
r_s (Å)	1.611	1.609	1.612	1.609	1.609	1.612	1.620	1.609
Δ (Å)	0.029	0.032	0.031	0.035	0.035	0.052	0.035	0.017
Vs (Å^3)	17.527	17.462	17.547	17.447	17.456	17.535	17.823	17.448
ECCv	0.0525	0.0590	0.0561	0.0645	0.0635	0.0930	0.0635	0.0307
SPHv	0.9999	1	1	0.9999	1	0.9998	1	0.9998

Table S11. Calculated distortion parameters for tetrahedra in the crystal structures of studied fedorite samples and fedorite, lalondeite, martinite and ellingsenite from literature. υ - volume distortion, BLD - bond length distortion, ELD - edge length distortion, TAV - tetrahedral angle variance, TQE - tetrahedral quadratic elongation.

	Gav-43	Yak-5	Irk-53	Fedorite, Murun [7]	Fedorite, Turiy [7]	Lalondeite [39]	Martinite [40]	Ellingsenite [41]
T1			**Si1**			**Si3**	**B**	**Si8**
υ	0.0003	0.0004	0.0002	0.0003	0.0002	0.0009	0.0014	0.0017
BLD (%)	0.3586	0.2495	0.3506	0.4130	0.2720	0.6089	0.7941	0.6504
ELD (%)	0.4647	0.5540	0.4135	0.4200	0.3087	0.8031	0.8625	1.0367
TAV	0.5196	1.0459	0.4139	0.4373	0.2859	0.8522	4.1803	4.4267
TQE	1.0004	1.0006	1.0000	1.0004	1.0001	1.0002	1.0015	1.0014
T2			**Si2**			**Si1**	**Si3**	
υ	0.0052	0.0053	0.0052	0.0052	0.0053	0.0058	0.0045	0.0064
BLD (%)	0.7430	0.7902	0.7816	0.6968	1.0261	1.4250	1.0530	0.9352
ELD (%)	2.0382	2.1037	2.0380	2.0457	2.1114	2.1679	1.7015	2.1038
TAV	21.0540	22.2419	21.4571	20.9800	25.7379	31.0480	20.5251	25.1115
TQE	1.0047	1.0049	1.0048	1.0053	1.0055	1.0066	1.0050	1.0058
T3			**Si3**			**Si4**		**Si5**
υ	0.0054	0.0058	0.0056	0.0055	0.0055	0.0067	0.0060	0.0075
BLD (%)	0.8978	0.9679	0.8821	0.9218	1.0394	1.0078	1.1639	1.1501
ELD (%)	2.0576	2.1541	2.0444	2.0276	2.0432	2.3598	2.1132	2.0413
TAV	23.0329	25.0887	23.2147	23.2741	25.0339	30.1033	28.1315	28.7083
TQE	1.0052	1.0057	1.0054	1.0054	1.0054	1.0078	1.0064	1.0066
T4			**Si4**			**Si8**	**Si5**	**Si6**
υ	0.0043	0.0046	0.0046	0.0041	0.0042	0.0052	0.0042	0.0033
BLD (%)	1.1139	1.1448	1.0823	1.1682	1.2384	1.5434	0.6803	1.3824
ELD (%)	1.9712	1.8794	1.7828	1.7271	1.7288	1.9678	1.5863	1.4607
TAV	20.9101	22.5819	21.1171	20.9471	21.9379	30.0642	16.3115	20.1531

TQE	1.0093	1.0053	1.0046	1.0053	1.0055	1.0065	1.0039	1.0042
T5				**Si5**			**Si6**	**Si4**
υ	0.0046	0.0047	0.0046	0.0042	0.0044	0.0053	0.0042	0.0036
BLD (%)	0.9452	1.0229	0.9831	1.0451	1.0856	1.2415	1.0048	0.6100
ELD (%)	1.8756	1.8952	1.8488	1.7982	1.8842	1.9678	1.6009	1.4448
TAV	20.4902	21.9339	20.5771	20.7159	22.2459	25.9998	18.1003	13.5907
TQE	1.0048	1.0048	1.0048	1.0047	1.0053	1.0056	1.0041	1.0035
T6				**Si6**			**Si7/B**	**Si1**
υ	0.0003	0.0005	0.0003	0.0002	0.0003	0.0005	0.0005	0.0010
BLD (%)	0.2563	0.2022	0.3729	0.2950	0.4194	0.1863	1.7087	1.0791
ELD (%)	0.3805	0.5143	0.4101	0.3338	0.4355	0.5070	0.5831	0.7790
TAV	0.4369	0.9819	0.3427	0.2298	0.4307	1.1753	5.0635	2.4027
TQE	1.0001	1.0003	1.0002	1.0002	1.0005	1.0002	1.0013	1.0007
T7			**Si7**			**Si2**	**Si1**	**Si2**
υ	0.0055	0.0054	0.0057	0.0052	0.0049	0.0060	0.0055	0.0033
BLD (%)	0.8880	0.9743	0.9113	0.9212	1.1028	0.8891	1.0905	1.5759
ELD (%)	2.0215	2.0434	2.0349	1.9501	1.9376	2.1573	2.1010	1.3609
TAV	23.0029	24.1059	23.9427	22.5859	24.3139	24.8598	26.3435	19.1651
TQE	1.0055	1.0056	1.0060	1.0052	1.0052	1.0059	1.0059	1.0043
T8			**Si8**			**Si7**	**Si2**	**Si7**
υ	0.0049	0.0052	0.0051	0.0041	0.0044	0.0056	0.0058	0.0017
BLD (%)	0.9147	1.0242	0.9761	1.1256	1.1097	1.5724	1.0865	0.5125
ELD (%)	1.8956	1.9615	1.8760	1.7459	1.8410	1.8767	1.8475	2.1720
TAV	21.5011	23.6319	22.1787	21.1637	22.5971	24.8598	26.1387	20.5691
TQE	1.0047	1.0055	1.0054	1.0046	1.0052	1.0068	1.0063	1.0049

Table S12. Calculated geometrical parameters for coordination polyhedra (M1, M2, M3, M4) in the crystal structures of fedorite, lalondeite, martinite and ellingsenite. Occ. – occypancy, m.a.n. – mean atomic number, BVS - bond-valence sum, ECoN - effective coordination number, Vp - volume of the coordination polyhedron, r_v - average distance from the volume center to the ligands, Δ_v - distance of the central atom to the volume center, r_s - average distance from the centroid to the ligands, Vs - volume of the sphere fitted to the positions of ligands, ECCv - volume eccentricity, SPHv – volume sphericity.

	Gav-43	Yak-5	Irk-53	Fedorite, Murun [7]	Fedorite, Turiy [7]	Lalondeite [39]	Martinite [40]	Ellingsenite [41]
			M1			**Ca1**	**Na5**	**Ca1**
<M-O,F> (Å)	2.464(5)	2.461(2)	2.466(2)	2.471(9)	2.474(9)	2.38(1)	2.419(9)	2.40(4)
Occ.	0.693 Na 0.311 Ca	0.719 Na 0.287 Ca	0.712 Na 0.290 Ca	0.771 Na 0.226 Ca	0.95 Na 0.05 Ca	1.00 Ca	0.51 Na 0.49 Ca	1.00 Ca
m.a.n. (e^-)	13.823	13.649	13.632	13.070	11.450	20.000	15.410	20.000
BVS (vu)	1.050	1.048	1.030	0.990	0.890	1.880	1.356	1.810
ECoN	5.6724	5.6480	5.7241	5.6660	5.6583	5.9784	5.7778	5.9300
Vp ($Å^3$)	18.939	18.884	19.023	19.092	19.207	17.613	19.350	17.918
r_v (Å)	2.463	2.461	2.466	2.470	2.474	2.382	2.474	2.399
Δ_v (Å)	0	0	0	0	0	0	0.090	0.055
r_s (Å)	2.463	2.461	2.466	2.470	2.474	2.382	2.479	2.400
Δ (Å)	0	0	0	0	0	0	0.181	0.064
Vs ($Å^3$)	62.621	62.442	62.824	63.124	63.440	56.604	63.793	57.890
ECCv	0	0	0	0	0	0	0.2037	0.0779
SPHv	0.8851	0.8817	0.8932	0.8839	0.8821	0.9673	0.9669	0.9801
			M2			**Ca2**	**Na1**	**Ca2**
<M-O,F> (Å)	2.429(5)	2.426(2)	2.428(2)	2.433(9)	2.433(9)	2.37(2)	2.462(8)	2.35(4)
Occ.	0.618 Ca 0.386 Na	0.591 Ca 0.415 Na	0.595 Ca 0.409 Na	0.567 Ca 0.433 Na	0.51 Ca 0.49 Na	1.00 Ca	1.00 Na	1.00 Ca
m.a.n. (e^-)	16.586	16.385	16.399	16.130	15.590	20.000	11.000	20.000
BVS (vu)	1.387	1.382	1.376	1.345	1.308	1.823	0.883	1.962
ECoN	5.7559	5.7634	5.7811	5.7170	5.7389	5.9882	5.8554	5.8362

Vp (Å^3)	18.384	18.344	18.382	18.503	18.517	17.573	18.280	16.815
r_v (Å)	2.427	2.424	2.426	2.431	2.431	2.376	2.438	2.350
Δ_V (Å)	0.104	0.105	0.103	0.104	0.108	0.053	0	0.141
r_s (Å)	2.427	2.425	2.426	2.431	2.431	2.376	2.438	2.352
Δ (Å)	0.097	0.096	0.091	0.107	0.109	0.025	0	0.098
Vs (Å^3)	59.882	59.711	59.843	60.215	60.201	56.218	60.680	54.475
ECCv	0.1157	0.1143	0.1088	0.1261	0.1281	0.0314	0.0001	0.1201
SPHv	0.9320	0.9325	0.9340	0.9258	0.9350	0.9840	0.8740	0.9749
			M3			**Ca3**	**Ca2**	**Ca3**
<M-O,F> (Å)	2.416(5)	2.413(2)	2.418(2)	2.413(9)	2.411(9)	2.41(2)	2.410(9)	2.43(4)
Occ.	0.891 Ca 0.118 Na	0.793 Ca 0.213 Na	0.848 Ca 0.171 Na	0.821 Ca 0.179 Na	0.792 Ca 0.208 Na	0.52 Ca 0.48 Na	0.80 Ca 0.20 Na	0.55 Ca 0.45 Na
m.a.n. (e^-)	18.160	18.203	18.841	18.380	18.110	15.680	18.200	15.950
BVS (vu)	1.600	1.614	1.646	1.628	1.616	1.345	1.629	1.418
ECoN	5.9831	5.9819	5.9835	5.9799	5.9775	5.8124	5.9285	5.6229
Vp (Å^3)	18.342	18.284	18.376	18.287	18.269	18.051	18.235	18.433
r_v (Å)	2.416	2.413	2.417	2.412	2.410	2.408	2.410	2.430
Δ_V (Å)	0.028	0.027	0.029	0.023	0.022	0.113	0.042	0.128
r_s (Å)	2.416	2.413	2.418	2.413	2.411	2.409	2.411	2.430
Δ (Å)	0.021	0.023	0.021	0.022	0.026	0.112	0.030	0.142
Vs (Å^3)	59.081	58.885	59.211	58.849	58.697	58.590	58.676	60.125
ECCv	0.0253	0.0284	0.0257	0.0266	0.0317	0.1330	0.0368	0.1648
SPHv	0.9758	0.9760	0.9766	0.9734	0.9734	0.9545	0.9486	0.9216
			M4			**Na1**	**Ca1**	**Na1**
<M-O,F> (Å)	2.407(5)	2.407(2)	2.408(2)	2.410(9)	2.409(9)	2.50(1)	2.362(9)	2.50(4)
Occ.	0.787 Ca 0.220 Na	0.716 Ca 0.293 Na	0.759 Ca 0.253 Na	0.74 Ca 0.26 Na	0.689 Ca 0.311 Na	1.00 Na	1.00 Ca	1.00 Na
m.a.n. (e^-)	16.586	17.543	17.963	17.660	17.210	11.000	20.000	11.000

BVS (vu)	1.460	1.530	1.554	1.527	1.499	0.785	1.901	0.921
ECoN	5.8153	5.8146	5.8315	5.8040	5.8106	5.8483	5.8717	5.5853
Vp (Å^3)	17.966	17.957	17.994	18.034	18.056	19.769	16.956	19.637
r_v (Å)	2.405	2.404	2.405	2.407	2.406	2.497	2.324	2.498
Δ_V (Å)	0.124	0.127	0.125	0.126	0.128	0.089	0.169	0
r_s (Å)	2.406	2.405	2.407	2.408	2.407	2.498	2.330	2.498
Δ (Å)	0.106	0.106	0.101	0.113	0.117	0.147	0.148	0
Vs (Å^3)	58.312	58.283	58.383	58.481	58.416	65.306	53.003	65.319
ECCv	0.1261	0.1262	0.1204	0.1347	0.1392	0.1660	0.1785	0
SPHv	0.9597	0.9581	0.9610	0.9608	0.9658	0.9464	0.9072	0.8632
		Na5			***A*1**		**Na4**	**Na2**
<M-O,F> (Å)	2.550(9)	2.552(5)	2.544(5)	2.554(9)	2.544(9)		2.542(9)	2.49(4)
Occ.	0.519 Na	0.476 Na	0.466 Na	0.643 Na	0.771 Na		1.00 Na	0.86 Na
BVS (vu)	0.999	1.006	1.026	1.000	1.023		1.039	1.231
ECoN	7.8873	7.8806	7.8337	7.9188	7.8724		7.6297	7.8130
Vp (Å^3)	28.112	28.140	27.934	28.007	27.816		27.830	25.852
r_v (Å)	2.538	2.539	2.533	2.535	2.530		2.537	2.481
Δ_V (Å)	0.216	0.228	0.194	0.285	0.231		0.163	0.213
r_s (Å)	2.554	2.554	2.550	2.552	2.548		2.554	2.489
Δ (Å)	0.041	0.023	0.067	0.022	0.042		0.101	0.040
Vs (Å^3)	69.802	69.804	69.428	69.619	63.317		69.752	64.627
ECCv	0.0478	0.0262	0.0771	0.0258	0.0482		0.1145	0.0475
SPHv	0.9489	0.9394	0.9494	0.9507	0.9467		0.9518	0.8843

Table S13. Calculated distortion parameters for for coordination polyhedra (M1, M2, M3, M4) in the crystal structures of fedorite, lalondeite, martinite and ellingsenite. υ - volume distortion, BLD - bond length distortion, ELD - edge length distortion, OAV - octahedral angle variance, OQE - octahedral quadratic elongation.

	Gav-43	Yak-5	Irk-53	Fedorite, Murun [7]	Fedorite, Turiy [7]	Lalondeite [39]	Martinite [40]	Ellingsenite [41]
			M1			**Ca1**	**Na5**	**Ca1**
υ	0.0498	0.0499	0.0487	0.0498	0.0488	0.0225	0.0471	0.0276
BLD (%)	3.1484	3.2507	2.8927	3.1579	3.1528	0.9048	2.1369	1.5769
ELD (%)	8.3929	8.3818	8.3265	8.3896	8.6099	5.4567	6.7902	5.9078
OAV	102.2187	102.1374	100.4776	102.0710	100.0664	51.0529	78.6325	59.8648
OQE	1.0372	1.0360	1.0350	1.0359	1.0374	1.0154	1.0273	1.0187
			M2			**Ca2**	**Na1**	**Ca2**
υ	0.0355	0.0349	0.0350	0.0346	0.0337	0.0180	0.0536	0.0303
BLD (%)	2.4522	2.3998	2.3249	2.6901	2.6400	0.5844	2.1479	2.4926
ELD (%)	7.0885	6.9193	7.0340	6.9821	6.9248	4.7940	7.5823	6.2743
OAV	80.9469	79.7176	79.9457	80.9469	77.4431	42.0068	84.5449	71.9887
OQE	1.0235	1.0314	1.0262	1.0261	1.0255	1.0124	1.0282	1.0230
			M3			**Ca3**	**Ca2**	**Ca3**
υ	0.0247	0.0245	0.0250	0.0238	0.0222	0.0321	0.0237	0.0368
BLD (%)	0.7106	0.6976	0.6550	0.7599	0.7329	3.1788	1.4936	3.2847
ELD (%)	5.8444	5.7992	5.8815	5.3802	5.5379	6.6418	5.5554	7.0733
OAV	53.8592	53.4450	54.5998	51.8168	48.3656	73.7755	51.0976	86.0676
OQE	1.0100	1.0165	1.0168	1.0077	1.0149	1.0344	1.0162	1.0287
			M4			**Na1**	**Ca1**	**Na1**
υ	0.0321	0.0321	0.0317	0.0312	0.0289	0.049	0.0365	0.0555
BLD (%)	2.4579	2.4650	2.3529	2.5726	2.5804	3.6402	2.2025	3.8210
ELD (%)	6.7584	6.7423	6.7115	6.6899	6.4655	8.2615	6.5274	8.7415
OAV	74.3663	74.7443	73.7474	72.9710	69.1074	103.6513	73.3287	113.1650

OQE	1.0242	1.0243	1.0239	1.0256	1.0290	1.0351	1.0236	1.0463
		Na5			**A1**		**-**	**Na4**	**Na2**
υ	0.0709	0.0700	0.0718	0.0719	0.0742		0.0796	0.0772
BLD (%)	1.1709	1.5501	1.4989	1.3408	1.3658		2.0983	3.0899
ELD (%)	13.6740	14.1081	14.1079	14.1120	14.0340		14.2221	12.9746

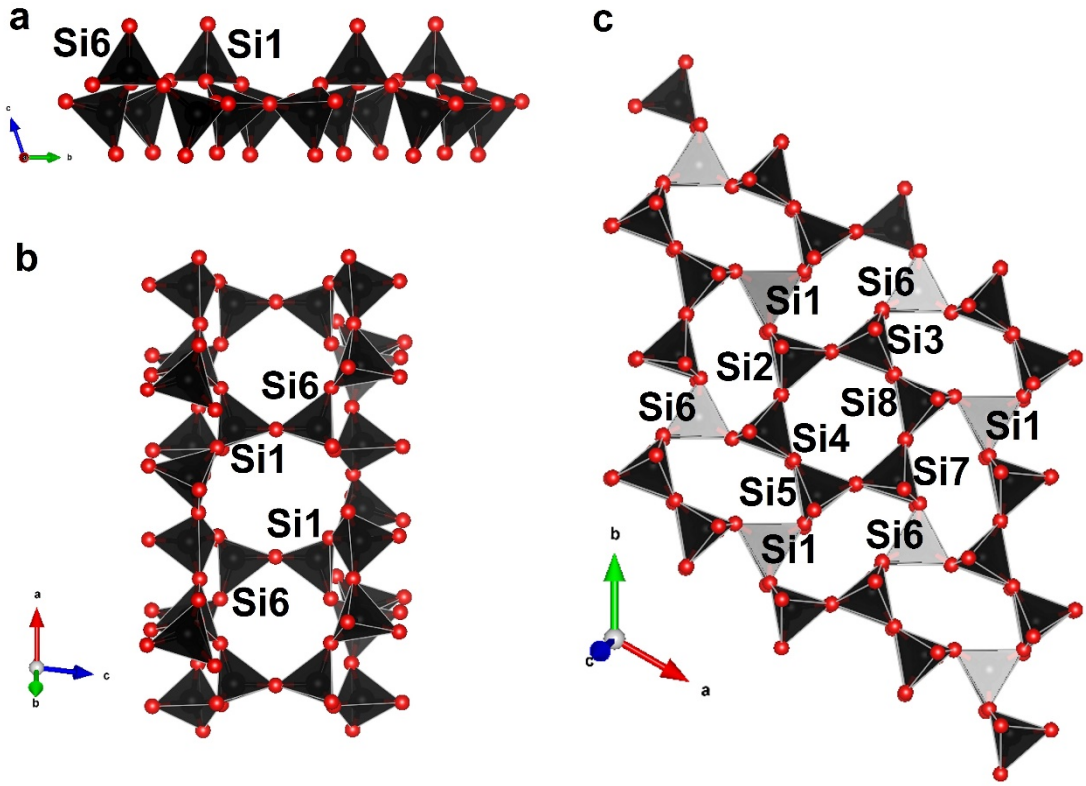

Figure S2. The fedorite tetrahedral sheet (*T*-layer): *a*) and *c*) – single layer, *b*) – double layer. Figure shows the tetrahedral pointing both ways.

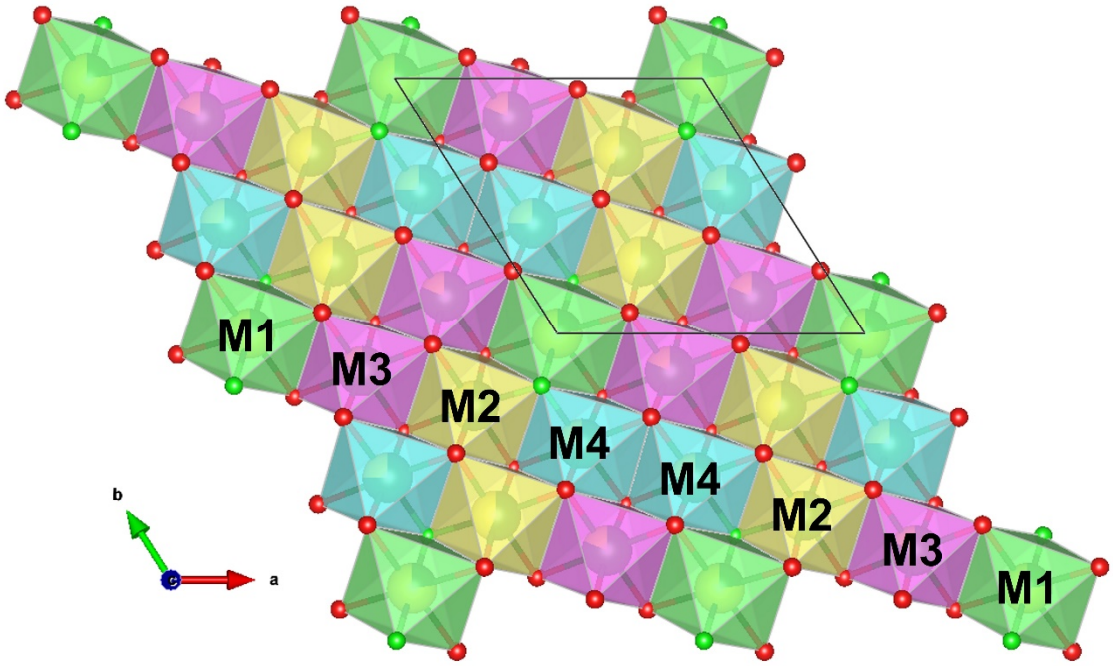

Figure S3. The fedorite octahedral sheet (*O*-layer). The four types of edge sharing octahedral are defined as: M1 (Na1Ca1 in Tables S1, S3, S5) – light green, M2 (Ca2Na2) – yellow, M3 (Ca3Na3) – lilac, M4 (Ca4Na4) – cyan. Oxygen and fluorine atoms are drawn in red and green, respectively. Unit cell edges are designated.

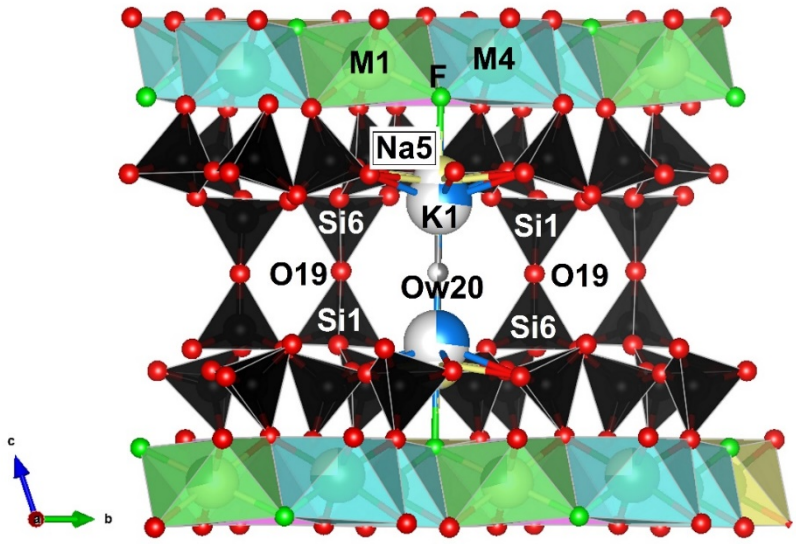

Figure S4. Fedorite structure fragment, showing the linkages between the *O* and T_2 sheets, T_2 and $\bar{T}_2$ sheets and interlayer Na5, K1 and Ow20 positions. K1 (blue) and Ow20 (grey) are designated, other K and Ow interlayer ions are omitted for clarity. Oxygen and fluorine atoms are drawn in red and green, respectively. Si-tetrahedra are black, Na5 are yellow spheres. M1 (Na1Ca1) – light green, M2 (Ca2Na2) – yellow, M3 (Ca3Na3) – lilac, M4 (Ca4Na4) – cyan octahedra. The partially white coloring of the spheres of K1, Na5 and Ow20 indicates a vacancy.

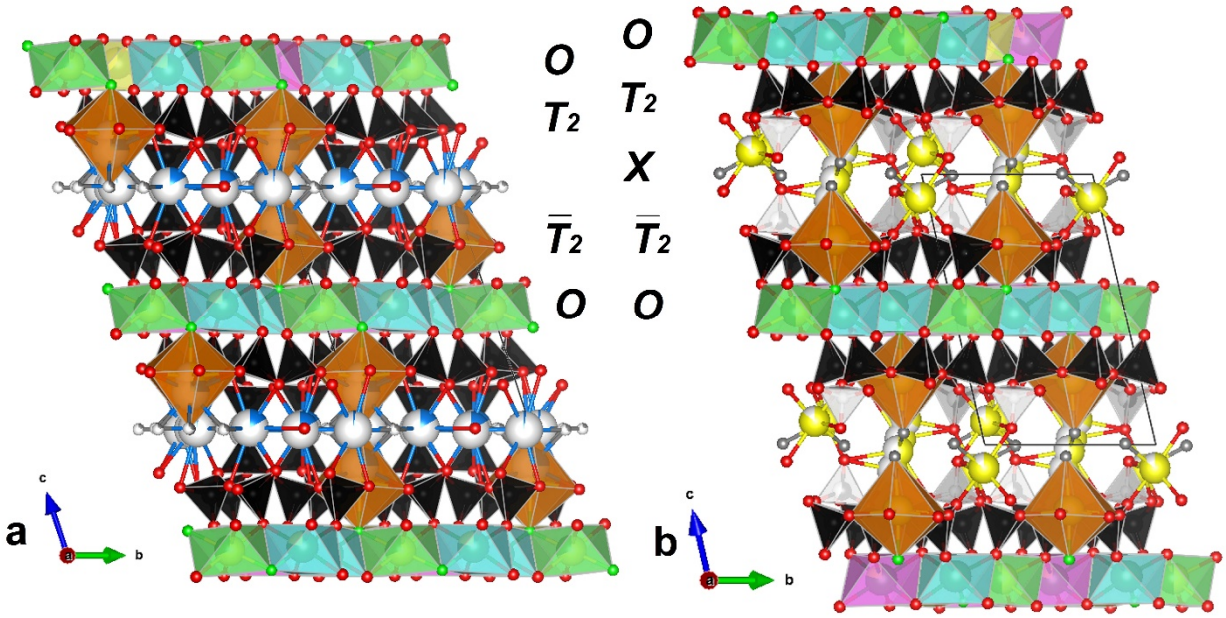

Figure S5. Crystal structures of fedorite (sample Gav-43) (*a*) and martinite [40] (*b*) projected along *a* axis. Oxygen and fluorine atoms are drawn in red and green, respectively. Si- and B-tetrahedra are black and white, respectively. M1– light green, M2– yellow, M3– lilac, M4– cyan octahedra. Interlayer potassium and sodium are designated as blue and yellow spheres. Ow atoms (oxygen of H_2O molecule) are drawn in grey. The partially white coloring of the spheres indicates a vacancy.

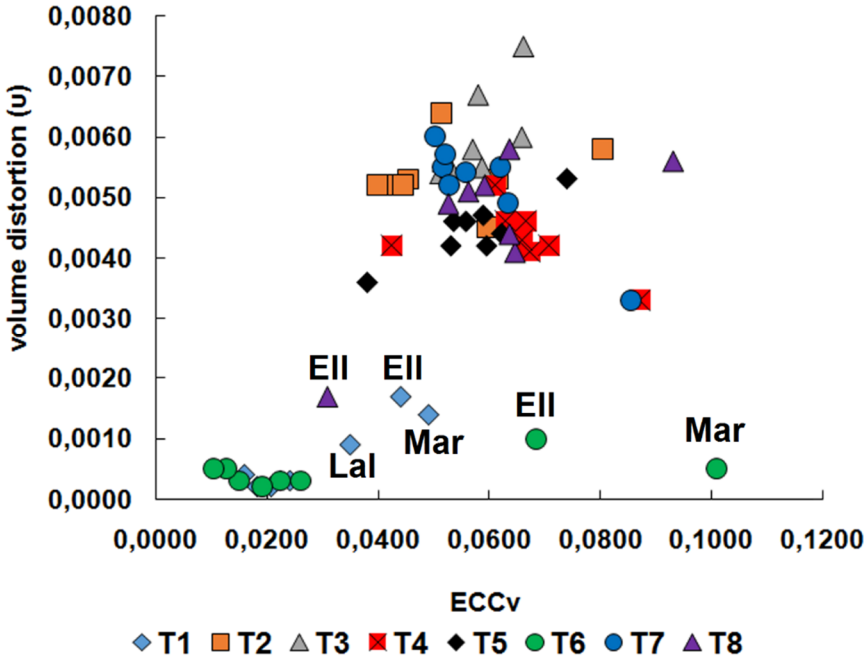

Figure S6. Volume distortion (υ) plotted against volume eccentricity (ECCv) for tetrahedra in fedorite under study (sample Gav-43, Yak-5, Irk-53, Murun complex), fedorite from Murun and Turiy complexes [7], lalondeite (Lal) [39], martinite (Mar) [40] and ellingsenite (Ell) [41]. Data were taken from Tables S10 and S11.

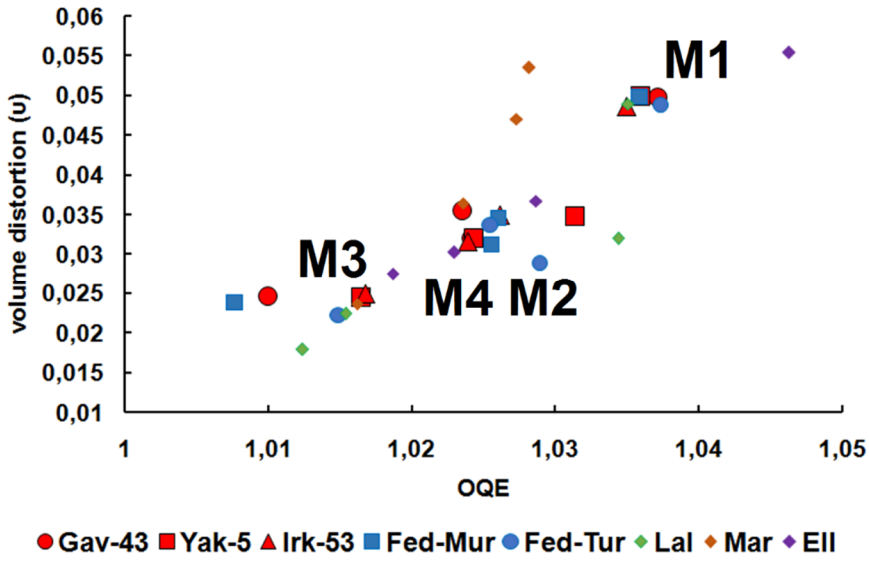

Figure S7. Volume distortion (υ) plotted against octahedral quadratic elongation (OQE) for M1-M4octahedra in fedorite under study (sample Gav-43, Yak-5, Irk-53, Murun complex), fedorite from Murun (Fed-Mur) and Turiy complexes (Fed-Tur) [7], lalondeite (Lal) [39], martinite (Mar) [40] and ellingsenite (Ell) [41]. Data were taken from Tables S12 and S13.

Table S13. The positions of the bands (cm^{-1}) in the IR spectra of the studied fedorite and structurally related minerals.

	Gav-43	Irk-53	Lalondeite [39]	Martinite [40]	Ellingsenite [41]
ν(O-H)	3656w, 3635, 3551		–	–	3600
ν(H-O-H)	3428, 3177	3177	3443	3437	3460
(Si-OH)	–	–	–	–	3260
δ(H-O-H)	1627		1631	1634	1630
$\nu(Si\text{-}O\text{-}Si)_{asym}$	1119, 1030		1121sh, 1025	–	1140, 1025, 880
$\nu(Si\text{-}O\text{-}Si)_{asym}$ and $\nu(B\text{-}O\text{-}B)_{asym}$	–	–	–	1137sh, 1011, 1081sh, 898sh, 862sh	–
L(O-H)	–	–	–	–	780
$\nu(Si\text{-}O\text{-}Si)_{sym}$	792, 615		787, 613, 466, 388	–	600, 480, 380
$\nu(Si\text{-}O\text{-}Si)_{sym}$ and $\nu(B\text{-}O\text{-}B)_{sym}$	–	–	–	786, 696, 621, 543, 498	–

Note: ν – stretching vibration, δ – bending vibrations, L – libration vibrations; sh – shoulder; w - weak

References:

7. Mitchell, R.H.; Burns, P.C. The structure of fedorite: a re-appraisal. *Can. Min.* **2001**, *39*, 769–777. [https://doi.org/10.2113/gscanmin.39.3.769]

39. McDonald, A.M.; Chao, G.Y. Lalondeite, a new hydrated Na-Ca fluorosilicate species from Mont Saint-Hilaire, Quebec: description and crystal structure. *Can. Min.* **2009**, *47*, 181–191. [https://doi.org/10.3749/canmin.47.1.181]

40. McDonald, A.M.; Chao, G.Y. Martinite, a new hydrated sodium calcium fluorborosilicate species from Mont Saint-Hilaire, Quebec: description, structure determination and genetic implication. *Can. Min.* **2007**, *45*, 1281–1292. [https://doi.org/10.2113/gscanmin.45.5.1281]

41. Yakovenchuk, V.N.; Ivanyuk, G.Yu.; Pakhomovsky, Y.A.; Selivanova, E.A.; Mikhailova J.A.; Krivovichev, S.V.; Zolotarev, A.A.; Zalkind, O.A. Ellingsenite, $Na_5Ca_6Si_{18}O_{38}(OH)_{13} \cdot 6H_2O$, a new martinite-related mineral species from phonolite of the Aris alkaline complex, Namibia. *Can. Min.* **2011**, *49*, 1099–1107. [https://doi.org/10.3749/canmin.49.5.1165]