Supplementary Material

Crystal-chemical characterization and spectroscopy of fluorcarletonite and carletonite

Ekaterina Kaneva*, Alexander Bogdanov, Tatiana Radomskaya, Olga Belozerova, and Roman Shendrik

Vinogradov Institute of Geochemistry, Siberian Branch of the Russian Academy of Sciences, Irkutsk, 664033, Russia

* Corresponding author.

E-mail address: kev604@mail.ru (E. Kaneva).

Table S1. Anisotropic atomic displacement parameters (Å^2) of fluorcarletonite sample.

Site	U11	U22	U33	U23	U13	U12
K1	0.0276(2)	0.0276(2)	0.0187(2)	0	0	–0.0090(2)
Na1	0.0150(2)	0.0150(2)	0.0213(4)	0	0	0
Na2	0.0274(2)	0.0274(2)	0.0243(4)	0.0072(2)	0.0072(2)	0.0097(3)
Na3	0.0203(3)	0.0203(3)	0.0143(4)	0	0	–0.0025(4)
Ca1	0.01163(8)	0.01147(7)	0.00997(7)	0.00035(6)	–0.00031(6)	0.00003(5)
Si1	0.0098(1)	0.0112(1)	0.0075(1)	–0.00098(8)	0.00001(8)	–0.00094(8)
Si2	0.0098(1)	0.0091(1)	0.0081(1)	0.00009(8)	–0.00047(8)	–0.00017(8)
O1	0.0190(4)	0.0194(4)	0.0188(3)	–0.0062(3)	0.0045(3)	0.0041(3)
O2	0.0192(4)	0.0131(3)	0.0139(3)	0.0047(3)	–0.0016(3)	0.0022(3)
O3	0.0131(3)	0.0133(3)	0.0106(3)	–0.0010(2)	–0.0024(2)	–0.0013(2)
O4	0.0142(3)	0.0142(3)	0.0128(4)	0.0008(3)	–0.0008(3)	–0.0050(4)
O5	0.0134(3)	0.0134(3)	0.0173(5)	0.0010(3)	–0.0010(3)	–0.0040(4)
O6	0.0195(5)	0.0179(5)	0.0080(4)	0	0	–0.0035(4)
O7	0.0198(4)	0.0165(3)	0.0093(3)	–0.0029(2)	–0.0008(3)	0.0012(3)
O8	0.0145(3)	0.0145(3)	0.0221(5)	–0.0047(3)	0.0047(3)	–0.0007(4)
O9	0.0114(5)	0.0412(8)	0.0119(4)	0	0	0.0013(5)
O10	0.0130(3)	0.0179(4)	0.0330(5)	–0.0053(3)	0.0056(3)	–0.0031(3)
Ow11	0.057(2)	0.057(2)	0.027(1)	0	0	0
Ow12	0.090(5)	0.090(5)	0.078(6)	0	0	–0.024(5)
F13	0.0186(4)	0.0186(4)	0.0242(7)	0	0	0
C1	0.0142(5)	0.0135(5)	0.0101(5)	0	0	0.0001(4)
C2	0.0134(3)	0.0134(3)	0.0153(5)	–0.0006(3)	0.0006(3)	–0.0012(4)

Table S2. Anisotropic atomic displacement parameters ($Å^2$) of carletonite sample.

Site	U11	U22	U33	U23	U13	U12
K1	0.0265(3)	0.0265(3)	0.0191(5)	0	0	–0.0096(3)
K2	0.0265(3)	0.0265(3)	0.0191(5)	0	0	–0.0096(3)
Na1	0.0126(3)	0.0126(3)	0.0226(6)	0	0	0
Na2	0.0245(3)	0.0245(3)	0.0218(5)	0.0069(3)	0.0069(3)	0.0095(4)
Na3	0.0169(3)	0.0169(3)	0.0118(5)	0	0	–0.0024(4)
Ca1	0.00986(9)	0.00978(9)	0.0081(1)	0.00043(7)	–0.00030(7)	–0.00009(7)
Si1	0.0078(1)	0.0094(1)	0.0055(1)	–0.0012(1)	0.0001(1)	–0.0012(1)
Si2	0.0078(1)	0.0069(1)	0.0062(1)	0.0000(1)	–0.0004(1)	–0.0003(1)
O1	0.0172(4)	0.0185(5)	0.0178(4)	–0.0066(4)	0.0043(4)	0.0047(4)
O2	0.0174(4)	0.0117(4)	0.0125(4)	0.0048(3)	–0.0021(3)	0.0020(3)
O3	0.0109(3)	0.0113(3)	0.0081(3)	–0.0012(3)	–0.0025(3)	–0.0014(3)
O4	0.0126(3)	0.0126(3)	0.0113(5)	0.0009(3)	–0.0009(3)	–0.0055(4)
O5	0.0123(3)	0.0123(3)	0.0176(6)	0.0007(3)	–0.0007(3)	–0.0048(4)
O6	0.0178(6)	0.0175(6)	0.0056(5)	0	0	–0.0031(5)
O7	0.0176(4)	0.0144(4)	0.0073(4)	–0.0028(3)	–0.0009(3)	0.0007(3)
O8	0.0130(3)	0.0130(3)	0.0202(7)	–0.0048(4)	0.0048(4)	–0.0012(4)
O9	0.0101(5)	0.0382(9)	0.0111(6)	0	0	0.0022(6)
O10	0.0113(4)	0.0158(4)	0.0311(6)	–0.0048(4)	0.0051(4)	–0.0033(3)
Ow11	0.052(2)	0.052(2)	0.030(2)	0	0	0
Ow12	0.081(4)	0.081(4)	0.088(6)	0	0	–0.019(5)
O13	0.0102(4)	0.0102(4)	0.0132(7)	0	0	0
C1	0.0125(6)	0.0115(6)	0.0077(6)	0	0	–0.0006(5)
C2	0.0111(4)	0.0111(4)	0.0134(7)	–0.0004(4)	0.0004(4)	–0.0011(5)

Table S3. Bond-valence sum for the studied fluorcarletonite. BVS for F13 site with mixed occupancy was calculated using the fractional site occupancies (i.e. 0.6F and 0.4O).

	Si1	**Si2**	**K1**	**Na1**	**Na2**	**Na3**	**Ca1**	**C1**	**C2**	**∑**
O1	1.077	0.992								**2.069**
O2	1.069	0.985	$0.054^{[\times4]}$							**2.108**
O3		1.128		$0.210^{[\times4]}$			0.320 0.271			**2.056**
O4		$0.978^{(\times2)}$			0.161					**2.117**
O5	$1.003^{(\times2)}$		$0.106^{[\times2]}$							**2.112**
O6	$1.026^{(\times2)}$									**2.052**
O7					$0.189^{[\times2]}$	$0.131^{[\times4]}$	0.221 0.206	$1.357^{[\times2]}$		**2.104**
O8						$0.186^{[\times2]}$	$0.262^{(\times2)}$		1.309	**2.019**
O9						$0.130^{[\times2]}$	$0.273^{(\times2)}$	1.365		**2.041**
O10			$0.151^{[\times4]}$		$0.212^{[\times2]}$		0.288		$1.400^{[\times2]}$	**2.051**
Ow11				0.216						**0.216**
Ow12					$0.065^{(\times2)}$					**0.130**
F13				0.090			$0.191^{(\times4)}$			**0.854**
∑	**4.175**	**4.083**	**1.032**	**1.133**	**1.028**	**1.156**	**2.032**	**4.079**	**4.109**	

$^{[\times2]}$, $^{[\times4]}$: for the calculation of the valence bond sum for cations.
$^{(\times2)}$, $^{(\times4)}$: for the calculation of the valence bond sum for anions.
BVS for F13 site with mixed occupancy was calculated using the fractional site occupancies (i.e. 0.6F and 0.4O)

Table S4. Bond-valence sum for the studied carletonite. BVS for O13 site with mixed occupancy was calculated using the fractional site occupancies (i.e. 0.61O and 0.39 F).

	Si1	**Si2**	**K1**	**K2**	**Na1**	**Na2**	**Na3**	**Ca**	**C1**	**C2**	**∑**
O1	1.077	0.997									**2.074**
O2	1.066	0.990	$0.055^{[\times4]}$								**2.056/ /2.111**
O3		1.131			$0.210^{[\times4]}$			0.320 0.276			**1.937**
O4		$0.982^{(\times2)}$				0.165					**2.129**
O5	$1.003^{(\times2)}$		$0.112^{[\times2]}$	$0.047^{[\times2]}$							**2.118/ /2.053**
O6	$1.032^{(\times2)}$										**2.064**
O7						$0.193^{[\times2]}$	$0.132^{[\times4]}$	0.216 0.206	$1.361^{[\times2]}$		**2.108**
O8							$0.190^{[\times2]}$	$0.261^{(\times2)}$		1.320	**2.032**
O9							$0.129^{[\times2]}$	$0.275^{(\times2)}$	1.376		**2.055**
O10			$0.157^{[\times4]}$	$0.354^{[\times4]}$		$0.213^{[\times2]}$		0.287		$1.376^{[\times2]}$	**2.033/ /2.230**
Ow11					0.206						**0.206**
Ow12						$0.058^{(\times2)}$					**0.116**
O13					0.090			$0.203^{(\times4)}$			**0.902**
∑	**4.178**	**4.100**	**0.758**	**1.463**	**1.147**	**1.035**	**1.166**	**2.069**	**4.098**	**4.072**	

$^{[\times2]}$, $^{[\times4]}$: for the calculation of the valence bond sum for cations.
$^{(\times2)}$, $^{(\times4)}$: for the calculation of the valence bond sum for anions.

Table S5. Calculated geometrical parameters for tetrahedra in the crystal structures of studied fluorcarletonite (Murun massif) and carletonite (Mt St Hilaire massif) samples. ECoN – effective coordination number [1–3], Vp – volume of the coordination polyhedron [4, 5], 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], Vs – volume of the sphere fitted to the positions of ligands [4, 5], ECCv – volume eccentricity [4, 5], SPHv – volume sphericity [4, 5].

parameter	Fluorcarletonite	Carletonite	Fluorcarletonite	Carletonite		
	Si1		**Si2**			
ECoN	3.993	3.994	3.968	3.969		
Vp (Å^3)	2.128	2.126	2.158	2.152		
r_v (Å)	1.607	1.607	1.615	1.613		
Δ_V (Å)	0.029	0.029	0.074	0.072		
r_s (Å)	1.607	1.607	1.615	1.614		
Δ (Å)	0.020	0.019	0.039	0.038		
Vs (Å^3)	17.396	17.378	17.661	17.610		
ECCv	0.0370	0.0358	0.0700	0.0691		
SPHv	1.0000	1.0000	1.0000	1.0000		
	Fluorcarletonite	**Carletonite**	**Fluorcarletonite**	**Carletonite**	**Fluorcarletonite**	**Carletonite**
	Na1		**Na2**		**K1**	
ECoN	5.671	5.621	5.250	5.180	8.407	8.312
Vp (Å^3)	16.826	16.945	19.115	19.152	47.655	47.013
r_v (Å)	2.335	2.341	2.445	2.445	2.993	2.979
Δ_V (Å)	0.487	0.499	0.319	0.336	0.003	0.002
r_s (Å)	2.373	2.381	2.451	2.450	3.007	2.993
Δ (Å)	0.121	0.123	0.184	0.212	0.258	0.263
Vs (Å^3)	55.955	56.543	61.645	61.638	113.899	112.315
ECCv	0.1456	0.1473	0.2088	0.2378	0.2360	0.2407
SPHv	0.8926	0.8745	0.8079	0.7914	0.8669	0.8588
	Fluorcarletonite	**Carletonite**	**Fluorcarletonite**	**Carletonite**		**Carletonite**
	Na3		**Ca1**			**K2**
ECoN	7.758	7.728	7.832	7.817		4.072
Vp (Å^3)	26.230	26.140	25.814	25.816		15.631
r_v (Å)	2.494	2.491	2.454	2.454		2.700
Δ_V (Å)	0.280	0.285	0.206	0.210		0.173
r_s (Å)	2.506	2.503	2.460	2.460		2.856
Δ (Å)	0.058	0.058	0.072	0.074		0.622
Vs (Å^3)	65.949	65.720	62.341	62.332		97.547
ECCv	0.0679	0.0678	0.0851	0.0875		0.5215
SPHv	0.9268	0.9223	0.9466	0.9437		1.0000

Table S6. Calculated distortion parameters for tetrahedra in the crystal structures of studied fluorcarletonite (Murun massif) and carletonite (Mt St Hilaire massif) samples.

parameter	Fluorcarletonite	Carletonite	Fluorcarletonite	Carletonite	Fluorcarletonite	Carletonite
	Si1		**Si2**		**K1**	
BLD (%)	0.681	0.632	1.223	1.207	5.828	6.081
ELD (%)	1.020	1.004	1.281	1.215	17.162	16.786
TAV	5.515	5.434	14.650	13.835		
TQE	1.0009	1.0013	1.0030	1.0030		
	Na1		**Na2**			**K2**
BLD (%)	3.211	3.529	5.158	5.732		13.040
ELD (%)	8.867	9.169	4.644	4.512		17.584
OAV	200.507	210.324	91.281	92.079		
OQE	1.0587	1.0623	1.0339	1.0361		
	Na3		**Ca1**			
BLD (%)	2.219	2.336	2.611	2.080		
ELD (%)	10.426	10.326	9.564	9.518		

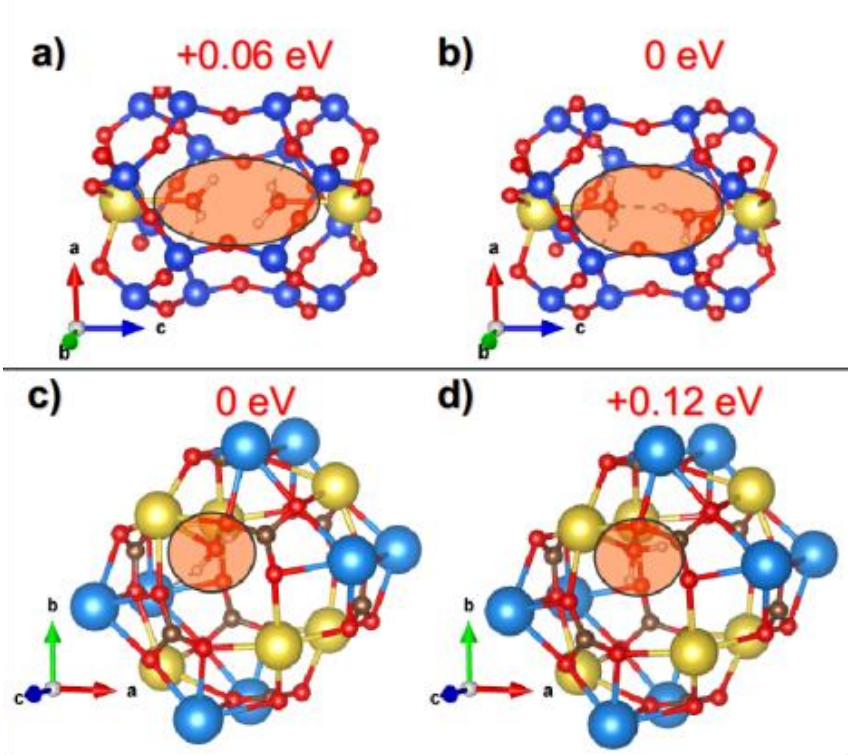

Figure S1. Calculated most stable orientations of H_2O in carletonite at O11 (a), (b) and O12 (c), (d) sites. Relative total energies are calculated for the O11 and O12 sites separately. The energies are given per 230-atomic cell.

Table S7. Crystallographic coordinates of the simulated structural model of fluorcarletonite. *The simulated crystal structure was examined in the space group P1. Position occupancies are taken as 1. Unit cell parameters are taken as: a* = 13.2256 Å, *b* = 13.2256 Å *c* = 16.7329 Å.

Site	x/a	y/b	z/c
K1	0.49908	0.00104	0.28876
K2	0.49747	0.00372	0.70867
K3	–0.00018	0.49794	0.29181
K4	–0.00579	0.49460	0.71048
Na1	0.00425	–0.00091	0.27591
Na2	0.00009	0.00299	0.72542
Na3	0.50183	0.49891	0.72313
Na4	0.50176	0.50334	0.27351
Na5	0.14177	0.64156	0.14446
Na6	0.84549	0.34547	0.85772
Na7	0.88150	0.38136	0.11355
Na8	0.14342	0.64347	0.85426
Na9	0.35170	0.15366	0.14052
Na10	0.64048	0.86054	0.85600
Na11	0.64428	0.85872	0.14366
Na12	0.37392	0.12548	0.87662
Na13	0.22300	0.27940	0.99921
Na14	0.77738	0.72482	0.00028
Na15	0.72324	0.22161	0.00104
Na16	0.27686	0.77668	0.99908
Ca1	0.06010	0.17782	0.14013
Ca2	0.94074	0.82459	0.85932
Ca3	0.94188	0.82435	0.13958
Ca4	0.06136	0.17768	0.86012
Ca5	0.82381	0.06080	0.14047
Ca6	0.17757	0.94088	0.85906
Ca7	0.17755	0.94140	0.13806
Ca8	0.82459	0.05950	0.86016
Ca9	0.44080	0.67719	0.85986
Ca10	0.56263	0.32396	0.14030
Ca11	0.55888	0.32292	0.86005
Ca12	0.44152	0.67717	0.13998
Ca13	0.67572	0.56057	0.86066
Ca14	0.32499	0.44268	0.13935
Ca15	0.32377	0.44091	0.85921
Ca16	0.67898	0.56082	0.14058
Si1	0.07498	0.26399	0.40752
Si2	0.92814	0.73355	0.59217
Si3	0.93013	0.73617	0.40769
Si4	0.07320	0.26549	0.59216
Si5	0.73837	0.07104	0.40752
Si6	0.26470	0.93086	0.59124
Si7	0.26815	0.93001	0.40615
Si8	0.73476	0.07215	0.59279
Si9	0.43007	0.76610	0.59231
Si10	0.57426	0.23549	0.40755
Si11	0.57067	0.23556	0.59292
Si12	0.43117	0.76592	0.40727

Si13	0.76336	0.57264	0.59115
Si14	0.23751	0.42887	0.40871
Si15	0.23522	0.42774	0.59347
Si16	0.76810	0.57240	0.40696
Si17	0.21848	0.12082	0.30562
Si18	0.78506	0.88087	0.69379
Si19	0.78686	0.88067	0.30563
Si20	0.21664	0.12064	0.69559
Si21	0.88353	0.21490	0.30624
Si22	0.11938	0.78651	0.69180
Si23	0.12170	0.78601	0.30604
Si24	0.88115	0.21593	0.69286
Si25	0.28620	0.61998	0.69241
Si26	0.71779	0.38136	0.30667
Si27	0.71456	0.38121	0.69315
Si28	0.28679	0.62040	0.30684
Si29	0.62010	0.71604	0.69346
Si30	0.38366	0.28663	0.30580
Si31	0.38020	0.28386	0.69601
Si32	0.62202	0.71622	0.30541
O1	0.15307	0.18245	0.37221
O2	0.85431	0.82119	0.62635
O3	0.85221	0.81732	0.37175
O4	0.14973	0.18398	0.62985
O5	0.82765	0.14458	0.37566
O6	0.17317	0.85810	0.62212
O7	0.18361	0.85474	0.37131
O8	0.82001	0.14681	0.62761
O9	0.35654	0.67663	0.62416
O10	0.64674	0.32663	0.37674
O11	0.64618	0.32051	0.62724
O12	0.35516	0.68173	0.37262
O13	0.68240	0.65141	0.62622
O14	0.32714	0.35623	0.37491
O15	0.31460	0.34964	0.63128
O16	0.68482	0.64741	0.36981
O17	0.28017	0.03234	0.35440
O18	0.72579	0.96806	0.64232
O19	0.72760	0.96852	0.35683
O20	0.27427	0.03271	0.64283
O21	0.97201	0.27457	0.35635
O22	0.03170	0.72472	0.64266
O23	0.03403	0.72818	0.35811
O24	0.96908	0.27503	0.64203
O25	0.22570	0.53250	0.64252
O26	0.77899	0.46862	0.35684
O27	0.77297	0.47035	0.64298
O28	0.22868	0.53232	0.35858
O29	0.53194	0.77725	0.64399
O30	0.47202	0.22649	0.35577
O31	0.46729	0.22577	0.64283
O32	0.53471	0.77508	0.35718

O33	0.15355	0.07841	0.23312
O34	0.85261	0.92330	0.76468
O35	0.85346	0.92301	0.23411
O36	0.14772	0.07712	0.76533
O37	0.92471	0.14745	0.23495
O38	0.07817	0.85211	0.76411
O39	0.08054	0.85134	0.23328
O40	0.92308	0.15145	0.76582
O41	0.35142	0.57917	0.76510
O42	0.64962	0.42340	0.23606
O43	0.65074	0.42255	0.76662
O44	0.35272	0.57860	0.23462
O45	0.57862	0.64873	0.76490
O46	0.42486	0.35375	0.23436
O47	0.42401	0.35221	0.76602
O48	0.57880	0.65062	0.23353
O49	0.30771	0.19774	0.27325
O50	0.69605	0.80538	0.72696
O51	0.69599	0.80687	0.27209
O52	0.30784	0.19248	0.73006
O53	0.80311	0.30081	0.27665
O54	0.19934	0.70023	0.72265
O55	0.19621	0.69484	0.27420
O56	0.80591	0.30661	0.72458
O57	0.12671	0.37626	0.40211
O58	0.87673	0.62223	0.59682
O59	0.88065	0.62294	0.40417
O60	0.12157	0.37923	0.59621
O61	0.62852	0.12594	0.39926
O62	0.37376	0.87519	0.59999
O63	0.38011	0.87827	0.40173
O64	0.62293	0.12367	0.59806
O65	0.04928	0.23676	0.49977
O66	0.95414	0.76443	0.50053
O67	0.76234	0.04611	0.50046
O68	0.24069	0.95664	0.49847
O69	0.45619	0.74069	0.50006
O70	0.54625	0.26069	0.49972
O71	0.73716	0.54668	0.49873
O72	0.26572	0.45221	0.50123
O73	0.20486	0.10637	0.06660
O74	0.78937	0.89547	0.93228
O75	0.78982	0.89535	0.06756
O76	0.20824	0.10617	0.93148
O77	0.89599	0.20866	0.06727
O78	0.10536	0.78887	0.93097
O79	0.10617	0.78878	0.06625
O80	0.89625	0.20379	0.93214
O81	0.28874	0.60639	0.93178
O82	0.70819	0.39596	0.06775
O83	0.70216	0.39572	0.93273
O84	0.28974	0.60624	0.06707

O85	0.60547	0.71191	0.93191
O86	0.39764	0.29824	0.06846
O87	0.39653	0.29373	0.93332
O88	0.60653	0.71229	0.06712
O89	0.18831	0.31570	0.13490
O90	0.81544	0.68663	0.86480
O91	0.81749	0.68614	0.13340
O92	0.18513	0.31783	0.86543
O93	0.68443	0.18363	0.13332
O94	0.31623	0.81498	0.86619
O95	0.31599	0.81589	0.13467
O96	0.68803	0.18616	0.86424
O97	0.04101	0.22131	0.99950
O98	0.95999	0.78600	0.99910
O99	0.78195	0.04096	0.00012
O100	0.21199	0.96065	–0.00091
O101	0.46020	0.71504	0.00019
O102	0.54099	0.27309	0.00080
O103	0.71466	0.54127	0.99989
O104	0.28176	0.46075	0.99929
O105	0.03171	0.35099	0.17717
O106	0.97156	0.64974	0.82217
O107	0.97296	0.65155	0.17878
O108	0.02523	0.35530	0.83372
O109	0.64911	0.02865	0.17880
O110	0.34991	0.96991	0.81981
O111	0.35967	0.97743	0.15446
O112	0.65241	0.02968	0.82121
O113	0.47190	0.85001	0.82141
O114	0.52766	0.14970	0.17573
O115	0.53141	0.15039	0.82213
O116	0.47375	0.85205	0.17353
O117	0.85536	0.52555	0.83906
O118	0.15271	0.47179	0.17867
O119	0.14871	0.47321	0.82106
O120	0.85201	0.53056	0.17807
O121	0.99221	0.01982	0.41224
O122	0.00412	0.97557	0.57761
O123	0.48541	0.51452	0.58681
O124	0.50377	0.47521	0.42181
O125	0.43298	0.06851	0.01268
O126	0.93270	0.43379	–0.02083
F1	0.00140	0.00014	0.12163
F2	0.00025	–0.00066	0.87704
F3	0.49958	0.50180	0.87810
F4	0.50227	0.50231	0.12232
C1	0.20873	0.05854	–0.00086
C2	0.78673	0.94333	0.00000
C3	0.94359	0.21132	–0.00034
C4	0.05786	0.78753	0.99882
C5	0.28638	0.55838	0.99937
C6	0.70852	0.44355	0.00008

C7	0.55806	0.71340	0.99980
C8	0.44406	0.28832	0.00078
C9	0.12299	0.38089	0.16342
C10	0.88226	0.62002	0.84194
C11	0.88230	0.62147	0.16322
C12	0.11889	0.38358	0.84004
C13	0.61918	0.11928	0.16255
C14	0.38081	0.87967	0.83604
C15	0.38461	0.88243	0.15422
C16	0.62264	0.12068	0.83599
H1	0.43400	0.56789	0.58225
H2	0.50284	0.49941	0.53036
H3	0.56292	0.42946	0.41938
H4	0.44476	0.42940	0.42282
H5	0.93766	0.07014	0.41644
H6	0.01090	0.00628	0.46858
H7	0.06146	0.92739	0.57981
H8	0.94408	0.93259	0.57022
H9	0.49463	0.10352	0.02966
H10	0.41496	0.02302	0.05781
H11	0.90425	0.48289	0.94039
H12	0.98616	0.40054	0.94763

Table S8. Crystallographic coordinates of the simulated structural model of carletonite.
The simulated crystal structure was examined in the space group P1. Position occupancies are taken as 1. Unit cell parameters are taken as: a = 13.2155 Å, b = 13.2155 Å c = 16.7067 Å.

Site	x/a	y/b	z/c
K1	0.49653	0.00066	0.29190
K2	0.49509	0.00323	0.70961
K3	0.99776	0.49737	0.29490
K4	0.99127	0.49366	0.71158
Na1	0.00220	–0.00140	0.27972
Na2	0.99774	0.00268	0.72614
Na3	0.49965	0.49818	0.72322
Na4	0.49968	0.50274	0.27695
Na5	0.13899	0.64022	0.14644
Na6	0.84418	0.34621	0.85953
Na7	0.88026	0.38165	0.11544
Na8	0.13938	0.64154	0.85604
Na9	0.35017	0.15238	0.14307
Na10	0.63739	0.86110	0.85801
Na11	0.64085	0.85927	0.14588
Na12	0.37249	0.12449	0.87867
Na13	0.22342	0.27716	0.00113
Na14	0.77208	0.72789	0.00234
Na15	0.72305	0.22324	0.00303
Na16	0.27118	0.77220	0.00094
Ca1	0.05787	0.17790	0.14292
Ca2	0.93810	0.82378	0.86008
Ca3	0.93941	0.82375	0.14247
Ca4	0.05886	0.17715	0.86181

Ca5	0.82139	0.06064	0.14328
Ca6	0.17557	0.94048	0.86021
Ca7	0.17550	0.94105	0.14111
Ca8	0.82171	0.05950	0.86164
Ca9	0.43828	0.67696	0.86070
Ca10	0.56043	0.32320	0.14269
Ca11	0.55658	0.32219	0.86178
Ca12	0.43908	0.67665	0.14311
Ca13	0.67331	0.55982	0.86232
Ca14	0.32258	0.44161	0.14149
Ca15	0.32096	0.43979	0.85984
Ca16	0.67763	0.56007	0.14395
Si1	0.07229	0.26378	0.40965
Si2	0.92652	0.73250	0.59425
Si3	0.92867	0.73501	0.40979
Si4	0.07039	0.26551	0.59429
Si5	0.73572	0.06988	0.40950
Si6	0.26298	0.93084	0.59326
Si7	0.26638	0.92995	0.40819
Si8	0.73223	0.07106	0.59484
Si9	0.42840	0.76610	0.59433
Si10	0.57168	0.23438	0.40948
Si11	0.56791	0.23468	0.59491
Si12	0.42974	0.76574	0.40926
Si13	0.76151	0.57150	0.59325
Si14	0.23499	0.42892	0.41071
Si15	0.23255	0.42781	0.59547
Si16	0.76645	0.57118	0.40912
Si17	0.21609	0.12068	0.30793
Si18	0.78299	0.88002	0.69561
Si19	0.78513	0.87971	0.30786
Si20	0.21404	0.12051	0.69753
Si21	0.88110	0.21411	0.30841
Si22	0.11754	0.78612	0.69366
Si23	0.11994	0.78560	0.30829
Si24	0.87854	0.21512	0.69488
Si25	0.28413	0.61986	0.69415
Si26	0.71557	0.38037	0.30884
Si27	0.71183	0.38035	0.69520
Si28	0.28499	0.62007	0.30895
Si29	0.61823	0.71515	0.69451
Si30	0.38124	0.28655	0.30786
Si31	0.37767	0.28343	0.69774
Si32	0.62042	0.71544	0.30772
O1	0.15062	0.18197	0.37483
O2	0.85256	0.82031	0.62820
O3	0.85067	0.81627	0.37397
O4	0.14702	0.18381	0.63169
O5	0.82487	0.14386	0.37787
O6	0.17154	0.85754	0.62380
O7	0.18159	0.85455	0.37373
O8	0.81784	0.14558	0.62951

O9	0.35420	0.67685	0.62576
O10	0.64465	0.32546	0.37907
O11	0.64317	0.32011	0.62907
O12	0.35389	0.68122	0.37469
O13	0.68043	0.65052	0.62795
O14	0.32492	0.35632	0.37711
O15	0.31198	0.34954	0.63310
O16	0.68310	0.64643	0.37221
O17	0.27868	0.03233	0.35634
O18	0.72290	0.96666	0.64406
O19	0.72498	0.96703	0.35908
O20	0.27227	0.03278	0.64489
O21	0.96919	0.27449	0.35855
O22	0.03026	0.72347	0.64463
O23	0.03273	0.72680	0.36027
O24	0.96619	0.27518	0.64424
O25	0.22281	0.53283	0.64430
O26	0.77745	0.46731	0.35899
O27	0.77122	0.46924	0.64527
O28	0.22595	0.53259	0.36076
O29	0.53033	0.77708	0.64610
O30	0.46934	0.22564	0.35764
O31	0.46419	0.22451	0.64448
O32	0.53357	0.77527	0.35940
O33	0.15085	0.07769	0.23574
O34	0.85082	0.92333	0.76609
O35	0.85203	0.92294	0.23680
O36	0.14480	0.07642	0.76692
O37	0.92301	0.14619	0.23760
O38	0.07565	0.85225	0.76550
O39	0.07815	0.85143	0.23594
O40	0.92111	0.15047	0.76757
O41	0.34998	0.57828	0.76629
O42	0.64688	0.42302	0.23869
O43	0.64777	0.42235	0.76839
O44	0.35112	0.57746	0.23706
O45	0.57617	0.64738	0.76646
O46	0.42296	0.35385	0.23663
O47	0.42233	0.35216	0.76725
O48	0.57642	0.64948	0.23626
O49	0.30465	0.19821	0.27511
O50	0.69478	0.80384	0.72939
O51	0.69504	0.80524	0.27366
O52	0.30471	0.19280	0.73240
O53	0.80027	0.29942	0.27819
O54	0.19802	0.70059	0.72526
O55	0.19526	0.69534	0.27584
O56	0.80251	0.30503	0.72697
O57	0.12426	0.37602	0.40412
O58	0.87493	0.62118	0.59887
O59	0.87908	0.62175	0.40648
O60	0.11884	0.37928	0.59822

O61	0.62565	0.12459	0.40123
O62	0.37229	0.87541	0.60186
O63	0.37834	0.87801	0.40374
O64	0.62050	0.12292	0.60016
O65	0.04605	0.23669	0.50192
O66	0.95292	0.76351	0.50262
O67	0.75987	0.04488	0.50258
O68	0.23893	0.95711	0.50049
O69	0.45498	0.74052	0.50209
O70	0.54333	0.25973	0.50164
O71	0.73529	0.54498	0.50086
O72	0.26323	0.45251	0.50326
O73	0.20634	0.10789	0.06879
O74	0.78321	0.89456	0.93426
O75	0.78349	0.89419	0.06971
O76	0.20959	0.10727	0.93351
O77	0.89225	0.21213	0.06965
O78	0.10368	0.78456	0.93278
O79	0.10450	0.78468	0.06823
O80	0.89187	0.20725	0.93435
O81	0.28234	0.60638	0.93333
O82	0.70984	0.39386	0.07012
O83	0.70382	0.39331	0.93493
O84	0.28348	0.60600	0.06881
O85	0.60409	0.71501	0.93386
O86	0.39332	0.29350	0.07033
O87	0.39288	0.28910	0.93505
O88	0.60497	0.71547	0.06926
O89	0.18481	0.31642	0.13575
O90	0.81419	0.68507	0.86920
O91	0.81702	0.68399	0.13305
O92	0.18154	0.31818	0.86858
O93	0.68063	0.18166	0.13379
O94	0.31574	0.8164	0.87112
O95	0.31472	0.81594	0.13424
O96	0.68437	0.18456	0.86725
O97	0.03786	0.21231	0.00167
O98	0.95878	0.79755	0.00098
O99	0.78785	0.04017	0.00233
O100	0.19731	0.96212	0.00126
O101	0.45932	0.70098	0.00216
O102	0.53852	0.27972	0.00279
O103	0.70184	0.53940	0.00237
O104	0.28773	0.46041	0.00072
O105	0.96871	0.64877	0.82245
O106	0.97122	0.65097	0.18208
O107	0.02174	0.35546	0.83622
O108	0.64639	0.02792	0.18256
O109	0.34796	0.96985	0.82084
O110	0.35763	0.97725	0.15632
O111	0.64958	0.02891	0.82171
O112	0.46990	0.84986	0.82225

O113	0.52459	0.14866	0.17854
O114	0.52849	0.14962	0.82278
O115	0.47110	0.85168	0.17704
O116	0.85307	0.52436	0.84092
O117	0.15027	0.47177	0.18194
O118	0.14573	0.47248	0.82134
O119	0.85051	0.52971	0.18131
O120	0.99845	0.00022	0.11499
O121	0.99822	–0.00082	0.88782
O122	0.49662	0.50051	0.88928
O123	0.50040	0.50105	0.11533
O124	0.02904	0.35109	0.18051
O125	0.989558	0.01997	0.41544
O126	0.00210	0.97438	0.57964
O127	0.48272	0.51482	0.58764
O128	0.50170	0.47396	0.42383
O129	0.43522	0.06295	0.01419
O130	0.93463	0.43747	–0.01797
C1	0.20509	0.06023	0.00127
C2	0.78427	0.94213	0.00212
C3	0.93959	0.21091	0.00190
C4	0.05662	0.78827	0.00073
C5	0.28385	0.55844	0.00096
C6	0.70564	0.44112	0.00241
C7	0.55712	0.71115	0.00181
C8	0.44042	0.28711	0.00266
C9	0.12013	0.38117	0.16591
C10	0.88013	0.61880	0.84410
C11	0.88109	0.62028	0.16528
C12	0.11560	0.38350	0.84200
C13	0.61602	0.11804	0.16492
C14	0.37935	0.88010	0.83832
C15	0.38264	0.88220	0.15589
C16	0.61951	0.11966	0.83737
H1	0.00054	–0.00042	0.05654
H2	0.99975	–0.00505	0.94620
H3	0.49173	0.50328	0.94759
H4	0.50500	0.50654	0.05712
H5	0.43120	0.56813	0.58291
H6	0.50020	0.49943	0.53111
H7	0.56088	0.42810	0.42171
H8	0.44251	0.42823	0.42484
H9	0.93487	0.07021	0.41963
H10	0.00801	0.00612	0.47191
H11	0.05984	0.92655	0.58156
H12	0.94223	0.93095	0.57248
H13	0.49544	0.09907	0.03286
H14	0.41373	0.02105	0.06066
H15	0.90311	0.48424	0.94289
H16	0.98501	0.40231	0.94850

Table S9. Selected bond distances (Å) for tetrahedra and polyhedra of the simulated structural models of fluorcarletonite and carletonite.

Fluorcarletonite		Carletonite		Fluorcarletonite		Carletonite	
Si1–O1	1.6059	Si1–O1	1.6059	Si17–O33	1.5886	Si17–O33	1.5877
Si1–O21	1.6146	Si1–O21	1.6142	Si17–O1	1.6291	Si17–O1	1.6290
Si1–O65	1.6212	Si1–O65	1.6200	Si17–O17	1.6435	Si17–O17	1.6436
Si1–O57	1.6374	Si1–O57	1.6372	Si17–O49	1.6496	Si17–O49	1.6493
<Si1–O>	1.6198	**<Si1–O>**	1.6193	**<Si17–O>**	1.6277	**<Si17–O>**	1.6274
Si2–O22	1.6134	Si2–O22	1.6133	Si18–O34	1.5876	Si18–O34	1.5867
Si2–O2	1.6199	Si2–O2	1.6198	Si18–O18	1.6389	Si18–O18	1.6380
Si2–O58	1.6235	Si2–O66	1.6228	Si18–O50	1.6403	Si18–O50	1.6404
Si2–O66	1.6238	Si2–O58	1.6232	Si18–O2	1.6538	Si18–O2	1.6542
<Si2–O>	1.6202	**<Si2–O>**	1.6198	**<Si18–O>**	1.6302	**<Si18–O>**	1.6298
Si3–O3	1.6049	Si3–O3	1.6044	Si19–O35	1.5880	Si19–O35	1.5868
Si3–O23	1.6086	Si3–O23	1.6085	Si19–O3	1.6349	Si19–O3	1.6349
Si3–O66	1.6290	Si3–O66	1.6278	Si19–O19	1.6428	Si19–O19	1.6419
Si3–O59	1.6354	Si3–O59	1.6349	Si19–O51	1.6468	Si19–O51	1.6469
<Si3–O>	1.6195	**<Si3–O>**	1.6189	**<Si19–O>**	1.6281	**<Si19–O>**	1.6276
Si4–O4	1.6075	Si4–O4	1.6067	Si20–O36	1.5887	Si20–O36	1.5875
Si4–O24	1.6150	Si4–O24	1.6152	Si20–O52	1.6402	Si20–O52	1.6394
Si4–O65	1.6231	Si4–O65	1.6218	Si20–O4	1.6417	Si20–O4	1.6414
Si4–O60	1.6361	Si4–O60	1.6356	Si20–O20	1.6470	Si20–O20	1.6462
<Si4–O>	1.6204	**<Si4–O>**	1.6198	**<Si20–O>**	1.6294	**<Si20–O>**	1.6286
Si5–O19	1.6056	Si5–O19	1.6053	Si21–O37	1.5860	Si21–O37	1.5849
Si5–O5	1.6199	Si5–O5	1.6196	Si21–O53	1.6332	Si21–O53	1.6332
Si5–O67	1.6209	Si5–O67	1.6198	Si21–O21	1.6418	Si21–O21	1.6412
Si5–O61	1.6301	Si5–O61	1.6304	Si21–O5	1.6615	Si21–O5	1.6616
<Si5–O>	1.6191	**<Si5–O>**	1.6188	**<Si21–O>**	1.6306	**<Si21–O>**	1.6302
Si6–O20	1.6050	Si6–O20	1.6043	Si22–O38	1.5854	Si22–O38	1.5845
Si6–O68	1.6207	Si6–O68	1.6199	Si22–O54	1.6392	Si22–O22	1.6391
Si6–O62	1.6261	Si6–O62	1.6261	Si22–O22	1.6397	Si22–O54	1.6393
Si6–O6	1.6305	Si6–O6	1.6307	Si22–O6	1.6619	Si22–O6	1.6620
<Si6–O>	1.6206	**<Si6–O>**	1.6203	**<Si22–O>**	1.6316	**<Si22–O>**	1.6312
Si7–O7	1.6066	Si7–O7	1.6062	Si23–O39	1.5891	Si23–O39	1.5884
Si7–O17	1.6145	Si7–O17	1.6147	Si23–O23	1.6397	Si23–O23	1.6391
Si7–O68	1.6255	Si7–O68	1.6242	Si23–O7	1.6400	Si23–O7	1.6400
Si7–O63	1.6330	Si7–O63	1.6328	Si23–O55	1.6457	Si23–O55	1.6453
<Si7–O>	1.6199	**<Si7–O>**	1.6195	**<Si23–O>**	1.6286	**<Si23–O>**	1.6282
Si8–O8	1.6081	Si8–O8	1.6079	Si24–O40	1.5891	Si24–O40	1.5879
Si8–O18	1.6111	Si8–O18	1.6109	Si24–O8	1.6375	Si24–O8	1.6373
Si8–O67	1.6245	Si8–O67	1.6230	Si24–O24	1.6392	Si24–O24	1.6394
Si8–O64	1.6309	Si8–O64	1.6303	Si24–O56	1.6462	Si24–O56	1.6458
<Si8–O>	1.6187	**<Si8–O>**	1.6180	**<Si24–O>**	1.6280	**<Si24–O>**	1.6276
Si9–O29	1.6077	Si9–O29	1.6174	Si25–O41	1.5858	Si25–O41	1.5849
Si9–O69	1.6171	Si9–O69	1.6162	Si25–O25	1.6358	Si25–O25	1.6349
Si9–O9	1.6216	Si9–O9	1.6213	Si25–O54	1.6439	Si25–O54	1.6442
Si9–O62	1.6288	Si9–O62	1.6287	Si25–O9	1.6525	Si25–O9	1.6523
<Si9–O>	1.6188	**<Si9–O>**	1.6209	**<Si25–O>**	1.6295	**<Si25–O>**	1.6291
Si10–O30	1.6104	Si10–O30	1.6101	Si26–O42	1.5868	Si26–O42	1.5860
Si10–O70	1.6207	Si10–O70	1.6196	Si26–O53	1.6311	Si26–O53	1.6308
Si10–O61	1.6227	Si10–O61	1.6226	Si26–O26	1.6407	Si26–O26	1.6404
Si10–O10	1.6240	Si10–O10	1.6238	Si26–O10	1.6678	Si26–O10	1.6678

<Si10–O>	1.6195	**<Si10–O>**	1.6190	**<Si26–O>**	1.6316	**<Si26–O>**	1.6313
Si11–O31	1.6074	Si11–O31	1.6070	Si27–O43	1.5884	Si27–O43	1.5874
Si11–O11	1.6092	Si11–O11	1.6092	Si27–O11	1.6365	Si27–O11	1.6365
Si11–O70	1.6271	Si11–O70	1.6258	Si27–O27	1.6406	Si27–O27	1.6405
Si11–O64	1.6354	Si11–O64	1.6348	Si27–O56	1.6462	Si27–O56	1.6458
<Si11–O>	1.6198	**<Si11–O>**	1.6192	**<Si27–O>**	1.6279	**<Si27–O>**	1.6276
Si12–O12	1.6083	Si12–O12	1.6081	Si28–O44	1.5895	Si28–O44	1.5885
Si12–O32	1.6100	Si12–O32	1.6102	Si28–O12	1.6392	Si28–O12	1.6396
Si12–O69	1.6222	Si12–O69	1.6210	Si28–O28	1.6423	Si28–O28	1.6415
Si12–O63	1.6348	Si12–O63	1.6344	Si28–O55	1.6440	Si28–O55	1.6436
<Si12–O>	1.6188	**<Si12–O>**	1.6184	**<Si28–O>**	1.6288	**<Si28–O>**	1.6283
Si13–O13	1.6050	Si13–O13	1.6046	Si29–O45	1.5882	Si29–O45	1.5876
Si13–O27	1.6120	Si13–O27	1.6119	Si29–O13	1.6357	Si29–O13	1.6357
Si13–O71	1.6215	Si13–O71	1.6205	Si29–O29	1.6432	Si29–O29	1.6425
Si13–O58	1.6392	Si13–O58	1.6390	Si29–O50	1.6491	Si29–O50	1.6491
<Si13–O>	1.6194	**<Si13–O>**	1.6190	**<Si29–O>**	1.6291	**<Si29–O>**	1.6287
Si14–O28	1.6090	Si14–O28	1.6087	Si30–O46	1.5856	Si30–O46	1.5814
Si14–O72	1.6222	Si14–O72	1.6208	Si30–O49	1.6394	Si30–O49	1.6390
Si14–O57	1.6259	Si14–O57	1.6255	Si30–O30	1.6424	Si30–O30	1.6418
Si14–O14	1.6273	Si14–O14	1.6273	Si30–O14	1.6563	Si30–O14	1.6562
<Si14–O>	1.6211	**<Si14–O>**	1.6206	**<Si30–O>**	1.6309	**<Si30–O>**	1.6296
Si15–O15	1.6029	Si15–O15	1.6023	Si31–O47	1.5891	Si31–O47	1.5880
Si15–O25	1.6153	Si15–O25	1.6150	Si31–O15	1.6379	Si31–O15	1.6380
Si15–O72	1.6277	Si15–O72	1.6262	Si31–O52	1.6436	Si31–O52	1.6429
Si15–O60	1.6349	Si15–O60	1.6345	Si31–O31	1.6457	Si31–O31	1.6449
<Si15–O>	1.6202	**<Si15–O>**	1.6195	**<Si31–O>**	1.6291	**<Si31–O>**	1.6285
Si16–O16	1.6073	Si16–O16	1.6070	Si32–O48	1.5893	Si32–O48	1.5885
Si16–O26	1.6150	Si16–O26	1.6146	Si32–O16	1.6369	Si32–O16	1.6367
Si16–O71	1.6253	Si16–O71	1.6243	Si32–O32	1.6400	Si32–O32	1.6396
Si16–O59	1.6324	Si16–O59	1.6321	Si32–O51	1.6448	Si32–O51	1.6445
<Si16–O>	1.6200	**<Si16–O>**	1.6195	**<Si32–O>**	1.6278	**<Si32–O>**	1.6273
K1–O109	2.7306	K1–O108	2.7182	K3–O120	2.7623	K3–O124	2.7495
K1–O114	2.7542	K1–O113	2.7477	K3–O105	2.7631	K3–O119	2.7515
K1–O116	2.7772	K1–O115	2.7698	K3–O118	2.7914	K3–O117	2.7817
K1–O111	2.9235	K1–O63	2.9255	K3–O107	2.7985	K3–O106	2.7921
K1–O63	2.9471	K1–O110	2.9319	K3–O59	2.9584	K3–O59	2.9390
K1–O61	3.0131	K1–O61	2.9884	K3–O57	2.9685	K3–O57	2.9489
K1–O17	3.1240	K1–O17	3.1021	K3–O26	3.1408	K3–O26	3.1274
K1–O30	3.2055	K1–O15	3.1432	K3–O21	3.1667	K3–O21	3.1542
K1–O32	3.2349	K1–O30	3.1899	K3–O28	3.2582	K3–O28	3.2437
K1–O19	3.2583	K1–O32	3.2224	K3–O23	3.2723	K3–O23	3.2558
<K1–O>	2.9968	**<K1–O>**	2.9739	**<K3–O>**	2.9880	**<K3–O>**	2.9744
K2–O110	2.7325	K2–O109	2.7255	K4–O119	2.7710	K4–O118	2.7582
K2–O115	2.7511	K2–O114	2.7409	K4–O106	2.7915	K4–O105	2.7788
K2–O113	2.7938	K2–O112	2.7857	K4–O108	2.7955	K4–O107	2.7989
K2–O112	2.8042	K2–O111	2.7913	K4–O117	2.8582	K4–O116	2.8583
K2–O64	2.9489	K2–O64	2.9313	K4–O60	2.9701	K4–O60	2.9518
K2–O62	2.9788	K2–O62	2.9542	K4–O58	2.9800	K4–O58	2.9580
K2–O31	3.1620	K2–O31	3.1468	K4–O24	3.1394	K4–O24	3.1164
K2–O20	3.1741	K2–O20	3.1611	K4–O27	3.1529	K4–O27	3.1286
K2–O29	3.2172	K2–O29	3.2055	K4–O22	3.2858	K4–O22	3.2772
K2–O18	3.2518	K2–O18	3.2399	K4–O25	3.3042	K4–O25	3.3007
<K2–O>	2.9814	**<K2–O>**	2.9682	**<K4–O>**	3.0049	**<K4–O>**	2.9927
Na1–O121	2.3031	Na1–O125	2.2910	Na9–O86	2.3408	Na9–O86	2.2978

Na1–O39	2.3120	Na1–O39	2.3077
Na1–O37	2.3294	Na1–O37	2.3226
Na1–O35	2.3407	Na1–O35	2.3350
Na1–O33	2.3477	Na1–O33	2.3435
Na1–F1	2.5818	Na1–O120	2.7527
<Na1–O,F>	2.3691	**<Na1–O>**	2.3921
Na2–O36	2.2847	Na2–O36	2.2783
Na2–O34	2.3123	Na2–O34	2.3055
Na2–O40	2.3130	Na2–O40	2.3063
Na2–O38	2.3382	Na2–O38	2.3335
Na2–O122	2.5002	Na2–O126	2.4766
Na2–F2	2.5375	Na2–O121	2.7016
<Na2–O,F>	2.3810	**<Na2–O>**	2.4003
Na3–O123	2.3006	Na3–O127	2.2867
Na3–O47	2.3106	Na3–O47	2.3041
Na3–O43	2.3299	Na3–O43	2.3250
Na3–O45	2.3337	Na3–O45	2.3307
Na3–O41	2.3615	Na3–O41	2.3559
Na3–F3	2.5935	Na3–O122	2.7748
<Na3–O,F>	2.3716	**<Na3–O>**	2.3962
Na4–O48	2.2979	Na4–O48	2.2915
Na4–O44	2.3020	Na4–O44	2.2965
Na4–O42	2.3097	Na4–O42	2.3028
Na4–O46	2.3189	Na4–O46	2.3137
Na4–O124	2.5093	Na4–O128	2.4834
Na4–F4	2.5299	Na4–O123	2.7003
<Na4–O,F>	2.3780	**<Na4–O>**	2.3980
Na5–O107	2.3091	Na5–O106	2.3001
Na5–O118	2.3216	Na5–O117	2.3086
Na5–O84	2.3926	Na5–O84	2.3522
Na5–O79	2.3928	Na5–O79	2.3579
Na5–O55	2.3934	Na5–O55	2.3996
<Na5–O>	2.3619	**<Na5–O>**	2.3437
Na6–O56	2.3453	Na6–O80	2.3092
Na6–O80	2.3479	Na6–O83	2.3271
Na6–O83	2.3687	Na6–O56	2.3461
Na6–O117	2.4056	Na6–O116	2.3776
Na6–O108	2.4144	Na6–O107	2.3818
Na6–O126	2.6124	Na6–O130	2.6593
<Na6–O>	2.4157	**<Na6–O>**	2.4002
Na7–O120	2.2827	Na7–O119	2.2790
Na7–O105	2.2894	Na7–O124	2.2827
Na7–O77	2.4194	Na7–O77	2.3727
Na7–O82	2.4246	Na7–O82	2.3816
Na7–O126	2.4486	Na7–O130	2.4553
<Na7–O>	2.3729	**<Na7–O>**	2.3543
Na8–O119	2.3204	Na8–O118	2.3097
Na8–O106	2.3370	Na8–O105	2.3263
Na8–O78	2.3662	Na8–O78	2.3321
Na8–O81	2.3700	Na8–O81	2.3351
Na8–O54	2.4414	Na8–O54	2.4462
<Na8–O>	2.3670	**<Na8–O>**	2.3499

Na9–O111	2.3448	Na9–O110	2.3270
Na9–O49	2.3686	Na9–O73	2.3450
Na9–O73	2.3859	Na9–O49	2.3654
Na9–O114	2.4012	Na9–O113	2.3693
Na9–O125	2.6458	Na9–O129	2.3805
<Na9–O>	2.4145	**<Na9–O>**	2.3475
Na10–O113	2.3077	Na10–O112	2.2974
Na10–O112	2.3169	Na10–O111	2.3048
Na10–O85	2.3858	Na10–O85	2.3508
Na10–O74	2.3917	Na10–O74	2.3520
Na10–O50	2.3947	Na10–O50	2.4011
<Na10–O>	2.3594	**<Na10–O>**	2.3412
Na11–O116	2.3117	Na11–O115	2.3052
Na11–O109	2.3240	Na11–O108	2.3126
Na11–O51	2.3571	Na11–O75	2.3207
Na11–O75	2.3584	Na11–O88	2.3397
Na11–O88	2.3748	Na11–O51	2.3622
<Na11–O>	2.3452	**<Na11–O>**	2.3281
Na12–O110	2.2885	Na12–O109	2.2837
Na12–O115	2.2973	Na12–O114	2.2874
Na12–O76	2.3895	Na12–O76	2.3506
Na12–O87	2.4374	Na12–O87	2.3858
Na12–O125	2.5221	Na12–O129	2.5445
Na12–O52	2.7501	Na12–O52	2.7549
<Na12–O>	2.4475	**<Na12–O>**	2.4345
Na13–O92	2.3496	Na13–O92	2.3462
Na13–O89	2.3656	Na13–O89	2.3639
Na13–O104	2.5212	Na13–O87	2.5018
Na13–O97	2.5266	Na13–O73	2.5166
Na13–O87	2.5532	Na13–O76	2.5200
Na13–O73	2.5624	Na13–O86	2.5348
Na13–O76	2.5636	Na13–O104	2.5665
Na13–O86	2.5961	Na13–O97	2.5977
<Na13–O>	2.5048	**<Na13–O>**	2.4934
Na14–O91	2.3461	Na14–O91	2.3363
Na14–O90	2.3765	Na14–O90	2.3618
Na14–O75	2.5261	Na14–O75	2.4737
Na14–O88	2.5267	Na14–O88	2.4808
Na14–O74	2.5325	Na14–O74	2.4833
Na14–O98	2.5472	Na14–O85	2.5034
Na14–O85	2.5510	Na14–O98	2.6335
Na14–O103	2.5655	Na14–O103	2.6584
<Na14–O>	2.4965	**<Na14–O>**	2.4914
Na15–O93	2.3270	Na15–O93	2.3213
Na15–O96	2.3825	Na15–O96	2.3809
Na15–O102	2.5046	Na15–O77	2.5020
Na15–O99	2.5123	Na15–O80	2.5177
Na15–O77	2.5452	Na15–O82	2.5241
Na15–O82	2.5696	Na15–O83	2.5319
Na15–O80	2.5730	Na15–O102	2.5503
Na15–O83	2.5857	Na15–O99	2.5666
<Na15–O>	2.5000	**<Na15–O>**	2.4869
Na16–O94	2.3393	Na16–O94	2.3221
Na16–O95	2.3842	Na16–O95	2.3716
Na16–O81	2.5229	Na16–O81	2.4698
Na16–O79	2.5269	Na16–O84	2.4771

				Na16–O84	2.5307	Na16–O79	2.4785
				Na16–O78	2.5436	Na16–O78	2.4947
				Na16–O101	2.5581	Na16–O101	2.6586
				Na16–O100	2.5799	Na16–O100	2.6930
				<Na16–O>	2.4982	**<Na16–O>**	2.4957
Ca1–O33	2.3828	Ca1–O33	2.3809	Ca9–O41	2.3648	Ca9–O41	2.3558
Ca1–O105	2.4021	Ca1–O124	2.4038	Ca9–O113	2.4099	Ca9–O101	2.4007
Ca1–O37	2.4259	Ca1–O97	2.4177	Ca9–O101	2.4144	Ca9–O112	2.4101
Ca1–O97	2.4354	Ca1–O37	2.4195	Ca9–O45	2.4472	Ca9–O45	2.4397
Ca1–O73	2.4643	Ca1–O89	2.4859	Ca9–O94	2.4590	Ca9–O94	2.4594
Ca1–O89	2.4916	Ca1–O73	2.4979	Ca9–F3	2.4654	Ca9–O122	2.5020
Ca1–F1	2.4942	Ca1–O120	2.5195	Ca9–O81	2.5237	Ca9–O85	2.5590
Ca1–O77	2.5225	Ca1–O77	2.5482	Ca9–O85	2.5312	Ca9–O81	2.5669
<Ca1–O,F>	2.4524	**<Ca1–O>**	2.4592	**<Ca9–O,F>**	2.4520	**<Ca9–O>**	2.4617
Ca2–O34	2.3601	Ca2–O34	2.3510	Ca10–O42	2.3708	Ca10–O42	2.3702
Ca2–O98	2.4074	Ca2–O98	2.3949	Ca10–O114	2.4243	Ca10–O102	2.4242
Ca2–O106	2.4290	Ca2–O105	2.4307	Ca10–O46	2.4398	Ca10–O113	2.4297
Ca2–O38	2.4442	Ca2–O38	2.4378	Ca10–O102	2.4461	Ca10–O46	2.4346
Ca2–F2	2.4594	Ca2–O90	2.4627	Ca10–O93	2.4602	Ca10–O93	2.4585
Ca2–O90	2.4665	Ca2–O121	2.4939	Ca10–O82	2.4670	Ca10–O82	2.4982
Ca2–O74	2.5252	Ca2–O78	2.5557	Ca10–F4	2.5083	Ca10–O123	2.5225
Ca2–O78	2.5300	Ca2–O74	2.5691	Ca10–O86	2.5145	Ca10–O86	2.5480
<Ca2–O,F>	2.4527	**<Ca2–O>**	2.4620	**<Ca10–O,F>**	2.4539	**<Ca10–O>**	2.4607
Ca3–O35	2.3605	Ca3–O35	2.3527	Ca11–O43	2.3783	Ca11–O43	2.3746
Ca3–O107	2.4128	Ca3–O98	2.4028	Ca11–O115	2.3960	Ca11–O114	2.4007
Ca3–O98	2.4168	Ca3–O106	2.4142	Ca11–O47	2.4099	Ca11–O47	2.4080
Ca3–O39	2.4389	Ca3–O39	2.4360	Ca11–O83	2.4488	Ca11–O102	2.4335
Ca3–O91	2.4614	Ca3–O91	2.4602	Ca11–O102	2.4570	Ca11–O83	2.4826
Ca3–F1	2.4729	Ca3–O120	2.5017	Ca11–O96	2.4887	Ca11–O96	2.4837
Ca3–O75	2.5256	Ca3–O79	2.5622	Ca11–O87	2.5025	Ca11–O87	2.5238
Ca3–O79	2.5393	Ca3–O75	2.5671	Ca11–F3	2.5106	Ca11–O122	2.5283
<Ca3–O,F>	2.4535	**<Ca3–O>**	2.4621	**<Ca11–O,F>**	2.4490	**<Ca11–O>**	2.4544
Ca4–O36	2.3641	Ca4–O36	2.3611	Ca12–O44	2.3636	Ca12–O44	2.3522
Ca4–O97	2.4176	Ca4–O97	2.3985	Ca12–O101	2.4048	Ca12–O101	2.3917
Ca4–O108	2.4376	Ca4–O40	2.4324	Ca12–O116	2.4178	Ca12–O48	2.4177
Ca4–O40	2.4402	Ca4–O107	2.4448	Ca12–O48	2.4230	Ca12–O115	2.4189
Ca4–O76	2.4686	Ca4–O92	2.4728	Ca12–F4	2.4661	Ca12–O95	2.4722
Ca4–O92	2.4745	Ca4–O76	2.5011	Ca12–O95	2.4759	Ca12–O123	2.5014
Ca4–F2	2.5093	Ca4–O121	2.5224	Ca12–O84	2.5293	Ca12–O88	2.5675
Ca4–O80	2.5179	Ca4–O80	2.5491	Ca12–O88	2.5425	Ca12–O84	2.5770
<Ca4–O,F>	2.4537	**<Ca4–O>**	2.4603	**<Ca12–O,F>**	2.4529	**<Ca12–O>**	2.4623
Ca5–O37	2.3651	Ca5–O37	2.3591	Ca13–O45	2.3614	Ca13–O45	2.3562
Ca5–O99	2.4271	Ca5–O99	2.4114	Ca13–O103	2.3995	Ca13–O103	2.3853
Ca5–O35	2.4351	Ca5–O35	2.4324	Ca13–O43	2.4326	Ca13–O43	2.4243
Ca5–O109	2.4352	Ca5–O108	2.4426	Ca13–O117	2.4474	Ca13–O116	2.4476
Ca5–O93	2.4600	Ca5–O93	2.4583	Ca13–F3	2.4731	Ca13–O90	2.4938
Ca5–O77	2.4971	Ca5–O120	2.5172	Ca13–O90	2.4898	Ca13–O122	2.5039
Ca5–F1	2.5019	Ca5–O77	2.5295	Ca13–O85	2.5080	Ca13–O85	2.5439
Ca5–O75	2.5452	Ca5–O75	2.5690	Ca13–O83	2.5160	Ca13–O83	2.5449
<Ca5–O,F>	2.4583	**<Ca5–O>**	2.4654	**<Ca13–O,F>**	2.4535	**<Ca13–O>**	2.4625
Ca6–O38	2.3730	Ca6–O38	2.3679	Ca14–O46	2.3781	Ca14–O46	2.3731
Ca6–O100	2.4011	Ca6–O100	2.3911	Ca14–O118	2.4027	Ca14–O117	2.4085
Ca6–O110	2.4029	Ca6–O109	2.4028	Ca14–O104	2.4241	Ca14–O104	2.4094
Ca6–O36	2.4212	Ca6–O36	2.4129	Ca14–O44	2.4306	Ca14–O44	2.4320
Ca6–O94	2.4799	Ca6–O94	2.4806	Ca14–O86	2.4452	Ca14–O89	2.4621
Ca6–F2	2.4875	Ca6–O121	2.5116	Ca14–O89	2.4686	Ca14–O86	2.4736
Ca6–O78	2.5301	Ca6–O76	2.5613	Ca14–F4	2.4900	Ca14–O123	2.5161

Ca6–O76	2.5321	Ca6–O78	2.5726	Ca14–O84	2.5218	Ca14–O84	2.5418
<Ca6–O,F>	2.4535	**<Ca6–O>**	2.4626	**<Ca14–O,F>**	2.4451	**<Ca14–O>**	2.4521
Ca7–O39	2.3671	Ca7–O39	2.3596	Ca15–O47	2.3591	Ca15–O47	2.3513
Ca7–O100	2.3833	Ca7–O100	2.3706	Ca15–O104	2.4231	Ca15–O104	2.4097
Ca7–O33	2.4320	Ca7–O33	2.4221	Ca15–O119	2.4394	Ca15–O41	2.4371
Ca7–O111	2.4706	Ca7–O110	2.4672	Ca15–O41	2.4407	Ca15–O118	2.4419
Ca7–F1	2.4712	Ca7–O95	2.4763	Ca15–O92	2.4541	Ca15–O92	2.4493
Ca7–O95	2.4720	Ca7–O120	2.5053	Ca15–F3	2.4809	Ca15–O122	2.5051
Ca7–O73	2.5142	Ca7–O73	2.5470	Ca15–O87	2.5006	Ca15–O87	2.5393
Ca7–O79	2.5317	Ca7–O79	2.5754	Ca15–O81	2.5453	Ca15–O81	2.5720
<Ca7–O,F>	2.4553	**<Ca7–O>**	2.4654	**<Ca15–O,F>**	2.4554	**<Ca15–O>**	2.4632
Ca8–O40	2.3806	Ca8–O40	2.3750	Ca16–O48	2.3633	Ca16–O48	2.3588
Ca8–O112	2.4012	Ca8–O111	2.4048	Ca16–O120	2.4063	Ca16–O119	2.4021
Ca8–O99	2.4213	Ca8–O99	2.4062	Ca16–O103	2.4148	Ca16–O103	2.4024
Ca8–O34	2.4360	Ca8–O34	2.4361	Ca16–O42	2.4508	Ca16–O42	2.4394
Ca8–O80	2.4475	Ca8–O96	2.4567	Ca16–O91	2.4733	Ca16–O91	2.4715
Ca8–O96	2.4643	Ca8–O80	2.4795	Ca16–F4	2.4808	Ca16–O123	2.5145
Ca8–F2	2.4719	Ca8–O121	2.5035	Ca16–O82	2.5275	Ca16–O82	2.5548
Ca8–O74	2.5258	Ca8–O74	2.5460	Ca16–O88	2.5381	Ca16–O88	2.5879
<Ca8–O,F>	2.4436	**<Ca8–O>**	2.4510	**<Ca16–O,F>**	2.4569	**<Ca16–O>**	2.4664
C1–O73	1.2949	C1–O73	1.2921	C9–O118	1.2903	C9–O117	1.2900
C1–O100	1.2954	C1–O76	1.2928	C9–O105	1.2909	C9–O124	1.2909
C1–O76	1.2955	C1–O100	1.3007	C9–O89	1.3106	C9–O89	1.3102
<C1–O>	1.2953	**<C1–O>**	1.2952	**<C9–O>**	1.2973	**<C9–O>**	1.2970
C2–O99	1.2927	C2–O75	1.2949	C10–O106	1.2879	C10–O105	1.2877
C2–O75	1.2970	C2–O74	1.2964	C10–O117	1.3000	C10–O116	1.2994
C2–O74	1.2985	C2–O99	1.2964	C10–O90	1.3052	C10–O90	1.3046
<C2–O>	1.2961	**<C2–O>**	1.2959	**<C10–O>**	1.2977	**<C10–O>**	1.2972
C3–O77	1.2952	C3–O77	1.2933	C11–O107	1.2898	C11–O106	1.2892
C3–O97	1.2952	C3–O80	1.2936	C11–O120	1.2915	C11–O119	1.2914
C3–O80	1.2956	C3–O97	1.2989	C11–O91	1.3097	C11–O91	1.3098
<C3–O>	1.2953	**<C3–O>**	1.2953	**<C11–O>**	1.2970	**<C11–O>**	1.2968
C4–O98	1.2945	C4–O79	1.2941	C12–O119	1.2890	C12–O118	1.2886
C4–O79	1.2966	C4–O78	1.2955	C12–O108	1.2982	C12–O107	1.2982
C4–O78	1.2977	C4–O98	1.2988	C12–O92	1.3055	C12–O92	1.3045
<C4–O>	1.2963	**<C4–O>**	1.2961	**<C12–O>**	1.2976	**<C12–O>**	1.2971
C5–O104	1.2927	C5–O81	1.2955	C13–O109	1.2913	C13–O108	1.2910
C5–O81	1.2975	C5–O84	1.2962	C13–O114	1.2944	C13–O113	1.2943
C5–O84	1.2984	C5–O104	1.2965	C13–O93	1.3070	C13–O93	1.3063
<C5–O>	1.2962	**<C5–O>**	1.2961	**<C13–O>**	1.2976	**<C13–O>**	1.2972
C6–O103	1.2949	C6–O83	1.2925	C14–O113	1.2903	C14–O112	1.2899
C6–O83	1.2950	C6–O82	1.2935	C14–O110	1.2905	C14–O109	1.2901
C6–O82	1.2956	C6–O103	1.2998	C14–O94	1.3099	C14–O94	1.3098
<C6–O>	1.2952	**<C6–O>**	1.2953	**<C14–O>**	1.2969	**<C14–O>**	1.2966
C7–O101	1.2945	C7–O88	1.2935	C15–O116	1.2868	C15–O115	1.2862
C7–O88	1.2961	C7–O85	1.2949	C15–O111	1.2990	C15–O110	1.2990
C7–O85	1.2978	C7–O101	1.2995	C15–O95	1.3057	C15–O95	1.3051
<C7–O>	1.2961	**<C7–O>**	1.2960	**<C15–O>**	1.2972	**<C15–O>**	1.2968
C8–O87	1.2941	C8–O87	1.2929	C16–O115	1.2901	C16–O114	1.2897
C8–O86	1.2948	C8–O86	1.2933	C16–O112	1.2901	C16–O111	1.2902
C8–O102	1.2977	C8–O102	1.3002	C16–O96	1.3119	C16–O96	1.3113
<C8–O>	1.2955	**<C8–O>**	1.2955	**<C16–O>**	1.2974	**<C16–O>**	1.2971

References

1. R. Hoppe, S. Voigt, H. Glaum, J. Kissel, H. P. Müller and K. Bernet, *J. Less-Common. Met.*, 1989, 156, 105–122.
2. M. Nespolo, G. Ferraris and H. Ohashi, *Acta Crystallogr*., 1999, B55, 902–916.
3. K. Momma and F. Izumi, *J. Appl. Crystallogr.*, 2011, 44, 1272–1276.
4. T. Balić-Žunić, and E. Makovicky, *Acta Crystallogr*., 1996, B52, 78–81.
5. T. Balić-Žunić and I. Vicković, *J. Appl. Cryst.*, 1996, 29, 305–306.