Supplementary data

Slyudyankaite, $Na_{28}Ca_4(Si_{24}Al_{24}O_{96})(SO_4)_6(S_6)_{1/3}(CO_2)\cdot 2H_2O$, a new sodalite-group mineral from the Malo-Bystrinskoe lazurite deposit, Baikal Lake area

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Historical background

Lazurite, along with other blue-, green- and violet-coloured sodalite-group minerals, is one of the main components of the lapis lazuli rock which is a valuable and beautiful ornamental gemstone known from prehistoric times. Currently, this stone, especially its blue varieties, is in unremitting demand on the world market.

Industrial deposits of lapis lazuli are not numerous and are situated on the territory of Afghanistan, Tajikistan, Russian Federation and Chile. All Russian deposits (Malo-Bystrinskoe, Slyudyanskoe, Tultuiskoe, Talinskoe, and Pokhabinskoe) belong to the Baikal Lake area. The most significant Malo-Bystrinskoe deposit is named after the Malaya Bystraya river which is the right tributary of Irkut River.

The first mention of the discovery of lapis lazuli in the alluvium of the Slyudyanka River was made by Academician E.G. Laksman in 1784. Three years later, a special expedition was sent to the Baikal Lake region, which collected 20 poods of low quality lapis lazuli in the form of boulders from river alluvium.

Further successes with the search for lapis lazuli in the Baikal Lake region are associated with the name of G.M. Permikin. In 1851, he sent 17 poods of good quality lapis lazuli collected from the banks of the rivers of the Lake Baikal basin to the Peterhof lapidary factory situated near St. Petersburg. In 1859 G.M. Permikin discovered the most significant primary Malo-Bystrinskoye deposit, which was operated with some interruptions until 1865 and gave about 25 tons of high-quality lapis lazuli. In addition to the extraction of lapis lazuli, he carried out significant volumes of exploration work at the Malo-Bystrinskoye deposit: the total volume of the mine and numerous pits was about 27,000 m^3.

After 1865, until the 30s of the XX century, mining operations were not carried out at the deposit. Regular work on the study and mining of lapis lazuli at the Malo-Bystrinskoye deposit was carried out intermittently in the 60-70s of the last century. The reserves of lazurite raw materials at the deposit were estimated at 13,300 tons (including 585 tons of ornamental quality material).

Subsequently, under the leadership of A.I. Zuev, prospecting work was carried out for lapis lazuli at the Slyudyanskoye deposit (in 1978 – 1979), at the Tultuiskoe deposit (in 1979-1980) and at the Chernushka occurrence (in 1983 – 1984). However, the reserves of lapis lazuli at these localities turned out to be insignificant. But the Malo-Bystrinskoye deposit was also mothballed in 1996 due to economic problems. This deposit is currently not being developed (Ivanov and Sapozhnikov 1985; http://lavrovit.ru/?page_id=551).

Work on the mineralogical and petrological study of lapis lazuli from the Baikal Lake region was resumed in 1922. It was supposed that lazurite crystallized as a result of metasomatic processes involving dolomite marbles and volatile components of hot pegmatites (Korzhinsky 1947). Based on optical data, it has been shown that there are isotropic and anisotropic (presumably orthorhombic) mineral related to lazurite (Voskoboinikova 1938). At the Malo-Bystrinskoe and Tultuiskoe deposits, anisotropic lazurite-related mineral associates with common isotropic lazurite.

Since 1972, investigations of lazurite occurrences were carried out with the participation of researchers from the Institute of Geochemistry, Siberian Branch of the Academy of Sciences of the USSR. A significant contribution to these investigations was made by Vladimir Georgievich Ivanov (1948 – 2002). He was assigned to work in the Institute on leaving Leningrad State University, after defense of the PhD thesis «Petrology, mineralogy and geochemistry of lazurite deposits of the Southern Baikal Lake region» based on investigations carried out under the guidance of Academician D.S. Korzhinsky.

Data on the geological structure, petrology, mineralogy and geochemistry for gem lazurite deposits of Russian Federation and Tajikistan obtained with active participation of V.G. Ivanov were summarized in the book by Ivanov and Sapozhnikov (1985). That time it was already obvious that the term “lazurite” used in numerous publications is actually related to a family of several mineral species and/or varieties which differ in chemical composition (including the contents of sulfide and sulfate sulfur), symmetry, character of structure modulation, optical properties, and color (deep blue, pale blue, green, violet, or lilac). In particular, “triclinic lazurite”, “monoclinic lazurite”, and “lazurite with cubic superstructure” have been characterized in the above-cited book.

Single-crystal X-ray diffraction (XRD) study of different lazurite-related minerals was carried out (Sapozhnikov 1990, 1992; Kaneva et al. 2010). The single-crystal XRD pattern of “orthorhombic lazurite” corresponds to the space group *Pnaa* and unit-cell parameters a = 9.066, b = 12.851, and c = 36.549 Å. The refined unit-cell parameters of the monoclinic (pseudo-orthorhombic, space group $P2_1/b$) mineral are: a = 36.36, $b = c$ = 51.40 Å, $\alpha = \beta = \gamma$ = 90º. The triclinic (pseudo-orthorhombic, space group $P1$ or $P\bar{1}$) lazurite-related mineral was characterized by the unit-cell parameters a = 9.091, b = 12.857, c = 25.719 Å, $\alpha = \beta = \gamma$ = 90º. Satellite reflections in the X-ray diffraction (XRD) patterns which are typical for these minerals have been explained by commensurate and incommensurate modulation of their crystal structures. The formation of superstructures may be caused by different laws of alternation of

extra-framework components in sodalite cages. In particular, this can result in modulation of the displacement of AlO_4 and SiO_4 tetrahedra from their positions in the cubic sub-cell with the parameter of $a \sim 9.07$ Å (Evsyunin et al. 1997, 1998). The structure modulation may arise as a result of lazurite recrystallization.

The orthorhombic lazurite-related mineral has been approved by the IMA Commission on New Minerals and Mineral Names as a new mineral species vladimirivanovite $Na_6Ca_2[Al_6Si_6O_{24}](SO_4,S_3,S_2,Cl)_2 \cdot H_2O$ (Sapozhnikov et al. 2012). The mineral was named after Vladimir G. Ivanov. Recently, lazurite *s.s.* has been approved as a cubic sodalite-group mineral with the idealized formula $Na_7Ca(Al_6Si_6O_{24})(SO_4)S_3^{\bullet-} \cdot H_2O$ where $S_3^{\bullet-}$ is trisulfide radical anion (Sapozhnikov et al. 2021b). The status of "triclinic lazurite" remained unknown for a long time. The investigation of the crystal structure of this mineral carried out in 2021 has confirmed its triclinic symmetry and "triclinic lazurite" got the status of a valid mineral species (with the name slyudyankaite) containing S_6 and CO_2 molecules as the species-defining components. Another lazurite-related mineral, "monoclinic lazurite" is still insufficiently studied.

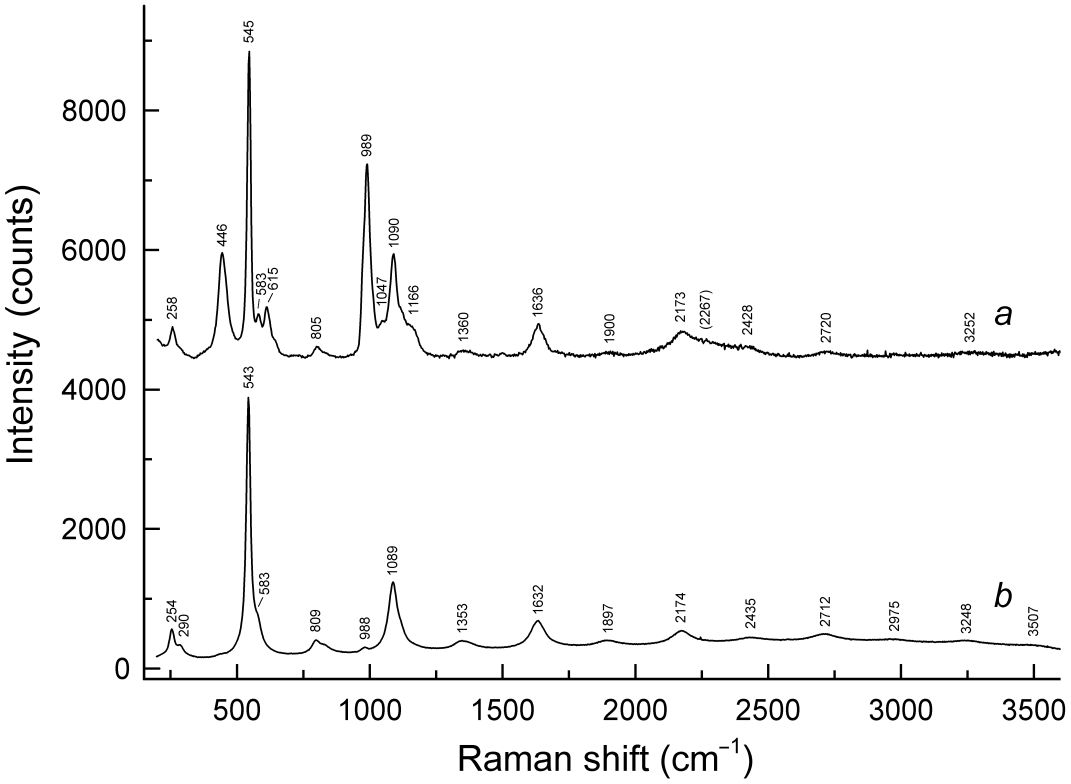

FIGURE S1. Raman spectra of (*a*) blue haüyne $(Na_{5.52}K_{0.35}Ca_{1.99})(Si_{6.10}Al_{5.81}Fe^{3+}_{0.09}O_{24})(SO_4)_{1.97}Cl_{0.11} \cdot nH_2O$ with trace amounts of the $S_3^{\bullet-}$ chromophore from the Laach Lake volcano, Eifel paleovolcanic region, Germany, and (*b*) lilac

sulfide-bearing haüyne $(Na_{6.45}Ca_{1.36}K_{0.01})(Al_{5.9}S4i_{6.06}O_{24})(SO_4)_{1.56}(S_4)_{0.09}(S_3^{\bullet-})_{0.035}Cl_{0.09}\cdot nH_2O$ containing both red (S_4) and blue ($S_3^{\bullet-}$) chromophores from the Malo-Bystrinskoe deposit, Baikal Lake area (Chukanov et al. 2020b).

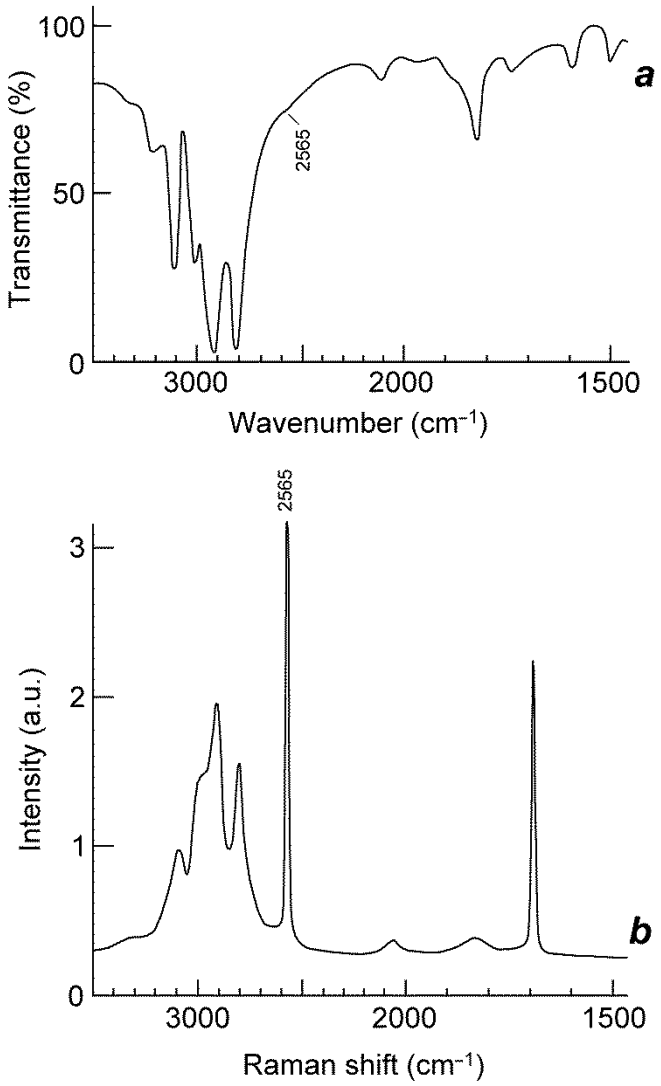

FIGURE S2. Infrared (***a***) and Raman (***b***) spectra of polycrystalline ammonium hydrosulfide $(NH_4)(HS)$ drawn using data from Bragin et al. (1977). The band at 2565 cm^{-1} corresponds to stretching vibrations of the HS^- anion.

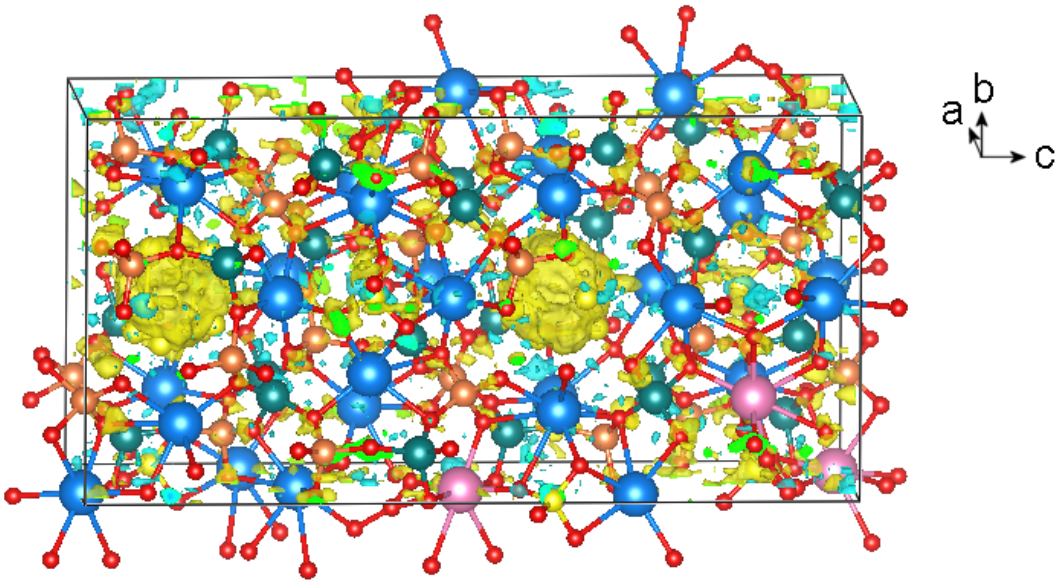

FIGURE S3. Residual electron density distribution in slyudyankaite (3D visualization of the difference Fourier synthesis); $\Delta\rho(\text{min}) / \Delta\rho(\text{max}) = -1.69 / 2.38$ e Å^{-3}. Balls represent atoms from the structure model. See the text for further explanation.

According to the spectroscopic data presented above, slyudyankaite contains impurities of chromophores S_4 (centers of red and lilac color), $S_3^{\bullet-}$ (centers of blue color), and S_6 (centers of yellow color). The search for S-bearing species other than S_6 was carried out as follows. The Fourier program lists the coordinates of the residual peaks, in descending order of magnitude. Each peak from the list was compared with its image in the Fourier map and carefully analyzed for distances to other peaks and angles between the resulting peak-to-peak segments. The coordinates of the peaks were taken from this list and were not further refined due to the disorder of the impurity components and low populations of corresponding sites. Some groups of residual peaks of electron density correspond to the $S_3^{\bullet-}$ radical anion and S_4 molecule having *cis*-conformation (Figs. S4 and S5). *Trans*-S_4 molecules were not identified, but it is to be noted that their configuration, bond lengths and covalent bond angles are close to those in the S_6 molecule having chair-like conformation. Consequently, overlapping of electron density belonging to the *trans*-S_4 and S_6 molecules is not excluded.

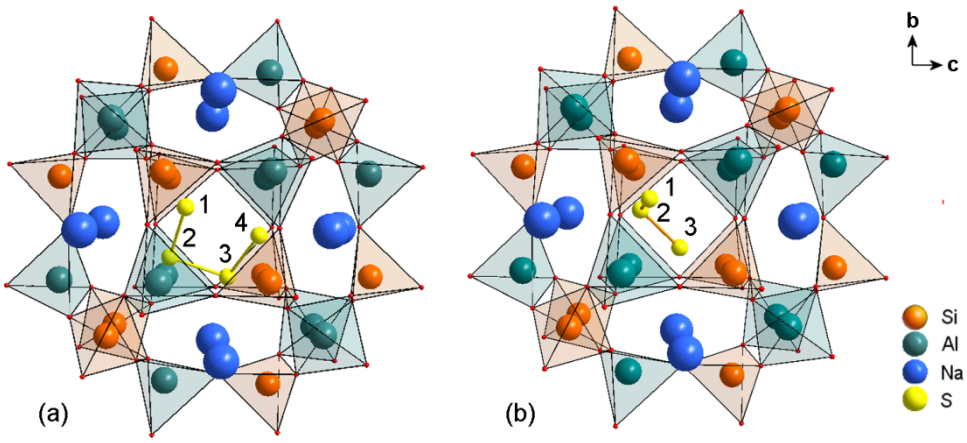

FIGURE S4. Possible locations of (a) S4 and (b) S3 molecules in the sodalite cage # 2, in projection along the *a*-axis. Sulfur positions are numbered. In S4, interatomic distances 1–2, 2–3, 3–4, and 4–1 are equal to 2.08(1), 1.98(1), 1.98(1), and 2.53(1) Å, respectively; angles 1–2–3 and 2–3–4 are equal to 101.1(5) and 94.1(5)°, respectively. The 1–2–3–4 torsion angle equals to 1.4(6)°. In S3, interatomic distances 1–2 and 2–3 are equal to 1.93(1) and 1.91(1) Å, respectively and the 1–2–3 angle equals 115.6(6)°.

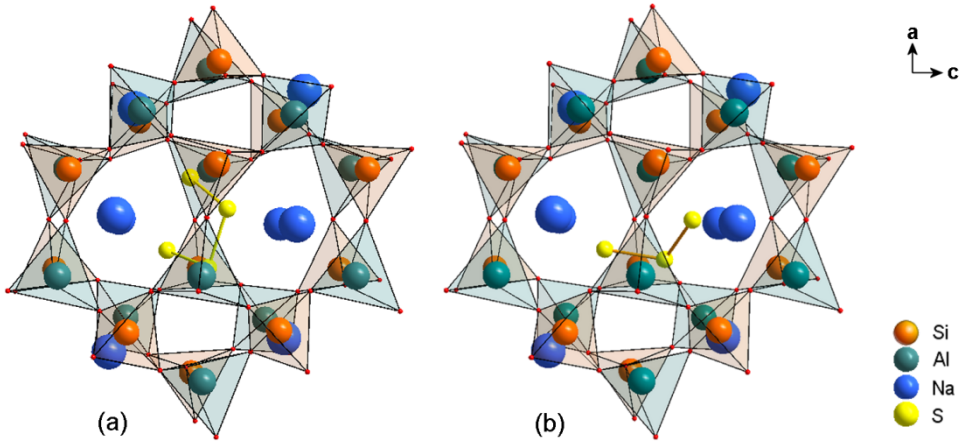

FIGURE S5. Possible locations of (a) S4 and (b) S3 molecules in the sodalite cage #2, in projection along the b-axis.

The rest of the residual electron density peaks are predominantly attributed to CO_2 and H_2O molecules, which, according to infrared and Raman spectroscopy data, occupy a number

of nonequivalent sites. The disorder of these molecules can be partially orientational, which makes it impossible to refine their positions in the structure.

TABLE S1. Site occupancies, positional (*x/a, y/b, z/c*) and equivalent atomic displacement parameters *U*(eq) of the framework atoms.

Atom	Occupancy	*x/a*	*y/b*	*z/c*	*U*(eq), Å^2
Si1	1	0.2499	0.248	0.4976	0.00479(12)
Si2	1	0.75025(9)	0.26032(6)	0.49950(3)	0.00548(12)
Si3	1	0.27915(9)	0.25947(6)	1.00196(3)	0.00366(11)
Si4	1	0.55550(10)	0.38033(6)	0.81384(3)	0.00394(11)
Si5	1	0.50420(10)	0.87730(7)	1.06252(3)	0.00513(12)
Si6	1	0.48378(10)	0.37578(6)	0.31266(3)	0.00390(11)
Si7	1	0.97997(10)	0.62612(7)	0.56651(3)	0.00508(12)
Si8	1	0.04864(10)	0.12336(6)	0.81254(3)	0.00397(11)
Si9	1	0.54555(10)	0.12173(7)	0.68928(3)	0.00468(12)
Si10	1	0.05207(10)	0.37782(6)	0.68659(3)	0.00410(11)
Si11	1	0.27222(10)	0.75134(6)	0.75081(3)	0.00400(11)
Si12	1	0.45892(10)	0.62287(6)	0.43888(3)	0.00445(11)
Si13	1	0.96916(10)	0.87823(6)	0.43785(3)	0.00416(11)
Si14	1	0.98957(10)	0.62824(7)	1.05993(3)	0.00524(12)
Si15	1	0.98786(10)	0.37674(7)	0.19125(3)	0.00474(12)
Si16	1	0.77386(9)	0.75127(6)	0.75174(3)	0.00446(11)
Si17	1	0.78143(10)	0.24969(7)	1.00416(3)	0.00401(11)
Si18	1	0.48351(10)	0.88087(6)	0.56544(3)	0.00444(12)
Si19	1	0.48321(10)	0.13010(7)	0.19147(3)	0.00464(12)
Si20	1	0.50690(10)	0.63165(6)	0.93494(3)	0.00419(11)
Si21	1	0.70931(9)	0.75489(7)	0.25189(3)	0.00447(11)
Si22	1	0.01261(9)	0.87683(6)	0.93565(3)	0.00379(11)
Si23	1	0.20747(10)	0.75440(6)	0.24756(3)	0.00410(11)
Si24	1	–0.01847(10)	0.13125(6)	0.31214(3)	0.00432(11)
Al1	1	0.49649(10)	0.13279(7)	0.56376(4)	0.00615(14)
Al2	1	0.54893(11)	0.38566(7)	0.94110(4)	0.00519(14)
Al3	1	0.02243(11)	0.37891(7)	1.06753(4)	0.00486(13)
Al4	1	–0.00791(10)	0.12970(7)	0.43583(3)	0.00465(13)
Al5	1	0.80072(10)	0.25293(7)	0.74831(3)	0.00420(13)
Al6	1	0.01308(10)	0.37753(7)	0.56090(4)	0.00669(14)

Al7	1	0.30131(10)	0.24804(7)	0.75246(4)	0.00437(13)
Al8	1	0.49861(10)	0.37499(7)	0.43664(3)	0.00490(13)
Al9	1	0.51436(11)	0.12860(7)	1.06622(4)	0.00563(14)
Al10	1	0.73383(11)	0.25457(7)	0.25140(3)	0.00486(13)
Al11	1	0.03379(10)	0.12698(7)	0.93769(4)	0.00433(13)
Al12	1	0.23419(11)	0.25349(7)	0.25281(4)	0.00472(13)
Al13	1	0.72173(10)	0.74850(7)	0.50158(3)	0.00418(13)
Al14	1	0.75142(10)	0.75814(7)	0.99630(3)	0.00530(14)
Al15	1	0.02471(10)	0.87442(7)	0.81157(4)	0.00409(13)
Al16	1	0.52333(10)	0.62965(7)	0.81132(3)	0.00394(13)
Al17	1	0.52446(11)	0.87407(7)	0.69116(4)	0.00483(13)
Al18	1	0.02090(11)	0.62776(7)	0.69060(4)	0.00529(14)
Al19	1	0.25407(10)	0.74511(7)	0.99838(4)	0.00522(14)
Al20	1	0.22268(10)	0.75341(7)	0.50417(3)	0.00465(13)
Al21	1	0.95636(10)	0.62712(7)	0.18545(4)	0.00475(13)
Al22	1	–0.03920(11)	0.88293(7)	0.31221(4)	0.00460(13)
Al23	1	0.45424(10)	0.62393(7)	0.31202(4)	0.00494(14)
Al24	1	0.46248(10)	0.88217(7)	0.18858(4)	0.00510(14)
O1	1	0.5353(2)	0.35555(15)	0.87554(7)	0.0094(3)
O2	1	0.1221(2)	0.15218(14)	0.27469(7)	0.0085(3)
O3	1	0.0441(3)	0.34690(17)	0.62572(8)	0.0149(4)
O4	1	0.9518(2)	0.00047(13)	0.44971(8)	0.0106(4)
O5	1	0.4264(2)	0.49303(13)	0.30159(7)	0.0090(3)
O6	1	0.4418(2)	0.50072(14)	0.44944(8)	0.0121(4)
O7	1	0.5447(2)	0.36049(15)	0.37159(7)	0.0087(3)
O8	1	0.3586(2)	0.28939(14)	0.45240(7)	0.0096(3)
O9	1	0.6593(2)	0.35361(14)	0.47234(7)	0.0096(3)
O10	1	0.8389(2)	0.20017(18)	0.45391(9)	0.0170(5)
O11	1	0.3460(2)	0.29762(14)	0.30374(7)	0.0079(3)
O12	1	0.0479(2)	0.35453(16)	0.13317(7)	0.0120(4)
O13	1	0.1484(2)	0.15805(15)	0.47189(8)	0.0115(4)
O14	1	0.1764(2)	0.33726(18)	1.03380(8)	0.0151(4)
O15	1	0.1916(2)	0.18922(16)	0.95979(7)	0.0131(4)
O16	1	0.6257(2)	0.15295(14)	0.22821(7)	0.0087(3)
O17	1	0.9693(2)	0.85581(15)	0.87578(7)	0.0101(4)
O18	1	0.4602(2)	0.64427(15)	0.87480(7)	0.0088(3)
O19	1	0.1236(2)	0.35549(14)	0.23104(7)	0.0086(3)

O20	1	0.8740(2)	0.65438(14)	0.73275(7)	0.0086(3)
O21	1	–0.0743(2)	0.01351(13)	0.30144(8)	0.0097(3)
O22	1	0.8425(2)	0.20771(14)	0.30198(7)	0.0080(3)
O23	1	0.9136(3)	0.16131(17)	0.77743(8)	0.0147(4)
O24	1	0.3424(2)	0.20467(15)	0.20244(7)	0.0096(3)
O25	1	0.6229(2)	0.35482(13)	0.27464(7)	0.0087(3)
O26	1	0.1917(2)	0.31412(15)	0.70939(8)	0.0128(4)
O27	1	0.3943(2)	0.32774(16)	0.96830(7)	0.0118(4)
O28	1	0.0114(3)	0.15132(16)	0.87246(7)	0.0126(4)
O29	1	0.7014(2)	0.31949(15)	0.79534(7)	0.0106(4)
O30	1	0.6053(2)	0.66878(17)	0.46643(8)	0.0142(4)
O31	1	0.0359(2)	0.15150(15)	0.37133(7)	0.0106(4)
O32	1	0.37204(20)	0.65562(13)	0.77131(7)	0.0073(3)
O33	1	0.5137(4)	0.14771(20)	0.62938(9)	0.0259(7)
O34	1	0.4281(2)	0.01197(14)	0.20163(8)	0.0114(4)
O35	1	0.8462(2)	0.30133(14)	0.20158(7)	0.0084(3)
O36	1	0.6375(2)	0.83504(16)	0.54389(9)	0.0144(4)
O37	1	0.3334(2)	0.19159(16)	0.54551(7)	0.0122(4)
O38	1	0.0509(2)	0.99657(14)	0.94967(8)	0.0123(4)
O39	1	0.1116(3)	0.84160(18)	0.27762(9)	0.0172(5)
O40	1	0.0780(2)	0.49953(13)	0.69881(8)	0.0107(4)
O41	1	0.1539(2)	0.80727(16)	0.95008(9)	0.0143(4)
O42	1	0.6370(2)	0.71395(14)	0.94734(7)	0.0103(4)
O43	1	0.6917(2)	0.18692(16)	0.70427(8)	0.0125(4)
O44	1	0.4870(2)	0.00200(14)	0.54860(8)	0.0125(4)
O45	1	0.6471(2)	0.17479(17)	0.52786(11)	0.0194(5)
O46	1	0.6139(2)	0.66861(16)	0.28325(9)	0.0147(4)
O47	1	0.3581(2)	0.64959(15)	0.96882(7)	0.0103(4)
O48	1	0.2042(2)	0.18270(17)	0.80143(8)	0.0144(4)
O49	1	0.3709(2)	0.84812(13)	0.72965(7)	0.0079(3)
O50	1	0.1128(2)	0.83640(17)	0.46815(8)	0.0144(4)
O51	1	0.3023(2)	0.69391(16)	0.29174(7)	0.0124(4)
O52	1	0.1738(2)	0.79317(14)	0.79945(7)	0.0076(3)
O53	1	0.9913(2)	0.85205(15)	0.37736(7)	0.0104(4)
O54	1	0.1569(2)	0.34413(15)	0.51997(8)	0.0124(4)
O55	1	0.8656(2)	0.85185(15)	0.96949(7)	0.0107(4)
O56	1	0.3993(3)	0.15147(17)	0.72193(11)	0.0194(5)

O57	1	0.4699(2)	0.85893(16)	0.62660(7)	0.0123(4)
O58	1	0.8358(2)	0.67267(16)	0.53802(8)	0.0128(4)
O59	1	0.9355(2)	0.49582(13)	0.19936(7)	0.0094(3)
O60	1	0.5784(2)	0.50144(13)	0.80098(7)	0.0096(3)
O61	1	0.8774(2)	0.16940(16)	0.96954(8)	0.0129(4)
O62	1	0.4060(2)	0.33821(16)	0.78728(8)	0.0133(4)
O63	1	0.67243(20)	0.71149(13)	0.80027(7)	0.0076(3)
O64	1	0.8738(2)	0.84860(13)	0.77194(7)	0.0080(3)
O65	1	0.6735(2)	0.79291(14)	0.70365(7)	0.0084(3)
O66	1	0.1690(2)	0.71085(13)	0.70309(7)	0.0076(3)
O67	1	0.6603(2)	0.82916(16)	1.04374(8)	0.0123(4)
O68	1	0.6626(2)	0.17482(15)	1.03271(9)	0.0137(4)
O69	1	0.9006(2)	0.34628(17)	0.71544(9)	0.0158(4)
O70	1	0.0788(2)	0.00208(13)	0.80083(8)	0.0100(4)
O71	1	0.3408(3)	0.83359(17)	0.53738(10)	0.0182(5)
O72	1	0.6153(3)	0.84436(17)	0.22407(10)	0.0189(5)
O73	1	0.5675(2)	0.51702(13)	0.94973(7)	0.0098(3)
O74	1	0.8156(2)	0.82623(15)	0.45720(7)	0.0109(4)
O75	1	0.3069(3)	0.6747(2)	0.45927(9)	0.0198(5)
O76	1	0.5812(2)	0.00143(13)	0.70108(8)	0.0103(4)
O77	1	0.0094(3)	0.50652(16)	1.04915(9)	0.0186(5)
O78	1	0.8051(3)	0.69494(17)	0.20938(9)	0.0174(5)
O79	1	0.5346(2)	0.14860(16)	0.13213(7)	0.0127(4)
O80	1	0.7137(2)	0.33434(17)	0.96554(9)	0.0150(4)
O81	1	0.1263(3)	0.6901(3)	0.55198(12)	0.0347(8)
O82	1	0.9603(3)	0.65920(17)	1.12018(7)	0.0142(4)
O83	1	0.8551(2)	0.30864(19)	0.54410(8)	0.0157(4)
O84	1	0.5143(2)	–0.00078(14)	1.04767(8)	0.0116(4)
O85	1	0.3518(2)	0.18150(16)	1.04385(8)	0.0142(4)
O86	1	0.4935(4)	0.85707(18)	1.12390(8)	0.0222(6)
O87	1	0.8503(2)	0.65939(16)	1.02403(8)	0.0132(4)
O88	1	0.3615(2)	0.83252(17)	1.03289(11)	0.0186(5)
O89	1	0.8020(3)	0.81482(19)	0.29659(9)	0.0189(5)
O90	1	0.9884(4)	0.50805(18)	0.54854(10)	0.0268(7)
O91	1	0.4716(2)	0.65273(15)	0.37796(7)	0.0110(4)
O92	1	0.8735(3)	0.3023(2)	1.05061(10)	0.0204(5)
O93	1	0.1392(2)	0.6880(2)	1.04376(8)	0.0168(5)

O94	1	0.3027(2)	0.81508(17)	0.20445(8)	0.0141(4)
O95	1	0.9579(3)	0.64662(19)	0.62771(8)	0.0183(5)
O96	1	0.1122(3)	0.66741(18)	0.21863(10)	0.0201(5)

TABLE S2. Harmonic atomic displacement parameters U_{ij} (Å^2) of the framework atoms.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Si1	0.0042(2)	0.0051(2)	0.0051(2)	–0.00047(16)	–0.00014(16)	0.00058(16)
Si2	0.0033(2)	0.0062(2)	0.0069(2)	0.00008(16)	0.00036(16)	0.00129(16)
Si3	0.00282(19)	0.00425(19)	0.00391(19)	0.00014(15)	0.00089(15)	0.00024(15)
Si4	0.0048(2)	0.00300(19)	0.00402(20)	0.00016(16)	0.00059(16)	–0.00056(15)
Si5	0.0051(2)	0.0049(2)	0.0054(2)	–0.00105(16)	0.00153(17)	–0.00106(16)
Si6	0.0051(2)	0.00361(19)	0.00301(19)	0.00009(16)	0.00009(15)	–0.00058(15)
Si7	0.0043(2)	0.0057(2)	0.0052(2)	0.00106(16)	–0.00011(16)	0.00266(16)
Si8	0.0052(2)	0.00341(19)	0.00324(19)	–0.00029(16)	–0.00062(16)	0.00043(15)
Si9	0.0047(2)	0.0045(2)	0.0048(2)	–0.00011(16)	–0.00157(16)	–0.00109(15)
Si10	0.0043(2)	0.00413(19)	0.00384(19)	–0.00030(16)	–0.00053(16)	0.00075(15)
Si11	0.0034(2)	0.00404(19)	0.00454(19)	0.00028(16)	0.00010(15)	–0.00004(15)
Si12	0.0049(2)	0.00377(19)	0.00467(20)	0.00040(16)	–0.00124(16)	–0.00099(15)
Si13	0.0048(2)	0.00395(19)	0.00375(19)	0.00004(16)	–0.00032(16)	0.00026(15)
Si14	0.0067(2)	0.0050(2)	0.00402(19)	0.00133(17)	0.00116(16)	0.00103(15)
Si15	0.0054(2)	0.0048(2)	0.0041(2)	0.00085(16)	0.00081(16)	0.00068(15)
Si16	0.0040(2)	0.0045(2)	0.0048(2)	–0.00009(16)	–0.00019(16)	0.00062(16)
Si17	0.0030(2)	0.00475(20)	0.00425(19)	0.00019(16)	0.00023(15)	0.00027(15)
Si18	0.0051(2)	0.0047(2)	0.00357(19)	0.00129(16)	–0.00076(16)	–0.00099(15)
Si19	0.0050(2)	0.0053(2)	0.00354(19)	0.00101(16)	–0.00016(16)	–0.00127(15)
Si20	0.0042(2)	0.00413(19)	0.00426(20)	0.00000(16)	–0.00049(16)	–0.00044(15)
Si21	0.0029(2)	0.0051(2)	0.0055(2)	–0.00014(16)	–0.00031(16)	0.00066(16)
Si22	0.0038(2)	0.00333(19)	0.00427(19)	0.00042(15)	0.00033(16)	0.00038(15)
Si23	0.0032(2)	0.00464(19)	0.00446(20)	0.00008(16)	0.00017(16)	–0.00008(15)
Si24	0.0052(2)	0.00376(19)	0.00404(19)	–0.00006(16)	–0.00015(16)	0.00071(15)
Al1	0.0060(3)	0.0060(2)	0.0064(2)	–0.0013(2)	–0.0021(2)	0.00235(19)
Al2	0.0061(3)	0.0044(2)	0.0051(2)	0.00092(19)	0.00235(19)	0.00118(18)
Al3	0.0052(2)	0.0052(2)	0.0041(2)	0.00045(19)	0.00006(18)	–0.00136(18)
Al4	0.0045(2)	0.0040(2)	0.0054(2)	–0.00059(18)	0.00004(19)	–0.00061(18)
Al5	0.0037(2)	0.0043(2)	0.0046(2)	0.00043(18)	–0.00010(18)	–0.00017(18)
Al6	0.0086(3)	0.0073(2)	0.0041(2)	0.0038(2)	–0.0021(2)	–0.00151(19)
Al7	0.0034(2)	0.0047(2)	0.0051(2)	0.00000(18)	–0.00047(18)	0.00023(18)
Al8	0.0053(2)	0.0049(2)	0.0045(2)	–0.00100(19)	0.00033(19)	0.00033(18)
Al9	0.0075(3)	0.0051(2)	0.0043(2)	0.0000(2)	0.00069(19)	0.00144(18)
Al10	0.0047(2)	0.0052(2)	0.0047(2)	0.00086(19)	–0.00004(18)	–0.00037(18)
Al11	0.0049(2)	0.0040(2)	0.0041(2)	–0.00013(18)	0.00087(18)	–0.00054(17)
Al12	0.0049(2)	0.0047(2)	0.0046(2)	0.00003(19)	–0.00006(18)	–0.00047(18)
Al13	0.0033(2)	0.0043(2)	0.0049(2)	0.00039(18)	–0.00039(18)	0.00007(18)
Al14	0.0042(2)	0.0063(2)	0.0054(2)	–0.00014(19)	0.00043(19)	–0.00099(18)

Al15	0.0044(2)	0.0039(2)	0.0040(2)	–0.00006(18)	0.00056(18)	–0.00030(17)
Al16	0.0045(2)	0.0033(2)	0.0040(2)	–0.00033(18)	0.00000(18)	0.00020(17)
Al17	0.0053(2)	0.0049(2)	0.0043(2)	0.00068(19)	0.00053(18)	0.00024(18)
Al18	0.0050(2)	0.0048(2)	0.0061(2)	0.00101(19)	–0.00162(19)	–0.00110(18)
Al19	0.0034(2)	0.0050(2)	0.0072(2)	–0.00004(19)	0.00077(19)	–0.00106(19)
Al20	0.0033(2)	0.0059(2)	0.0048(2)	–0.00023(18)	0.00019(18)	–0.00012(18)
Al21	0.0053(2)	0.0046(2)	0.0044(2)	–0.00065(19)	0.00064(18)	–0.00105(18)
Al22	0.0064(3)	0.0035(2)	0.0040(2)	0.00009(19)	0.00081(19)	–0.00037(17)
Al23	0.0060(3)	0.0039(2)	0.0049(2)	–0.00015(19)	–0.00058(19)	0.00086(18)
Al24	0.0052(2)	0.0053(2)	0.0048(2)	0.00080(19)	0.00079(19)	0.00119(18)
O1	0.0121(7)	0.0116(6)	0.0044(5)	–0.0009(5)	0.0011(5)	0.0006(4)
O2	0.0076(6)	0.0085(6)	0.0095(6)	–0.0023(5)	0.0028(5)	0.0001(4)
O3	0.0226(9)	0.0168(7)	0.0053(6)	0.0059(7)	–0.0030(6)	–0.0033(5)
O4	0.0153(7)	0.0037(5)	0.0128(6)	–0.0003(5)	0.0054(5)	–0.0002(4)
O5	0.0104(6)	0.0041(5)	0.0126(6)	0.0005(4)	–0.0002(5)	–0.0009(4)
O6	0.0179(8)	0.0045(5)	0.0138(7)	0.0011(5)	0.0035(6)	0.0016(5)
O7	0.0095(6)	0.0122(6)	0.0042(5)	–0.0009(5)	–0.0008(4)	0.0005(4)
O8	0.0094(6)	0.0101(6)	0.0093(6)	–0.0034(5)	0.0034(5)	0.0004(5)
O9	0.0081(6)	0.0090(6)	0.0117(6)	0.0012(5)	–0.0034(5)	0.0014(5)
O10	0.0111(7)	0.0200(8)	0.0200(8)	0.0070(6)	0.0008(6)	–0.0112(7)
O11	0.0076(6)	0.0088(6)	0.0073(5)	–0.0031(5)	–0.0015(4)	0.0001(4)
O12	0.0142(7)	0.0163(7)	0.0056(6)	0.0043(6)	0.0042(5)	0.0015(5)
O13	0.0124(7)	0.0110(6)	0.0110(6)	–0.0072(5)	–0.0057(5)	0.0037(5)
O14	0.0140(8)	0.0196(8)	0.0117(7)	0.0077(6)	0.0066(6)	–0.0038(6)
O15	0.0153(7)	0.0147(7)	0.0092(6)	–0.0100(6)	–0.0005(5)	–0.0037(5)
O16	0.0080(6)	0.0080(6)	0.0100(6)	–0.0015(5)	–0.0028(5)	–0.0022(4)
O17	0.0124(7)	0.0148(7)	0.0032(5)	–0.0025(5)	0.0011(5)	–0.0012(5)
O18	0.0097(6)	0.0143(6)	0.0024(5)	0.0002(5)	–0.0008(4)	0.0011(4)
O19	0.0076(6)	0.0084(6)	0.0098(6)	0.0019(5)	–0.0022(5)	0.0006(4)
O20	0.0066(6)	0.0078(5)	0.0116(6)	0.0031(4)	0.0019(5)	–0.0012(5)
O21	0.0102(6)	0.0036(5)	0.0152(7)	–0.0008(4)	–0.0010(5)	–0.0001(5)
O22	0.0091(6)	0.0073(5)	0.0076(5)	0.0034(5)	–0.0031(4)	0.0007(4)
O23	0.0158(8)	0.0157(7)	0.0127(7)	0.0093(6)	–0.0073(6)	0.0007(6)
O24	0.0088(6)	0.0115(6)	0.0085(6)	0.0043(5)	0.0005(5)	–0.0018(5)
O25	0.0098(6)	0.0068(5)	0.0093(6)	0.0007(5)	0.0048(5)	–0.0004(4)
O26	0.0100(7)	0.0109(6)	0.0176(7)	0.0025(5)	–0.0060(6)	0.0041(5)
O27	0.0096(6)	0.0168(7)	0.0088(6)	–0.0080(5)	0.0011(5)	0.0032(5)
O28	0.0196(8)	0.0136(7)	0.0047(6)	0.0033(6)	0.0016(5)	0.0014(5)
O29	0.0115(7)	0.0127(6)	0.0076(6)	0.0067(5)	0.0036(5)	–0.0013(5)
O30	0.0101(7)	0.0211(8)	0.0114(7)	–0.0074(6)	–0.0038(5)	–0.0039(6)
O31	0.0127(7)	0.0137(7)	0.0052(5)	–0.0038(5)	–0.0029(5)	0.0016(5)

O32	0.0066(5)	0.0065(5)	0.0087(6)	0.0015(4)	–0.0022(4)	0.0005(4)
O33	0.0497(17)	0.0186(9)	0.0093(7)	–0.0044(10)	–0.0153(9)	0.0032(6)
O34	0.0135(7)	0.0053(5)	0.0154(7)	–0.0011(5)	0.0019(6)	–0.0012(5)
O35	0.0070(6)	0.0093(6)	0.0088(6)	–0.0024(5)	0.0010(5)	0.0006(4)
O36	0.0113(7)	0.0136(7)	0.0183(8)	0.0052(6)	0.0051(6)	–0.0031(6)
O37	0.0078(6)	0.0184(7)	0.0105(6)	0.0024(5)	–0.0022(5)	0.0066(5)
O38	0.0190(8)	0.0035(5)	0.0146(7)	–0.0008(5)	–0.0078(6)	–0.0002(5)
O39	0.0162(8)	0.0184(8)	0.0172(8)	0.0086(7)	0.0062(6)	–0.0039(6)
O40	0.0106(6)	0.0036(5)	0.0179(7)	–0.0005(5)	–0.0018(5)	–0.0012(5)
O41	0.0107(7)	0.0138(7)	0.0184(8)	0.0083(6)	–0.0014(6)	0.0034(6)
O42	0.0122(7)	0.0085(6)	0.0102(6)	–0.0048(5)	–0.0033(5)	–0.0002(5)
O43	0.0099(7)	0.0121(7)	0.0155(7)	–0.0046(5)	–0.0047(5)	–0.0025(5)
O44	0.0172(8)	0.0054(5)	0.0150(7)	0.0012(5)	0.0056(6)	0.0015(5)
O45	0.0095(7)	0.0121(7)	0.0367(12)	0.0009(6)	0.0084(7)	0.0134(7)
O46	0.0106(7)	0.0127(7)	0.0207(8)	–0.0061(6)	0.0038(6)	0.0053(6)
O47	0.0089(6)	0.0116(6)	0.0105(6)	0.0031(5)	0.0041(5)	–0.0015(5)
O48	0.0155(8)	0.0167(7)	0.0111(6)	–0.0124(6)	0.0034(6)	–0.0006(5)
O49	0.0063(5)	0.0069(5)	0.0104(6)	–0.0023(4)	0.0037(4)	0.0012(4)
O50	0.0122(7)	0.0156(7)	0.0154(7)	0.0059(6)	–0.0060(6)	0.0023(6)
O51	0.0132(7)	0.0155(7)	0.0086(6)	0.0078(6)	–0.0017(5)	0.0029(5)
O52	0.0075(6)	0.0086(5)	0.0067(5)	0.0024(4)	0.0028(4)	–0.0004(4)
O53	0.0168(7)	0.0115(6)	0.0031(5)	0.0033(5)	–0.0004(5)	–0.0005(4)
O54	0.0123(7)	0.0114(6)	0.0135(7)	0.0064(5)	0.0041(5)	0.0006(5)
O55	0.0082(6)	0.0140(7)	0.0097(6)	–0.0050(5)	0.0049(5)	–0.0029(5)
O56	0.0113(7)	0.0124(7)	0.0345(11)	0.0039(6)	0.0091(7)	–0.0090(7)
O57	0.0183(8)	0.0140(7)	0.0045(5)	0.0010(6)	–0.0007(5)	0.0027(5)
O58	0.0137(7)	0.0132(7)	0.0115(6)	0.0060(6)	–0.0071(5)	0.0000(5)
O59	0.0108(6)	0.0041(5)	0.0132(6)	0.0009(5)	0.0008(5)	0.0010(4)
O60	0.0129(7)	0.0044(5)	0.0115(6)	0.0005(5)	0.0015(5)	0.0001(4)
O61	0.0127(7)	0.0128(7)	0.0134(7)	0.0049(5)	0.0063(6)	0.0000(5)
O62	0.0086(6)	0.0144(7)	0.0169(8)	–0.0041(5)	–0.0027(6)	–0.0042(6)
O63	0.0062(5)	0.0087(6)	0.0078(5)	–0.0027(4)	0.0021(4)	0.0015(4)
O64	0.0065(5)	0.0069(5)	0.0104(6)	–0.0018(4)	–0.0022(5)	0.0010(4)
O65	0.0070(6)	0.0106(6)	0.0077(5)	0.0027(5)	–0.0012(4)	0.0001(4)
O66	0.0084(6)	0.0077(5)	0.0068(5)	–0.0013(4)	–0.0027(4)	–0.0004(4)
O67	0.0089(6)	0.0148(7)	0.0131(7)	0.0024(5)	0.0023(5)	–0.0060(5)
O68	0.0133(7)	0.0091(6)	0.0188(8)	0.0016(5)	0.0101(6)	0.0051(5)
O69	0.0094(7)	0.0139(7)	0.0240(9)	–0.0012(5)	0.0078(6)	0.0071(6)
O70	0.0101(6)	0.0040(5)	0.0159(7)	–0.0002(5)	0.0027(5)	0.0001(5)
O71	0.0145(8)	0.0147(7)	0.0254(9)	0.0010(6)	–0.0145(7)	–0.0087(7)
O72	0.0140(8)	0.0143(8)	0.0283(10)	0.0041(6)	–0.0092(7)	0.0079(7)

O73	0.0119(6)	0.0051(5)	0.0123(6)	0.0018(5)	–0.0018(5)	0.0007(4)
O74	0.0123(7)	0.0101(6)	0.0102(6)	–0.0059(5)	0.0031(5)	0.0006(5)
O75	0.0140(8)	0.0302(11)	0.0152(8)	0.0138(8)	–0.0044(6)	–0.0133(7)
O76	0.0111(6)	0.0046(5)	0.0151(7)	0.0003(5)	–0.0019(5)	0.0018(5)
O77	0.0339(12)	0.0068(6)	0.0151(8)	0.0065(7)	0.0049(8)	0.0023(5)
O78	0.0193(9)	0.0131(7)	0.0199(8)	0.0032(6)	0.0101(7)	–0.0040(6)
O79	0.0178(8)	0.0164(7)	0.0039(5)	0.0020(6)	0.0027(5)	0.0000(5)
O80	0.0112(7)	0.0170(7)	0.0168(7)	0.0061(6)	0.0022(6)	0.0098(6)
O81	0.0184(10)	0.0557(19)	0.0299(13)	–0.0126(11)	0.0016(9)	0.0264(13)
O82	0.0231(9)	0.0151(7)	0.0044(6)	0.0038(6)	0.0036(6)	0.0018(5)
O83	0.0100(7)	0.0273(9)	0.0096(6)	–0.0028(6)	–0.0042(5)	–0.0027(6)
O84	0.0145(7)	0.0049(5)	0.0154(7)	–0.0020(5)	–0.0038(6)	0.0006(5)
O85	0.0123(7)	0.0145(7)	0.0157(7)	0.0015(6)	–0.0047(6)	0.0085(6)
O86	0.0448(15)	0.0166(8)	0.0053(6)	0.0001(9)	0.0117(8)	–0.0014(6)
O87	0.0096(6)	0.0157(7)	0.0144(7)	0.0050(5)	–0.0033(5)	0.0014(6)
O88	0.0085(7)	0.0137(7)	0.0336(11)	–0.0020(6)	–0.0069(7)	–0.0086(7)
O89	0.0222(9)	0.0208(9)	0.0135(7)	–0.0170(8)	–0.0064(7)	0.0029(6)
O90	0.0500(17)	0.0116(7)	0.0190(9)	0.0161(9)	–0.0189(10)	–0.0068(7)
O91	0.0155(7)	0.0121(6)	0.0055(6)	–0.0017(5)	–0.0021(5)	0.0018(5)
O92	0.0200(9)	0.0227(9)	0.0185(9)	–0.0087(8)	–0.0059(7)	–0.0031(7)
O93	0.0113(7)	0.0286(10)	0.0105(7)	–0.0076(7)	0.0048(5)	0.0001(6)
O94	0.0131(7)	0.0153(7)	0.0138(7)	–0.0034(6)	0.0057(6)	0.0037(6)
O95	0.0224(9)	0.0245(9)	0.0082(7)	0.0123(8)	–0.0075(6)	–0.0056(6)
O96	0.0159(8)	0.0149(8)	0.0295(11)	–0.0062(6)	–0.0104(8)	–0.0065(7)

TABLE S3. Selected interatomic distances in the SiO_4 and AlO_4 tetrahedra.

Si1–O8	1.612(2)		Si1–O13	1.616(2)		Si1–O37	1.617(2)		Si1–O54	1.606(2)
Si2–O9	1.617(2)		Si2–O10	1.619(2)		Si2–O45	1.615(2)		Si2–O83	1.611(2)
Si3–O14	1.596(2)		Si3–O15	1.617(2)		Si3–O27	1.613(2)		Si3–O85	1.613(2)
Si4–O1	1.627(2)		Si4–O29	1.610(2)		Si4–O60	1.607(2)		Si4–O62	1.607(2)
Si5–O67	1.619(2)		Si5–O84(i)	1.618(2)		Si5–O86	1.601(2)		Si5–O88	1.604(2)
Si6–O5	1.624(2)		Si6–O7	1.623(2)		Si6–O11	1.616(2)		Si6–O25	1.618(2)
Si7–O58	1.614(2)		Si7–O81(ii)	1.602(3)		Si7–O90	1.591(2)		Si7–O95	1.606(2)
Si8–O23(iii)	1.597(2)		Si8–O28	1.617(2)		Si8–O48	1.625(2)		Si8–O70	1.615(2)
Si9–O33	1.600(3)		Si9–O43	1.611(2)		Si9–O56	1.615(3)		Si9–O76	1.613(2)
Si10–O3	1.615(2)		Si10–O26	1.618(2)		Si10–O40	1.6151(2)		Si10–O69(iii)	1.610(2)
Si11–O32	1.619(2)		Si11–O49	1.624(2)		Si11–O52	1.628(2)		Si11–O66	1.625(2)
Si12–O6	1.603(2)		Si12–O30	1.612(2)		Si12–O75	1.619(3)		Si12–O91	1.615(2)
Si13–O4(i)	1.612(2)		Si13–O50(ii)	1.609(2)		Si13–O53	1.603(2)		Si13–O74	1.619(2)
Si14–O77(ii)	1.603(2)		Si14–O82	1.620(2)		Si14–O87	1.613(2)		Si14–O93(ii)	1.610(2)
Si15–O12(ii)	1.614(2)		Si15–O19(ii)	1.621(2)		Si15–O35	1.628(2)		Si15–O59	1.621(2)
Si16–O20	1.621(2)		Si16–O63	1.630(2)		Si16–O64	1.628(2)		Si16–O65	1.625(2)
Si17–O61	1.620(2)		Si17–O68	1.618(2)		Si17–O80	1.597(2)		Si17–O92	1.604(3)
Si18–O36	1.614(2)		Si18–O44(i	1.619(2)		Si18–O57	1.601(2)		Si18–O71	1.597(2)
Si19–O16	1.623(2)		Si19–O24	1.624(2)		Si19–O34	1.621(2)		Si19–O79	1.611(2)
Si20–O18	1.609(2)		Si20–O42	1.613(2)		Si20–O47	1.621(2)		Si20–O73	1.622(2)
Si21–O46	1.620(2)		Si21–O72	1.603(3)		Si21–O78	1.596(3)		Si21–O89	1.616(2)
Si22–O17(iii)	1.609(2)		Si22–O38	1.620(2)		Si22–O41	1.607(2)		Si22–O55(iii)	1.621(2)
Si23–O39	1.618(3)		Si23–O51	1.623(2)		Si23–O94	1.605(2)		Si23–O96	1.595(3)
Si24–O2	1.617(2)		Si24–O21	1.620(2)		Si24–O22(iii)	1.622(2)		Si24– O31	1.618(2)
Al1–O33	1.703(2)		Al1–O37	1.727(2)		Al1–O44	1.731(2)		Al1–O45	1.732(3)
Al2–O1	1.732(2)		Al2–O27	1.731(2)		Al2–O73	1.714(2)		Al2–O80	1.750(2)
Al3–O12(iv)	1.730(2)		Al3–O14	1.729(2)		Al3–O77	1.714(2)		Al3–O92(iii)	1.723(3)
Al4–O4(iii)	1.740(2)		Al4–O10(iii)	1.725(2)		Al4–O13	1.729(2)		Al4–O31	1.726(2)
Al5–O23	1.733(2)		Al5–O29	1.735(2)		Al5–O43	1.723(2)		Al5–O69	1.723(2)

Al6–O3	1.733(2)		Al6–O54	1.730(2)		Al6–O83(iii)	1.734(2)		Al6–O90(iii)	1.726(3)
Al7–O26	1.714(2)		Al7–O48	1.749(2)		Al7–O56	1.720(3)		Al7–O62	1.743(2)
Al8–O6	1.733(2)		Al8–O7	1.7326(19)		Al8–O8	1.725(2)		Al8–O9	1.741(2)
Al9–O68	1.701(2)		Al9–O79(iv)	1.722(2)		Al9–O84	1.733(2)		Al9–O85	1.722(2)
Al10–O16	1.737(2)		Al10–O22	1.738(2)		Al10–O25	1.744(2)		Al10–O35	1.741(2)
Al11–O15	1.730(2)		Al11–O28	1.716(2)		Al11–O38(v)	1.715(2)		Al11–O61(iii)	1.726(2)
Al12–O2	1.743(2)		Al12–O11	1.747(2)		Al12–O19	1.746(2)		Al12–O24	1.742(2)
Al13–O30	1.723(2)		Al13–O36	1.736(2)		Al13–O58	1.703(2)		Al13–O74	1.737(2)
Al14–O42	1.723(2)		Al14–O55	1.729(2)		Al14–O67	1.735(2)		Al14–O87	1.713(2)
Al15–O17(iii)	1.740(2)		Al15–O52	1.739(2)		Al15–O64(iii)	1.734(2)		Al15–O70(i)	1.736(2)
Al16–O18	1.738(2)		Al16–O32	1.745(2)		Al16–O60	1.747(2)		Al16–O63	1.733(2)
Al17–O49	1.738(2)		Al17–O57	1.740(2)		Al17–O65	1.740(2)		Al17–O76(i)	1.736(2)
Al18–O20(iii)	1.751(2)		Al18–O40	1.745(2)		Al18–O66	1.742(2)		Al18–O95(iii)	1.730(2)
Al19–O41	1.734(2)		Al19–O47	1.729(2)		Al19–O88	1.729(2)		Al19–O93	1.725(2)
Al20–O50	1.730(2)		Al20–O71	1.711(2)		Al20–O75	1.716(3)		Al20–O81	1.712(3)
Al21–O59	1.738(2)		Al21–O78	1.740(3)		Al21–O82(vi)	1.727(2)		Al21–O96(ii)	1.725(3)
Al22–O21(i)	1.735(2)		Al22–O39	1.716(3)		Al22–O53(iii)	1.742(2)		Al22–O89(iii)	1.728(3)
Al23–O5	1.725(2)		Al23–O46	1.721(2)		Al23–O51	1.727(2)		Al23–O91	1.741(2)
Al24–O34(i)	1.735(2)		Al24–O72	1.727(3)		Al24–O86(vi)	1.716(2)		Al24–O94	1.731(2)

(i) *x, y*+1, *z*; (ii) *x*+1, *y, z*; (iii) *x*–1, *y, z*; (iv) *x, y, z*+1; (v) *x, y*–1, *z*; (vi) *x, y, z*–1

TABLE S4. Selected interatomic distances (Å) in the SO_4 tetrahedra.

S1–Os11(i)	1.463(3)		S6–Os67	1.492(8)
S2–Os21	1.484(3)		S1–Os12	1.457(4)
S3–Os31(ii)	1.451(4)		S2–Os22	1.475(3)
S3–Os35	1.512(14)		S3–Os32	1.485(4)
S4–Os41	1.495(3)		S3–Os36(ii)	1.532(13)
S5–Os51	1.457(4)		S4–Os42	1.471(3)
S6–Os61	1.448(4)		S5–Os52(iii)	1.471(3)
S6–Os65(ii)	1.488(9)		S6–Os62(ii)	1.484(9)
S1–Os13(ii)	1.469(3)		S6–Os66	1.438(9)
S2–Os23	1.459(4)		S1–Os14	1.473(3)
S3–Os33	1.507(5)		S2–Os24	1.473(3)
S3–Os37	1.385(15)		S3–Os34	1.465(4)
S4–Os43	1.460(4)		S4–Os44(i)	1.475(3)
S5–Os53(iv)	1.466(3)		S5–Os54(v)	1.475(3)
S6–Os63	1.489(10)		S6–Os64	1.500(13)

(i) x+1, y, z; (ii) x, y–1, z; (iii) x–1, y+1, z; (iv) x, y+1, z+1; (v) x, y, z+1

TABLE S5. The site occupancies, positional (*x/a, y/b, z/c*) and isotropic/equivalent atomic displacement parameters for the sulfate (S, Os) and sulfide (Ss) groups.

Atom	Occupancy	*x/a*	*y/b*	*z/c*	*U*(iso*/eq), Å^2
S1	1	0.98658(10)	0.00439(7)	0.61028(3)	0.01232(9)*
Os11	1	0.1337(3)	–0.0069(3)	0.58744(14)	0.0342(8)
Os12	1	0.8758(4)	0.0214(3)	0.56999(13)	0.0387(10)
Os13	1	0.9525(3)	0.9111(2)	0.64099(11)	0.0255(6)
Os14	1	0.9839(5)	0.0946(2)	0.64552(13)	0.0367(9)
S2	1	0.05780(10)	0.46740(7)	0.87680(3)	0.01223(9)*
Os21	1	0.0640(4)	0.5431(3)	0.92030(11)	0.0352(9)
Os22	1	0.0909(3)	0.5236(2)	0.82814(9)	0.0238(6)
Os23	1	0.1700(4)	0.3891(3)	0.88731(17)	0.0388(10)
Os24	1	–0.0917(3)	0.4222(3)	0.87353(12)	0.0296(7)
S3	1	0.52821(10)	0.03527(7)	0.88757(4)	0.01377(10)*
Os31	1	0.5246(5)	0.9588(3)	0.84609(13)	0.0398(10)
Os32	0.75	0.5702(5)	0.1416(3)	0.8707(2)	0.0371(13)
Os33	0.75	0.3767(5)	0.0501(4)	0.9107(2)	0.0425(14)
Os34	0.75	0.6332(5)	–0.0048(3)	0.92602(15)	0.0308(10)
Os35	0.25	0.6828(14)	0.0760(15)	0.8971(7)	0.053(5)
Os36	0.25	0.4850(18)	0.9906(12)	0.9407(5)	0.040(4)
Os37	0.25	0.4226(18)	0.1040(11)	0.8695(6)	0.042(4)
S4	1	0.95418(10)	0.53721(7)	0.37700(3)	0.01346(10)*
Os41	1	0.9593(4)	0.4563(3)	0.41870(12)	0.0360(9)
Os42	1	0.9160(3)	0.4839(2)	0.32813(10)	0.0251(6)
Os43	1	0.8405(4)	0.6121(3)	0.39126(17)	0.0390(10)
Os44	1	0.1016(3)	0.5856(3)	0.37258(14)	0.0367(9)
S5	1	0.01418(10)	1.00076(7)	1.11055(3)	0.01210(9)*
Os51	1	0.1311(4)	0.9824(3)	1.07270(15)	0.0425(11)
Os52	1	0.8707(3)	0.0176(3)	1.08505(13)	0.0300(7)
Os53	1	0.0478(4)	0.0924(2)	0.14235(12)	0.0278(7)
Os54	1	0.0059(5)	0.9108(2)	0.14602(15)	0.0413(11)
S6	1	0.47322(10)	–0.02916(7)	0.38684(4)	0.01520(10)*
Os61	1	0.4703(5)	0.0529(3)	0.34832(13)	0.0398(10)
Os62	0.5	0.4377(14)	0.8660(6)	0.3663(5)	0.067(4)
Os63	0.5	0.3516(12)	0.0066(8)	0.4214(3)	0.060(3)
Os64	0.5	0.6246(15)	–0.0415(10)	0.4098(6)	0.089(5)
Os65	0.5	0.5831(10)	0.8999(6)	0.3628(3)	0.046(2)
Os66	0.5	0.3362(9)	–0.0834(8)	0.3953(5)	0.063(3)
Os67	0.5	0.5394(12)	0.0081(7)	0.4367(3)	0.050(3)
Ss10	0.1219	0.4350(10)	0.3721(7)	0.6048(3)	0.0291(5)*

Ss11	0.1219	0.5206(10)	0.4053(7)	0.6784(3)	0.0291(5)*
Ss12	0.1219	0.6864(10)	0.5021(7)	0.6607(3)	0.0291(5)*
Ss13	0.1219	0.5695(10)	0.6301(7)	0.6384(3)	0.0291(5)*
Ss14	0.1219	0.4941(10)	0.5960(7)	0.5723(3)	0.0291(5)*
Ss15	0.1219	0.3257(10)	0.5021(7)	0.5887(3)	0.0291(5)*
Ss20	0.2188	0.6713(7)	0.4910(5)	0.0862(2)	0.0387(5)*
Ss21	0.2188	0.3195(7)	0.5092(5)	0.1611(2)	0.0387(5)*
Ss22	0.1094	0.4999(15)	0.5910(10)	0.0692(5)	0.0387(5)*
Ss23	0.1094	0.4189(15)	0.6358(10)	0.1401(5)	0.0387(5)*
Ss24	0.1094	0.5000(15)	0.4171(10)	0.1792(5)	0.0387(5)*
Ss25	0.1094	0.5677(15)	0.3745(10)	0.1089(5)	0.0387(5)*
Ss26	0.1094	0.5635(14)	0.6232(10)	0.0946(5)	0.0387(5)*
Ss27	0.1094	0.4807(15)	0.6080(9)	0.1732(5)	0.0387(5)*
Ss28	0.1094	0.4188(15)	0.3814(10)	0.1482(5)	0.0387(5)*
Ss29	0.1094	0.5220(15)	0.4020(10)	0.0756(5)	0.0387(5)*

TABLE S6. The site occupancies, positional (*x/a, y/b, z/c*) and isotropic/equivalent atomic displacement parameters for the extra-framework cations.

Atom	Occupancy	x/a	y/b	z/c	u(eq), Å^2
Na1	1	–0.19173(15)	0.31830(10)	0.37490(5)	0.0145(3)
Na2	1	0.30447(16)	0.18251(11)	0.37469(5)	0.0157(3)
Na3	1	0.15573(15)	0.50919(10)	0.28072(5)	0.0161(3)
Na4	1	0.17786(16)	0.49512(11)	0.46802(7)	0.0216(3)
Na5	1	0.69832(16)	0.82803(11)	0.87228(5)	0.0163(3)
Na6	1	0.22866(18)	0.49604(11)	0.98725(7)	0.0242(4)
Na7	1	0.21754(17)	0.19037(12)	0.63225(5)	0.0195(3)
Na8	1	0.26832(16)	0.49197(10)	0.76090(6)	0.0187(3)
Na9	1	0.81192(16)	0.19132(11)	0.12885(5)	0.0164(3)
Na10	1	0.22443(18)	0.22212(14)	1.12320(5)	0.0228(4)
Na11	1	0.34750(16)	0.99768(10)	0.78291(6)	0.0179(3)
Na12	1	0.80643(19)	0.21886(16)	0.62196(6)	0.0300(4)
Na13	1	0.19925(14)	0.68712(10)	0.87470(5)	0.0130(2)
Na14	1	0.65346(17)	0.00616(11)	0.28424(6)	0.0189(3)
Na15	1	0.84822(15)	0.49767(10)	0.78213(5)	0.0152(3)
Na16	1	0.84816(15)	0.00407(10)	0.72185(5)	0.0142(3)
Na17	1	0.15986(16)	0.00334(10)	0.22198(5)	0.0161(3)
Na18	1	0.77836(18)	0.51319(10)	0.48455(7)	0.0220(3)
Na19	1	0.78046(17)	0.81087(13)	0.13135(6)	0.0213(3)
Na20	1	0.83342(16)	0.51095(11)	0.96678(6)	0.0188(3)
Na21	1	0.19632(16)	0.81805(11)	0.62904(6)	0.0187(3)
Na22	1	0.19394(18)	0.79241(14)	1.11886(6)	0.0249(4)
Na23	1	0.77838(17)	0.78003(13)	0.62168(5)	0.0208(3)
Na24	1	0.74221(17)	0.51136(10)	0.26041(6)	0.0196(3)
Ca25	0.75	0.32023(9)	0.24277(6)	0.87974(3)	0.01542(13)
Na25	0.25	0.32023(9)	0.24277(6)	0.87974(3)	0.01542(13)
Ca26	0.5	0.69924(12)	0.75691(8)	0.37732(3)	0.0227(2)
Na26	0.5	0.69924(12)	0.75691(8)	0.37732(3)	0.0227(2)
Ca27	0.75	0.76119(9)	0.00609(5)	1.00183(3)	0.01392(12)
Na27	0.25	0.76119(9)	0.00609(5)	1.00183(3)	0.01392(12)
Ca28	0.5	0.22524(10)	0.76011(7)	0.37589(3)	0.01693(17)
Na28	0.5	0.22524(10)	0.76011(7)	0.37589(3)	0.01693(17)
Ca29	0.5	0.72064(8)	0.00462(6)	0.49602(3)	0.01017(13)
Na29	0.5	0.72064(8)	0.00462(6)	0.49602(3)	0.01017(13)
Ca30	0.5	0.23748(13)	–0.00142(7)	0.50217(4)	0.0223(2)
Na30	0.5	0.23748(13)	–0.00142(7)	0.50217(4)	0.0223(2)
Na31	0.75	0.78328(13)	0.24868(9)	0.87676(4)	0.0181(2)
Ca31	0.25	0.78328(13)	0.24868(9)	0.87676(4)	0.0181(2)
Na32	0.75	0.28125(12)	0.00261(8)	0.99585(4)	0.0153(2)
Ca32	0.25	0.28125(12)	0.00261(8)	0.99585(4)	0.0153(2)