Electronic Supplementary Information

Effects of intervalence charge transfer interaction between π-stacked mixed valent tetrathiafulvalene ligands on the electrical conductivity of 3D metal–organic frameworks

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Experimental Section:

General Materials and Methods.

Starting materials, reagents, and solvents, such as ethylene trithiocarbonate, dimethyl acetylenedicarboxylate, triethyl phosphite, NaOH, KOH, RbOH, CsOH, and electrolytes were purchased from Sigma-Aldrich / Millipore-Sigma, Acros Organic, TCI America, and EMD Chemicals. The electrodes (Ag/AgCl, Pt-wire, Pt-disk, and glassy-carbon) and electrochemical cells were procured from BASi. The ^{1}H NMR spectra of the ligand was recorded on a Bruker 500 MHz NMR spectrometer. The MALDI-TOF mass spectra were recorded on a Bruker Autoflex instrument. The FT-IR spectra of the MOFs were recorded on a Shimadzu IRAffinity-1S spectrometer. Raman spectra were collected in a backscattering geometry and analyzed by spectrograph (Triplemate 1377, Spex) equipped with a CCD camera (Andor, IDus) the samples were excited with a Kr^+ laser (Innova 100, Coherent) line at 530.9 nm. The power at the sample was 50 mW and the total spectra collection time was 100 s.

The single crystal and powder X-ray diffraction (SXRD and PXRD) analyses of MOFs **1–4** were performed at 100 K on a Bruker D8 Venture dual source diffractometer equipped with a CMOS detector using MoKα radiation (λ = 0.71073 Å). Structures were refined by full-matrix least-squares against F^2 using all data (SHELX97).[S1] All non-hydrogen atoms were refined anisotropically if not stated otherwise and the hydrogen atoms were constrained in geometric positions to their parent atoms. The PXRD patterns of these MOFs were recorded on a Rigaku Ultima IV X-ray diffractometer equipped with Cu Kα radiation source (λ = 1.5406 Å) and a CCD area detector. The solvent-accessible void space inside these MOFs was calculated by using Mercury software.[S2]

The surface area and pore volume of evacuated MOFs were determined from the N_2 sorption isotherms (77 K) measured with a Quantachrome Autosorb iQ Gas Sorption Analyzer.

Thermogravimetric analysis was conducted under a N_2 atmosphere using an SDT Q600 instrument.

The solid-state ESR spectra of MOFs were recorded on a Bruker EMX EPR X-band spectrometer at room temperature. Powdered samples of each freshly prepared and air-exposed were inserted into precision-bore 4 mm quartz tube, and the sample weight and height were measured in order to determine the amount and volume. The spin was quantified by performing double integration of the obtained spectrum using the following equation:[S3,S4]

$$n_s = \frac{DI}{\frac{c}{f(B_1, B_m)} \times \{G_R \times C_t \times n\} \times \left\{\sqrt{P} \times B_m \times Q \times n_B \times S(S+1)\right\}}$$

where, c = point sample calibration factor; B_1 = microwave magnetic field; B_m = modulation amplitude; G_R = the receiver gain, C_t = conversion time; n = number of scans; P = microwave power; Q = quality factor of the resonator; n_B = Boltzmann temperature correction; S = electronic spin; and n_s = absolute number of spins. The total number of spins/mg MOF was calculated by obtained spins/mm^3. From this value, the spins/mole and spins/TTFTC values were calculated using its molecular formula and formula weight.

Cyclic voltammograms of the ligand and MOFs were recorded on a Princeton Applied Research VersaStat 3-450 instrument using a glassy carbon disc (for the ligand solutions) or Pt-disc (for drop-cast MOF films) working electrode, Ag/AgCl reference electrode, Pt-wire counter electrode, in a 0.1 M Bu_4NPF_6 / MeCN supporting electrolyte solution. The suspension of each MOF in the electrolyte solution was drop-cast (one drop) on a Pt-disc working electrode and the solvent was allowed to evaporate to obtain the MOF film attached to the electrode surface, which was used to record its solid-state CV. The solution-phase CVs of the ligand was recorded using 0.2 mM solutions in the same supporting electrolyte solution.

Diffuse-reflectance spectra of the materials were recorded on a Shimadzu UV-2600 spectrophotometer coupled with a Shimadzu ISR-2600 Plus integrating sphere (400–1400 nm) and on a Cary 7000 universal measurement spectrophotometer (up to 2400 nm). The direct optical band gaps of these materials were determined from respective Tauc plots.

Density functional theory (DFT) calculations were performed using the Quantum-Espresso package.[S5] Norm conserving pseudopotentials with Perdew-Burke-Ernzerhof (PBE) exchange correlation were used. A cutoff energy of 544 eV and an appropriate k-point mesh (3×3×3, 2×3×6, and 6×3×2 for Na-MOF **1**, K-MOF **2**, and Cs-MOF **4**, respectively, generated using the Monkhosrt-Pack scheme) were used and found to be enough for total energy to converge within 0.01 meV/atom. All calculations were carried out on the primitive cell of the MOF crystals. The structure was first fully optimized with respect to atomic coordinates. Then, single-point calculation on the DFT/PBE-optimized structures was performed using the higher-level hybrid HSE06 functional, which is known to predict band gaps more accurately than DFT/PBE. Due to the significant computational cost associated with the hybrid functional, no further structural optimizations were performed on the MOF structure. The band structure and partial density of states were directly derived from the single-point calculation.

Electrical conductivity of these MOF materials was determined from current-voltage (*I-V*) measurements under ambient conditions (293 K) using in-situ pressed pellets of each material.[S3,S6] A homemade two-probe device consisting of two precision-cut stainless-steel rods with flat round tips (radius = 0.135 cm) partially inserted into a snugly fit Teflon tube securing the pellet sandwiched between the two steel rods was used for two-probe electrical measurements. The tips of the steel rods were precoated with silver paint for better electrical contact between the electrodes and sandwiched MOF materials. Each pellet was prepared from 3.5 mg of respective material placed between the two silver-coated steel rods inserted in a Teflon tube and then pressed under a constant 260 MPa pressure for 1 min using a digital Parr pellet press. The thickness (L ≈ 0.02 cm) of MOF pellets was measured from the difference in the total length of two steel rods with and without the sandwiched materials using a digital caliper, and the area (A = 0.057 cm^2) was defined by the radius of the steel rods inserted inside the Teflon tube. The corresponding conductivities were calculated using the equation: σ = L/RA (R = total resistance of the pellet obtained from the slope of the corresponding *I-V* plots). The average (and standard deviation) of 3–5 devices of each material is reported. For temperature-dependent *I-V* measurements, the same setup was immersed in a temperature-controlled sand bath, and the temperature was measured precisely by a pair of digital thermocouples. The devices were held at each temperature for 30 min before measuring their *I-V* plots to ensure the accuracy of the measurements. The activation energy (E_a) was calculated from the temperature-dependent conductivity data using the Arrhenius equation: $\sigma = Aexp(\frac{Ea}{RT})$ where A = a pre-exponential factor, R = gas constant, and T = temperature in Kelvin.

Material Synthesis and Characterization.

TTFTC-Me_4. TTFTC-Me_4 was synthesized in two steps according to a modified literature protocol:[S8,S9] Ethylene trithiocarbonate (11 g, 0.0807 mol) was dissolved in toluene (40 mL) and dimethyl acetylenedicarboxylate (11.47 g, ~ 9.92 mL, 0.0807 mol) was added to it. The mixture solution was refluxed for 8 h. After cooling down to room temperature, the mixture solution was kept in the refrigerator for overnight to allow 4,5-bis(carbomethoxy)-1,3-dithiole-2-thione to precipitate, which was filtered and rinsed with cold Et_2O. The yellow crystals were further dried under vacuum. Yield: 13.22 g (70 %). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 3.93 (s, 6H). 4,5-bis(carbomethoxy)-1,3-dithiole-2-thione (2 g, 0.008 mol) was dissolved in benzene (16 mL) and triethyl phosphite (2 g, ~ 2.08 mL, 0.012 mol) was added to it. The mixture solution was heated under reflux for overnight. After cooling the reaction mixture to room temperature, the solution was concentrated under reduced pressure. Then EtOH (10 mL) was added to the residue to precipitate TTFTC-Me_4, which was filtered, rinsed with EtOH and dried under vacuum.

Recrystallization from MeOH gave black-brown crystals. Yield: 0.68 g (20 %). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 3.88 (s, 12H). MALDI-TOF MS (*m/z*): calc. for $C_{14}H_{12}O_8S_4$ 436.48, obs. 436.44 [M^-].

TTFTC-H$_4$. TTFTC-H_4 was synthesized as previously reported:[S7,S9] A mixture of TTFTC-Me_4 ester (0.34 g, 0.0008 mol) and KOH/EtOH solution (~0.01 mol in 20 mL) was heated under reflux for 1 h. After allowing the reaction mixture to cool down to room temperature, the orange suspension was filtered and rinsed with EtOH. The resulting orange-brown solid was dissolved in deionized H_2O (7 mL) and the solution was acidified slowly with conc. HCl (37 %) until the pH reached 1. The resulting purple solid was filtered, rinsed with H_2O and dried under vacuum to obtain blackish-purple colored TTFTC-H_4. MALDI-TOF MS (*m/z*): calc. 188.93 $[M - 2H]^{2-}$, observed: 188.84.

Na-MOF. To a solution of TTFTC-Me_4 (20 mg, 0.046 mmol) in a 1:2 THF / MeOH mixture (6 mL) placed in a 20 mL vial, a 0.5 M NaOH solution (1.6 mL) was added slowly. After sonicating the resulting reaction mixture for 5 min and then standing it at 65 °C for 12 h, the SXRD-quality brown colored needle-shaped crystals precipitated out. The resulting crystals were filtered, rinsed thoroughly with MeCN three times, and then soaked in MeCN for 12 h. Finally, the resulting crystals were filtered and dried under vacuum for 24 h to obtain brown colored crystalline bulk material (**1-ox**). Yield: 21.40 mg (91%). Elemental analysis of Na-MOF ($C_{11}H_{16}Na_4O_{15}S_4$): calc. C: 21.69, H: 2.62, S: 21.03; found C: 21.42, H: 1.20, S: 20.44. FT-IR (cm^{-1}): 1581, 1558, 1350, 1103, 972, 914, 790, 752, 690, 601. Raman shift (cm^{-1}): 1408, 1498, 1561.

K-MOF. To a solution of TTFTC-Me_4 (20 mg, 0.046 mmol) in a 1:2 THF / MeOH mixture (6 mL) placed in a 20 mL vial, a 0.5 M KOH solution (0.6 mL) was added slowly. After sonicating the resulting reaction mixture for 5 min and then standing it at 80 °C for 2 h, the SXRD-quality reddish orange colored needle-shaped crystals precipitated out of the solution. The resulting crystals were filtered, rinsed with CH_3CN three times, and then soaked in MeCN for 12 h. Finally, the resulting crystals were filtered and dried under vacuum for 24 h to obtain reddish orange colored crystalline bulk material (**2**). Upon exposing this material to air for 7 d, it gradually turned black crystalline powder (**2-ox**) due to aerobic oxidation of a significant population of TTFTC ligands to $TTFTC^{\bullet+}$ radical cations. Yield: 21.35 mg (77%). Elemental analysis of K-MOF ($C_{10}H_8K_4O_{12}S_4$): calc. C: 19.85, H: 1.33, S: 21.20; found: C: 19.84, H: 1.20, S: 20.98. FT-IR (cm^{-1}): 1578, 1559, 1351, 1095, 1031, 909, 794, 757, 698 for **2** and 1581, 1557, 1344, 1217, 1094, 1027, 955, 908, 793, 754, 692 for **2-ox**. Raman shift (cm^{-1}): 1531, 1555, 1588 for **2** and 1401, 1483, 1538 for **2-ox**.

Rb-MOF. To a solution of TTFTC-Me_4 (20 mg, 0.046 mmol) in a 1:2 THF / MeOH mixture (6 mL) placed in a 20 mL vial, a 0.5 M RbOH solution (0.6 mL) was added slowly. After sonicating the resulting reaction mixture for 5 min and then standing it at 65 °C for 12 h, the SXRD-quality orange colored needle-shaped crystals precipitated out of the solution. The resulting crystals were filtered, rinsed with MeCN three times, and then soaked in MeCN for 12 h. Finally, the resulting orange crystals were filtered and dried under vacuum for 24 h to obtain the crystalline bulk material (**3**). Upon exposing this material to air for 7 d, it gradually turned black crystalline powder (**3-ox**) due to aerobic oxidation of a significant population of TTFTC ligands to $TTFTC^{\bullet+}$ radical cations. Yield: 27.25 mg (75%). Elemental analysis of Rb-MOF ($C_{10}H_8Rb_4O_{12}S_4$): calc. C: 15.19, H: 1.02, S: 16.22; found: C: 14.75, H: 1.06, S: 15.63. FT-IR (cm^{-1}): 1574, 1551, 1342, 1099, 1026, 904, 796, 753, 691 for **3** and 1579, 1548, 1339, 1303, 1216, 1096, 1026, 970, 904, 798, 753, 691 for **3-ox**. Raman shift (cm^{-1}): 1395, 1533, 1593 for **3** and 1401, 1434, 1529 for **3-ox**.

Cs-MOF. To a solution of TTFTC-Me_4 (5 mg, 0.0115 mmol) in a 1:2 THF / MeOH mixture (1.5 mL) placed in a 5 mL vial, a 0.5 M CsOH solution (0.15 mL) was added slowly. After sonicating the reaction mixture for 5 min, the smaller 5 mL vial without the cap was placed inside a screw-capped 20 mL vial containing a 1:1 THF/MeOH (5 mL) mixture to allow solvent vapor diffusion at 20 °C for 3 d, which yielded the SXRD-quality orange-colored needle-shaped crystals. The resulting crystals were filtered, rinsed with MeCN three times, and then soaked in MeCN for 12 h. Finally, the resulting crystals were filtered and dried under vacuum for 24 h to obtain orange crystalline bulk material (**4**). It remained unchanged upon prolonged exposure to air. Yield: 10.91 mg (84%). Elemental analysis of Cs-MOF

($C_{10}H_4Cs_4O_{12}S_4$): calc. C: 12.72, H: 0.43, S: 13.58; observed: C: 12.71, H: 0.42, S: 13.43. FT-IR (cm^{-1}): 1566, 1554, 1334, 1087, 1026, 902, 856, 794, 748, 709, 682, 602. Raman shift (cm^{-1}): 1351, 1528, 1555, 1583.

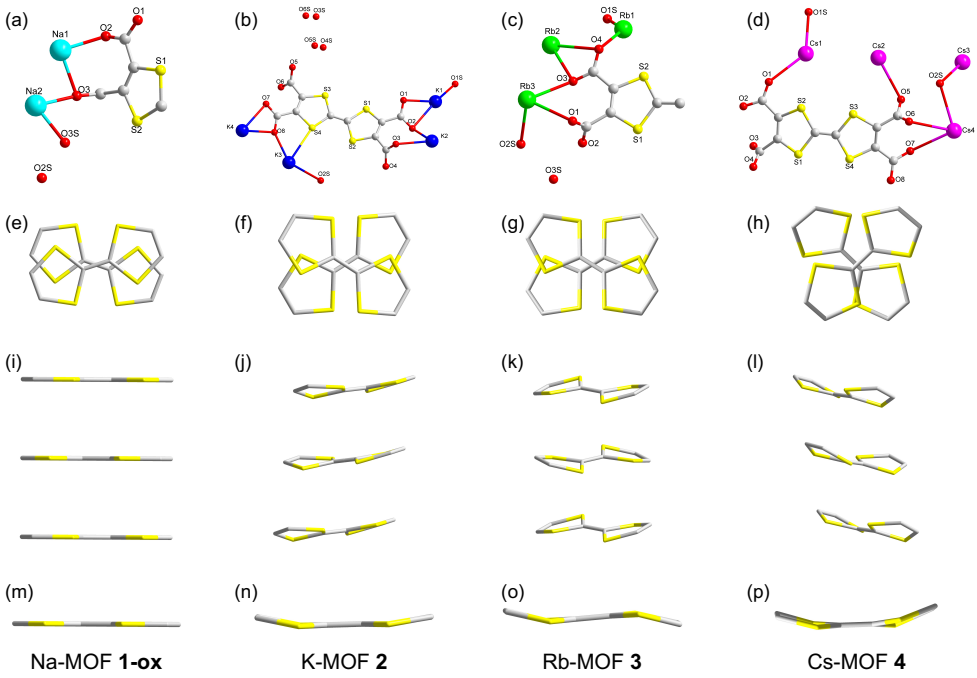

Fig. S1. (a–d) The asymmetric units, (e–f) the top-view of two consecutive TTFTC cores showing their relative orientation, (i–l) the side-view of three consecutive TTF layers showing their alignments, and (m–p) the side-view of each TTF-core showing their uniform shapes in MOFs.

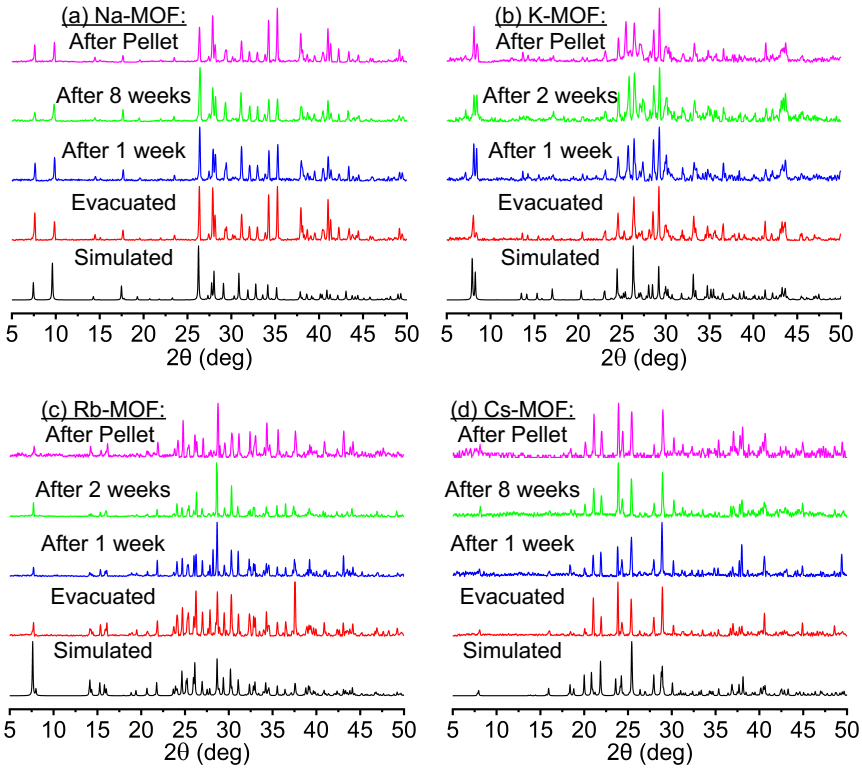

Fig. S2 The PXRD patterns of evacuated and air-exposed (a) Na-MOF, (b) K-MOF, (c) Rb-MOF, and (d) Cs-MOF at different stages.

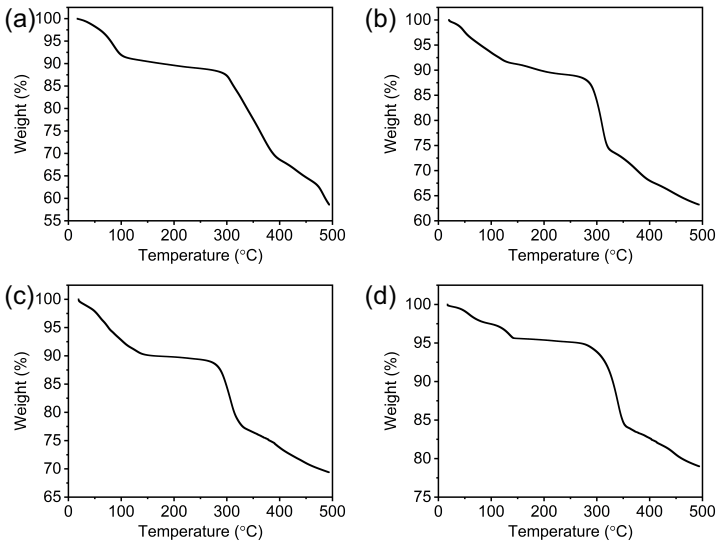

Fig. S3 The TGA profiles of (a) Na-MOF, (b) K-MOF, (c) Rb-MOF, and (d) Cs-MOF.

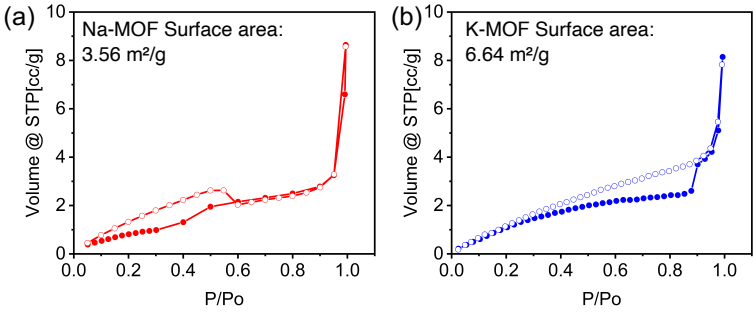

Fig. S4 The N_2 sorption isotherms of (a) Na-MOF and (b) K-MOF measured at 77 K.

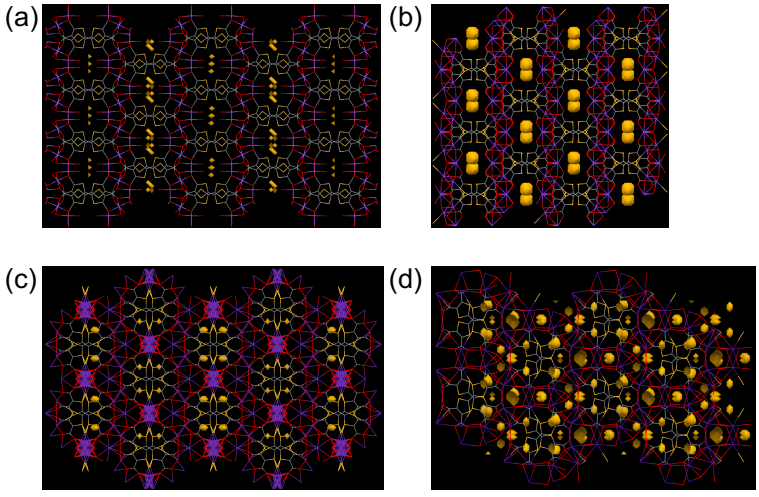

Fig. S5 The representations of the solvent-accessible voids in (a) Na-MOF packing cavity exhibiting 0.5 % void with a probe radius of 0.4 Å, (b) K-MOF packing cavity exhibiting 1.4 % void with a probe radius of 1.2 Å, (c) Rb-MOF packing cavity exhibiting 1.0 % void with a probe radius of 0.4 Å, and (d) Cs-MOF packing cavity exhibiting 2 % void with a probe radius of 0.5 Å.

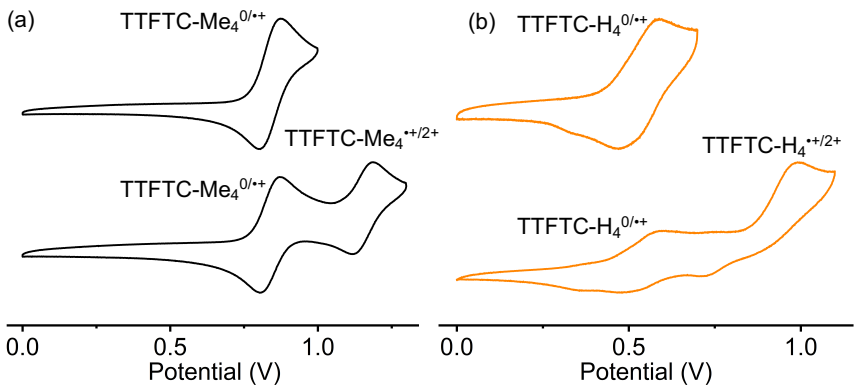

Fig. S6 The solution-phase CVs of (a) TTFTC-Me_4 and (b) TTFTC-H_4 in 0.1 M $TBAPF_6$ (glassy carbon working electrode, Pt-wire counter electrode, and Ag/AgCl reference electrode).

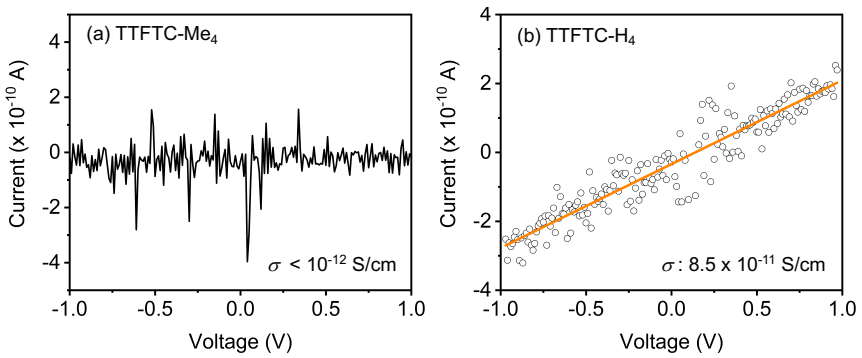

Fig. S7 The *I-V* plots of insulting / poorly conducting (a) TTFTC-Me_4 and (b) TTFTC-H_4 (at 293 K).

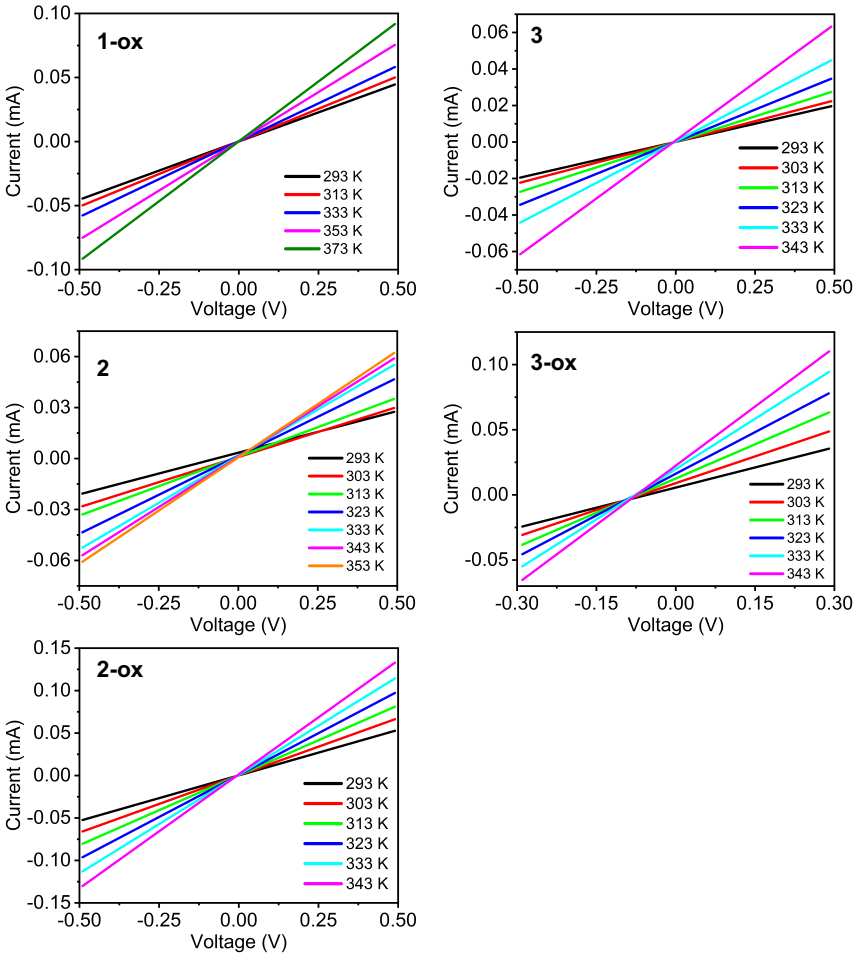

Fig. S8. The temperature-dependent *I-V* plots of freshly prepared and aerobically oxidized MOFs.

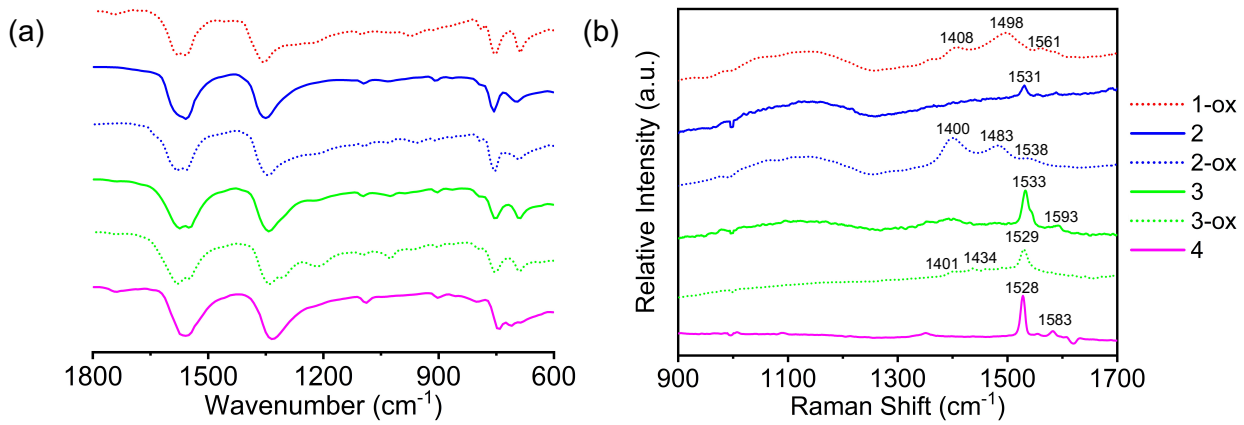

Fig. S9. (a) IR and (b) Raman spectra of MOFs.

Table S1. The crystallographic data of Na-MOF and K-MOF.

MOF	**1: $[Na_4(TTFTC)(H_2O)_2]\cdot 0.5H_2O$**	**2: $[K_4(TTFTC)(H_2O)_2]\cdot 2H_2O$**
Chemical formula	$C_{20}H_{10}Na_8O_{21}S_8$	$C_{10}H_8K_4O_{12}S_4$
Formula weight	1026.68	604.80
Temperature	100(2) K	208(2) K
Crystal system	Orthorhombic	Monoclinic
Space group	*I b a m*	*P 2₁ / c*
a(Å);α(°)	9.9733(6); 90	21.6112(12); 90
b(Å);β(°)	23.7417(16); 90	13.0967(7); 97.934(2)
c (Å); γ (°)	6.7824(4); 90	7.3463(4); 90
V(Å^3); Z	1605.96(17); 2	2059.36(19); 4
ρ(calc.) mgm^{-3}	2.123	1.951
μ(MoK$_\alpha$) mm^{-1}	0.760	1.328
2θ$_{max}$ (°)	50.052	50.054
R(int)	0.0488	0.0449
Completeness to θ	99.2 %	99.9 %
Data/param.	769 / 88	3643 / 355
GOF	1.155	1.079
R1[I>2sigma(I)]	0.0380	0.0682
wR2 (all data)	0.1041	0.2006
max. peak/hole (e.Å^{-3})	0.705 / -0.606	0.717 / -0.758

Table S2. The crystallographic data of Rb-MOF and Cs-MOF.

MOF	**3: $[Rb_4(TTFTC)(H_2O)_3]\cdot H_2O$**	**4: $[Cs_4(TTFTC)(H_2O)_2]$**
Chemical formula	$C_5H_4Rb_2O_6S_2$	$C_{10}H_4Cs_4O_{12}S_4$
Formula weight	395.14	944.01
Temperature	100(2) K	100(2) K
Crystal system	Orthorhombic	Orthorhombic
Space group	*P b c n*	*P n a 2₁*
a(Å);α(°)	12.5218(11); 90	7.3641(5); 90
b(Å);β(°)	23.348(2); 90	12.7617(8); 90
c (Å); γ (°)	7.3314(6); 90	22.6074(14); 90
V(Å^3); Z	2143.4(3); 8	2124.6(2); 4
ρ(calc.) mgm^{-3}	2.449	2.951
μ(MoK$_\alpha$) mm^{-1}	9.525	7.247
2θ$_{max}$ (°)	50.056	61.092
R(int)	0.0510	0.0497
Completeness to θ	99.5 %	99.7 %
Data/param.	1891 / 146	5935 / 255
GOF	1.074	1.088
R1[I>2sigma(I)]	0.0418	0.0443
wR2 (all data)	0.1095	0.1050
max. peak/hole (e.Å^{-3})	1.319 / -1.237	2.055 / -1.754

Crystallographic Data of MOFs.

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Na-MOF. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Na(1)	7500	2500	2500	16(1)
Na(2)	9286(2)	3350(1)	5000	27(1)
S(1)	4147(1)	4142(1)	0	17(1)
S(2)	6933(1)	4566(1)	0	19(1)
O(1)	3779(3)	2945(1)	0	15(1)
O(2)	5936(3)	2665(1)	0	14(1)
O(3)	8487(2)	3385(1)	1660(4)	19(1)
C(1)	5020(5)	3035(2)	0	12(1)
C(2)	5446(4)	3642(2)	0	14(1)
C(3)	6698(5)	3842(2)	0	15(1)
C(4)	7997(4)	3504(2)	0	17(1)
C(5)	5213(5)	4732(2)	0	16(1)
O(2S)	10000	5000	7500	51(3)
O(3S)	9261(6)	4339(2)	5698(9)	42(2)

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for K-MOF. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
K(1)	10752(1)	2566(1)	-22(2)	27(1)
K(2)	10474(1)	-411(1)	2655(2)	23(1)
K(3)	5469(1)	415(1)	2701(2)	21(1)
K(4)	4287(1)	2468(1)	5147(2)	24(1)
C(5)	7733(3)	2251(5)	1903(11)	6(2)
C(6)	7214(3)	2790(5)	2088(12)	6(2)
S(1)	8434(1)	2798(2)	1426(6)	11(1)
S(2)	7759(2)	915(2)	2112(6)	12(1)

S(3)	7175(1)	4133(2)	1858(6)	12(1)
S(4)	6516(1)	2226(2)	2475(5)	9(1)
C(5')	7781(16)	2250(30)	2840(50)	39(6)
C(6')	7250(14)	2800(30)	2980(60)	37(6)
S(1')	8475(6)	2810(11)	2320(40)	52(4)
S(2')	7820(7)	878(13)	2920(30)	48(4)
S(3')	7230(7)	4115(12)	2690(30)	47(4)
S(4')	6551(6)	2192(10)	3340(30)	46(3)
O(1)	9805(2)	2625(3)	2092(6)	24(1)
O(2)	9813(2)	1055(3)	946(6)	22(1)
O(3)	9296(2)	-324(4)	3786(6)	34(1)
O(4)	8632(4)	-919(7)	1238(18)	34(3)
O(4')	8546(5)	-994(9)	2170(20)	27(4)
O(5)	6394(3)	5923(4)	3597(10)	57(2)
O(6)	5712(2)	5468(4)	1175(7)	32(1)
O(7)	5237(2)	3991(3)	4033(6)	21(1)
O(8)	5236(2)	2390(3)	3021(6)	21(1)
C(1)	9552(2)	1786(4)	1611(7)	14(1)
C(2)	8879(3)	1676(4)	1862(8)	16(1)
C(3)	8572(3)	816(4)	2200(8)	19(1)
C(4)	8848(3)	-230(5)	2560(9)	22(1)
C(7)	6423(3)	4229(4)	2534(8)	16(1)
C(8)	6127(2)	3372(4)	2834(8)	14(1)
C(9)	5480(2)	3253(4)	3341(7)	12(1)
C(10)	6146(3)	5295(4)	2415(9)	22(1)
O(1S)	8573(3)	8877(4)	7278(8)	48(1)
O(2S)	6393(2)	-1113(4)	2542(8)	43(1)
O(3S)	7633(6)	8496(8)	4220(20)	54(3)
O(5S)	7415(9)	6518(18)	5240(30)	91(7)
O(4S)	7645(7)	6458(12)	4510(20)	49(4)
O(6S)	7362(12)	8420(20)	5420(40)	156(10)

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Rb-MOF. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rb(1)	6708(1)	7748(1)	3657(1)	29(1)
Rb(2)	5000	6870(1)	7500	45(1)
Rb(31)	5795(5)	4906(3)	8066(10)	79(1)
Rb(32)	5925(2)	5291(2)	9307(5)	79(1)
S(1)	10268(1)	5929(1)	4820(2)	21(1)
S(2)	8393(1)	5247(1)	5912(2)	21(1)
O(1)	8607(3)	7013(2)	2703(5)	23(1)
O(2)	9468(3)	7251(2)	5269(6)	27(1)
O(3)	6958(3)	6727(2)	5619(6)	27(1)
O(4)	6357(3)	5833(2)	5907(7)	32(1)
O(5)	5000	5757(7)	12500	112(5)
O(6)	10000	8433(6)	7500	101(4)
O(7)	8063(5)	8566(4)	5886(9)	85(2)
C(1)	9027(4)	6903(2)	4220(7)	20(1)
C(2)	9032(4)	6278(2)	4808(7)	18(1)
C(3)	7073(5)	6199(2)	5620(8)	22(1)
C(4)	8186(4)	5974(2)	5350(7)	18(1)
C(5)	9725(4)	5239(2)	5159(7)	20(1)

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Cs-MOF. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cs(1)	5312(2)	6420(1)	5416(1)	28(1)
Cs(2)	2454(1)	3989(1)	6788(1)	21(1)
Cs(3)	4784(1)	1324(1)	8672(1)	22(1)
Cs(4)	2901(1)	-1117(1)	7185(1)	19(1)
S(1)	4993(5)	2751(3)	3473(1)	18(1)
S(2)	3844(5)	4419(3)	4286(2)	19(1)

S(3)	2619(5)	2582(3)	5255(1)	17(1)
S(4)	4230(5)	993(3)	4472(2)	17(1)
O(1)	5200(30)	6449(9)	4105(6)	55(5)
O(2)	6207(15)	6302(8)	3174(5)	22(2)
O(3)	8543(14)	4520(9)	2818(5)	22(2)
O(4)	6337(15)	3665(8)	2335(4)	21(2)
O(5)	3317(18)	1706(9)	6594(4)	28(3)
O(6)	1248(14)	564(8)	6278(4)	20(2)
O(7)	4803(16)	-524(9)	5968(4)	26(2)
O(8)	4940(20)	-1061(9)	5039(5)	39(3)
C(1)	5630(30)	5935(11)	3659(7)	29(4)
C(2)	5311(19)	4789(11)	3701(6)	18(3)
C(3)	5837(18)	3998(10)	3330(5)	12(2)
C(4)	7060(20)	4080(11)	2783(6)	17(3)
C(5)	4080(20)	3060(11)	4174(6)	17(3)
C(6)	3690(20)	2332(10)	4567(6)	20(3)
C(7)	3090(20)	1362(10)	5568(6)	17(3)
C(8)	2532(19)	1171(11)	6193(7)	16(3)
C(9)	3940(19)	659(11)	5226(6)	18(3)
C(10)	4650(20)	-392(10)	5423(6)	18(3)
O(1S)	7155(15)	7990(8)	6302(5)	25(2)
O(2S)	2183(17)	1123(10)	7671(5)	29(3)

Table S7. Bond lengths [Å] and angles [°] for Na-MOF.

Na(1)-O(2)	2.337(2)
Na(1)-O(2)#1	2.337(2)
Na(1)-O(1)#2	2.370(2)
Na(1)-O(1)#3	2.370(2)
Na(1)-O(3)	2.390(2)
Na(1)-O(3)#1	2.390(2)
Na(1)-C(4)	2.967(4)
Na(1)-C(4)#1	2.967(4)
Na(1)-Na(2)	3.1821(17)
Na(1)-Na(2)#1	3.1821(17)

Na(1)-Na(1)#4	3.3912(2)
Na(1)-Na(1)#5	3.3912(2)
Na(2)-O(3S)	2.395(6)
Na(2)-O(3S)#6	2.395(6)
Na(2)-O(3)	2.403(2)
Na(2)-O(3)#6	2.403(2)
Na(2)-O(2)#1	2.421(4)
Na(2)-O(3)#7	2.491(3)
Na(2)-O(3)#8	2.491(3)
Na(2)-C(4)#8	2.734(5)
Na(2)-Na(2)#9	3.6779(16)
Na(2)-Na(2)#8	3.6779(16)
S(1)-C(2)	1.757(4)
S(1)-C(5)	1.758(5)
S(2)-C(3)	1.736(4)
S(2)-C(5)	1.759(5)
O(1)-C(1)	1.256(6)
O(2)-C(1)	1.268(5)
O(3)-C(4)	1.259(3)
C(1)-C(2)	1.503(6)
C(2)-C(3)	1.334(7)
C(3)-C(4)	1.523(6)
C(5)-C(5)#10	1.342(9)
O(3S)-O(3S)#6	0.947(12)

O(2)-Na(1)-O(2)#1	180.0
O(2)-Na(1)-O(1)#2	85.11(8)
O(2)#1-Na(1)-O(1)#2	94.89(8)
O(2)-Na(1)-O(1)#3	94.89(8)
O(2)#1-Na(1)-O(1)#3	85.11(8)
O(1)#2-Na(1)-O(1)#3	180.0
O(2)-Na(1)-O(3)	87.40(9)
O(2)#1-Na(1)-O(3)	92.61(9)
O(1)#2-Na(1)-O(3)	89.99(9)
O(1)#3-Na(1)-O(3)	90.01(9)
O(2)-Na(1)-O(3)#1	92.60(9)

O(2)#1-Na(1)-O(3)#1	87.39(9)
O(1)#2-Na(1)-O(3)#1	90.01(9)
O(1)#3-Na(1)-O(3)#1	89.99(9)
O(3)-Na(1)-O(3)#1	180.0
O(2)-Na(1)-C(4)	64.03(10)
O(2)#1-Na(1)-C(4)	115.98(10)
O(1)#2-Na(1)-C(4)	81.93(9)
O(1)#3-Na(1)-C(4)	98.07(9)
O(3)-Na(1)-C(4)	24.27(8)
O(3)#1-Na(1)-C(4)	155.73(8)
O(2)-Na(1)-C(4)#1	115.97(10)
O(2)#1-Na(1)-C(4)#1	64.03(10)
O(1)#2-Na(1)-C(4)#1	98.07(9)
O(1)#3-Na(1)-C(4)#1	81.93(9)
O(3)-Na(1)-C(4)#1	155.73(8)
O(3)#1-Na(1)-C(4)#1	24.27(8)
C(4)-Na(1)-C(4)#1	180.0
O(2)-Na(1)-Na(2)	130.84(8)
O(2)#1-Na(1)-Na(2)	49.16(8)
O(1)#2-Na(1)-Na(2)	111.28(8)
O(1)#3-Na(1)-Na(2)	68.72(8)
O(3)-Na(1)-Na(2)	48.58(6)
O(3)#1-Na(1)-Na(2)	131.42(6)
C(4)-Na(1)-Na(2)	72.62(6)
C(4)#1-Na(1)-Na(2)	107.38(6)
O(2)-Na(1)-Na(2)#1	49.16(8)
O(2)#1-Na(1)-Na(2)#1	130.84(8)
O(1)#2-Na(1)-Na(2)#1	68.72(8)
O(1)#3-Na(1)-Na(2)#1	111.28(8)
O(3)-Na(1)-Na(2)#1	131.42(6)
O(3)#1-Na(1)-Na(2)#1	48.58(6)
C(4)-Na(1)-Na(2)#1	107.38(6)
C(4)#1-Na(1)-Na(2)#1	72.62(6)
Na(2)-Na(1)-Na(2)#1	180.00(6)
O(2)-Na(1)-Na(1)#4	136.52(5)
O(2)#1-Na(1)-Na(1)#4	43.48(5)

O(1)#2-Na(1)-Na(1)#4	135.67(5)
O(1)#3-Na(1)-Na(1)#4	44.33(5)
O(3)-Na(1)-Na(1)#4	103.80(6)
O(3)#1-Na(1)-Na(1)#4	76.20(6)
C(4)-Na(1)-Na(1)#4	124.86(5)
C(4)#1-Na(1)-Na(1)#4	55.14(5)
Na(2)-Na(1)-Na(1)#4	57.801(19)
Na(2)#1-Na(1)-Na(1)#4	122.198(19)
O(2)-Na(1)-Na(1)#5	43.48(5)
O(2)#1-Na(1)-Na(1)#5	136.52(5)
O(1)#2-Na(1)-Na(1)#5	44.33(5)
O(1)#3-Na(1)-Na(1)#5	135.67(5)
O(3)-Na(1)-Na(1)#5	76.20(6)
O(3)#1-Na(1)-Na(1)#5	103.80(6)
C(4)-Na(1)-Na(1)#5	55.14(5)
C(4)#1-Na(1)-Na(1)#5	124.86(5)
Na(2)-Na(1)-Na(1)#5	122.199(19)
Na(2)#1-Na(1)-Na(1)#5	57.802(19)
Na(1)#4-Na(1)-Na(1)#5	180.0
O(3S)-Na(2)-O(3S)#6	22.8(3)
O(3S)-Na(2)-O(3)	98.59(16)
O(3S)#6-Na(2)-O(3)	77.09(16)
O(3S)-Na(2)-O(3)#6	77.09(16)
O(3S)#6-Na(2)-O(3)#6	98.59(16)
O(3)-Na(2)-O(3)#6	141.06(14)
O(3S)-Na(2)-O(2)#1	167.19(15)
O(3S)#6-Na(2)-O(2)#1	167.19(15)
O(3)-Na(2)-O(2)#1	90.21(8)
O(3)#6-Na(2)-O(2)#1	90.21(8)
O(3S)-Na(2)-O(3)#7	83.54(15)
O(3S)#6-Na(2)-O(3)#7	93.80(16)
O(3)-Na(2)-O(3)#7	136.10(10)
O(3)#6-Na(2)-O(3)#7	82.44(8)
O(2)#1-Na(2)-O(3)#7	96.59(11)
O(3S)-Na(2)-O(3)#8	93.80(16)
O(3S)#6-Na(2)-O(3)#8	83.54(15)

O(3)-Na(2)-O(3)#8	82.44(8)
O(3)#6-Na(2)-O(3)#8	136.10(10)
O(2)#1-Na(2)-O(3)#8	96.59(11)
O(3)#7-Na(2)-O(3)#8	53.73(12)
O(3S)-Na(2)-C(4)#8	83.08(18)
O(3S)#6-Na(2)-C(4)#8	83.08(18)
O(3)-Na(2)-C(4)#8	108.91(7)
O(3)#6-Na(2)-C(4)#8	108.91(7)
O(2)#1-Na(2)-C(4)#8	102.93(14)
O(3)#7-Na(2)-C(4)#8	27.39(6)
O(3)#8-Na(2)-C(4)#8	27.39(6)
O(3S)-Na(2)-Na(1)	136.18(15)
O(3S)#6-Na(2)-Na(1)	120.72(15)
O(3)-Na(2)-Na(1)	48.22(6)
O(3)#6-Na(2)-Na(1)	109.78(8)
O(2)#1-Na(2)-Na(1)	46.90(6)
O(3)#7-Na(2)-Na(1)	139.54(9)
O(3)#8-Na(2)-Na(1)	106.22(6)
C(4)#8-Na(2)-Na(1)	129.75(9)
O(3S)-Na(2)-Na(1)#4	120.72(15)
O(3S)#6-Na(2)-Na(1)#4	136.18(16)
O(3)-Na(2)-Na(1)#4	109.78(8)
O(3)#6-Na(2)-Na(1)#4	48.22(6)
O(2)#1-Na(2)-Na(1)#4	46.90(6)
O(3)#7-Na(2)-Na(1)#4	106.22(6)
O(3)#8-Na(2)-Na(1)#4	139.54(9)
C(4)#8-Na(2)-Na(1)#4	129.75(9)
Na(1)-Na(2)-Na(1)#4	64.40(4)
O(3S)-Na(2)-Na(2)#9	79.73(14)
O(3S)#6-Na(2)-Na(2)#9	100.74(15)
O(3)-Na(2)-Na(2)#9	176.08(11)
O(3)#6-Na(2)-Na(2)#9	42.18(5)
O(2)#1-Na(2)-Na(2)#9	92.04(3)
O(3)#7-Na(2)-Na(2)#9	40.38(6)
O(3)#8-Na(2)-Na(2)#9	94.11(10)
C(4)#8-Na(2)-Na(2)#9	67.44(6)

Na(1)-Na(2)-Na(2)#9	135.07(3)
Na(1)#4-Na(2)-Na(2)#9	74.06(3)
O(3S)-Na(2)-Na(2)#8	100.74(15)
O(3S)#6-Na(2)-Na(2)#8	79.73(14)
O(3)-Na(2)-Na(2)#8	42.18(5)
O(3)#6-Na(2)-Na(2)#8	176.08(11)
O(2)#1-Na(2)-Na(2)#8	92.04(3)
O(3)#7-Na(2)-Na(2)#8	94.11(10)
O(3)#8-Na(2)-Na(2)#8	40.38(6)
C(4)#8-Na(2)-Na(2)#8	67.44(6)
Na(1)-Na(2)-Na(2)#8	74.06(3)
Na(1)#4-Na(2)-Na(2)#8	135.07(3)
Na(2)#9-Na(2)-Na(2)#8	134.46(12)
C(2)-S(1)-C(5)	95.3(2)
C(3)-S(2)-C(5)	95.2(2)
C(1)-O(1)-Na(1)#11	127.30(13)
C(1)-O(1)-Na(1)#3	127.30(13)
Na(1)#11-O(1)-Na(1)#3	91.34(10)
C(1)-O(2)-Na(1)	126.66(13)
C(1)-O(2)-Na(1)#5	126.66(13)
Na(1)-O(2)-Na(1)#5	93.05(11)
C(1)-O(2)-Na(2)#1	128.6(3)
Na(1)-O(2)-Na(2)#1	83.94(9)
Na(1)#5-O(2)-Na(2)#1	83.94(9)
C(4)-O(3)-Na(1)	104.5(2)
C(4)-O(3)-Na(2)	168.3(2)
Na(1)-O(3)-Na(2)	83.20(9)
C(4)-O(3)-Na(2)#8	87.1(2)
Na(1)-O(3)-Na(2)#8	116.50(10)
Na(2)-O(3)-Na(2)#8	97.43(8)
O(1)-C(1)-O(2)	126.3(4)
O(1)-C(1)-C(2)	116.2(4)
O(2)-C(1)-C(2)	117.5(4)
C(3)-C(2)-C(1)	127.2(4)
C(3)-C(2)-S(1)	116.8(3)
C(1)-C(2)-S(1)	116.0(3)

C(2)-C(3)-C(4)	127.5(4)
C(2)-C(3)-S(2)	118.5(3)
C(4)-C(3)-S(2)	114.0(3)
O(3)#12-C(4)-O(3)	126.7(4)
O(3)#12-C(4)-C(3)	116.6(2)
O(3)-C(4)-C(3)	116.6(2)
O(3)#12-C(4)-Na(2)#8	65.5(2)
O(3)-C(4)-Na(2)#8	65.5(2)
C(3)-C(4)-Na(2)#8	155.9(3)
O(3)#12-C(4)-Na(1)#5	51.25(18)
O(3)-C(4)-Na(1)#5	113.3(3)
C(3)-C(4)-Na(1)#5	106.3(2)
Na(2)#8-C(4)-Na(1)#5	93.34(13)
O(3)#12-C(4)-Na(1)	113.3(3)
O(3)-C(4)-Na(1)	51.24(18)
C(3)-C(4)-Na(1)	106.3(2)
Na(2)#8-C(4)-Na(1)	93.34(13)
Na(1)#5-C(4)-Na(1)	69.71(10)
C(5)#10-C(5)-S(1)	124.3(5)
C(5)#10-C(5)-S(2)	121.4(5)
S(1)-C(5)-S(2)	114.3(2)
O(3S)#6-O(3S)-Na(2)	78.60(14)

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,-y+1/2,-z+1/2 #2 x+1/2,-y+1/2,z #3 -x+1,y+0,-z+1/2
#4 -x+3/2,-y+1/2,z+1/2 #5 -x+3/2,-y+1/2,z-1/2
#6 x,y,-z+1 #7 -x+2,y,z+1/2 #8 -x+2,y+0,-z+1/2
#9 -x+2,y+0,-z+3/2 #10 -x+1,-y+1,-z #11 x-1/2,-y+1/2,-z
#12 x,y,-z

Table S8. Bond lengths [Å] and angles [°] for K-MOF.

K(1)-O(1)	2.736(4)
K(1)-O(4)#1	2.747(10)
K(1)-O(1)#2	2.747(5)
K(1)-O(1S)#3	2.914(6)

K(1)-O(3)#4	2.916(5)
K(1)-O(2)	2.989(4)
K(1)-O(1S)#5	2.992(6)
K(1)-O(4')#4	3.063(13)
K(1)-O(4')#1	3.111(14)
K(1)-C(1)	3.172(5)
K(1)-C(1)#2	3.434(6)
K(1)-C(4)#4	3.452(6)
K(2)-O(2)	2.609(4)
K(2)-O(1)#3	2.654(4)
K(2)-O(2)#1	2.764(4)
K(2)-O(3)#6	2.767(5)
K(2)-O(3)	2.789(5)
K(2)-O(1S)#5	2.873(6)
K(2)-S(1')#3	3.252(13)
K(2)-S(1)#3	3.329(3)
K(2)-C(4)	3.513(6)
K(2)-C(1)	3.525(6)
K(3)-O(7)#7	2.625(4)
K(3)-O(8)	2.652(4)
K(3)-O(7)#2	2.783(4)
K(3)-O(6)#8	2.785(5)
K(3)-O(6)#7	2.789(5)
K(3)-O(2S)	2.841(6)
K(3)-S(4')	3.287(14)
K(3)-S(4)	3.298(3)
K(3)-C(10)#7	3.482(6)
K(3)-C(9)#7	3.518(5)
K(3)-K(4)#2	4.0506(19)
K(3)-K(4)#9	4.0994(19)
K(4)-O(8)#8	2.739(4)
K(4)-O(8)	2.746(4)
K(4)-O(6)#7	2.794(5)
K(4)-O(5)#10	2.799(5)
K(4)-O(2S)#11	2.952(6)
K(4)-O(2S)#9	2.981(6)

K(4)-O(7)	3.055(4)
K(4)-C(9)	3.227(6)
K(4)-C(9)#8	3.373(5)
K(4)-C(10)#7	3.468(6)
K(4)-K(4)#8	3.6741(2)
K(4)-K(4)#2	3.6741(2)
C(5)-C(6)	1.347(10)
C(5)-S(1)	1.755(7)
C(5)-S(2)	1.756(8)
C(6)-S(4)	1.739(7)
C(6)-S(3)	1.768(8)
S(1)-C(2)	1.761(6)
S(2)-C(3)	1.754(6)
S(3)-C(7)	1.768(6)
S(4)-C(8)	1.758(6)
C(5')-C(6')	1.37(5)
C(5')-S(1')	1.76(4)
C(5')-S(2')	1.79(4)
C(6')-S(3')	1.74(4)
C(6')-S(4')	1.76(3)
S(1')-C(2)	1.780(15)
S(2')-C(3)	1.780(17)
S(3')-C(7)	1.738(15)
S(4')-C(8)	1.809(15)
O(1)-C(1)	1.256(7)
O(2)-C(1)	1.246(7)
O(3)-C(4)	1.233(8)
O(4)-C(4)	1.360(12)
O(4')-C(4)	1.207(13)
O(5)-C(10)	1.260(8)
O(6)-C(10)	1.235(8)
O(7)-C(9)	1.242(7)
O(8)-C(9)	1.256(7)
C(1)-C(2)	1.497(7)
C(2)-C(3)	1.347(8)
C(3)-C(4)	1.503(8)

C(7)-C(8)	1.325(8)
C(7)-C(10)	1.517(8)
C(8)-C(9)	1.502(7)
O(3S)-O(6S)	1.12(3)
O(5S)-O(4S)	0.79(2)

O(1)-K(1)-O(4)#1	129.8(3)
O(1)-K(1)-O(1)#2	84.52(12)
O(4)#1-K(1)-O(1)#2	91.2(2)
O(1)-K(1)-O(1S)#3	141.17(15)
O(4)#1-K(1)-O(1S)#3	88.5(3)
O(1)#2-K(1)-O(1S)#3	89.60(15)
O(1)-K(1)-O(3)#4	74.65(13)
O(4)#1-K(1)-O(3)#4	152.2(2)
O(1)#2-K(1)-O(3)#4	105.79(14)
O(1S)#3-K(1)-O(3)#4	70.16(15)
O(1)-K(1)-O(2)	45.43(12)
O(4)#1-K(1)-O(2)	86.1(2)
O(1)#2-K(1)-O(2)	70.46(12)
O(1S)#3-K(1)-O(2)	159.22(16)
O(3)#4-K(1)-O(2)	119.97(13)
O(1)-K(1)-O(1S)#5	88.23(15)
O(4)#1-K(1)-O(1S)#5	60.7(3)
O(1)#2-K(1)-O(1S)#5	134.81(15)
O(1S)#3-K(1)-O(1S)#5	121.3(2)
O(3)#4-K(1)-O(1S)#5	115.06(16)
O(2)-K(1)-O(1S)#5	72.88(14)
O(1)-K(1)-O(4')#4	86.1(3)
O(4)#1-K(1)-O(4')#4	119.3(2)
O(1)#2-K(1)-O(4')#4	146.1(2)
O(1S)#3-K(1)-O(4')#4	77.7(3)
O(3)#4-K(1)-O(4')#4	40.4(2)
O(2)-K(1)-O(4')#4	122.2(3)
O(1S)#5-K(1)-O(4')#4	77.2(2)
O(1)-K(1)-O(4')#1	139.6(3)
O(4)#1-K(1)-O(4')#1	12.6(2)

O(1)#2-K(1)-O(4')#1	85.0(2)
O(1S)#3-K(1)-O(4')#1	77.5(3)
O(3)#4-K(1)-O(4')#1	145.6(3)
O(2)-K(1)-O(4')#1	94.4(3)
O(1S)#5-K(1)-O(4')#1	72.3(3)
O(1)-K(1)-C(1)	23.05(13)
O(4)#1-K(1)-C(1)	109.2(3)
O(1)#2-K(1)-C(1)	72.64(14)
O(1S)#3-K(1)-C(1)	154.74(16)
O(3)#4-K(1)-C(1)	97.00(14)
O(2)-K(1)-C(1)	23.08(13)
O(1S)#5-K(1)-C(1)	83.71(15)
O(4')#4-K(1)-C(1)	107.0(3)
O(4')#1-K(1)-C(1)	117.4(3)
O(1)-K(1)-C(1)#2	81.51(13)
O(4)#1-K(1)-C(1)#2	108.1(2)
O(1)#2-K(1)-C(1)#2	19.71(13)
O(1S)#3-K(1)-C(1)#2	80.35(15)
O(3)#4-K(1)-C(1)#2	86.25(14)
O(2)-K(1)-C(1)#2	82.26(12)
O(1S)#5-K(1)-C(1)#2	153.01(15)
C(1)-K(1)-C(1)#2	77.09(13)
O(1)-K(1)-C(4)#4	80.31(13)
O(4)#1-K(1)-C(4)#4	136.8(2)
O(1)#2-K(1)-C(4)#4	125.90(14)
O(1S)#3-K(1)-C(4)#4	72.35(16)
O(3)#4-K(1)-C(4)#4	20.15(14)
O(2)-K(1)-C(4)#4	123.92(13)
O(1S)#5-K(1)-C(4)#4	96.39(16)
C(1)-K(1)-C(4)#4	103.28(14)
C(1)#2-K(1)-C(4)#4	106.28(14)
O(2)-K(2)-O(1)#3	129.21(14)
O(2)-K(2)-O(2)#1	74.22(14)
O(1)#3-K(2)-O(2)#1	75.43(13)
O(2)-K(2)-O(3)#6	102.34(14)
O(1)#3-K(2)-O(3)#6	106.50(15)

O(2)#1-K(2)-O(3)#6	176.43(14)
O(2)-K(2)-O(3)	69.57(13)
O(1)#3-K(2)-O(3)	78.08(14)
O(2)#1-K(2)-O(3)	101.76(14)
O(3)#6-K(2)-O(3)	75.91(17)
O(2)-K(2)-O(1S)#5	80.62(15)
O(1)#3-K(2)-O(1S)#5	147.77(15)
O(2)#1-K(2)-O(1S)#5	107.20(16)
O(3)#6-K(2)-O(1S)#5	72.86(16)
O(3)-K(2)-O(1S)#5	130.39(16)
O(2)-K(2)-S(1')#3	149.9(4)
O(1)#3-K(2)-S(1')#3	58.1(3)
O(2)#1-K(2)-S(1')#3	81.4(5)
O(3)#6-K(2)-S(1')#3	102.1(5)
O(3)-K(2)-S(1')#3	134.0(3)
O(1S)#5-K(2)-S(1')#3	90.1(3)
O(2)-K(2)-S(1)#3	160.33(12)
O(1)#3-K(2)-S(1)#3	57.62(10)
O(2)#1-K(2)-S(1)#3	92.22(11)
O(3)#6-K(2)-S(1)#3	91.35(12)
O(3)-K(2)-S(1)#3	128.28(12)
O(1S)#5-K(2)-S(1)#3	90.19(13)
O(2)-K(2)-C(4)	57.39(14)
O(1)#3-K(2)-C(4)	80.24(13)
O(2)#1-K(2)-C(4)	84.80(14)
O(3)#6-K(2)-C(4)	92.53(15)
O(3)-K(2)-C(4)	18.34(14)
O(1S)#5-K(2)-C(4)	131.74(16)
S(1')#3-K(2)-C(4)	138.1(3)
S(1)#3-K(2)-C(4)	136.92(12)
O(2)-K(2)-C(1)	16.01(13)
O(1)#3-K(2)-C(1)	132.80(13)
O(2)#1-K(2)-C(1)	89.71(13)
O(3)#6-K(2)-C(1)	86.79(13)
O(3)-K(2)-C(1)	61.23(13)
O(1S)#5-K(2)-C(1)	79.34(15)

S(1')#3-K(2)-C(1)	163.7(4)
S(1)#3-K(2)-C(1)	169.45(11)
C(4)-K(2)-C(1)	53.59(13)
O(2)-K(2)-K(1)#8	64.61(10)
O(1)#3-K(2)-K(1)#8	150.63(11)
O(2)#1-K(2)-K(1)#8	132.44(10)
O(3)#6-K(2)-K(1)#8	45.15(10)
O(3)-K(2)-K(1)#8	85.74(11)
O(1S)#5-K(2)-K(1)#8	45.18(12)
S(1)#3-K(2)-K(1)#8	119.74(6)
C(4)-K(2)-K(1)#8	92.02(11)
C(1)-K(2)-K(1)#8	52.80(9)
O(2)-K(2)-K(1)#1	90.24(10)
O(1)#3-K(2)-K(1)#1	40.45(10)
O(2)#1-K(2)-K(1)#1	45.87(9)
O(3)#6-K(2)-K(1)#1	134.05(12)
O(3)-K(2)-K(1)#1	67.49(11)
O(1S)#5-K(2)-K(1)#1	153.06(13)
S(1)#3-K(2)-K(1)#1	90.25(6)
C(4)-K(2)-K(1)#1	57.68(10)
C(1)-K(2)-K(1)#1	98.50(10)
K(1)#8-K(2)-K(1)#1	148.81(4)
O(7)#7-K(3)-O(8)	129.14(14)
O(7)#7-K(3)-O(7)#2	73.38(14)
O(8)-K(3)-O(7)#2	78.60(13)
O(7)#7-K(3)-O(6)#8	99.97(13)
O(8)-K(3)-O(6)#8	109.74(14)
O(7)#2-K(3)-O(6)#8	171.63(13)
O(7)#7-K(3)-O(6)#7	70.54(13)
O(8)-K(3)-O(6)#7	75.94(13)
O(7)#2-K(3)-O(6)#7	103.32(14)
O(6)#8-K(3)-O(6)#7	78.66(16)
O(7)#7-K(3)-O(2S)	81.08(15)
O(8)-K(3)-O(2S)	146.48(15)
O(7)#2-K(3)-O(2S)	100.98(15)
O(6)#8-K(3)-O(2S)	72.58(15)

O(6)#7-K(3)-O(2S)	134.97(16)
O(7)#7-K(3)-S(4')	158.0(4)
O(8)-K(3)-S(4')	55.7(2)
O(7)#2-K(3)-S(4')	88.3(4)
O(6)#8-K(3)-S(4')	97.0(4)
O(6)#7-K(3)-S(4')	127.0(3)
O(2S)-K(3)-S(4')	90.8(2)
O(7)#7-K(3)-S(4)	147.50(12)
O(8)-K(3)-S(4)	56.14(10)
O(7)#2-K(3)-S(4)	77.48(11)
O(6)#8-K(3)-S(4)	107.50(12)
O(6)#7-K(3)-S(4)	131.23(11)
O(2S)-K(3)-S(4)	90.76(12)
O(7)#7-K(3)-C(10)#7	56.12(14)
O(8)-K(3)-C(10)#7	81.05(13)
O(7)#2-K(3)-C(10)#7	86.75(14)
O(6)#8-K(3)-C(10)#7	93.74(15)
O(6)#7-K(3)-C(10)#7	18.88(14)
O(2S)-K(3)-C(10)#7	132.47(15)
S(4)-K(3)-C(10)#7	136.33(11)
O(7)#7-K(3)-C(9)#7	16.33(12)
O(8)-K(3)-C(9)#7	133.81(13)
O(7)#2-K(3)-C(9)#7	89.59(12)
O(6)#8-K(3)-C(9)#7	84.02(13)
O(6)#7-K(3)-C(9)#7	63.54(13)
O(2S)-K(3)-C(9)#7	79.43(14)
S(4)-K(3)-C(9)#7	162.06(12)
C(10)#7-K(3)-C(9)#7	53.57(13)
O(7)#7-K(3)-K(4)#2	88.53(10)
O(8)-K(3)-K(4)#2	42.11(9)
O(7)#2-K(3)-K(4)#2	48.91(9)
O(6)#8-K(3)-K(4)#2	137.36(11)
O(6)#7-K(3)-K(4)#2	64.92(11)
O(2S)-K(3)-K(4)#2	149.88(13)
S(4)-K(3)-K(4)#2	82.96(6)
C(10)#7-K(3)-K(4)#2	56.90(10)

C(9)#7-K(3)-K(4)#2	97.97(9)
O(7)#7-K(3)-K(4)#9	64.41(10)
O(8)-K(3)-K(4)#9	151.66(11)
O(7)#2-K(3)-K(4)#9	128.85(9)
O(6)#8-K(3)-K(4)#9	42.80(10)
O(6)#7-K(3)-K(4)#9	89.01(11)
O(2S)-K(3)-K(4)#9	46.64(11)
S(4)-K(3)-K(4)#9	128.99(7)
C(10)#7-K(3)-K(4)#9	92.47(10)
C(9)#7-K(3)-K(4)#9	51.89(9)
K(4)#2-K(3)-K(4)#9	148.05(4)
O(8)#8-K(4)-O(8)	84.40(11)
O(8)#8-K(4)-O(6)#7	107.16(14)
O(8)-K(4)-O(6)#7	74.39(13)
O(8)#8-K(4)-O(5)#10	93.82(15)
O(8)-K(4)-O(5)#10	133.11(17)
O(6)#7-K(4)-O(5)#10	147.82(16)
O(8)#8-K(4)-O(2S)#11	136.36(15)
O(8)-K(4)-O(2S)#11	89.14(14)
O(6)#7-K(4)-O(2S)#11	112.46(16)
O(5)#10-K(4)-O(2S)#11	60.69(19)
O(8)#8-K(4)-O(2S)#9	88.69(14)
O(8)-K(4)-O(2S)#9	140.15(14)
O(6)#7-K(4)-O(2S)#9	70.36(15)
O(5)#10-K(4)-O(2S)#9	86.41(18)
O(2S)#11-K(4)-O(2S)#9	121.1(2)
O(8)#8-K(4)-O(7)	72.70(12)
O(8)-K(4)-O(7)	44.71(11)
O(6)#7-K(4)-O(7)	119.10(13)
O(5)#10-K(4)-O(7)	90.00(15)
O(2S)#11-K(4)-O(7)	72.59(13)
O(2S)#9-K(4)-O(7)	160.78(14)
O(8)#8-K(4)-C(9)	74.89(13)
O(8)-K(4)-C(9)	22.48(13)
O(6)#7-K(4)-C(9)	96.71(14)
O(5)#10-K(4)-C(9)	112.46(17)

O(2S)#11-K(4)-C(9)	82.92(14)
O(2S)#9-K(4)-C(9)	155.37(15)
O(7)-K(4)-C(9)	22.59(12)
O(8)#8-K(4)-C(9)#8	20.55(12)
O(8)-K(4)-C(9)#8	79.97(13)
O(6)#7-K(4)-C(9)#8	86.67(14)
O(5)#10-K(4)-C(9)#8	111.58(16)
O(2S)#11-K(4)-C(9)#8	154.68(15)
O(2S)#9-K(4)-C(9)#8	80.04(14)
O(7)-K(4)-C(9)#8	83.76(12)
C(9)-K(4)-C(9)#8	78.31(13)
O(8)#8-K(4)-C(10)#7	126.24(14)
O(8)-K(4)-C(10)#7	80.06(13)
O(6)#7-K(4)-C(10)#7	19.13(14)
O(5)#10-K(4)-C(10)#7	133.01(15)
O(2S)#11-K(4)-C(10)#7	94.67(16)
O(2S)#9-K(4)-C(10)#7	72.74(15)
O(7)-K(4)-C(10)#7	122.09(13)
C(9)-K(4)-C(10)#7	102.08(14)
C(9)#8-K(4)-C(10)#7	105.71(14)
O(8)#8-K(4)-K(4)#8	48.03(9)
O(8)-K(4)-K(4)#8	132.27(9)
O(6)#7-K(4)-K(4)#8	111.65(12)
O(5)#10-K(4)-K(4)#8	65.21(15)
O(2S)#11-K(4)-K(4)#8	125.85(12)
O(2S)#9-K(4)-K(4)#8	51.39(11)
O(7)-K(4)-K(4)#8	110.23(9)
C(9)-K(4)-K(4)#8	120.93(10)
C(9)#8-K(4)-K(4)#8	54.31(9)
C(10)#7-K(4)-K(4)#8	121.61(12)
O(8)#8-K(4)-K(4)#2	131.73(9)
O(8)-K(4)-K(4)#2	47.87(9)
O(6)#7-K(4)-K(4)#2	70.97(11)
O(5)#10-K(4)-K(4)#2	112.64(16)
O(2S)#11-K(4)-K(4)#2	52.08(11)
O(2S)#9-K(4)-K(4)#2	130.63(12)

O(7)-K(4)-K(4)#2	67.94(9)
C(9)-K(4)-K(4)#2	58.09(10)
C(9)#8-K(4)-K(4)#2	126.60(10)
C(10)#7-K(4)-K(4)#2	60.88(11)
K(4)#8-K(4)-K(4)#2	177.38(9)
C(6)-C(5)-S(1)	124.0(6)
C(6)-C(5)-S(2)	122.1(6)
S(1)-C(5)-S(2)	113.9(4)
C(5)-C(6)-S(4)	123.1(6)
C(5)-C(6)-S(3)	122.8(6)
S(4)-C(6)-S(3)	114.0(4)
C(5)-S(1)-C(2)	95.1(3)
C(5)-S(1)-K(2)#4	148.7(3)
C(2)-S(1)-K(2)#4	101.4(2)
C(3)-S(2)-C(5)	95.6(3)
C(6)-S(3)-C(7)	94.4(3)
C(6)-S(4)-C(8)	96.1(3)
C(6)-S(4)-K(3)	158.6(3)
C(8)-S(4)-K(3)	105.1(2)
C(6')-C(5')-S(1')	123(3)
C(6')-C(5')-S(2')	124(3)
S(1')-C(5')-S(2')	112.8(18)
C(5')-C(6')-S(3')	121(3)
C(5')-C(6')-S(4')	121(3)
S(3')-C(6')-S(4')	117.2(19)
C(5')-S(1')-C(2)	98.4(13)
C(2)-S(1')-K(2)#4	103.7(5)
C(3)-S(2')-C(5')	94.5(13)
C(7)-S(3')-C(6')	95.9(13)
C(6')-S(4')-C(8)	90.3(13)
C(6')-S(4')-K(3)	155.0(13)
C(8)-S(4')-K(3)	104.2(6)
C(1)-O(1)-K(2)#4	140.6(4)
C(1)-O(1)-K(1)	98.4(3)
K(2)#4-O(1)-K(1)	105.19(15)
C(1)-O(1)-K(1)#8	112.8(4)

K(2)#4-O(1)-K(1)#8	100.74(14)
K(1)-O(1)-K(1)#8	84.23(12)
C(1)-O(2)-K(2)	128.7(4)
C(1)-O(2)-K(2)#1	123.7(4)
K(2)-O(2)-K(2)#1	105.78(14)
C(1)-O(2)-K(1)	86.7(3)
K(2)-O(2)-K(1)	104.91(14)
K(2)#1-O(2)-K(1)	92.55(12)
C(4)-O(3)-K(2)#6	132.6(4)
C(4)-O(3)-K(2)	116.3(4)
K(2)#6-O(3)-K(2)	104.10(17)
C(4)-O(3)-K(1)#3	105.3(4)
K(2)#6-O(3)-K(1)#3	92.57(13)
K(2)-O(3)-K(1)#3	97.26(14)
C(4)-O(4)-K(1)#1	128.3(6)
C(4)-O(4')-K(1)#3	98.4(7)
C(4)-O(4')-K(1)#1	112.6(9)
K(1)#3-O(4')-K(1)#1	73.1(2)
C(10)-O(5)-K(4)#10	121.7(4)
C(10)-O(6)-K(3)#2	128.9(4)
C(10)-O(6)-K(3)#11	114.2(4)
K(3)#2-O(6)-K(3)#11	101.34(16)
C(10)-O(6)-K(4)#11	113.0(4)
K(3)#2-O(6)-K(4)#11	94.58(14)
K(3)#11-O(6)-K(4)#11	99.83(14)
C(9)-O(7)-K(3)#11	127.2(3)
C(9)-O(7)-K(3)#8	125.7(3)
K(3)#11-O(7)-K(3)#8	106.62(14)
C(9)-O(7)-K(4)	86.5(3)
K(3)#11-O(7)-K(4)	103.09(14)
K(3)#8-O(7)-K(4)	87.75(11)
C(9)-O(8)-K(3)	144.5(3)
C(9)-O(8)-K(4)#2	109.5(3)
K(3)-O(8)-K(4)#2	97.41(13)
C(9)-O(8)-K(4)	100.8(3)
K(3)-O(8)-K(4)	104.62(14)

K(4)#2-O(8)-K(4)	84.10(11)
O(2)-C(1)-O(1)	125.5(5)
O(2)-C(1)-C(2)	118.3(5)
O(1)-C(1)-C(2)	116.2(5)
O(2)-C(1)-K(1)	70.2(3)
O(1)-C(1)-K(1)	58.6(3)
C(2)-C(1)-K(1)	159.4(4)
O(2)-C(1)-K(1)#8	97.7(3)
O(1)-C(1)-K(1)#8	47.5(3)
C(2)-C(1)-K(1)#8	125.8(3)
K(1)-C(1)-K(1)#8	67.51(11)
O(2)-C(1)-K(2)	35.3(3)
O(1)-C(1)-K(2)	116.2(3)
C(2)-C(1)-K(2)	115.1(3)
K(1)-C(1)-K(2)	82.98(12)
K(1)#8-C(1)-K(2)	72.36(11)
C(3)-C(2)-C(1)	127.9(5)
C(3)-C(2)-S(1)	117.4(4)
C(1)-C(2)-S(1)	114.4(4)
C(3)-C(2)-S(1')	113.3(6)
C(1)-C(2)-S(1')	117.0(6)
C(2)-C(3)-C(4)	126.9(5)
C(2)-C(3)-S(2)	116.6(5)
C(4)-C(3)-S(2)	116.4(4)
C(2)-C(3)-S(2')	120.7(7)
C(4)-C(3)-S(2')	110.2(7)
O(4')-C(4)-O(3)	115.9(8)
O(3)-C(4)-O(4)	127.8(6)
O(4')-C(4)-C(3)	121.7(7)
O(3)-C(4)-C(3)	118.1(5)
O(4)-C(4)-C(3)	113.0(6)
O(3)-C(4)-K(1)#3	54.6(3)
O(4)-C(4)-K(1)#3	81.7(5)
C(3)-C(4)-K(1)#3	156.8(4)
O(4')-C(4)-K(2)	117.1(7)
O(3)-C(4)-K(2)	45.4(3)

O(4)-C(4)-K(2)	102.3(5)
C(3)-C(4)-K(2)	115.9(3)
K(1)#3-C(4)-K(2)	75.86(12)
C(8)-C(7)-C(10)	126.4(5)
C(8)-C(7)-S(3')	114.8(7)
C(10)-C(7)-S(3')	117.9(7)
C(8)-C(7)-S(3)	118.1(4)
C(10)-C(7)-S(3)	114.8(4)
C(7)-C(8)-C(9)	128.0(5)
C(7)-C(8)-S(4)	116.5(4)
C(9)-C(8)-S(4)	115.4(4)
C(7)-C(8)-S(4')	121.0(6)
C(9)-C(8)-S(4')	108.7(6)
O(7)-C(9)-O(8)	125.9(5)
O(7)-C(9)-C(8)	118.7(5)
O(8)-C(9)-C(8)	115.4(5)
O(7)-C(9)-K(4)	70.9(3)
O(8)-C(9)-K(4)	56.7(3)
C(8)-C(9)-K(4)	163.3(3)
O(7)-C(9)-K(4)#2	100.2(3)
O(8)-C(9)-K(4)#2	49.9(3)
C(8)-C(9)-K(4)#2	120.3(3)
K(4)-C(9)-K(4)#2	67.60(11)
O(7)-C(9)-K(3)#11	36.5(3)
O(8)-C(9)-K(3)#11	117.8(3)
C(8)-C(9)-K(3)#11	113.4(3)
K(4)-C(9)-K(3)#11	82.57(12)
K(4)#2-C(9)-K(3)#11	72.97(10)
O(6)-C(10)-O(5)	126.6(6)
O(6)-C(10)-C(7)	117.6(5)
O(5)-C(10)-C(7)	115.7(6)
O(6)-C(10)-K(4)#11	47.9(3)
O(5)-C(10)-K(4)#11	84.0(4)
C(7)-C(10)-K(4)#11	149.4(4)
O(6)-C(10)-K(3)#11	47.0(3)
O(5)-C(10)-K(3)#11	108.5(4)

C(7)-C(10)-K(3)#11	115.4(3)
K(4)#11-C(10)-K(3)#11	75.85(13)
K(2)#5-O(1S)-K(1)#4	90.44(16)
K(2)#5-O(1S)-K(1)#5	98.52(18)
K(1)#4-O(1S)-K(1)#5	77.00(14)
K(3)-O(2S)-K(4)#7	100.53(17)
K(3)-O(2S)-K(4)#9	89.48(15)
K(4)#7-O(2S)-K(4)#9	76.52(13)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z #2 x,-y+1/2,z-1/2 #3 -x+2,y-1/2,-z+1/2

#4 -x+2,y+1/2,-z+1/2 #5 -x+2,-y+1,-z+1 #6 -x+2,-y,-z+1

#7 -x+1,y-1/2,-z+1/2 #8 x,-y+1/2,z+1/2 #9 -x+1,-y,-z+1

#10 -x+1,-y+1,-z+1 #11 -x+1,y+1/2,-z+1/2

Table S9. Bond lengths [Å] and angles [°] for Rb-MOF.

Rb(1)-O(3)	2.802(4)
Rb(1)-O(2)#1	2.887(4)
Rb(1)-O(2)#2	2.913(4)
Rb(1)-O(1)	3.015(4)
Rb(1)-O(7)	3.033(8)
Rb(1)-O(3)#1	3.042(4)
Rb(1)-O(1)#3	3.044(4)
Rb(1)-C(1)#1	3.477(5)
Rb(1)-C(1)	3.535(5)
Rb(1)-O(6)#1	3.591(11)
Rb(1)-C(3)#1	3.652(6)
Rb(1)-C(2)#1	3.740(5)
Rb(2)-O(3)	2.833(4)
Rb(2)-O(3)#4	2.833(4)
Rb(2)-O(2)#3	2.962(4)
Rb(2)-O(2)#2	2.962(4)
Rb(2)-O(1)#3	3.140(4)
Rb(2)-O(1)#2	3.140(4)
Rb(2)-O(4)	3.181(4)

Rb(2)-O(4)#4	3.182(4)
Rb(2)-C(3)#4	3.331(6)
Rb(2)-C(3)	3.331(6)
Rb(2)-C(1)#3	3.359(5)
Rb(2)-C(1)#2	3.359(5)
Rb(31)-O(5)#5	1.887(16)
Rb(31)-Rb(31)#4	2.158(12)
Rb(31)-O(4)	2.772(7)
Rb(31)-O(4)#6	2.794(7)
Rb(31)-Rb(31)#5	3.493(15)
Rb(31)-O(4)#4	3.538(8)
Rb(31)-C(3)#6	3.566(8)
Rb(31)-O(6)#7	3.604(16)
Rb(31)-Rb(31)#8	3.6920(18)
Rb(31)-Rb(31)#6	3.6920(18)
Rb(31)-S(2)	3.702(6)
Rb(31)-S(2)#6	3.881(6)
Rb(32)-O(5)	2.830(8)
Rb(32)-O(4)	2.847(5)
Rb(32)-Rb(32)#5	2.870(6)
Rb(32)-O(4)#6	2.923(5)
Rb(32)-O(5)#5	3.013(14)
Rb(32)-O(4)#4	3.129(5)
Rb(32)-O(7)#3	3.173(9)
Rb(32)-Rb(32)#4	3.519(7)
Rb(32)-S(2)#6	3.537(3)
Rb(32)-C(3)	3.724(6)
Rb(32)-Rb(32)#8	3.909(3)
Rb(32)-Rb(32)#6	3.909(3)
S(1)-C(2)	1.749(5)
S(1)-C(5)	1.766(5)
S(2)-C(5)	1.758(5)
S(2)-C(4)	1.766(5)
O(1)-C(1)	1.257(7)
O(2)-C(1)	1.248(7)
O(3)-C(3)	1.241(7)

O(4)-C(3)	1.256(7)
C(1)-C(2)	1.521(7)
C(2)-C(4)	1.335(8)
C(3)-C(4)	1.502(8)
C(5)-C(5)#9	1.332(11)

O(3)-Rb(1)-O(2)#1	119.96(12)
O(3)-Rb(1)-O(2)#2	88.26(11)
O(2)#1-Rb(1)-O(2)#2	75.03(13)
O(3)-Rb(1)-O(1)	63.04(11)
O(2)#1-Rb(1)-O(1)	101.72(11)
O(2)#2-Rb(1)-O(1)	145.35(11)
O(3)-Rb(1)-O(7)	101.34(18)
O(2)#1-Rb(1)-O(7)	138.44(17)
O(2)#2-Rb(1)-O(7)	113.12(16)
O(1)-Rb(1)-O(7)	92.40(17)
O(3)-Rb(1)-O(3)#1	131.09(7)
O(2)#1-Rb(1)-O(3)#1	69.50(11)
O(2)#2-Rb(1)-O(3)#1	136.59(11)
O(1)-Rb(1)-O(3)#1	68.05(10)
O(7)-Rb(1)-O(3)#1	80.41(14)
O(3)-Rb(1)-O(1)#3	70.73(11)
O(2)#1-Rb(1)-O(1)#3	140.55(11)
O(2)#2-Rb(1)-O(1)#3	67.15(11)
O(1)-Rb(1)-O(1)#3	115.62(10)
O(7)-Rb(1)-O(1)#3	55.40(14)
O(3)#1-Rb(1)-O(1)#3	135.31(11)
O(3)-Rb(1)-C(1)#1	135.18(13)
O(2)#1-Rb(1)-C(1)#1	19.99(12)
O(2)#2-Rb(1)-C(1)#1	89.90(12)
O(1)-Rb(1)-C(1)#1	97.18(12)
O(7)-Rb(1)-C(1)#1	120.28(17)
O(3)#1-Rb(1)-C(1)#1	50.64(12)
O(1)#3-Rb(1)-C(1)#1	146.56(12)
O(3)-Rb(1)-C(1)	51.17(12)
O(2)#1-Rb(1)-C(1)	121.31(12)

O(2)#2-Rb(1)-C(1)	139.43(12)
O(1)-Rb(1)-C(1)	20.18(11)
O(7)-Rb(1)-C(1)	80.16(18)
O(3)#1-Rb(1)-C(1)	81.92(11)
O(1)#3-Rb(1)-C(1)	95.44(11)
C(1)#1-Rb(1)-C(1)	117.21(15)
O(3)-Rb(1)-O(6)#1	62.27(15)
O(2)#1-Rb(1)-O(6)#1	59.59(13)
O(2)#2-Rb(1)-O(6)#1	59.41(13)
O(1)-Rb(1)-O(6)#1	88.74(15)
O(7)-Rb(1)-O(6)#1	160.75(15)
O(3)#1-Rb(1)-O(6)#1	117.61(8)
O(1)#3-Rb(1)-O(6)#1	107.07(8)
C(1)#1-Rb(1)-O(6)#1	78.56(13)
C(1)-Rb(1)-O(6)#1	95.05(17)
O(3)-Rb(1)-C(3)#1	147.04(12)
O(2)#1-Rb(1)-C(3)#1	71.83(12)
O(2)#2-Rb(1)-C(3)#1	124.54(12)
O(1)-Rb(1)-C(3)#1	84.94(11)
O(7)-Rb(1)-C(3)#1	70.76(16)
O(3)#1-Rb(1)-C(3)#1	18.67(12)
O(1)#3-Rb(1)-C(3)#1	121.68(12)
C(1)#1-Rb(1)-C(3)#1	51.85(13)
C(1)-Rb(1)-C(3)#1	95.95(12)
O(6)#1-Rb(1)-C(3)#1	128.46(11)
O(3)-Rb(1)-C(2)#1	158.79(12)
O(2)#1-Rb(1)-C(2)#1	39.14(11)
O(2)#2-Rb(1)-C(2)#1	88.01(11)
O(1)-Rb(1)-C(2)#1	111.48(11)
O(7)-Rb(1)-C(2)#1	99.33(17)
O(3)#1-Rb(1)-C(2)#1	48.60(11)
O(1)#3-Rb(1)-C(2)#1	126.29(11)
C(1)#1-Rb(1)-C(2)#1	23.98(12)
C(1)-Rb(1)-C(2)#1	129.11(12)
O(6)#1-Rb(1)-C(2)#1	98.12(14)
C(3)#1-Rb(1)-C(2)#1	40.02(12)

O(3)-Rb(2)-O(3)#4	166.44(16)
O(3)-Rb(2)-O(2)#3	102.75(12)
O(3)#4-Rb(2)-O(2)#3	86.73(12)
O(3)-Rb(2)-O(2)#2	86.73(12)
O(3)#4-Rb(2)-O(2)#2	102.75(12)
O(2)#3-Rb(2)-O(2)#2	92.32(16)
O(3)-Rb(2)-O(1)#3	68.93(11)
O(3)#4-Rb(2)-O(1)#3	123.75(11)
O(2)#3-Rb(2)-O(1)#3	42.91(11)
O(2)#2-Rb(2)-O(1)#3	65.31(11)
O(3)-Rb(2)-O(1)#2	123.76(11)
O(3)#4-Rb(2)-O(1)#2	68.93(11)
O(2)#3-Rb(2)-O(1)#2	65.31(11)
O(2)#2-Rb(2)-O(1)#2	42.91(11)
O(1)#3-Rb(2)-O(1)#2	67.75(14)
O(3)-Rb(2)-O(4)	43.03(11)
O(3)#4-Rb(2)-O(4)	123.45(11)
O(2)#3-Rb(2)-O(4)	131.21(12)
O(2)#2-Rb(2)-O(4)	113.33(12)
O(1)#3-Rb(2)-O(4)	110.67(10)
O(1)#2-Rb(2)-O(4)	155.72(11)
O(3)-Rb(2)-O(4)#4	123.44(11)
O(3)#4-Rb(2)-O(4)#4	43.03(11)
O(2)#3-Rb(2)-O(4)#4	113.33(12)
O(2)#2-Rb(2)-O(4)#4	131.21(12)
O(1)#3-Rb(2)-O(4)#4	155.72(11)
O(1)#2-Rb(2)-O(4)#4	110.67(10)
O(4)-Rb(2)-O(4)#4	80.81(15)
O(3)-Rb(2)-C(3)#4	145.12(13)
O(3)#4-Rb(2)-C(3)#4	21.34(13)
O(2)#3-Rb(2)-C(3)#4	102.57(13)
O(2)#2-Rb(2)-C(3)#4	115.75(13)
O(1)#3-Rb(2)-C(3)#4	143.50(12)
O(1)#2-Rb(2)-C(3)#4	88.72(12)
O(4)-Rb(2)-C(3)#4	102.11(12)
O(4)#4-Rb(2)-C(3)#4	22.09(12)

O(3)-Rb(2)-C(3)	21.33(13)
O(3)#4-Rb(2)-C(3)	145.12(13)
O(2)#3-Rb(2)-C(3)	115.75(13)
O(2)#2-Rb(2)-C(3)	102.57(13)
O(1)#3-Rb(2)-C(3)	88.72(12)
O(1)#2-Rb(2)-C(3)	143.50(12)
O(4)-Rb(2)-C(3)	22.09(12)
O(4)#4-Rb(2)-C(3)	102.11(12)
C(3)#4-Rb(2)-C(3)	123.85(19)
O(3)-Rb(2)-C(1)#3	88.24(13)
O(3)#4-Rb(2)-C(1)#3	103.42(13)
O(2)#3-Rb(2)-C(1)#3	21.62(12)
O(2)#2-Rb(2)-C(1)#3	75.42(12)
O(1)#3-Rb(2)-C(1)#3	21.96(12)
O(1)#2-Rb(2)-C(1)#3	60.74(11)
O(4)-Rb(2)-C(1)#3	126.40(12)
O(4)#4-Rb(2)-C(1)#3	134.87(13)
C(3)#4-Rb(2)-C(1)#3	121.92(14)
C(3)-Rb(2)-C(1)#3	105.90(13)
O(3)-Rb(2)-C(1)#2	103.42(13)
O(3)#4-Rb(2)-C(1)#2	88.24(13)
O(2)#3-Rb(2)-C(1)#2	75.42(12)
O(2)#2-Rb(2)-C(1)#2	21.62(12)
O(1)#3-Rb(2)-C(1)#2	60.74(11)
O(1)#2-Rb(2)-C(1)#2	21.96(12)
O(4)-Rb(2)-C(1)#2	134.87(13)
O(4)#4-Rb(2)-C(1)#2	126.40(12)
C(3)#4-Rb(2)-C(1)#2	105.90(13)
C(3)-Rb(2)-C(1)#2	121.92(14)
C(1)#3-Rb(2)-C(1)#2	62.96(17)
O(5)#5-Rb(31)-Rb(31)#4	55.1(3)
O(5)#5-Rb(31)-O(4)	130.5(4)
Rb(31)#4-Rb(31)-O(4)	90.8(3)
O(5)#5-Rb(31)-O(4)#6	77.9(3)
Rb(31)#4-Rb(31)-O(4)#6	121.3(3)
O(4)-Rb(31)-O(4)#6	147.5(3)

O(5)#5-Rb(31)-Rb(31)#5	88.9(3)
Rb(31)#4-Rb(31)-Rb(31)#5	77.6(3)
O(4)-Rb(31)-Rb(31)#5	120.7(4)
O(4)#6-Rb(31)-Rb(31)#5	67.4(2)
O(5)#5-Rb(31)-O(4)#4	98.4(3)
Rb(31)#4-Rb(31)-O(4)#4	51.6(2)
O(4)-Rb(31)-O(4)#4	80.6(2)
O(4)#6-Rb(31)-O(4)#4	114.2(2)
Rb(31)#5-Rb(31)-O(4)#4	46.82(18)
O(5)#5-Rb(31)-C(3)#6	76.1(3)
Rb(31)#4-Rb(31)-C(3)#6	128.03(19)
O(4)-Rb(31)-C(3)#6	138.6(2)
O(4)#6-Rb(31)-C(3)#6	18.06(14)
Rb(31)#5-Rb(31)-C(3)#6	85.4(2)
O(4)#4-Rb(31)-C(3)#6	132.3(2)
O(5)#5-Rb(31)-O(6)#7	17.5(3)
Rb(31)#4-Rb(31)-O(6)#7	72.58(11)
O(4)-Rb(31)-O(6)#7	138.5(3)
O(4)#6-Rb(31)-O(6)#7	64.32(17)
Rb(31)#5-Rb(31)-O(6)#7	93.2(2)
O(4)#4-Rb(31)-O(6)#7	113.42(18)
C(3)#6-Rb(31)-O(6)#7	59.63(15)
O(5)#5-Rb(31)-Rb(31)#8	83.1(3)
Rb(31)#4-Rb(31)-Rb(31)#8	67.5(4)
O(4)-Rb(31)-Rb(31)#8	48.70(16)
O(4)#6-Rb(31)-Rb(31)#8	144.5(4)
Rb(31)#5-Rb(31)-Rb(31)#8	142.3(2)
O(4)#4-Rb(31)-Rb(31)#8	97.96(17)
C(3)#6-Rb(31)-Rb(31)#8	127.4(3)
O(6)#7-Rb(31)-Rb(31)#8	90.0(3)
O(5)#5-Rb(31)-Rb(31)#6	108.4(2)
Rb(31)#4-Rb(31)-Rb(31)#6	112.5(4)
O(4)-Rb(31)-Rb(31)#6	118.3(4)
O(4)#6-Rb(31)-Rb(31)#6	48.19(14)
Rb(31)#5-Rb(31)-Rb(31)#6	34.8(2)
O(4)#4-Rb(31)-Rb(31)#6	73.5(2)

C(3)#6-Rb(31)-Rb(31)#6	64.21(16)
O(6)#7-Rb(31)-Rb(31)#6	103.2(2)
Rb(31)#8-Rb(31)-Rb(31)#6	166.3(5)
O(5)#5-Rb(31)-S(2)	123.1(4)
Rb(31)#4-Rb(31)-S(2)	130.3(4)
O(4)-Rb(31)-S(2)	50.60(13)
O(4)#6-Rb(31)-S(2)	103.27(18)
Rb(31)#5-Rb(31)-S(2)	145.1(4)
O(4)#4-Rb(31)-S(2)	128.9(2)
C(3)#6-Rb(31)-S(2)	89.17(16)
O(6)#7-Rb(31)-S(2)	113.5(2)
Rb(31)#8-Rb(31)-S(2)	63.31(10)
Rb(31)#6-Rb(31)-S(2)	113.45(18)
O(5)#5-Rb(31)-S(2)#6	119.0(4)
Rb(31)#4-Rb(31)-S(2)#6	168.6(4)
O(4)-Rb(31)-S(2)#6	99.6(2)
O(4)#6-Rb(31)-S(2)#6	48.03(13)
Rb(31)#5-Rb(31)-S(2)#6	93.0(3)
O(4)#4-Rb(31)-S(2)#6	125.5(3)
C(3)#6-Rb(31)-S(2)#6	43.54(11)
O(6)#7-Rb(31)-S(2)#6	101.87(15)
Rb(31)#8-Rb(31)-S(2)#6	123.01(10)
Rb(31)#6-Rb(31)-S(2)#6	58.48(10)
S(2)-Rb(31)-S(2)#6	60.85(9)
O(5)-Rb(32)-O(4)	129.1(3)
O(5)-Rb(32)-Rb(32)#5	63.8(3)
O(4)-Rb(32)-Rb(32)#5	132.4(2)
O(5)-Rb(32)-O(4)#6	95.1(3)
O(4)-Rb(32)-O(4)#6	135.6(2)
O(5)-Rb(32)-O(5)#5	121.3(2)
O(4)-Rb(32)-O(5)#5	92.8(2)
O(4)#6-Rb(32)-O(5)#5	61.3(2)
O(5)-Rb(32)-O(4)#4	60.80(14)
O(4)-Rb(32)-O(4)#4	87.14(15)
O(4)#6-Rb(32)-O(4)#4	123.52(12)
O(5)#5-Rb(32)-O(4)#4	87.45(18)

O(5)-Rb(32)-O(7)#3	62.5(3)
O(4)-Rb(32)-O(7)#3	82.50(17)
O(4)#6-Rb(32)-O(7)#3	122.3(2)
O(5)#5-Rb(32)-O(7)#3	175.3(2)
O(4)#4-Rb(32)-O(7)#3	92.45(19)
O(5)-Rb(32)-Rb(32)#4	110.71(13)
O(4)-Rb(32)-Rb(32)#4	57.74(14)
O(4)#6-Rb(32)-Rb(32)#4	115.10(12)
O(5)#5-Rb(32)-Rb(32)#4	54.28(19)
O(4)#4-Rb(32)-Rb(32)#4	50.31(11)
O(7)#3-Rb(32)-Rb(32)#4	122.51(15)
O(5)-Rb(32)-S(2)#6	102.64(14)
O(4)-Rb(32)-S(2)#6	106.42(12)
O(4)#6-Rb(32)-S(2)#6	52.13(10)
O(5)#5-Rb(32)-S(2)#6	101.18(19)
O(4)#4-Rb(32)-S(2)#6	163.35(16)
O(7)#3-Rb(32)-S(2)#6	80.11(16)
O(5)-Rb(32)-C(3)	122.6(3)
O(4)-Rb(32)-C(3)	15.87(13)
Rb(32)#5-Rb(32)-C(3)	146.90(18)
O(4)#6-Rb(32)-C(3)	136.92(17)
O(5)#5-Rb(32)-C(3)	106.95(18)
O(4)#4-Rb(32)-C(3)	94.93(14)
O(7)#3-Rb(32)-C(3)	68.39(16)
Rb(32)#4-Rb(32)-C(3)	73.00(13)
S(2)#6-Rb(32)-C(3)	96.10(11)
O(5)-Rb(32)-Rb(32)#8	155.43(6)
O(4)-Rb(32)-Rb(32)#8	48.19(9)
O(4)#6-Rb(32)-Rb(32)#8	93.7(2)
O(5)#5-Rb(32)-Rb(32)#8	46.05(15)
O(4)#4-Rb(32)-Rb(32)#8	95.36(10)
O(7)#3-Rb(32)-Rb(32)#8	129.34(15)
S(2)#6-Rb(32)-Rb(32)#8	100.89(11)
C(3)-Rb(32)-Rb(32)#8	61.11(10)
O(5)-Rb(32)-Rb(32)#6	50.0(3)
O(4)-Rb(32)-Rb(32)#6	167.21(14)

O(4)#6-Rb(32)-Rb(32)#6	46.55(11)
O(5)#5-Rb(32)-Rb(32)#6	97.50(18)
O(4)#4-Rb(32)-Rb(32)#6	100.80(11)
O(7)#3-Rb(32)-Rb(32)#6	87.12(17)
S(2)#6-Rb(32)-Rb(32)#6	64.20(6)
C(3)-Rb(32)-Rb(32)#6	151.44(14)
C(2)-S(1)-C(5)	94.9(3)
C(2)-S(1)-Rb(1)#10	92.50(18)
C(5)-S(1)-Rb(1)#10	153.55(18)
C(5)-S(2)-C(4)	94.4(3)
C(5)-S(2)-Rb(32)#8	136.15(19)
C(4)-S(2)-Rb(32)#8	97.79(19)
C(5)-S(2)-Rb(31)	164.9(2)
C(4)-S(2)-Rb(31)	100.2(2)
C(5)-S(2)-Rb(31)#8	128.7(2)
C(4)-S(2)-Rb(31)#8	80.8(2)
Rb(31)-S(2)-Rb(31)#8	58.21(9)
C(5)-S(2)-Rb(32)	159.45(19)
C(4)-S(2)-Rb(32)	90.45(18)
Rb(32)#8-S(2)-Rb(32)	62.44(6)
C(1)-O(1)-Rb(1)	103.9(3)
C(1)-O(1)-Rb(1)#1	162.6(3)
Rb(1)-O(1)-Rb(1)#1	91.12(10)
C(1)-O(1)-Rb(2)#1	88.9(3)
Rb(1)-O(1)-Rb(2)#1	88.66(10)
Rb(1)#1-O(1)-Rb(2)#1	82.75(9)
C(1)-O(2)-Rb(1)#3	107.7(3)
C(1)-O(2)-Rb(1)#10	126.4(3)
Rb(1)#3-O(2)-Rb(1)#10	104.96(13)
C(1)-O(2)-Rb(2)#1	97.4(3)
Rb(1)#3-O(2)-Rb(2)#1	134.73(15)
Rb(1)#10-O(2)-Rb(2)#1	88.18(11)
C(3)-O(3)-Rb(1)	149.1(4)
C(3)-O(3)-Rb(2)	102.5(3)
Rb(1)-O(3)-Rb(2)	93.00(12)
C(3)-O(3)-Rb(1)#3	109.7(4)

Rb(1)-O(3)-Rb(1)#3	95.43(12)
Rb(2)-O(3)-Rb(1)#3	94.10(12)
C(3)-O(4)-Rb(31)	143.9(4)
C(3)-O(4)-Rb(31)#8	118.3(4)
Rb(31)-O(4)-Rb(31)#8	83.11(13)
C(3)-O(4)-Rb(32)	125.8(4)
C(3)-O(4)-Rb(32)#8	132.5(4)
Rb(31)-O(4)-Rb(32)#8	58.8(2)
Rb(31)#8-O(4)-Rb(32)#8	25.92(18)
C(3)-O(4)-Rb(32)#4	156.7(4)
Rb(31)-O(4)-Rb(32)#4	58.74(18)
Rb(31)#8-O(4)-Rb(32)#4	58.87(16)
C(3)-O(4)-Rb(2)	85.7(3)
Rb(31)-O(4)-Rb(2)	104.4(2)
Rb(31)#8-O(4)-Rb(2)	127.5(2)
Rb(32)-O(4)-Rb(2)	85.15(14)
Rb(32)#8-O(4)-Rb(2)	137.00(16)
Rb(32)#4-O(4)-Rb(2)	80.71(11)
C(3)-O(4)-Rb(31)#4	174.5(4)
Rb(31)-O(4)-Rb(31)#4	37.6(3)
Rb(31)#8-O(4)-Rb(31)#4	65.8(2)
Rb(2)-O(4)-Rb(31)#4	88.89(14)
Rb(31)#5-O(5)-Rb(31)#6	69.8(7)
Rb(31)#5-O(5)-Rb(32)#11	69.5(4)
Rb(31)#6-O(5)-Rb(32)#11	73.6(4)
Rb(32)#11-O(5)-Rb(32)	134.7(6)
Rb(31)#5-O(5)-Rb(32)#5	15.1(2)
Rb(31)#6-O(5)-Rb(32)#5	68.5(5)
Rb(31)#5-O(5)-Rb(32)#6	68.5(5)
Rb(31)#6-O(5)-Rb(32)#6	15.1(2)
Rb(1)#3-O(6)-Rb(1)#10	79.7(3)
Rb(1)#3-O(6)-Rb(31)#12	157.6(2)
Rb(1)#10-O(6)-Rb(31)#12	122.75(12)
Rb(1)#3-O(6)-Rb(31)#13	122.75(12)
Rb(1)#10-O(6)-Rb(31)#13	157.6(2)
Rb(31)#12-O(6)-Rb(31)#13	34.8(2)

Rb(1)-O(7)-Rb(32)#1	123.8(2)
Rb(1)-O(7)-Rb(2)#1	80.10(17)
O(2)-C(1)-O(1)	126.6(5)
O(2)-C(1)-C(2)	116.6(5)
O(1)-C(1)-C(2)	116.7(5)
O(2)-C(1)-Rb(2)#1	61.0(3)
O(1)-C(1)-Rb(2)#1	69.2(3)
C(2)-C(1)-Rb(2)#1	157.3(3)
O(2)-C(1)-Rb(1)#3	52.3(3)
O(1)-C(1)-Rb(1)#3	132.0(3)
C(2)-C(1)-Rb(1)#3	87.8(3)
Rb(2)#1-C(1)-Rb(1)#3	104.32(14)
O(2)-C(1)-Rb(1)	94.1(3)
O(1)-C(1)-Rb(1)	55.9(3)
C(2)-C(1)-Rb(1)	124.9(3)
Rb(2)#1-C(1)-Rb(1)	77.18(11)
Rb(1)#3-C(1)-Rb(1)	76.19(10)
C(4)-C(2)-C(1)	126.2(5)
C(4)-C(2)-S(1)	116.9(4)
C(1)-C(2)-S(1)	116.8(4)
C(4)-C(2)-Rb(1)#3	84.4(3)
C(1)-C(2)-Rb(1)#3	68.3(3)
S(1)-C(2)-Rb(1)#3	119.9(2)
O(3)-C(3)-O(4)	126.4(5)
O(3)-C(3)-C(4)	117.0(5)
O(4)-C(3)-C(4)	116.5(5)
O(3)-C(3)-Rb(2)	56.1(3)
O(4)-C(3)-Rb(2)	72.2(3)
C(4)-C(3)-Rb(2)	160.3(4)
O(3)-C(3)-Rb(31)#8	131.8(4)
O(4)-C(3)-Rb(31)#8	43.6(3)
C(4)-C(3)-Rb(31)#8	95.4(3)
Rb(2)-C(3)-Rb(31)#8	102.01(17)
O(3)-C(3)-Rb(1)#3	51.7(3)
O(4)-C(3)-Rb(1)#3	130.9(4)
C(4)-C(3)-Rb(1)#3	85.8(3)

Rb(2)-C(3)-Rb(1)#3	75.91(11)
Rb(31)#8-C(3)-Rb(1)#3	174.1(2)
O(3)-C(3)-Rb(32)	121.4(4)
O(4)-C(3)-Rb(32)	38.3(3)
C(4)-C(3)-Rb(32)	104.8(3)
Rb(2)-C(3)-Rb(32)	70.53(12)
Rb(1)#3-C(3)-Rb(32)	95.87(15)
C(2)-C(4)-C(3)	126.1(5)
C(2)-C(4)-S(2)	117.6(4)
C(3)-C(4)-S(2)	116.1(4)
C(5)#9-C(5)-S(2)	123.6(6)
C(5)#9-C(5)-S(1)	122.8(6)
S(2)-C(5)-S(1)	113.6(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,-y+3/2,z-1/2 #2 x-1/2,-y+3/2,-z+1
#3 -x+3/2,-y+3/2,z+1/2 #4 -x+1,y,-z+3/2 #5 -x+1,-y+1,-z+2
#6 x,-y+1,z+1/2 #7 x-1/2,y-1/2,-z+3/2 #8 x,-y+1,z-1/2
#9 -x+2,-y+1,-z+1 #10 x+1/2,-y+3/2,-z+1 #11 -x+1,y,-z+5/2
#12 x+1/2,y+1/2,-z+3/2 #13 -x+3/2,y+1/2,z

Table S10. Bond lengths [Å] and angles [°] for Cs-MOF.

Cs(1)-O(1)	2.966(13)
Cs(1)-O(1S)	3.140(10)
Cs(1)-O(1S)#1	3.159(12)
Cs(1)-O(6)#2	3.268(10)
Cs(1)-O(8)#3	3.337(12)
Cs(1)-C(10)#2	3.451(15)
Cs(1)-O(8)#2	3.546(16)
Cs(1)-O(7)#2	3.715(12)
Cs(1)-S(2)	3.770(4)
Cs(1)-C(9)#2	3.790(14)
Cs(1)-Cs(4)#2	4.4461(14)
Cs(1)-Cs(1)#1	4.5996(12)
Cs(2)-O(5)	3.015(11)

Cs(2)-O(6)#2	3.076(11)
Cs(2)-O(3)#4	3.095(11)
Cs(2)-O(5)#5	3.203(13)
Cs(2)-O(2)#4	3.306(10)
Cs(2)-O(7)#5	3.329(11)
Cs(2)-C(4)#4	3.356(14)
Cs(2)-O(4)#4	3.359(10)
Cs(2)-C(8)	3.841(14)
Cs(2)-C(8)#5	3.871(14)
Cs(2)-S(3)	3.905(3)
Cs(2)-Cs(4)#5	4.4068(13)
Cs(3)-O(2S)	2.975(11)
Cs(3)-O(1)#4	3.007(12)
Cs(3)-O(8)#6	3.115(12)
Cs(3)-O(2)#7	3.159(12)
Cs(3)-O(3)#7	3.246(11)
Cs(3)-O(2)#4	3.313(10)
Cs(3)-C(1)#7	3.41(2)
Cs(3)-C(1)#4	3.511(15)
Cs(3)-S(4)#6	3.542(3)
Cs(3)-O(1)#8	3.81(2)
Cs(3)-S(2)#8	3.870(4)
Cs(4)-O(3)#7	3.093(10)
Cs(4)-O(2S)	3.108(12)
Cs(4)-O(4)#8	3.151(11)
Cs(4)-O(1S)#5	3.162(11)
Cs(4)-O(7)	3.178(10)
Cs(4)-O(6)	3.208(10)
Cs(4)-O(4)#6	3.316(10)
Cs(4)-C(8)	3.692(15)
Cs(4)-C(3)#8	3.782(13)
Cs(4)-S(1)#8	3.887(4)
Cs(4)-S(1)#6	3.903(3)
Cs(4)-C(4)#8	3.908(16)
S(1)-C(3)	1.739(13)
S(1)-C(5)	1.766(14)

S(2)-C(5)	1.762(14)
S(2)-C(2)	1.771(14)
S(3)-C(7)	1.745(13)
S(3)-C(6)	1.772(15)
S(4)-C(6)	1.768(14)
S(4)-C(9)	1.770(14)
O(1)-C(1)	1.244(19)
O(2)-C(1)	1.264(18)
O(3)-C(4)	1.227(18)
O(4)-C(4)	1.264(18)
O(5)-C(8)	1.274(18)
O(6)-C(8)	1.238(18)
O(7)-C(10)	1.248(16)
O(8)-C(10)	1.238(17)
C(1)-C(2)	1.48(2)
C(2)-C(3)	1.369(18)
C(3)-C(4)	1.535(18)
C(5)-C(6)	1.318(17)
C(7)-C(9)	1.34(2)
C(7)-C(8)	1.49(2)
C(9)-C(10)	1.507(19)

O(1)-Cs(1)-O(1S)	129.8(4)
O(1)-Cs(1)-O(1S)#1	127.6(4)
O(1S)-Cs(1)-O(1S)#1	76.2(2)
O(1)-Cs(1)-O(6)#2	127.7(3)
O(1S)-Cs(1)-O(6)#2	91.3(3)
O(1S)#1-Cs(1)-O(6)#2	87.8(3)
O(1)-Cs(1)-O(8)#3	74.3(3)
O(1S)-Cs(1)-O(8)#3	65.4(3)
O(1S)#1-Cs(1)-O(8)#3	82.7(3)
O(6)#2-Cs(1)-O(8)#3	156.4(3)
O(1)-Cs(1)-C(10)#2	91.9(4)
O(1S)-Cs(1)-C(10)#2	80.8(3)
O(1S)#1-Cs(1)-C(10)#2	140.2(3)
O(6)#2-Cs(1)-C(10)#2	60.5(3)

O(8)#3-Cs(1)-C(10)#2	116.3(4)
O(1)-Cs(1)-O(8)#2	77.7(4)
O(1S)-Cs(1)-O(8)#2	79.6(3)
O(1S)#1-Cs(1)-O(8)#2	153.1(3)
O(6)#2-Cs(1)-O(8)#2	80.8(3)
O(8)#3-Cs(1)-O(8)#2	98.1(4)
C(10)#2-Cs(1)-O(8)#2	20.3(3)
O(1)-Cs(1)-O(7)#2	111.3(4)
O(1S)-Cs(1)-O(7)#2	66.3(3)
O(1S)#1-Cs(1)-O(7)#2	121.1(2)
O(6)#2-Cs(1)-O(7)#2	51.2(2)
O(8)#3-Cs(1)-O(7)#2	117.0(3)
C(10)#2-Cs(1)-O(7)#2	19.6(3)
O(8)#2-Cs(1)-O(7)#2	35.4(2)
O(1)-Cs(1)-S(2)	47.4(3)
O(1S)-Cs(1)-S(2)	171.1(2)
O(1S)#1-Cs(1)-S(2)	112.3(2)
O(6)#2-Cs(1)-S(2)	86.54(18)
O(8)#3-Cs(1)-S(2)	117.1(2)
C(10)#2-Cs(1)-S(2)	90.6(2)
O(8)#2-Cs(1)-S(2)	91.4(2)
O(7)#2-Cs(1)-S(2)	105.93(17)
O(1)-Cs(1)-C(9)#2	85.1(4)
O(1S)-Cs(1)-C(9)#2	102.4(3)
O(1S)#1-Cs(1)-C(9)#2	139.3(3)
O(6)#2-Cs(1)-C(9)#2	51.4(3)
O(8)#3-Cs(1)-C(9)#2	134.6(3)
C(10)#2-Cs(1)-C(9)#2	23.4(3)
O(8)#2-Cs(1)-C(9)#2	37.3(3)
O(7)#2-Cs(1)-C(9)#2	36.4(3)
S(2)-Cs(1)-C(9)#2	69.6(2)
O(1)-Cs(1)-Cs(4)#2	155.7(4)
O(1S)-Cs(1)-Cs(4)#2	45.3(2)
O(1S)#1-Cs(1)-Cs(4)#2	76.51(19)
O(6)#2-Cs(1)-Cs(4)#2	46.08(18)
O(8)#3-Cs(1)-Cs(4)#2	110.4(2)

C(10)#2-Cs(1)-Cs(4)#2	64.3(2)
O(8)#2-Cs(1)-Cs(4)#2	78.0(2)
O(7)#2-Cs(1)-Cs(4)#2	44.72(15)
S(2)-Cs(1)-Cs(4)#2	132.34(6)
C(9)#2-Cs(1)-Cs(4)#2	74.9(2)
O(1)-Cs(1)-Cs(1)#1	88.4(4)
O(1S)-Cs(1)-Cs(1)#1	87.91(19)
O(1S)#1-Cs(1)-Cs(1)#1	42.94(19)
O(6)#2-Cs(1)-Cs(1)#1	129.28(18)
O(8)#3-Cs(1)-Cs(1)#1	50.0(3)
C(10)#2-Cs(1)-Cs(1)#1	165.5(2)
O(8)#2-Cs(1)-Cs(1)#1	147.94(19)
O(7)#2-Cs(1)-Cs(1)#1	153.77(16)
S(2)-Cs(1)-Cs(1)#1	100.15(6)
C(9)#2-Cs(1)-Cs(1)#1	169.7(2)
Cs(4)#2-Cs(1)-Cs(1)#1	113.288(19)
O(5)-Cs(2)-O(6)#2	86.2(3)
O(5)-Cs(2)-O(3)#4	138.9(3)
O(6)#2-Cs(2)-O(3)#4	112.6(3)
O(5)-Cs(2)-O(5)#5	85.0(2)
O(6)#2-Cs(2)-O(5)#5	149.8(3)
O(3)#4-Cs(2)-O(5)#5	92.7(3)
O(5)-Cs(2)-O(2)#4	88.1(3)
O(6)#2-Cs(2)-O(2)#4	96.1(3)
O(3)#4-Cs(2)-O(2)#4	55.0(3)
O(5)#5-Cs(2)-O(2)#4	112.5(3)
O(5)-Cs(2)-O(7)#5	127.7(3)
O(6)#2-Cs(2)-O(7)#5	102.4(3)
O(3)#4-Cs(2)-O(7)#5	85.3(3)
O(5)#5-Cs(2)-O(7)#5	61.9(3)
O(2)#4-Cs(2)-O(7)#5	140.2(3)
O(5)-Cs(2)-C(4)#4	141.7(3)
O(6)#2-Cs(2)-C(4)#4	91.1(3)
O(3)#4-Cs(2)-C(4)#4	21.4(3)
O(5)#5-Cs(2)-C(4)#4	113.3(3)
O(2)#4-Cs(2)-C(4)#4	54.2(3)

O(7)#5-Cs(2)-C(4)#4	90.2(3)
O(5)-Cs(2)-O(4)#4	149.2(3)
O(6)#2-Cs(2)-O(4)#4	74.4(3)
O(3)#4-Cs(2)-O(4)#4	40.4(3)
O(5)#5-Cs(2)-O(4)#4	123.3(3)
O(2)#4-Cs(2)-O(4)#4	70.9(2)
O(7)#5-Cs(2)-O(4)#4	80.5(3)
C(4)#4-Cs(2)-O(4)#4	21.7(3)
O(5)-Cs(2)-C(8)	16.4(3)
O(6)#2-Cs(2)-C(8)	91.6(3)
O(3)#4-Cs(2)-C(8)	147.4(3)
O(5)#5-Cs(2)-C(8)	73.0(3)
O(2)#4-Cs(2)-C(8)	102.8(3)
O(7)#5-Cs(2)-C(8)	111.4(3)
C(4)#4-Cs(2)-C(8)	157.1(4)
O(4)#4-Cs(2)-C(8)	163.6(3)
O(5)-Cs(2)-C(8)#5	95.5(3)
O(6)#2-Cs(2)-C(8)#5	136.9(3)
O(3)#4-Cs(2)-C(8)#5	94.1(3)
O(5)#5-Cs(2)-C(8)#5	17.7(3)
O(2)#4-Cs(2)-C(8)#5	127.1(3)
O(7)#5-Cs(2)-C(8)#5	44.7(3)
C(4)#4-Cs(2)-C(8)#5	111.8(3)
O(4)#4-Cs(2)-C(8)#5	115.0(3)
C(8)-Cs(2)-C(8)#5	81.0(3)
O(5)-Cs(2)-S(3)	54.5(2)
O(6)#2-Cs(2)-S(3)	73.98(19)
O(3)#4-Cs(2)-S(3)	163.3(2)
O(5)#5-Cs(2)-S(3)	77.3(2)
O(2)#4-Cs(2)-S(3)	141.28(18)
O(7)#5-Cs(2)-S(3)	78.16(18)
C(4)#4-Cs(2)-S(3)	158.3(3)
O(4)#4-Cs(2)-S(3)	136.72(18)
C(8)-Cs(2)-S(3)	42.1(2)
C(8)#5-Cs(2)-S(3)	72.3(2)
O(5)-Cs(2)-Cs(4)#5	141.8(2)

O(6)#2-Cs(2)-Cs(4)#5	130.78(19)
O(3)#4-Cs(2)-Cs(4)#5	44.58(19)
O(5)#5-Cs(2)-Cs(4)#5	58.3(2)
O(2)#4-Cs(2)-Cs(4)#5	95.93(19)
O(7)#5-Cs(2)-Cs(4)#5	45.94(18)
C(4)#4-Cs(2)-Cs(4)#5	59.4(3)
O(4)#4-Cs(2)-Cs(4)#5	65.01(19)
C(8)-Cs(2)-Cs(4)#5	131.3(2)
C(8)#5-Cs(2)-Cs(4)#5	52.5(2)
S(3)-Cs(2)-Cs(4)#5	119.19(6)
O(2S)-Cs(3)-O(1)#4	109.3(4)
O(2S)-Cs(3)-O(8)#6	141.9(4)
O(1)#4-Cs(3)-O(8)#6	77.2(3)
O(2S)-Cs(3)-O(2)#7	109.3(3)
O(1)#4-Cs(3)-O(2)#7	97.0(4)
O(8)#6-Cs(3)-O(2)#7	107.0(4)
O(2S)-Cs(3)-O(3)#7	74.4(3)
O(1)#4-Cs(3)-O(3)#7	149.6(4)
O(8)#6-Cs(3)-O(3)#7	119.3(3)
O(2)#7-Cs(3)-O(3)#7	55.1(3)
O(2S)-Cs(3)-O(2)#4	71.3(3)
O(1)#4-Cs(3)-O(2)#4	41.1(3)
O(8)#6-Cs(3)-O(2)#4	116.7(3)
O(2)#7-Cs(3)-O(2)#4	95.3(3)
O(3)#7-Cs(3)-O(2)#4	122.0(3)
O(2S)-Cs(3)-C(1)#7	128.2(3)
O(1)#4-Cs(3)-C(1)#7	97.9(5)
O(8)#6-Cs(3)-C(1)#7	85.9(4)
O(2)#7-Cs(3)-C(1)#7	21.7(3)
O(3)#7-Cs(3)-C(1)#7	61.1(3)
O(2)#4-Cs(3)-C(1)#7	110.4(3)
O(2S)-Cs(3)-C(1)#4	91.4(4)
O(1)#4-Cs(3)-C(1)#4	20.1(3)
O(8)#6-Cs(3)-C(1)#4	97.0(3)
O(2)#7-Cs(3)-C(1)#4	95.0(4)
O(3)#7-Cs(3)-C(1)#4	137.2(3)

O(2)#4-Cs(3)-C(1)#4	21.1(3)
C(1)#7-Cs(3)-C(1)#4	103.3(4)
O(2S)-Cs(3)-S(4)#6	116.7(2)
O(1)#4-Cs(3)-S(4)#6	128.5(2)
O(8)#6-Cs(3)-S(4)#6	52.4(2)
O(2)#7-Cs(3)-S(4)#6	89.02(19)
O(3)#7-Cs(3)-S(4)#6	68.52(19)
O(2)#4-Cs(3)-S(4)#6	169.11(19)
C(1)#7-Cs(3)-S(4)#6	71.4(3)
C(1)#4-Cs(3)-S(4)#6	148.6(3)
O(2S)-Cs(3)-O(1)#8	65.0(3)
O(1)#4-Cs(3)-O(1)#8	83.1(4)
O(8)#6-Cs(3)-O(1)#8	79.1(4)
O(2)#7-Cs(3)-O(1)#8	173.8(3)
O(3)#7-Cs(3)-O(1)#8	123.3(3)
O(2)#4-Cs(3)-O(1)#8	80.6(3)
C(1)#7-Cs(3)-O(1)#8	164.4(3)
C(1)#4-Cs(3)-O(1)#8	82.9(4)
S(4)#6-Cs(3)-O(1)#8	95.82(19)
O(2S)-Cs(3)-S(2)#8	77.0(2)
O(1)#4-Cs(3)-S(2)#8	118.6(4)
O(8)#6-Cs(3)-S(2)#8	67.7(3)
O(2)#7-Cs(3)-S(2)#8	140.12(19)
O(3)#7-Cs(3)-S(2)#8	91.7(2)
O(2)#4-Cs(3)-S(2)#8	123.0(2)
C(1)#7-Cs(3)-S(2)#8	126.5(3)
C(1)#4-Cs(3)-S(2)#8	124.7(3)
S(4)#6-Cs(3)-S(2)#8	55.51(8)
O(1)#8-Cs(3)-S(2)#8	42.90(19)
O(2S)-Cs(3)-Cs(2)#2	64.8(2)
O(1)#4-Cs(3)-Cs(2)#2	112.0(3)
O(8)#6-Cs(3)-Cs(2)#2	149.5(3)
O(2)#7-Cs(3)-Cs(2)#2	44.52(19)
O(3)#7-Cs(3)-Cs(2)#2	40.86(19)
O(2)#4-Cs(3)-Cs(2)#2	82.11(19)
C(1)#7-Cs(3)-Cs(2)#2	64.3(3)

C(1)#4-Cs(3)-Cs(2)#2	96.5(3)
S(4)#6-Cs(3)-Cs(2)#2	107.80(6)
O(1)#8-Cs(3)-Cs(2)#2	129.78(19)
S(2)#8-Cs(3)-Cs(2)#2	124.06(6)
O(3)#7-Cs(4)-O(2S)	74.8(3)
O(3)#7-Cs(4)-O(4)#8	144.3(3)
O(2S)-Cs(4)-O(4)#8	82.8(3)
O(3)#7-Cs(4)-O(1S)#5	129.7(3)
O(2S)-Cs(4)-O(1S)#5	152.7(3)
O(4)#8-Cs(4)-O(1S)#5	80.2(3)
O(3)#7-Cs(4)-O(7)	88.0(3)
O(2S)-Cs(4)-O(7)	99.3(3)
O(4)#8-Cs(4)-O(7)	123.4(3)
O(1S)#5-Cs(4)-O(7)	73.1(3)
O(3)#7-Cs(4)-O(6)	116.2(3)
O(2S)-Cs(4)-O(6)	63.0(3)
O(4)#8-Cs(4)-O(6)	75.6(3)
O(1S)#5-Cs(4)-O(6)	92.1(3)
O(7)-Cs(4)-O(6)	57.0(3)
O(3)#7-Cs(4)-O(4)#6	93.9(3)
O(2S)-Cs(4)-O(4)#6	153.4(3)
O(4)#8-Cs(4)-O(4)#6	94.0(2)
O(1S)#5-Cs(4)-O(4)#6	49.7(2)
O(7)-Cs(4)-O(4)#6	104.3(3)
O(6)-Cs(4)-O(4)#6	141.7(2)
O(3)#7-Cs(4)-C(8)	97.8(3)
O(2S)-Cs(4)-C(8)	58.3(3)
O(4)#8-Cs(4)-C(8)	93.6(3)
O(1S)#5-Cs(4)-C(8)	101.6(3)
O(7)-Cs(4)-C(8)	47.0(3)
O(6)-Cs(4)-C(8)	19.1(3)
O(4)#6-Cs(4)-C(8)	148.2(3)
O(3)#7-Cs(4)-C(3)#8	106.8(3)
O(2S)-Cs(4)-C(3)#8	66.3(3)
O(4)#8-Cs(4)-C(3)#8	37.7(3)
O(1S)#5-Cs(4)-C(3)#8	109.6(3)

O(7)-Cs(4)-C(3)#8	154.7(3)
O(6)-Cs(4)-C(3)#8	97.8(3)
O(4)#6-Cs(4)-C(3)#8	95.2(3)
C(8)-Cs(4)-C(3)#8	109.4(3)
O(3)#7-Cs(4)-S(1)#8	102.4(2)
O(2S)-Cs(4)-S(1)#8	89.1(2)
O(4)#8-Cs(4)-S(1)#8	48.98(18)
O(1S)#5-Cs(4)-S(1)#8	95.6(2)
O(7)-Cs(4)-S(1)#8	168.1(2)
O(6)-Cs(4)-S(1)#8	121.28(19)
O(4)#6-Cs(4)-S(1)#8	69.64(19)
C(8)-Cs(4)-S(1)#8	135.1(2)
C(3)#8-Cs(4)-S(1)#8	26.2(2)
O(3)#7-Cs(4)-S(1)#6	57.2(2)
O(2S)-Cs(4)-S(1)#6	107.2(2)
O(4)#8-Cs(4)-S(1)#6	105.43(19)
O(1S)#5-Cs(4)-S(1)#6	97.84(19)
O(7)-Cs(4)-S(1)#6	126.7(2)
O(6)-Cs(4)-S(1)#6	170.1(2)
O(4)#6-Cs(4)-S(1)#6	48.15(17)
C(8)-Cs(4)-S(1)#6	154.8(2)
C(3)#8-Cs(4)-S(1)#6	78.4(2)
S(1)#8-Cs(4)-S(1)#6	57.34(4)
O(3)#7-Cs(4)-C(4)#8	128.0(3)
O(2S)-Cs(4)-C(4)#8	70.1(3)
O(4)#8-Cs(4)-C(4)#8	16.6(3)
O(1S)#5-Cs(4)-C(4)#8	96.0(3)
O(7)-Cs(4)-C(4)#8	134.2(3)
O(6)-Cs(4)-C(4)#8	79.8(3)
O(4)#6-Cs(4)-C(4)#8	100.7(3)
C(8)-Cs(4)-C(4)#8	95.2(3)
C(3)#8-Cs(4)-C(4)#8	22.9(3)
S(1)#8-Cs(4)-C(4)#8	41.5(2)
S(1)#6-Cs(4)-C(4)#8	98.5(2)
C(3)-S(1)-C(5)	95.7(6)
C(3)-S(1)-Cs(4)#9	73.5(4)

C(5)-S(1)-Cs(4)#9	112.4(5)
C(3)-S(1)-Cs(4)#10	102.0(4)
C(5)-S(1)-Cs(4)#10	160.1(5)
Cs(4)#9-S(1)-Cs(4)#10	81.79(7)
C(5)-S(2)-C(2)	95.4(7)
C(5)-S(2)-Cs(1)	137.4(5)
C(2)-S(2)-Cs(1)	98.7(5)
C(5)-S(2)-Cs(3)#9	129.4(5)
C(2)-S(2)-Cs(3)#9	89.2(5)
Cs(1)-S(2)-Cs(3)#9	90.92(8)
C(7)-S(3)-C(6)	96.1(7)
C(7)-S(3)-Cs(2)	93.3(5)
C(6)-S(3)-Cs(2)	151.2(5)
C(6)-S(4)-C(9)	95.1(7)
C(6)-S(4)-Cs(3)#10	156.3(5)
C(9)-S(4)-Cs(3)#10	108.4(5)
C(1)-O(1)-Cs(1)	142.9(12)
C(1)-O(1)-Cs(3)#11	103.5(10)
Cs(1)-O(1)-Cs(3)#11	109.7(4)
C(1)-O(1)-Cs(3)#9	90.7(13)
Cs(1)-O(1)-Cs(3)#9	106.4(5)
Cs(3)#11-O(1)-Cs(3)#9	87.6(4)
C(1)-O(2)-Cs(3)#12	90.5(10)
C(1)-O(2)-Cs(2)#11	151.6(9)
Cs(3)#12-O(2)-Cs(2)#11	93.4(3)
C(1)-O(2)-Cs(3)#11	88.3(8)
Cs(3)#12-O(2)-Cs(3)#11	94.4(3)
Cs(2)#11-O(2)-Cs(3)#11	119.3(3)
C(4)-O(3)-Cs(4)#12	126.9(9)
C(4)-O(3)-Cs(2)#11	91.3(8)
Cs(4)#12-O(3)-Cs(2)#11	90.8(3)
C(4)-O(3)-Cs(3)#12	134.4(9)
Cs(4)#12-O(3)-Cs(3)#12	98.1(3)
Cs(2)#11-O(3)-Cs(3)#12	95.8(3)
C(4)-O(4)-Cs(4)#9	118.0(9)
C(4)-O(4)-Cs(4)#10	114.9(9)

Cs(4)#9-O(4)-Cs(4)#10	104.1(3)
C(4)-O(4)-Cs(2)#11	79.0(8)
Cs(4)#9-O(4)-Cs(2)#11	98.3(3)
Cs(4)#10-O(4)-Cs(2)#11	142.3(3)
C(8)-O(5)-Cs(2)	121.7(9)
C(8)-O(5)-Cs(2)#2	112.4(9)
Cs(2)-O(5)-Cs(2)#2	116.6(4)
C(8)-O(6)-Cs(2)#5	129.5(9)
C(8)-O(6)-Cs(4)	103.1(9)
Cs(2)#5-O(6)-Cs(4)	103.2(3)
C(8)-O(6)-Cs(1)#5	123.6(9)
Cs(2)#5-O(6)-Cs(1)#5	100.1(3)
Cs(4)-O(6)-Cs(1)#5	86.7(2)
C(10)-O(7)-Cs(4)	147.7(10)
C(10)-O(7)-Cs(2)#2	121.6(9)
Cs(4)-O(7)-Cs(2)#2	85.2(2)
C(10)-O(7)-Cs(1)#5	68.2(9)
Cs(4)-O(7)-Cs(1)#5	79.9(3)
Cs(2)#2-O(7)-Cs(1)#5	152.9(3)
C(10)-O(8)-Cs(3)#10	141.5(10)
C(10)-O(8)-Cs(1)#13	119.9(9)
Cs(3)#10-O(8)-Cs(1)#13	98.3(3)
C(10)-O(8)-Cs(1)#5	75.5(10)
Cs(3)#10-O(8)-Cs(1)#5	106.7(4)
Cs(1)#13-O(8)-Cs(1)#5	83.8(3)
O(1)-C(1)-O(2)	126.3(14)
O(1)-C(1)-C(2)	115.3(14)
O(2)-C(1)-C(2)	118.3(13)
O(1)-C(1)-Cs(3)#12	99.5(14)
O(2)-C(1)-Cs(3)#12	67.7(10)
C(2)-C(1)-Cs(3)#12	107.4(10)
O(1)-C(1)-Cs(3)#11	56.4(8)
O(2)-C(1)-Cs(3)#11	70.6(8)
C(2)-C(1)-Cs(3)#11	165.3(12)
Cs(3)#12-C(1)-Cs(3)#11	86.6(4)
C(3)-C(2)-C(1)	129.9(13)

C(3)-C(2)-S(2)	115.7(10)
C(1)-C(2)-S(2)	114.0(11)
C(2)-C(3)-C(4)	127.6(12)
C(2)-C(3)-S(1)	117.4(10)
C(4)-C(3)-S(1)	115.0(9)
C(2)-C(3)-Cs(4)#9	104.0(9)
C(4)-C(3)-Cs(4)#9	83.1(8)
S(1)-C(3)-Cs(4)#9	80.3(5)
O(3)-C(4)-O(4)	128.3(13)
O(3)-C(4)-C(3)	120.2(13)
O(4)-C(4)-C(3)	111.6(12)
O(3)-C(4)-Cs(2)#11	67.2(8)
O(4)-C(4)-Cs(2)#11	79.3(8)
C(3)-C(4)-Cs(2)#11	130.7(9)
O(3)-C(4)-Cs(4)#9	151.8(10)
O(4)-C(4)-Cs(4)#9	45.4(7)
C(3)-C(4)-Cs(4)#9	73.9(7)
Cs(2)#11-C(4)-Cs(4)#9	85.1(3)
C(6)-C(5)-S(2)	125.1(11)
C(6)-C(5)-S(1)	122.1(11)
S(2)-C(5)-S(1)	112.8(7)
C(5)-C(6)-S(4)	123.3(11)
C(5)-C(6)-S(3)	124.3(11)
S(4)-C(6)-S(3)	112.4(7)
C(9)-C(7)-C(8)	124.5(12)
C(9)-C(7)-S(3)	117.2(11)
C(8)-C(7)-S(3)	118.3(10)
O(6)-C(8)-O(5)	124.8(14)
O(6)-C(8)-C(7)	117.4(13)
O(5)-C(8)-C(7)	117.5(13)
O(6)-C(8)-Cs(4)	57.8(8)
O(5)-C(8)-Cs(4)	87.6(9)
C(7)-C(8)-Cs(4)	133.2(9)
O(6)-C(8)-Cs(2)	121.3(9)
O(5)-C(8)-Cs(2)	41.9(7)
C(7)-C(8)-Cs(2)	100.6(8)

Cs(4)-C(8)-Cs(2)	121.9(4)
O(6)-C(8)-Cs(2)#2	129.0(10)
O(5)-C(8)-Cs(2)#2	49.9(8)
C(7)-C(8)-Cs(2)#2	94.6(8)
Cs(4)-C(8)-Cs(2)#2	71.2(3)
Cs(2)-C(8)-Cs(2)#2	86.7(3)
C(7)-C(9)-C(10)	125.9(12)
C(7)-C(9)-S(4)	116.8(11)
C(10)-C(9)-S(4)	117.3(10)
C(7)-C(9)-Cs(1)#5	94.3(9)
C(10)-C(9)-Cs(1)#5	65.6(8)
S(4)-C(9)-Cs(1)#5	111.3(6)
O(8)-C(10)-O(7)	125.7(13)
O(8)-C(10)-C(9)	117.8(13)
O(7)-C(10)-C(9)	116.4(12)
O(8)-C(10)-Cs(1)#5	84.2(10)
O(7)-C(10)-Cs(1)#5	92.2(9)
C(9)-C(10)-Cs(1)#5	91.0(8)
Cs(1)-O(1S)-Cs(1)#14	93.8(3)
Cs(1)-O(1S)-Cs(4)#2	89.7(3)
Cs(1)#14-O(1S)-Cs(4)#2	116.9(3)
Cs(3)-O(2S)-Cs(4)	103.8(4)

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+3/2,z #2 x+1/2,-y+1/2,z #3 x,y+1,z

#4 -x+1,-y+1,z+1/2 #5 x-1/2,-y+1/2,z #6 -x+1,-y,z+1/2

#7 -x+3/2,y-1/2,z+1/2 #8 -x+1/2,y-1/2,z+1/2

#9 -x+1/2,y+1/2,z-1/2 #10 -x+1,-y,z-1/2 #11 -x+1,-y+1,z-1/2

#12 -x+3/2,y+1/2,z-1/2 #13 x,y-1,z #14 x+1/2,-y+3/2,z

Table S11. Anisotropic displacement parameters ($Å^2$ x 10^3) for Na-MOF. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
Na(1)	18(1)	15(1)	14(1)	2(1)	-1(1)	5(1)
Na(2)	29(1)	24(1)	27(1)	0	0	-5(1)
S(1)	15(1)	11(1)	24(1)	0	0	2(1)
S(2)	17(1)	11(1)	28(1)	0	0	-1(1)
O(1)	15(2)	14(2)	16(2)	0	0	-5(1)
O(2)	15(2)	12(2)	15(2)	0	0	4(1)
O(3)	17(1)	19(1)	22(1)	2(1)	-5(1)	1(1)
C(1)	17(2)	12(2)	7(2)	0	0	-1(2)
C(2)	17(2)	12(2)	13(2)	0	0	3(2)
C(3)	20(2)	13(2)	13(2)	0	0	2(2)
C(4)	13(2)	13(2)	24(3)	0	0	-4(2)
C(5)	21(2)	13(2)	16(2)	0	0	2(2)
O(2S)	49(7)	56(8)	48(8)	0	0	0
O(3S)	49(3)	34(3)	43(4)	8(2)	-3(3)	8(2)

Table S12. Anisotropic displacement parameters ($Å^2$ x 10^3) for K-MOF. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
K(1)	23(1)	35(1)	24(1)	-1(1)	8(1)	-2(1)
K(2)	24(1)	17(1)	26(1)	3(1)	2(1)	5(1)
K(3)	24(1)	12(1)	28(1)	-1(1)	4(1)	-5(1)
K(4)	24(1)	26(1)	24(1)	-2(1)	8(1)	1(1)
C(5)	6(2)	6(2)	7(2)	0(1)	0(1)	1(1)
C(6)	6(2)	6(2)	7(2)	0(1)	1(1)	-1(1)
S(1)	4(1)	4(1)	26(2)	2(1)	4(1)	2(1)
S(2)	4(1)	4(1)	30(2)	-2(1)	2(1)	1(1)
S(3)	5(1)	4(1)	26(2)	-2(1)	6(1)	0(1)
S(4)	5(1)	3(1)	21(2)	0(1)	5(1)	2(1)

C(5')	44(13)	42(13)	31(13)	-14(11)	12(11)	2(11)
C(6')	29(11)	47(12)	35(13)	-14(11)	6(11)	-2(10)
S(1')	32(5)	53(6)	73(11)	-9(7)	16(7)	-3(4)
S(2')	34(6)	47(6)	62(10)	-7(7)	6(7)	0(4)
S(3')	35(6)	48(6)	61(10)	-5(7)	11(7)	1(4)
S(4')	31(5)	41(5)	69(10)	4(7)	16(7)	7(4)
O(1)	16(2)	22(2)	34(3)	-9(2)	5(2)	-4(2)
O(2)	22(2)	20(2)	25(2)	3(2)	9(2)	6(2)
O(3)	42(3)	37(3)	24(2)	11(2)	7(2)	13(2)
O(4)	34(3)	33(3)	35(3)	-1(1)	4(1)	1(1)
O(4')	27(4)	27(4)	28(4)	0(1)	3(1)	0(1)
O(5)	40(3)	25(3)	103(5)	-35(3)	-6(3)	4(2)
O(6)	31(3)	30(3)	35(3)	15(2)	6(2)	16(2)
O(7)	22(2)	18(2)	24(2)	4(2)	11(2)	9(2)
O(8)	14(2)	16(2)	32(2)	-5(2)	5(2)	-4(2)
C(1)	10(3)	17(3)	15(3)	-1(2)	5(2)	3(2)
C(2)	14(3)	14(3)	18(3)	-5(2)	-3(2)	3(2)
C(3)	8(3)	18(3)	29(3)	-10(2)	1(2)	1(2)
C(4)	9(3)	17(3)	41(4)	0(3)	6(3)	-1(2)
C(7)	15(3)	14(3)	21(3)	-6(2)	4(2)	2(2)
C(8)	12(3)	8(3)	20(3)	-4(2)	2(2)	4(2)
C(9)	15(3)	10(3)	10(3)	1(2)	0(2)	5(2)
C(10)	19(3)	14(3)	36(4)	-3(3)	15(3)	1(2)
O(1S)	35(3)	47(3)	64(4)	3(3)	18(3)	1(3)
O(2S)	37(3)	43(3)	52(3)	-6(3)	13(2)	-5(2)
O(3S)	49(7)	25(6)	84(9)	19(6)	-8(6)	-14(5)
O(5S)	78(16)	60(11)	130(20)	-14(13)	-17(12)	16(11)
O(4S)	41(9)	32(7)	73(11)	19(7)	9(6)	-10(6)
O(6S)	151(13)	144(13)	164(13)	6(9)	-6(9)	15(9)

Table S13. Anisotropic displacement parameters ($Å^2$ x 10^3) for Rb-MOF. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
Rb(1)	25(1)	37(1)	24(1)	11(1)	6(1)	14(1)
Rb(2)	31(1)	20(1)	86(1)	0	36(1)	0
Rb(31)	51(1)	95(2)	90(2)	61(2)	-2(2)	3(2)
Rb(32)	51(1)	95(2)	90(2)	61(2)	-2(2)	3(2)
S(1)	17(1)	21(1)	24(1)	4(1)	1(1)	2(1)
S(2)	20(1)	20(1)	24(1)	2(1)	4(1)	1(1)
O(1)	23(2)	24(2)	22(2)	5(2)	3(2)	8(2)
O(2)	30(2)	25(2)	27(2)	-3(2)	4(2)	-7(2)
O(3)	24(2)	21(2)	37(2)	-4(2)	13(2)	3(2)
O(4)	18(2)	27(2)	51(3)	0(2)	3(2)	-1(2)
O(5)	91(8)	197(14)	47(6)	0	8(6)	0
O(6)	40(5)	146(11)	118(10)	0	16(6)	0
O(7)	62(4)	155(7)	40(3)	6(4)	2(3)	-14(5)
C(1)	15(3)	23(3)	21(3)	-1(2)	9(2)	2(2)
C(2)	18(3)	22(3)	14(2)	-1(2)	1(2)	6(2)
C(3)	21(3)	23(3)	22(3)	0(2)	0(2)	1(2)
C(4)	20(3)	17(3)	16(2)	1(2)	1(2)	1(2)
C(5)	21(3)	23(3)	16(2)	2(2)	2(2)	-1(2)

Table S14. Anisotropic displacement parameters ($Å^2$ x 10^3) for Cs-MOF. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
Cs(1)	38(1)	21(1)	24(1)	-3(1)	2(1)	2(1)
Cs(2)	22(1)	16(1)	26(1)	-6(1)	0(1)	0(1)
Cs(3)	30(1)	15(1)	22(1)	1(1)	-5(1)	0(1)
Cs(4)	21(1)	16(1)	21(1)	1(1)	-1(1)	-2(1)
S(1)	25(2)	10(2)	18(1)	0(1)	1(1)	-2(1)
S(2)	26(2)	12(2)	19(2)	1(1)	5(1)	1(1)
S(3)	21(2)	14(2)	17(1)	1(1)	1(1)	2(1)
S(4)	24(2)	12(1)	16(1)	0(1)	0(1)	0(1)

O(1)	127(16)	12(6)	26(6)	-1(5)	24(7)	-6(8)
O(2)	23(6)	14(5)	28(5)	1(4)	4(4)	3(4)
O(3)	17(6)	20(5)	30(5)	4(4)	3(4)	-1(4)
O(4)	21(6)	22(5)	20(5)	-1(4)	2(4)	-1(4)
O(5)	44(8)	20(5)	21(5)	0(4)	-2(5)	-1(5)
O(6)	19(5)	18(5)	23(5)	4(4)	3(4)	-3(4)
O(7)	39(7)	23(6)	16(5)	0(4)	2(4)	9(5)
O(8)	77(11)	16(6)	26(6)	2(5)	-2(6)	2(6)
C(1)	56(12)	12(6)	19(7)	1(6)	4(7)	-2(7)
C(2)	18(7)	14(6)	22(6)	3(5)	5(6)	1(5)
C(3)	11(6)	14(6)	12(6)	0(4)	4(5)	3(5)
C(4)	23(8)	12(6)	14(6)	3(5)	7(5)	1(6)
C(5)	22(7)	14(6)	15(6)	4(5)	-4(5)	-3(6)
C(6)	26(8)	12(6)	22(7)	3(5)	-2(6)	1(6)
C(7)	16(7)	10(6)	25(7)	5(5)	-6(5)	4(5)
C(8)	14(7)	15(6)	20(7)	-3(5)	-1(5)	5(5)
C(9)	17(7)	16(7)	20(6)	1(5)	-2(5)	1(6)
C(10)	31(8)	7(5)	16(6)	0(5)	2(6)	-2(5)
O(1S)	32(6)	16(5)	27(5)	-6(4)	-8(5)	10(5)
O(2S)	30(7)	37(7)	20(5)	2(4)	2(4)	-3(5)

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