Synthesis and structure of $[Na_4(DMSO)_{15}][(I_3)_3(I)]$. Self-assembly of hexacoordinated sodium.

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Materials and Methods. The reagents, dimethyl sulfoxide (DMSO, 99.9%, Carlo Erba), iodomethane (98%, stabilized with silver, Merck) and sodium hydroxide (≥97%, pellets, Merck), were used without further purification. ^{1}H NMR and ^{13}C NMR spectra were acquired at 25°C on a Bruker Avance 400 MHz spectrometer, using the solvent residual signal as the reference for chemical shifts. FT-IR spectra were obtained using a Perkin-Elmer, Paragon 500, Serial 1000 (4000 - 400 cm^{-1}) using KBr disks. Thermogravimetric analysis (TG) and differential scanning calorimetry (DSC) were performed on a Rheometrics Scientific STA instrument in a nitrogen atmosphere with a continuous flow of 40 ml/min +/- 2 ml/min and a heating rate of 2 K/min, from 25°C to 400°C.

Synthesis of $[Na_4(DMSO)_{15}][(I)(I_3)_3]$ (1). NaOH powder (0.170 g, 4.24 mmol) was added to a DMSO (11.010 g, 140.91 mmol) and distilled water (0.130 g, 7.20 mmol) solution. The resulting mixture was ultrasonicated for 30 min, CH_3I (3.420 g, 24.09 mmol) was added, and ultrasonication was continued for 1.5 h. The obtained yellow solution was kept at 20°C for 6 d, with continuous agitation. The color of the solution changed from yellow to red, and a white precipitate formed. The precipitate was filtered, washed with ethanol and identified as $[(CH_3)_3SO]I$ (**2**). The filtrate was, refrigerated at 4°C for 8 d, where green crystals with a metallic luster formed for **1**. The crystals of **1** were filtered and dried in a vacuum. Compound **1** is hygroscopic, soluble in water, methanol, ethanol, DMSO and acetonitrile, partially soluble in dichloromethane and insoluble in toluene. The yield obtained was 0.762 g, 28%. ^{1}H NMR (DMSO-d_6): δ 2.54(s, 6H). ^{13}C NMR (DMSO-d_6): δ 40.34 (CH_3). ^{1}H NMR ($CDCl_3$): δ 2.63 (s, 6H). ^{13}C NMR ($CDCl_3$): δ 40.99 (CH_3). ^{1}H NMR (D_2O): δ 2.80 (s, 6H). ^{13}C NMR (D_2O): δ 39.04 (CH_3). IR (KBr, cm^{-1}): 2986 (m), 2906 (m), ν(C-H); 1436 (s), 1403 (m), 1313 (m), δ(C-H); 1017 (vs), ν(S=O); 952 (s), 934(m), 897 (w), δ(C-H); 704 (s), 674 (m), ν(C-S).

Compound **2** was identified as trimethyl sulfoxonium iodide[1-4] (0.694 g, 13%). ^{1}H NMR (DMSO-d_6): δ 3.87 (s, 9H). ^{13}C NMR (DMSO-d_6): δ 39.02 (CH_3). IR (KBr, cm^{-1}): 2962 (vs), 2880 (s), ν(C-H); 1402 (s), 1339 (w), 1312 (m), δ(C-H); 1229 (vs), ν(S=O); 1039 (vs), 952(s), δ(C-H); 757 (m),ν(C-S).

Additional experiments were conducted under similar conditions as the synthesis of **1**. We used LiOH, KOH, RbOH and CsOH instead of NaOH, but the reactions did not yield the complexes containing the cations Li^+, K^+, Rb^+ or Cs^+ ions. Subsequently, NaI (4.24 mmol) was added to the final solutions of each experiment, and the mixture was kept refrigerated at 4°C for 3 d. Crystals of **1** were formed in all solutions.

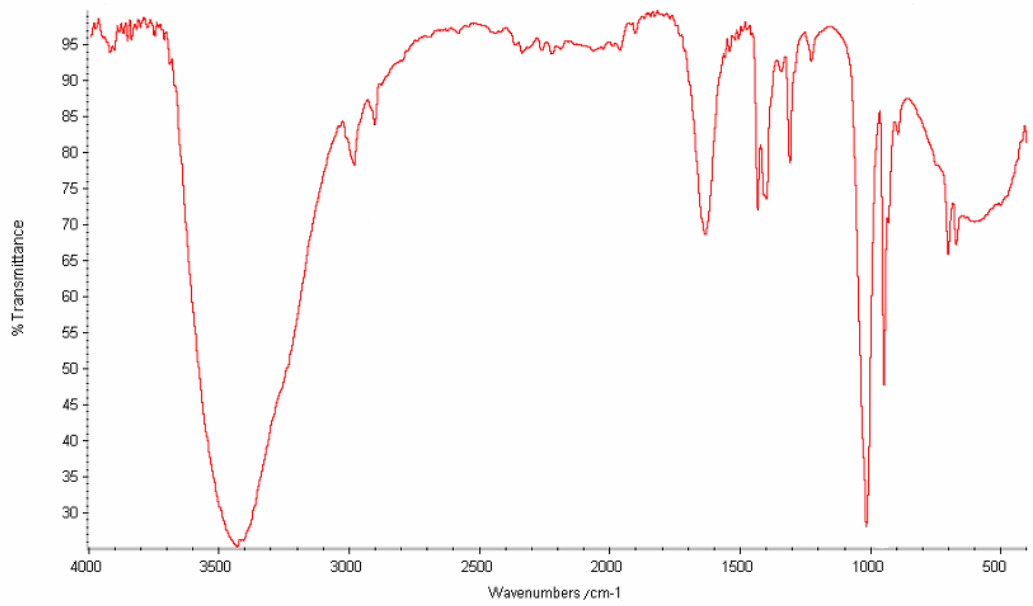

Figure SI.1 IR spectrum of **1**.

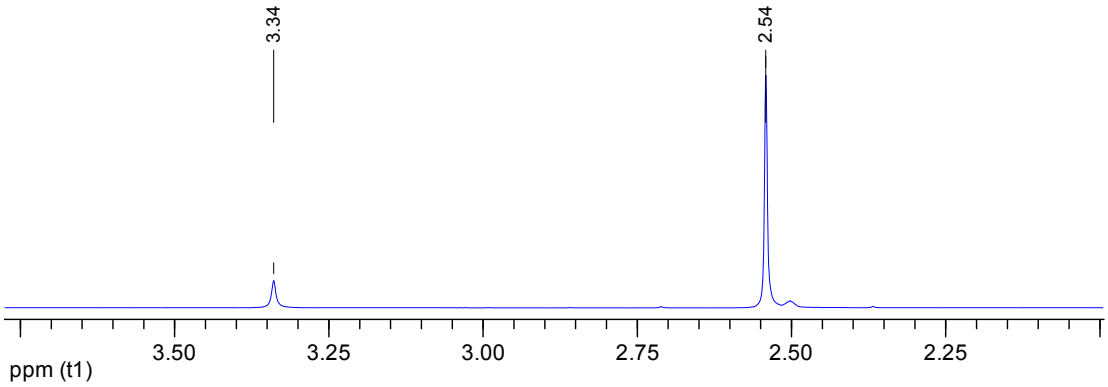

Figure SI.2 ^{1}H NMR (DMSO-d_6) spectrum of **1**.

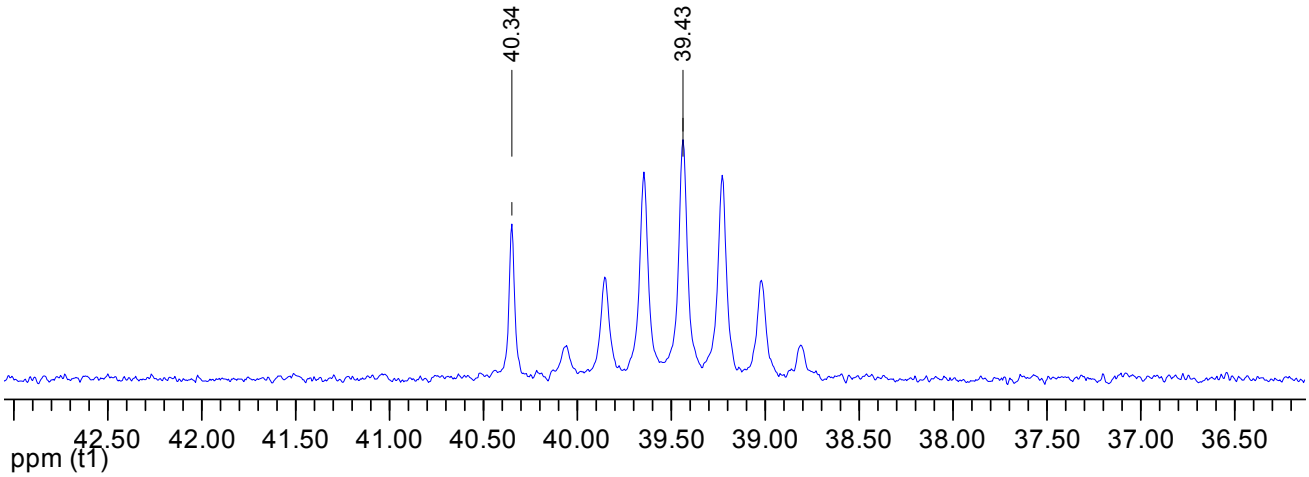

Figure SI.3 ^{13}C NMR (DMSO-d_6) spectrum of **1**.

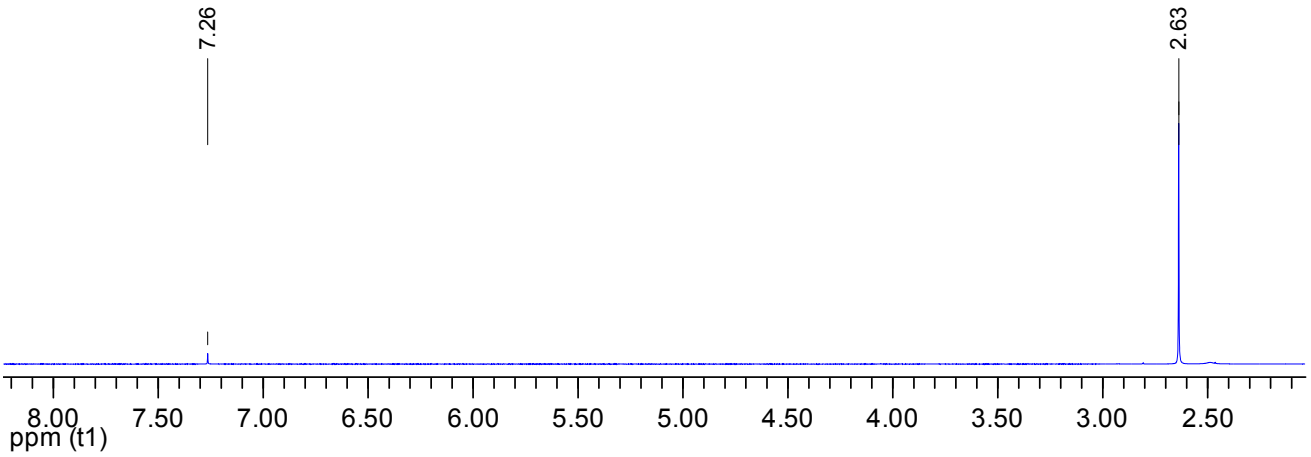

Figure SI.4 ^{1}H NMR ($CDCl_3$) spectrum of **1**.

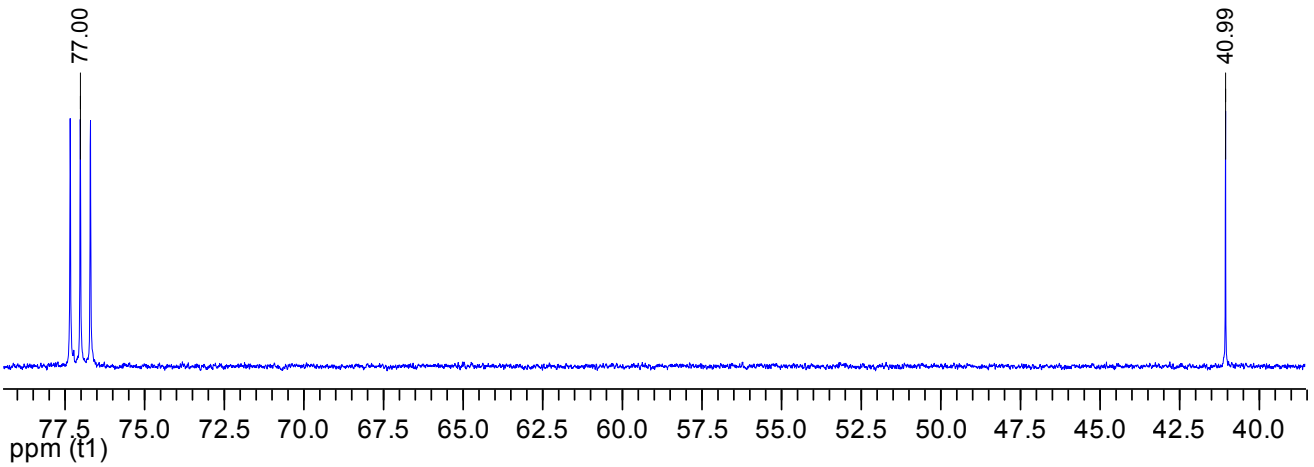

Figure SI.5 ^{13}C NMR ($CDCl_3$) spectrum of **1**.

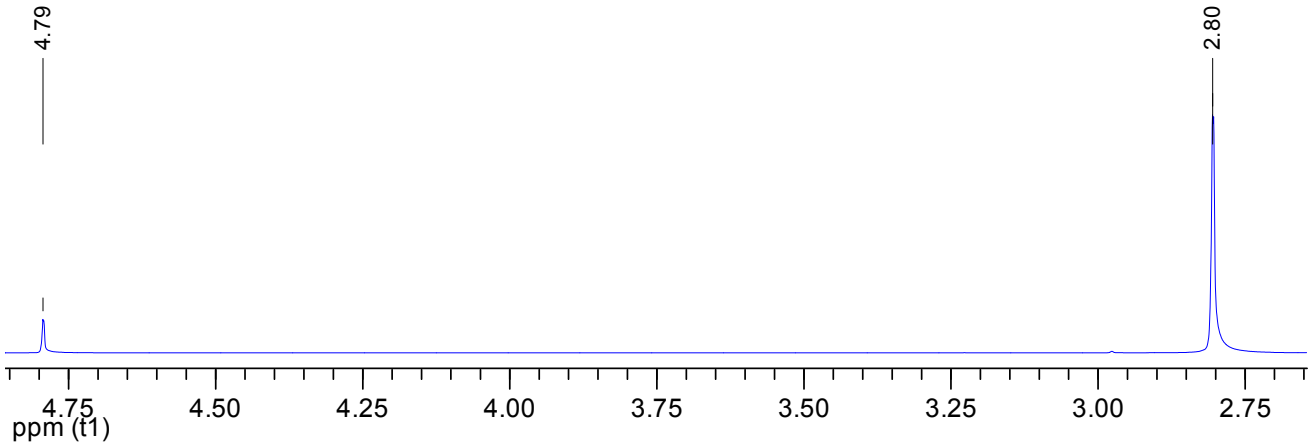

Figure SI.6 ^{1}H NMR (D_2O) spectrum of **1**.

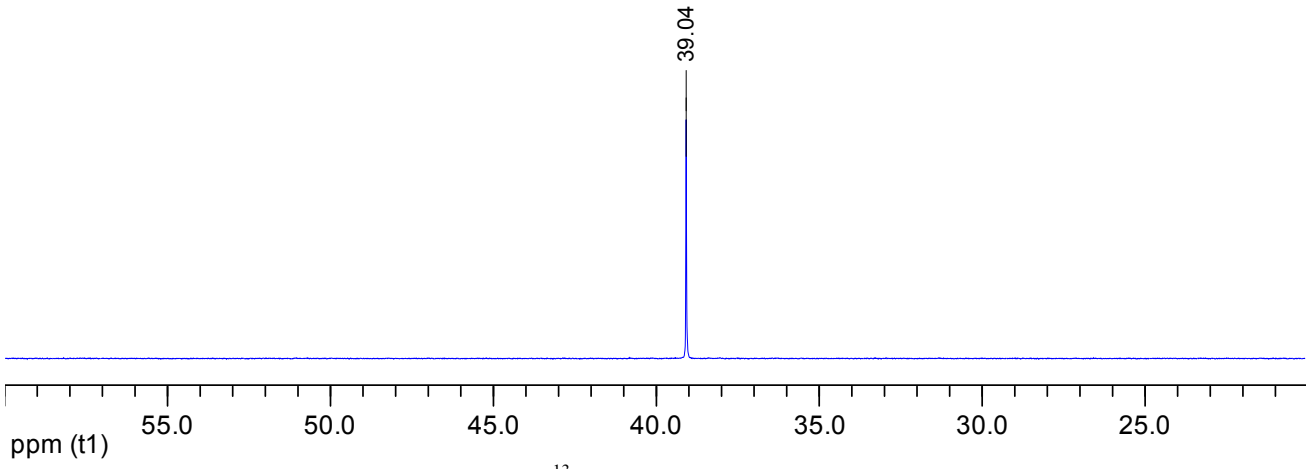

Figure SI.7 ^{13}C NMR (D_2O) spectrum of **1**.

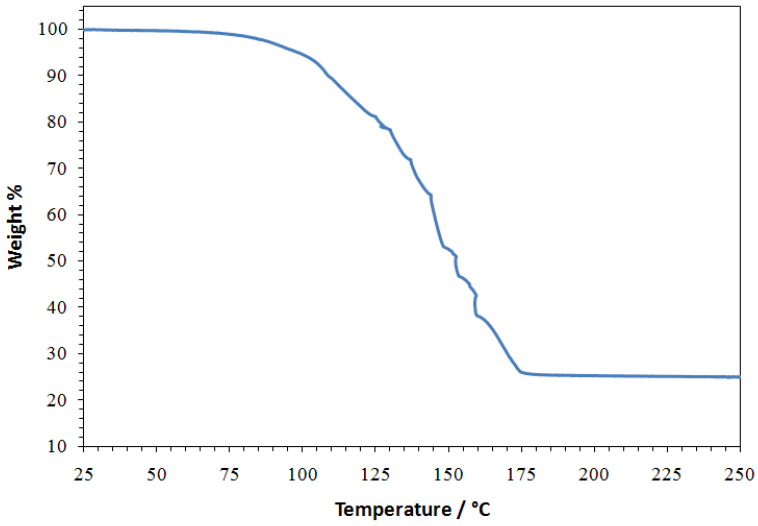

Figure SI.8 Thermogravimetric analyses of **1**.

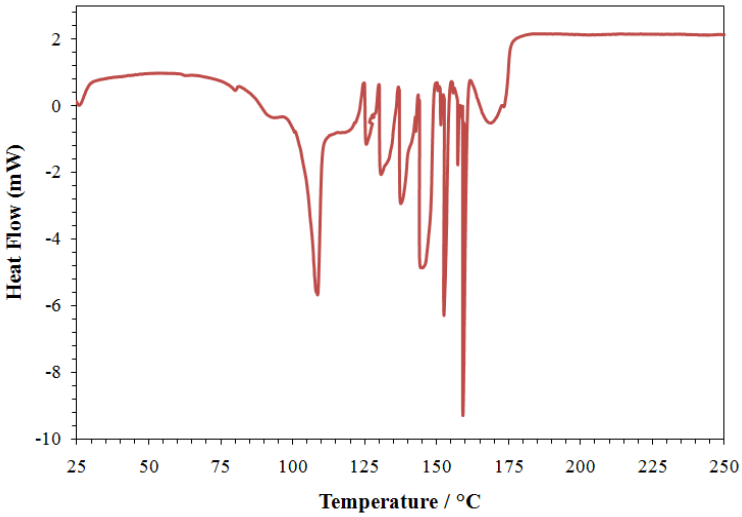

Figure SI.9 Differential scanning calorimetry (DSC) image of **1**.

X-ray Measurement and Structure Determination of 1: Data collection was performed on a Nonius Kappa CCD equipped with graphite-monochromatized Mo-K_α-radiation (λ=0.71073 Å) and a nominal crystal to area detector distance of 36 mm. Intensities were integrated using DENZO and scaled with SCALEPACK[5]. Several scans in ϕ and ω directions were taken to increase the number of redundant reflections, which were averaged in the refinement cycles. This procedure replaces, in approximation, an empirical absorption correction. The structures were solved with direct method SHELXS86 and refined against F^2 SHELX97[6]. All non-hydrogen atoms were refined with anisotropic displacement parameters, except O(3), O(4) and O(5), which were split positions for a disordered oxygen atom with occupations of 0.7, 0.15 and 0.15, respectively. Hydrogen atoms were calculated and refined using a riding model. The Na(2) and Na(3) positions show occupation disorders with occupation factors of 0.2833 for Na(2) and 0.0500 for Na(3). Further information about these disorders is included in the cif-file.

Table 1. Crystal data and structure refinement for **1**.

Empirical formula	C30 H90 I10 Na4 O15 S15	
Formula weight	2532.88	
Temperature	233(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	$P6_3/m$ (no. 176)	
Unit cell dimensions	a = 12.0292(4) Å	□= 90°.
	b = 12.0292(3) Å	□= 90°.
	c = 32.9777(7) Å	□ = 120°.
Volume	4132.61(19) $Å^3$	
Z	2	
Density (calculated)	2.035 Mg/m^3	
Absorption coefficient	4.193 mm^{-1}	
F(000)	2408	
Crystal size	0.35 x 0.15 x 0.08 mm^3	
Theta range for data collection	1.95 to 26.00°.	
Index ranges	-12<=h<=14, -14<=k<=13, -40<=l<=40	
Reflections collected	16891	
Independent reflections	2729 [R(int) = 0.0499]	
Reflections [I>2sigma(I)]	1915	
Completeness to theta = 26.00°	98.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2729 / 0 / 121	
Goodness-of-fit on F^2	1.081	
Final R indices [I>2sigma(I)]	R1 = 0.0352, wR2 = 0.0833	
R indices (all data)	R1 = 0.0548, wR2 = 0.0902	
Largest diff. peak and hole	0.659 and -0.622 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **1**. U(eq) is defined as one third of the trace for the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	3333	6667	2500	49(1)
I(2)	3333	6667	1407(1)	44(1)
I(3)	3333	6667	532(1)	43(1)
I(4)	3333	6667	-409(1)	49(1)
I(5)	3333	6667	-1605(1)	46(1)
I(6)	3333	6667	-2500	40(1)
Na(1)	0	10000	2001(1)	32(1)
Na(2)	0	10000	1006(1)	32(1)
Na(3)	0	10000	0	45(3)
S(1)	2783(1)	10581(1)	2500	34(1)
S(2)	572(1)	7808(1)	1503(1)	36(1)
S(3)	2699(1)	10472(1)	542(1)	47(1)
O(1)	1342(3)	9677(3)	2500	39(1)
O(2)	-364(3)	8297(3)	1531(1)	46(1)
O(3)	1327(4)	9396(5)	654(1)	47(1)
O(4)	1313(18)	9626(18)	542(7)	24(4)
O(5)	1330(20)	9430(20)	371(6)	55(6)
C(1)	3395(4)	10079(4)	2094(1)	49(1)
C(2)	222(5)	6741(5)	1917(1)	53(1)
C(3)	13(4)	6655(4)	1106(1)	50(1)
C(4)	3598(5)	10181(5)	904(1)	66(1)
C(5)	3233(5)	10033(5)	106(1)	66(2)

Table 3. Bond lengths [Å] and angles [°] for **1**.

I(2)-I(3)	2.8842(7)
I(3)-I(4)	3.1037(6)
I(5)-I(6)	2.9526(4)
I(6)-I(5)#1	2.9526(4)
Na(1)-O(2)#2	2.427(3)
Na(1)-O(2)	2.427(3)
Na(1)-O(2)#3	2.427(3)
Na(1)-O(1)#3	2.469(3)
Na(1)-O(1)	2.469(3)
Na(1)-O(1)#2	2.469(3)
Na(1)-Na(2)	3.281(3)
Na(1)-Na(1)#4	3.294(4)
Na(2)-O(3)#2	2.363(5)
Na(2)-O(3)#3	2.363(5)
Na(2)-O(3)	2.363(5)
Na(2)-O(4)#2	2.40(2)
Na(2)-O(4)	2.40(2)
Na(2)-O(4)#3	2.40(2)
Na(2)-O(2)#3	2.549(3)
Na(2)-O(2)#2	2.549(3)
Na(2)-O(2)	2.549(3)
Na(2)-O(5)#2	2.92(2)
Na(2)-O(5)	2.92(2)
Na(2)-O(5)#3	2.92(2)
Na(3)-O(5)#3	2.37(2)
Na(3)-O(5)#2	2.37(2)
Na(3)-O(5)#5	2.37(2)
Na(3)-O(5)#6	2.37(2)
Na(3)-O(5)	2.37(2)
Na(3)-O(5)#7	2.37(2)
Na(3)-O(4)#6	2.57(2)
Na(3)-O(4)#5	2.57(2)
Na(3)-O(4)#7	2.57(2)
Na(3)-O(4)#3	2.57(2)
Na(3)-O(4)	2.57(2)
Na(3)-O(4)#2	2.57(2)
S(1)-O(1)	1.517(4)

S(1)-C(1)	1.773(4)
S(1)-C(1)#4	1.773(4)
S(2)-O(2)	1.511(3)
S(2)-C(2)	1.774(4)
S(2)-C(3)	1.776(4)
S(3)-O(4)	1.456(19)
S(3)-O(3)	1.549(5)
S(3)-O(5)	1.60(2)
S(3)-C(5)	1.758(5)
S(3)-C(4)	1.761(5)
O(1)-Na(1)#4	2.469(3)
O(3)-O(5)	0.93(2)
O(4)-O(5)	0.62(2)

I(2)-I(3)-I(4)	180.0
I(5)#1-I(6)-I(5)	180.0
O(2)#2-Na(1)-O(2)	83.67(11)
O(2)#2-Na(1)-O(2)#3	83.67(11)
O(2)-Na(1)-O(2)#3	83.67(11)
O(2)#2-Na(1)-O(1)#3	97.39(9)
O(2)-Na(1)-O(1)#3	177.62(10)
O(2)#3-Na(1)-O(1)#3	98.55(9)
O(2)#2-Na(1)-O(1)	177.62(10)
O(2)-Na(1)-O(1)	98.55(9)
O(2)#3-Na(1)-O(1)	97.39(9)
O(1)#3-Na(1)-O(1)	80.36(9)
O(2)#2-Na(1)-O(1)#2	98.55(9)
O(2)-Na(1)-O(1)#2	97.39(9)
O(2)#3-Na(1)-O(1)#2	177.62(10)
O(1)#3-Na(1)-O(1)#2	80.36(9)
O(1)-Na(1)-O(1)#2	80.36(9)
O(2)#2-Na(1)-Na(2)	50.37(7)
O(2)-Na(1)-Na(2)	50.37(7)
O(2)#3-Na(1)-Na(2)	50.37(7)
O(1)#3-Na(1)-Na(2)	131.84(6)
O(1)-Na(1)-Na(2)	131.84(6)
O(1)#2-Na(1)-Na(2)	131.84(6)
O(2)#2-Na(1)-Na(1)#4	129.63(7)
O(2)-Na(1)-Na(1)#4	129.63(7)

O(2)#3-Na(1)-Na(1)#4	129.63(7)
O(1)#3-Na(1)-Na(1)#4	48.16(6)
O(1)-Na(1)-Na(1)#4	48.16(6)
O(1)#2-Na(1)-Na(1)#4	48.16(6)
Na(2)-Na(1)-Na(1)#4	180.0
O(3)#2-Na(2)-O(3)#3	97.93(16)
O(3)#2-Na(2)-O(3)	97.93(16)
O(3)#3-Na(2)-O(3)	97.93(16)
O(3)#2-Na(2)-O(4)#2	11.2(5)
O(3)#3-Na(2)-O(4)#2	94.4(5)
O(3)-Na(2)-O(4)#2	87.9(5)
O(3)#2-Na(2)-O(4)	94.4(5)
O(3)#3-Na(2)-O(4)	87.9(5)
O(3)-Na(2)-O(4)	11.2(5)
O(4)#2-Na(2)-O(4)	83.6(8)
O(3)#2-Na(2)-O(4)#3	87.9(5)
O(3)#3-Na(2)-O(4)#3	11.2(5)
O(3)-Na(2)-O(4)#3	94.4(5)
O(4)#2-Na(2)-O(4)#3	83.6(8)
O(4)-Na(2)-O(4)#3	83.6(8)
O(3)#2-Na(2)-O(2)#3	165.73(15)
O(3)#3-Na(2)-O(2)#3	87.56(13)
O(3)-Na(2)-O(2)#3	94.32(13)
O(4)#2-Na(2)-O(2)#3	176.8(5)
O(4)-Na(2)-O(2)#3	99.0(5)
O(4)#3-Na(2)-O(2)#3	98.5(5)
O(3)#2-Na(2)-O(2)#2	87.56(13)
O(3)#3-Na(2)-O(2)#2	94.32(13)
O(3)-Na(2)-O(2)#2	165.73(15)
O(4)#2-Na(2)-O(2)#2	98.5(5)
O(4)-Na(2)-O(2)#2	176.8(5)
O(4)#3-Na(2)-O(2)#2	99.0(5)
O(2)#3-Na(2)-O(2)#2	78.86(10)
O(3)#2-Na(2)-O(2)	94.32(13)
O(3)#3-Na(2)-O(2)	165.73(15)
O(3)-Na(2)-O(2)	87.56(13)
O(4)#2-Na(2)-O(2)	99.0(5)
O(4)-Na(2)-O(2)	98.5(5)
O(4)#3-Na(2)-O(2)	176.8(5)

O(2)#3-Na(2)-O(2)	78.86(10)
O(2)#2-Na(2)-O(2)	78.86(10)
O(3)#2-Na(2)-O(5)#2	16.5(4)
O(3)#3-Na(2)-O(5)#2	87.5(4)
O(3)-Na(2)-O(5)#2	86.7(4)
O(4)#2-Na(2)-O(5)#2	7.2(7)
O(4)-Na(2)-O(5)#2	81.2(6)
O(4)#3-Na(2)-O(5)#2	76.6(7)
O(2)#3-Na(2)-O(5)#2	175.1(4)
O(2)#2-Na(2)-O(5)#2	101.1(4)
O(2)-Na(2)-O(5)#2	106.0(4)
O(3)#2-Na(2)-O(5)	87.5(4)
O(3)#3-Na(2)-O(5)	86.7(4)
O(3)-Na(2)-O(5)	16.5(4)
O(4)#2-Na(2)-O(5)	76.6(7)
O(4)-Na(2)-O(5)	7.2(7)
O(4)#3-Na(2)-O(5)	81.2(6)
O(2)#3-Na(2)-O(5)	106.0(4)
O(2)#2-Na(2)-O(5)	175.1(4)
O(2)-Na(2)-O(5)	101.1(4)
O(5)#2-Na(2)-O(5)	74.1(6)
O(3)#2-Na(2)-O(5)#3	86.7(4)
O(3)#3-Na(2)-O(5)#3	16.5(4)
O(3)-Na(2)-O(5)#3	87.5(4)
O(4)#2-Na(2)-O(5)#3	81.2(6)
O(4)-Na(2)-O(5)#3	76.6(7)
O(4)#3-Na(2)-O(5)#3	7.2(7)
O(2)#3-Na(2)-O(5)#3	101.1(4)
O(2)#2-Na(2)-O(5)#3	106.0(4)
O(2)-Na(2)-O(5)#3	175.1(4)
O(5)#2-Na(2)-O(5)#3	74.1(6)
O(5)-Na(2)-O(5)#3	74.1(6)
O(5)#3-Na(3)-O(5)#2	95.8(7)
O(5)#3-Na(3)-O(5)#5	180.0(9)
O(5)#2-Na(3)-O(5)#5	84.2(7)
O(5)#3-Na(3)-O(5)#6	84.2(7)
O(5)#2-Na(3)-O(5)#6	84.2(7)
O(5)#5-Na(3)-O(5)#6	95.8(7)
O(5)#3-Na(3)-O(5)	95.8(7)

O(5)#2-Na(3)-O(5)	95.8(7)
O(5)#5-Na(3)-O(5)	84.2(7)
O(5)#6-Na(3)-O(5)	180.0(9)
O(5)#3-Na(3)-O(5)#7	84.2(7)
O(5)#2-Na(3)-O(5)#7	180.0(9)
O(5)#5-Na(3)-O(5)#7	95.8(7)
O(5)#6-Na(3)-O(5)#7	95.8(7)
O(5)-Na(3)-O(5)#7	84.2(7)
O(5)#3-Na(3)-O(4)#6	95.6(7)
O(5)#2-Na(3)-O(4)#6	90.4(8)
O(5)#5-Na(3)-O(4)#6	84.4(7)
O(5)#6-Na(3)-O(4)#6	13.5(6)
O(5)-Na(3)-O(4)#6	166.5(6)
O(5)#7-Na(3)-O(4)#6	89.6(8)
O(5)#3-Na(3)-O(4)#5	166.5(6)
O(5)#2-Na(3)-O(4)#5	95.6(7)
O(5)#5-Na(3)-O(4)#5	13.5(6)
O(5)#6-Na(3)-O(4)#5	89.6(8)
O(5)-Na(3)-O(4)#5	90.4(8)
O(5)#7-Na(3)-O(4)#5	84.4(7)
O(4)#6-Na(3)-O(4)#5	77.0(7)
O(5)#3-Na(3)-O(4)#7	90.4(8)
O(5)#2-Na(3)-O(4)#7	166.5(6)
O(5)#5-Na(3)-O(4)#7	89.6(8)
O(5)#6-Na(3)-O(4)#7	84.4(7)
O(5)-Na(3)-O(4)#7	95.6(7)
O(5)#7-Na(3)-O(4)#7	13.5(6)
O(4)#6-Na(3)-O(4)#7	77.0(7)
O(4)#5-Na(3)-O(4)#7	77.0(7)
O(5)#3-Na(3)-O(4)#3	13.5(6)
O(5)#2-Na(3)-O(4)#3	84.4(7)
O(5)#5-Na(3)-O(4)#3	166.5(6)
O(5)#6-Na(3)-O(4)#3	90.4(8)
O(5)-Na(3)-O(4)#3	89.6(8)
O(5)#7-Na(3)-O(4)#3	95.6(7)
O(4)#6-Na(3)-O(4)#3	103.0(7)
O(4)#5-Na(3)-O(4)#3	180.0(7)
O(4)#7-Na(3)-O(4)#3	103.0(7)
O(5)#3-Na(3)-O(4)	84.4(7)

O(5)#2-Na(3)-O(4)	89.6(8)
O(5)#5-Na(3)-O(4)	95.6(7)
O(5)#6-Na(3)-O(4)	166.5(6)
O(5)-Na(3)-O(4)	13.5(6)
O(5)#7-Na(3)-O(4)	90.4(8)
O(4)#6-Na(3)-O(4)	180.0(7)
O(4)#5-Na(3)-O(4)	103.0(7)
O(4)#7-Na(3)-O(4)	103.0(7)
O(4)#3-Na(3)-O(4)	77.0(7)
O(5)#3-Na(3)-O(4)#2	89.6(8)
O(5)#2-Na(3)-O(4)#2	13.5(6)
O(5)#5-Na(3)-O(4)#2	90.4(8)
O(5)#6-Na(3)-O(4)#2	95.6(7)
O(5)-Na(3)-O(4)#2	84.4(7)
O(5)#7-Na(3)-O(4)#2	166.5(6)
O(4)#6-Na(3)-O(4)#2	103.0(7)
O(4)#5-Na(3)-O(4)#2	103.0(7)
O(4)#7-Na(3)-O(4)#2	180.000(2)
O(4)#3-Na(3)-O(4)#2	77.0(7)
O(4)-Na(3)-O(4)#2	77.0(7)
O(1)-S(1)-C(1)	106.02(17)
O(1)-S(1)-C(1)#4	106.02(17)
C(1)-S(1)-C(1)#4	98.2(3)
O(2)-S(2)-C(2)	106.32(19)
O(2)-S(2)-C(3)	106.49(17)
C(2)-S(2)-C(3)	98.1(2)
O(4)-S(3)-O(3)	17.5(8)
O(4)-S(3)-O(5)	22.7(9)
O(3)-S(3)-O(5)	34.5(8)
O(4)-S(3)-C(5)	104.7(8)
O(3)-S(3)-C(5)	109.9(2)
O(5)-S(3)-C(5)	82.3(8)
O(4)-S(3)-C(4)	117.6(9)
O(3)-S(3)-C(4)	100.1(2)
O(5)-S(3)-C(4)	125.5(8)
C(5)-S(3)-C(4)	98.2(3)
O(4)-S(3)-Na(2)	38.0(8)
O(3)-S(3)-Na(2)	38.44(18)
O(5)-S(3)-Na(2)	59.8(8)

C(5)-S(3)-Na(2)	141.83(17)
C(4)-S(3)-Na(2)	107.07(18)
S(1)-O(1)-Na(1)	119.34(14)
S(1)-O(1)-Na(1)#4	119.34(14)
Na(1)-O(1)-Na(1)#4	83.68(12)
S(2)-O(2)-Na(1)	120.84(15)
S(2)-O(2)-Na(2)	114.15(15)
Na(1)-O(2)-Na(2)	82.46(9)
O(5)-O(3)-S(3)	75.4(13)
O(5)-O(3)-Na(2)	117.6(14)
S(3)-O(3)-Na(2)	117.5(3)
O(5)-O(3)-Na(3)	41.9(13)
S(3)-O(3)-Na(3)	95.8(2)
Na(2)-O(3)-Na(3)	75.76(14)
O(5)-O(4)-S(3)	92(3)
O(5)-O(4)-Na(2)	144(3)
S(3)-O(4)-Na(2)	120.0(11)
O(5)-O(4)-Na(3)	64(3)
S(3)-O(4)-Na(3)	117.9(11)
Na(2)-O(4)-Na(3)	83.7(6)
O(4)-O(5)-O(3)	26(2)
O(4)-O(5)-S(3)	66(3)
O(3)-O(5)-S(3)	70.0(12)
O(4)-O(5)-Na(3)	102(3)
O(3)-O(5)-Na(3)	122.9(17)
S(3)-O(5)-Na(3)	122.5(12)
O(4)-O(5)-Na(2)	29(3)
O(3)-O(5)-Na(2)	45.9(11)
S(3)-O(5)-Na(2)	91.9(9)
Na(3)-O(5)-Na(2)	77.0(6)

Symmetry transformations used to generate equivalent atoms:

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

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

#7 x-y+1,x+1,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	45(1)	45(1)	56(1)	0	0	22(1)
I(2)	42(1)	42(1)	49(1)	0	0	21(1)
I(3)	38(1)	38(1)	53(1)	0	0	19(1)
I(4)	53(1)	53(1)	43(1)	0	0	26(1)
I(5)	48(1)	48(1)	42(1)	0	0	24(1)
I(6)	35(1)	35(1)	52(1)	0	0	17(1)
Na(1)	33(1)	33(1)	32(1)	0	0	16(1)
Na(2)	32(1)	32(1)	32(1)	0	0	16(1)
Na(3)	44(5)	44(5)	48(6)	0	0	22(2)
S(1)	33(1)	31(1)	38(1)	0	0	16(1)
S(2)	35(1)	31(1)	42(1)	-2(1)	-3(1)	16(1)
S(3)	47(1)	37(1)	61(1)	-4(1)	-3(1)	24(1)
O(1)	29(2)	45(2)	40(2)	0	0	17(2)
O(2)	53(2)	41(2)	55(2)	-10(1)	-7(1)	32(2)
C(1)	37(3)	55(3)	46(2)	-7(2)	7(2)	17(2)
C(2)	62(3)	68(3)	45(2)	11(2)	6(2)	44(3)
C(3)	60(3)	60(3)	41(2)	-13(2)	-8(2)	38(2)
C(4)	77(4)	62(3)	46(2)	8(2)	-8(2)	25(3)
C(5)	81(4)	59(3)	42(2)	-9(2)	3(2)	23(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **1**.

	x	y	z	U(eq)
H(1A)	3141	10285	1838	74
H(1B)	3053	9160	2111	74
H(1C)	4324	10519	2110	74
H(2A)	476	7225	2168	80
H(2B)	691	6284	1885	80
H(2C)	-692	6131	1923	80
H(3A)	134	7086	848	75
H(3B)	-892	6047	1146	75
H(3C)	491	6202	1108	75
H(4A)	3424	10391	1172	99
H(4B)	4505	10710	845	99
H(4C)	3360	9283	896	99
H(5A)	2809	10123	-131	99
H(5B)	3032	9148	131	99
H(5C)	4154	10586	79	99

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