

Bis[aqua(2,3-naphtho-15-crown-5)-sodium] tetrakis(thiocyanato- κN)-cobaltate(II)

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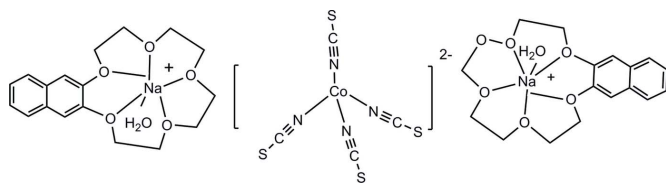
Received 9 September 2009; accepted 24 September 2009

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.046; wR factor = 0.110; data-to-parameter ratio = 14.8.

The title complex, $[\text{Na}(\text{C}_{18}\text{H}_{22}\text{O}_5)(\text{H}_2\text{O})]_2[\text{Co}(\text{NCS})_4]$, consists of two aqua(2,3-naphtho-15-crown-5)sodium complex cations and one $[\text{Co}(\text{NCS})_4]^{2-}$ complex anion, which has crystallographic $\bar{1}$ symmetry. In the anion, the Co^{II} centre is coordinated by the N atoms of four NCS^- ligands in a distorted tetrahedral geometry. In the complex cations, the Na^{I} centre is coordinated by five O atoms of the 2,3-naphtho-15-crown-5 ligand and one water O atom. The complex molecules form a two-dimensional network *via* weak $\text{O}-\text{H}\cdots\text{S}$ interactions between adjacent cations and anions

Related literature

For crown ether complexes, see: Pedersen (1967); Zhang *et al.* (1996). For $\pi-\pi$ interactions of the naphtho crown ether, see: Gao *et al.* (2005). For structural information on compounds with similar features, see Fan *et al.* (1985); Dou *et al.* (2004); Yu *et al.* (2005); Zhang *et al.* (2006).



Experimental

Crystal data

 $[\text{Na}(\text{C}_{18}\text{H}_{22}\text{O}_5)(\text{H}_2\text{O})]_2[\text{Co}(\text{NCS})_4]$
 $M_r = 1009.97$

 Monoclinic, $C2/c$
 $a = 23.030$ (5) Å

 $b = 13.170$ (3) Å
 $c = 17.469$ (4) Å
 $\beta = 115.255$ (3) $^\circ$
 $V = 4792.0$ (18) Å 3
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 0.61$ mm $^{-1}$
 $T = 298$ K
 $0.39 \times 0.36 \times 0.18$ mm

Data collection

 Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.796$, $T_{\text{max}} = 0.898$
 12300 measured reflections
 4232 independent reflections
 2150 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.110$
 $S = 1.00$
 4232 reflections
 285 parameters

 6 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.25$ e Å $^{-3}$
 $\Delta\rho_{\text{min}} = -0.28$ e Å $^{-3}$
Table 1

 Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O6}-\text{H1}\cdots\text{S2}^{\text{i}}$	0.84	2.62	3.458 (3)	173
$\text{O6}-\text{H3}\cdots\text{S1}^{\text{ii}}$	0.84	2.57	3.389 (3)	165

 Symmetry codes: (i) $x, -y + 1, z - \frac{1}{2}$; (ii) $-x + \frac{3}{2}, -y + \frac{1}{2}, -z + 1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We acknowledge the Science Foundation of Liaocheng University, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2189).

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supplementary materials

Acta Cryst. (2009). E65, m1314 [doi:10.1107/S1600536809038641]

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Comment

Due to the unusual coordination numbers and arrangements with various metal ions, crown ethers have attracted much attention (Pedersen, 1967; Zhang *et al.*, 1996). In particular, the naphtho crown ethers play an important role in crystal engineering of supramolecular interactions, such as $\pi\cdots\pi$ interactions (Dou *et al.*, 2004; Gao *et al.*, 2005). In order to study the weak interactions of the naphtho crown ether, we have synthesized the title complex by the reaction of naphtho-15-crown-5 with CoCl_2 and NaSCN . The title complex, $[\text{Na}(\text{N15C5})\text{H}_2\text{O}]_2[\text{Co}(\text{NCS})_4]$ is made up of two $[\text{Na}(\text{N15C5})\text{H}_2\text{O}]^+$ complex cations and one $[\text{Co}(\text{NCS})_4]^{2-}$ complex anion. In the complex anion, the Co is coordinated by four N atoms of the NCS ligands and exhibits a distorted tetrahedral geometry. The average Co—N bond length is 1.945 (4) Å, which is consistent with that of $[\text{K}(\text{18C6})]_2[\text{Co}(\text{SCN})_4]$ (1.94 Å) (Fan *et al.*, 1985). In the complex cation, the Na is coordinated by five O atoms of the crown ether and one O atom of the H_2O . The Na—O(crown ether) distances are in the range 2.329 (3) to 2.361 (3) Å, average 2.344 (3) Å, which is shorter than that of $[\text{Na}(\text{N15C5})][\text{Pd}(\text{SCN})_4]$ (Dou *et al.*, 2004). The Na—O(H_2O) bond length is 2.278 (3) Å, which is comparable to that of $[\{\text{Na}(\text{18C6})\}_2(\text{H}_2\text{O})][\text{Ni}(\text{i-mnt})_2]$ (Yu *et al.*, 2005). For the neighboring complex cations and the complex anions, the distances of O(6) \cdots S(2) and O(6)—S(1) are 3.46 (3) Å and 3.39 (4) Å respectively, which are shorter than those in the complex $\{[(\text{Me}_3\text{Sn})(\mu\text{-OH})][\text{Me}_2\text{Sn}(\mu_3\text{-SCH}_2\text{CO}_2)]\}_n$ (Zhang *et al.*, 2006), indicating that there are O—H \cdots S weak interactions between the neighboring complex cations and complex anions. The title complex is assembled into two-dimensional network by virtue of O—H \cdots S weak interactions.

Experimental

The title complex was prepared by adding 10 ml of an aqueous mixture of CoCl_2 (0.032 g, 0.25 mmol) and NaSCN (0.81 g, 10 mmol) to a solution of 2,3-naphtho-15-crown-5 (0.16 g, 0.5 mmol) in 10 ml dichloromethane. The reaction mixture was stirred for 2 hrs at room temperature and filtered. The precipitate was dissolved in the CH_3CN , and the crystal was obtained a week later. m.p.: 470–472. Anal. Calcd (%) for $\text{C}_{40}\text{H}_{48}\text{CoN}_4\text{Na}_2\text{O}_{12}\text{S}_4$: C, 47.45; H, 4.82; N, 5.62. Found (%): C, 47.52; H, 4.75; N, 5.54.

Refinement

The C—H H atoms were positioned with idealized geometry and were refined as isotropic with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{O})$ for all H atoms using a riding model with C—H = 0.93 Å for aromatic H, and C—H = 0.97 Å for CH_2 . The S2 atom was refined using an approximately isotropic model (ISOR in SHELXL).

Figures

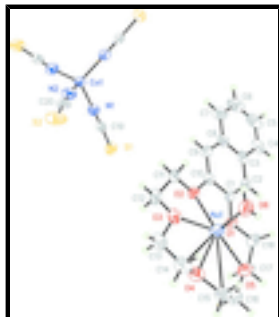


Fig. 1. The molecular structure of the compound, showing 40% probability displacement ellipsoids.

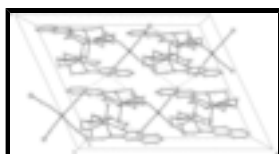


Fig. 2. View of the two-dimensional network structure in the crystal structure of the title complex. Intermolecular O—H...S are shown. H atoms have been omitted.

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Crystal data

[Na(C₁₈H₂₂O₅)(H₂O)]₂[Co(NCS)₄]

$M_r = 1009.97$

Monoclinic, *C*2/*c*

Hall symbol: -*C* 2yc

$a = 23.030 (5) \text{ \AA}$

$b = 13.170 (3) \text{ \AA}$

$c = 17.469 (4) \text{ \AA}$

$\beta = 115.255 (3)^\circ$

$V = 4792.0 (18) \text{ \AA}^3$

$Z = 4$

$F_{000} = 2100$

$D_x = 1.400 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1972 reflections

$\theta = 2.5\text{--}21.9^\circ$

$\mu = 0.61 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Block, red

$0.39 \times 0.36 \times 0.18 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298 \text{ K}$

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.796$, $T_{\max} = 0.898$

12300 measured reflections

4232 independent reflections

2150 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 1.8^\circ$

$h = -23 \rightarrow 27$

$k = -15 \rightarrow 10$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2 + 7.4253P]$
$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
4232 reflections	$(\Delta/\sigma)_{\max} = 0.001$
285 parameters	$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$
6 restraints	$\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	0.51700 (7)	0.7500	0.0623 (3)
Na1	0.81291 (7)	0.28279 (13)	0.32041 (10)	0.0657 (5)
N1	0.57146 (16)	0.4339 (3)	0.8270 (2)	0.0680 (10)
N2	0.53079 (17)	0.5994 (3)	0.6834 (3)	0.0808 (12)
O1	0.80689 (12)	0.1597 (2)	0.41499 (16)	0.0580 (7)
O2	0.73752 (11)	0.3173 (2)	0.37301 (15)	0.0534 (7)
O3	0.77894 (13)	0.4521 (2)	0.28951 (16)	0.0632 (8)
O4	0.90108 (13)	0.3783 (2)	0.32829 (17)	0.0680 (8)
O5	0.90001 (12)	0.1712 (2)	0.36137 (18)	0.0690 (8)
O6	0.75231 (14)	0.2494 (2)	0.18076 (19)	0.0952 (11)
H1	0.7131	0.2636	0.1564	0.114*
H3	0.7649	0.2381	0.1427	0.114*
S1	0.67314 (6)	0.32131 (10)	0.94135 (7)	0.0739 (4)
S2	0.58936 (6)	0.70155 (14)	0.59663 (10)	0.1164 (6)
C1	0.74760 (18)	0.1464 (3)	0.4142 (2)	0.0472 (10)
C2	0.72491 (19)	0.0597 (3)	0.4328 (2)	0.0558 (11)
H2	0.7506	0.0020	0.4480	0.067*
C3	0.6622 (2)	0.0558 (3)	0.4292 (2)	0.0580 (11)
C4	0.6371 (2)	-0.0332 (4)	0.4494 (3)	0.0766 (14)
H4	0.6617	-0.0920	0.4647	0.092*
C5	0.5771 (3)	-0.0328 (5)	0.4463 (3)	0.0969 (18)

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H5	0.5613	-0.0916	0.4601	0.116*
C6	0.5395 (3)	0.0523 (6)	0.4234 (3)	0.1004 (19)
H6	0.4988	0.0508	0.4221	0.121*
C7	0.5614 (2)	0.1392 (4)	0.4024 (3)	0.0862 (15)
H7	0.5352	0.1963	0.3861	0.103*
C8	0.62357 (19)	0.1435 (4)	0.4052 (3)	0.0596 (11)
C9	0.64775 (18)	0.2321 (3)	0.3848 (2)	0.0579 (11)
H9	0.6220	0.2898	0.3678	0.070*
C10	0.70851 (18)	0.2349 (3)	0.3896 (2)	0.0459 (9)
C11	0.69937 (19)	0.4050 (3)	0.3348 (3)	0.0606 (11)
H11A	0.6762	0.4263	0.3672	0.073*
H11B	0.6684	0.3891	0.2777	0.073*
C12	0.7428 (2)	0.4878 (3)	0.3330 (3)	0.0668 (12)
H12A	0.7177	0.5467	0.3042	0.080*
H12B	0.7715	0.5073	0.3903	0.080*
C13	0.8307 (2)	0.5175 (4)	0.2980 (3)	0.0770 (14)
H13A	0.8541	0.5386	0.3564	0.092*
H13B	0.8145	0.5777	0.2632	0.092*
C14	0.8738 (2)	0.4593 (4)	0.2697 (3)	0.0778 (14)
H14A	0.8495	0.4326	0.2132	0.093*
H14B	0.9074	0.5031	0.2688	0.093*
C15	0.9376 (2)	0.3071 (4)	0.3053 (3)	0.0813 (15)
H15A	0.9754	0.3398	0.3055	0.098*
H15B	0.9121	0.2808	0.2490	0.098*
C16	0.9568 (2)	0.2230 (4)	0.3686 (3)	0.0842 (15)
H16A	0.9851	0.1761	0.3580	0.101*
H16B	0.9796	0.2502	0.4253	0.101*
C17	0.91031 (19)	0.1114 (4)	0.4336 (3)	0.0762 (14)
H17A	0.9302	0.1522	0.4845	0.091*
H17B	0.9387	0.0551	0.4378	0.091*
C18	0.84685 (19)	0.0722 (3)	0.4251 (3)	0.0689 (13)
H18A	0.8279	0.0279	0.3762	0.083*
H18B	0.8520	0.0343	0.4752	0.083*
C19	0.61400 (19)	0.3861 (3)	0.8744 (3)	0.0535 (11)
C20	0.55531 (19)	0.6421 (4)	0.6479 (3)	0.0719 (14)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0459 (5)	0.0642 (6)	0.0740 (6)	0.000	0.0228 (4)	0.000
Na1	0.0605 (10)	0.0661 (12)	0.0759 (11)	0.0079 (8)	0.0344 (9)	0.0094 (9)
N1	0.052 (2)	0.066 (3)	0.084 (3)	-0.0012 (19)	0.027 (2)	0.006 (2)
N2	0.059 (2)	0.090 (3)	0.091 (3)	-0.008 (2)	0.030 (2)	0.013 (2)
O1	0.0525 (17)	0.0562 (19)	0.0705 (19)	0.0140 (14)	0.0311 (14)	0.0077 (14)
O2	0.0524 (16)	0.0422 (17)	0.0665 (18)	0.0095 (13)	0.0263 (14)	0.0088 (14)
O3	0.0724 (19)	0.056 (2)	0.0596 (18)	-0.0050 (15)	0.0268 (16)	-0.0006 (14)
O4	0.0646 (18)	0.088 (2)	0.0551 (18)	-0.0045 (17)	0.0291 (15)	-0.0010 (17)
O5	0.0531 (18)	0.083 (2)	0.072 (2)	0.0075 (16)	0.0281 (15)	-0.0001 (17)

O6	0.088 (2)	0.099 (3)	0.084 (2)	0.0186 (19)	0.0222 (19)	-0.0222 (19)
S1	0.0733 (8)	0.0708 (9)	0.0714 (8)	0.0126 (6)	0.0250 (6)	0.0094 (6)
S2	0.0666 (9)	0.1589 (17)	0.1127 (12)	-0.0027 (9)	0.0277 (8)	0.0643 (11)
C1	0.051 (2)	0.044 (3)	0.045 (2)	0.006 (2)	0.0192 (19)	-0.0018 (19)
C2	0.067 (3)	0.043 (3)	0.051 (3)	0.004 (2)	0.019 (2)	-0.001 (2)
C3	0.071 (3)	0.057 (3)	0.047 (3)	-0.016 (2)	0.026 (2)	-0.012 (2)
C4	0.089 (4)	0.074 (4)	0.058 (3)	-0.025 (3)	0.022 (3)	-0.006 (2)
C5	0.097 (5)	0.116 (6)	0.076 (4)	-0.052 (4)	0.035 (3)	-0.005 (4)
C6	0.071 (4)	0.139 (6)	0.092 (4)	-0.034 (4)	0.036 (3)	-0.014 (4)
C7	0.063 (3)	0.103 (5)	0.098 (4)	-0.013 (3)	0.039 (3)	-0.011 (3)
C8	0.057 (3)	0.065 (3)	0.061 (3)	-0.012 (2)	0.029 (2)	-0.010 (2)
C9	0.052 (3)	0.057 (3)	0.062 (3)	0.006 (2)	0.021 (2)	-0.008 (2)
C10	0.053 (2)	0.039 (2)	0.046 (2)	-0.001 (2)	0.0214 (19)	-0.0018 (19)
C11	0.063 (3)	0.043 (3)	0.072 (3)	0.011 (2)	0.025 (2)	0.004 (2)
C12	0.089 (3)	0.043 (3)	0.066 (3)	0.006 (2)	0.031 (3)	0.002 (2)
C13	0.099 (4)	0.064 (3)	0.068 (3)	-0.013 (3)	0.035 (3)	0.009 (3)
C14	0.085 (3)	0.090 (4)	0.059 (3)	-0.019 (3)	0.031 (3)	0.013 (3)
C15	0.063 (3)	0.114 (5)	0.079 (4)	-0.009 (3)	0.042 (3)	-0.011 (3)
C16	0.056 (3)	0.105 (4)	0.097 (4)	0.007 (3)	0.038 (3)	-0.009 (3)
C17	0.053 (3)	0.081 (4)	0.090 (4)	0.024 (2)	0.026 (3)	0.013 (3)
C18	0.067 (3)	0.063 (3)	0.077 (3)	0.025 (2)	0.031 (2)	0.015 (2)
C19	0.053 (3)	0.049 (3)	0.069 (3)	-0.010 (2)	0.035 (2)	-0.006 (2)
C20	0.041 (3)	0.085 (4)	0.071 (3)	0.003 (2)	0.005 (2)	0.010 (3)

Geometric parameters (Å, °)

Co1—N2	1.934 (4)	C4—C5	1.360 (6)
Co1—N2 ⁱ	1.934 (4)	C4—H4	0.9300
Co1—N1 ⁱ	1.956 (4)	C5—C6	1.367 (7)
Co1—N1	1.956 (4)	C5—H5	0.9300
Na1—O6	2.278 (3)	C6—C7	1.363 (7)
Na1—O2	2.329 (3)	C6—H6	0.9300
Na1—O5	2.339 (3)	C7—C8	1.412 (5)
Na1—O4	2.343 (3)	C7—H7	0.9300
Na1—O3	2.348 (3)	C8—C9	1.404 (5)
Na1—O1	2.361 (3)	C9—C10	1.366 (5)
N1—C19	1.162 (5)	C9—H9	0.9300
N2—C20	1.147 (5)	C11—C12	1.488 (5)
O1—C1	1.371 (4)	C11—H11A	0.9700
O1—C18	1.438 (4)	C11—H11B	0.9700
O2—C10	1.369 (4)	C12—H12A	0.9700
O2—C11	1.432 (4)	C12—H12B	0.9700
O3—C12	1.425 (4)	C13—C14	1.494 (6)
O3—C13	1.427 (5)	C13—H13A	0.9700
O4—C14	1.425 (5)	C13—H13B	0.9700
O4—C15	1.427 (5)	C14—H14A	0.9700
O5—C17	1.420 (5)	C14—H14B	0.9700
O5—C16	1.432 (5)	C15—C16	1.493 (6)
O6—H1	0.8393	C15—H15A	0.9700

supplementary materials

O6—H3	0.8435	C15—H15B	0.9700
S1—C19	1.610 (5)	C16—H16A	0.9700
S2—C20	1.622 (5)	C16—H16B	0.9700
C1—C2	1.351 (5)	C17—C18	1.496 (5)
C1—C10	1.423 (5)	C17—H17A	0.9700
C2—C3	1.420 (5)	C17—H17B	0.9700
C2—H2	0.9300	C18—H18A	0.9700
C3—C8	1.407 (6)	C18—H18B	0.9700
C3—C4	1.416 (6)		
N2—Co1—N2 ⁱ	111.7 (3)	C8—C7—H7	119.7
N2—Co1—N1 ⁱ	108.47 (16)	C9—C8—C3	119.3 (4)
N2 ⁱ —Co1—N1 ⁱ	108.11 (15)	C9—C8—C7	122.0 (5)
N2—Co1—N1	108.11 (15)	C3—C8—C7	118.7 (5)
N2 ⁱ —Co1—N1	108.47 (16)	C10—C9—C8	120.9 (4)
N1 ⁱ —Co1—N1	112.0 (2)	C10—C9—H9	119.5
O6—Na1—O2	103.94 (11)	C8—C9—H9	119.5
O6—Na1—O5	105.07 (12)	C9—C10—O2	126.0 (4)
O2—Na1—O5	133.49 (12)	C9—C10—C1	119.7 (4)
O6—Na1—O4	106.64 (12)	O2—C10—C1	114.2 (3)
O2—Na1—O4	130.18 (12)	O2—C11—C12	108.4 (3)
O5—Na1—O4	73.18 (12)	O2—C11—H11A	110.0
O6—Na1—O3	86.87 (11)	C12—C11—H11A	110.0
O2—Na1—O3	70.98 (10)	O2—C11—H11B	110.0
O5—Na1—O3	145.58 (12)	C12—C11—H11B	110.0
O4—Na1—O3	72.47 (11)	H11A—C11—H11B	108.4
O6—Na1—O1	115.14 (13)	O3—C12—C11	108.7 (3)
O2—Na1—O1	65.28 (9)	O3—C12—H12A	110.0
O5—Na1—O1	69.71 (11)	C11—C12—H12A	110.0
O4—Na1—O1	129.50 (12)	O3—C12—H12B	110.0
O3—Na1—O1	134.41 (11)	C11—C12—H12B	110.0
C19—N1—Co1	178.3 (4)	H12A—C12—H12B	108.3
C20—N2—Co1	172.3 (4)	O3—C13—C14	107.4 (4)
C1—O1—C18	118.8 (3)	O3—C13—H13A	110.2
C1—O1—Na1	115.9 (2)	C14—C13—H13A	110.2
C18—O1—Na1	114.2 (2)	O3—C13—H13B	110.2
C10—O2—C11	118.7 (3)	C14—C13—H13B	110.2
C10—O2—Na1	116.3 (2)	H13A—C13—H13B	108.5
C11—O2—Na1	112.7 (2)	O4—C14—C13	107.4 (3)
C12—O3—C13	113.5 (3)	O4—C14—H14A	110.2
C12—O3—Na1	113.8 (2)	C13—C14—H14A	110.2
C13—O3—Na1	111.6 (2)	O4—C14—H14B	110.2
C14—O4—C15	115.0 (3)	C13—C14—H14B	110.2
C14—O4—Na1	104.7 (2)	H14A—C14—H14B	108.5
C15—O4—Na1	103.3 (3)	O4—C15—C16	107.7 (4)
C17—O5—C16	112.7 (3)	O4—C15—H15A	110.2
C17—O5—Na1	114.6 (2)	C16—C15—H15A	110.2
C16—O5—Na1	111.1 (3)	O4—C15—H15B	110.2
Na1—O6—H1	122.3	C16—C15—H15B	110.2

Na1—O6—H3	128.2	H15A—C15—H15B	108.5
H1—O6—H3	107.3	O5—C16—C15	108.5 (4)
C2—C1—O1	126.3 (4)	O5—C16—H16A	110.0
C2—C1—C10	120.3 (4)	C15—C16—H16A	110.0
O1—C1—C10	113.4 (4)	O5—C16—H16B	110.0
C1—C2—C3	120.7 (4)	C15—C16—H16B	110.0
C1—C2—H2	119.7	H16A—C16—H16B	108.4
C3—C2—H2	119.7	O5—C17—C18	108.5 (3)
C8—C3—C4	118.7 (4)	O5—C17—H17A	110.0
C8—C3—C2	119.0 (4)	C18—C17—H17A	110.0
C4—C3—C2	122.3 (4)	O5—C17—H17B	110.0
C5—C4—C3	120.2 (5)	C18—C17—H17B	110.0
C5—C4—H4	119.9	H17A—C17—H17B	108.4
C3—C4—H4	119.9	O1—C18—C17	106.4 (3)
C4—C5—C6	121.3 (6)	O1—C18—H18A	110.4
C4—C5—H5	119.3	C17—C18—H18A	110.4
C6—C5—H5	119.3	O1—C18—H18B	110.4
C7—C6—C5	120.5 (5)	C17—C18—H18B	110.4
C7—C6—H6	119.8	H18A—C18—H18B	108.6
C5—C6—H6	119.8	N1—C19—S1	178.9 (4)
C6—C7—C8	120.6 (5)	N2—C20—S2	179.2 (5)
C6—C7—H7	119.7		

Symmetry codes: (i) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O6—H1 \cdots S2 ⁱⁱ	0.84	2.62	3.458 (3)	173
O6—H3 \cdots S1 ⁱⁱⁱ	0.84	2.57	3.389 (3)	165

Symmetry codes: (ii) $x, -y+1, z-1/2$; (iii) $-x+3/2, -y+1/2, -z+1$.

Fig. 1

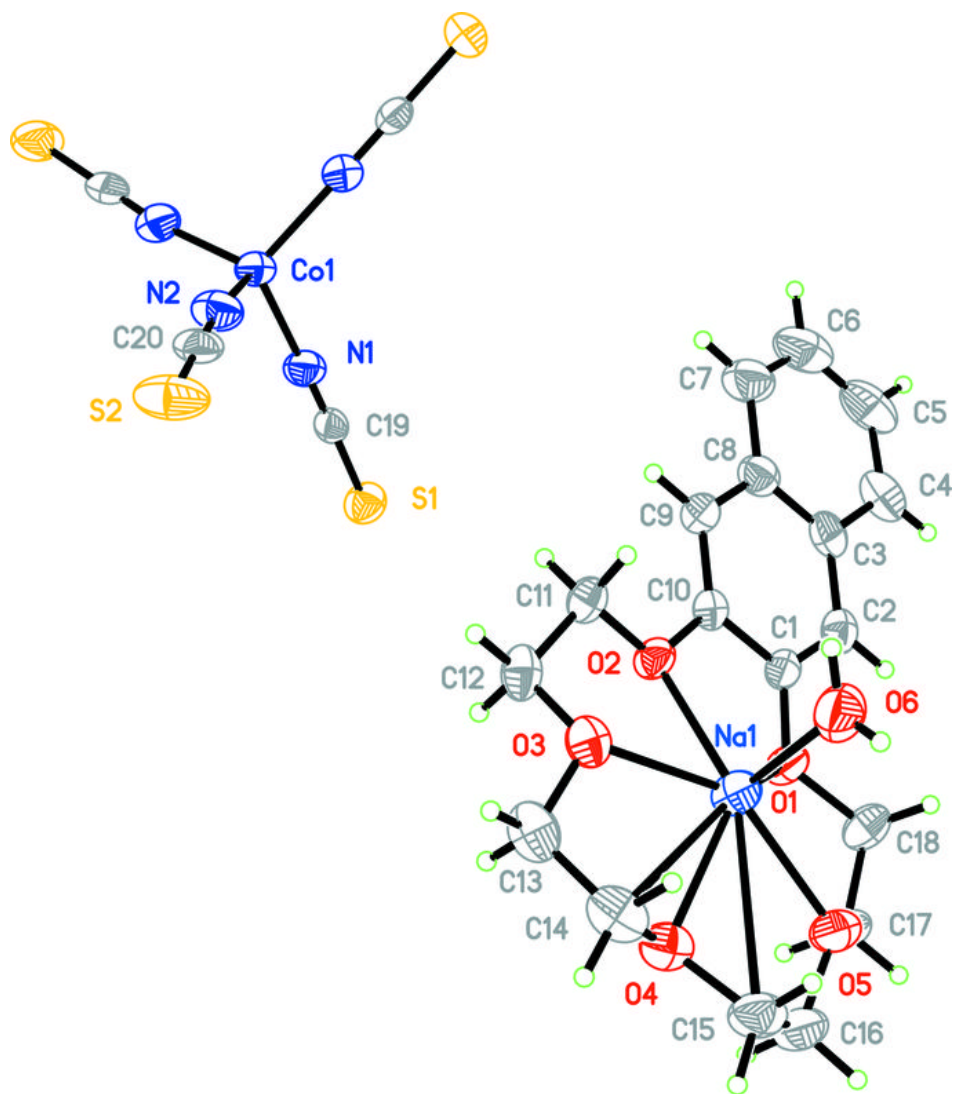


Fig. 2

