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

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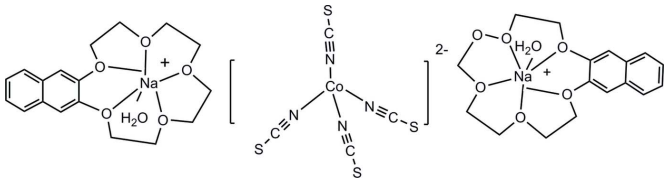
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.046; wR factor = 0.110; data-to-parameter ratio = 14.8.

The title complex, $[Na(C_{18}H_{22}O_5)(H_2O)]_2[Co(NCS)_4]$, consists of two aqua(2,3-naphtho-15-crown-5)sodium complex cations and one $[Co(NCS)_4]^{2-}$ 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 O—H···S interactions between adjacent cations and anions

Related literature

For crown ether complexes, see: Pedersen (1967); Zhang *et al.* (1996). For π–π 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

$[Na(C_{18}H_{22}O_5)(H_2O)]_2[Co(NCS)_4]$
M_r = 1009.97
Monoclinic, $C2/c$
a = 23.030 (5) Å
b = 13.170 (3) Å
c = 17.469 (4) Å
β = 115.255 (3)°
V = 4792.0 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 298 K
0.39 × 0.36 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
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_{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
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O6—H1···S2^{i}	0.84	2.62	3.458 (3)	173
O6—H3···S1^{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*.

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

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supporting information

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S1. 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, $[Na(N15C5)H_2O]_2[Co(NCS)_4]$ is made up of two $[Na(N15C5)H_2O]^+$ complex cations and one $[Co(NCS)_4]^{2-}$ 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 $[K(18C6)]_2[Co(SCN)_4]$(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 $[Na(N15C5)][Pd(SCN)_4]$ (Dou *et al.*, 2004). The Na—O(H_2O) bond length is 2.278 (3) Å, which is comparable to that of $[\{Na(18C6)\}_2(H_2O)][Ni(i\text{-}mnt)_2]$ (Yu *et al.*, 2005). For the neighboring complex cations and the complex anions, the distances of O(6)···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 $\{[(Me_3Sn)(\mu\text{-}OH)][Me_2Sn(\mu_3\text{-}SCH_2CO_2)]\}_n$ (Zhang *et al.*, 2006), indicating that there are O—H···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···S weak interactions.

S2. 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 precipite was dissolved in the CH_3CN, and the crystal was obtained a week later. m.p.: 470–472. Anal. Calcd (%) for $C_{40}H_{48}CoN_4Na_2O_{12}S_4$: C, 47.45; H, 4.82; N, 5.62. Found (%): C, 47.52; H, 4.75; N, 5.54.

S3. Refinement

The C—H H atoms were positioned with idealized geometry and were refined as isotropic with U_{iso}(H) = 1.2 U_{eq}(C, 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).

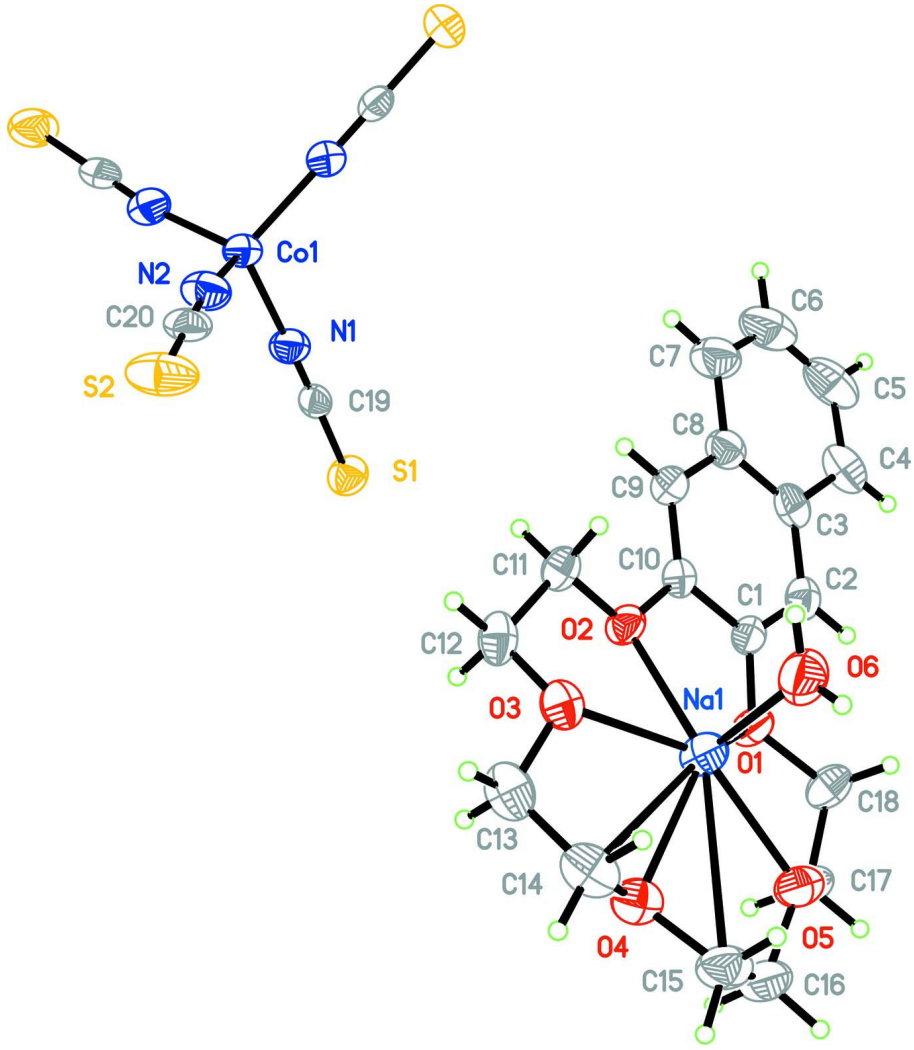

Figure 1

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

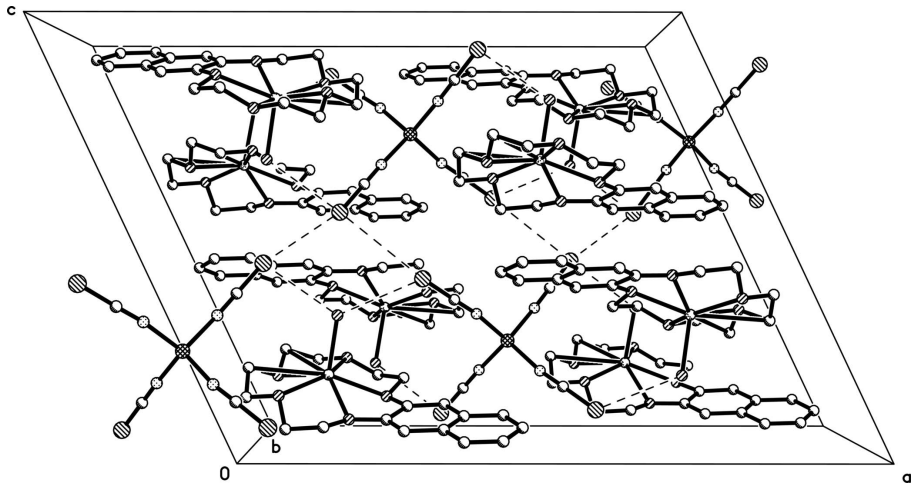

Figure 2

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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$c = 17.469\ (4)$ Å
$\beta = 115.255\ (3)°$
$V = 4792.0\ (18)$ Å^3
$Z = 4$
$F(000) = 2100$
$D_x = 1.400$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1972 reflections
$\theta = 2.5–21.9°$
$\mu = 0.61$ mm^{-1}
$T = 298$ K
Block, red
0.39 × 0.36 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and φ 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 $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -23\rightarrow27$
$k = -15\rightarrow10$
$l = -20\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.110$
$S = 1.00$
4232 reflections
285 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2 + 7.4253P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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)
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 (Å²)

	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, º)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H1···S2^{ii}	0.84	2.62	3.458 (3)	173
O6—H3···S1^{iii}	0.84	2.57	3.389 (3)	165

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