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Tris(4-morpholinecarbodithioato-κ^2S,S')-cobalt(III)

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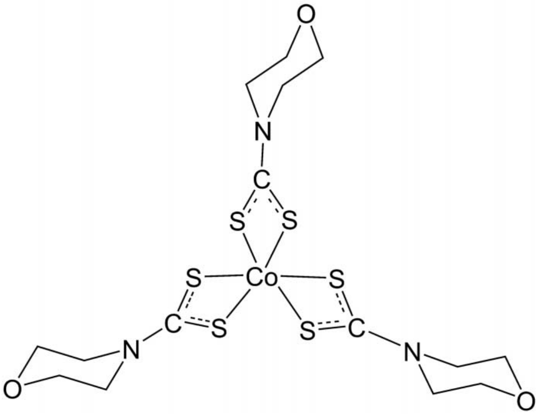
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.131; data-to-parameter ratio = 17.9.

In the unsolvated title compound, $[Co(C_5H_8NOS_2)_3]$, the Co^{III} ion is coordinated by three chelating dithiocarbamate ligands. The central CoS_6 core forms a trigonally distorted octahedron.

Related literature

For related literature, see: Zhang *et al.* (2001); Butcher & Sinn (1976); Healy & Sinn (1975); Cadore *et al.* (2005); Healy *et al.* (1990); Hulanicki (1967); Kropidłowska *et al.* (2007); Nasirov (2003); Sakla *et al.* (1979).



Experimental

Crystal data

$[Co(C_5H_8NOS_2)_3]$
M_r = 545.66
Monoclinic, $P2_1/c$
a = 13.1952 (6) Å
b = 11.4668 (5) Å
c = 15.7281 (9) Å
β = 101.006 (5)°
V = 2336.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 120 (2) K
0.19 × 0.10 × 0.02 mm

Data collection

Oxford Diffraction KM4 CCD area-detector diffractometer
Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2006); analytical numerical absorption correction using a multifaceted crystal model (Clark & Reid, 1995)]
T_{min} = 0.74, T_{max} = 0.9
12971 measured reflections
4538 independent reflections
4094 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.131
S = 1.13
4538 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2018).

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supplementary materials

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Tris(4-morpholinecarbodithioato-κ^2S,S')cobalt(III)

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Comment

Dithiocarbamates (dtc) react with many metallic ions and the complexing properties of these ligands are directly related to the presence of two donor S atoms. The dithiocarbamates serve different analytical purposes-the more interesting properties occur with disubstituted dithiocarbamates since the monosubstituted compounds show stronger reducing properties and tend to decompose to hydrogen sulfide (Hulanicki, 1967). Microdetermination of some metals such as Ni, Co, Fe, Cd or Zn using 4-morpholinecarbodithioate have been described (Sakla *et al.* 1979, Cadore *et al.*, 2005.). What more, cobalt dithiocarbamates, such as aforementioned morpholine derivative, were used as catalyst systems for producing polybutadiene of a high degree of polymerization (Nasirov, 2003).

The structures of solvated tris(4-morpholinecarbodithioato-κ^2S,S')cobalt(III) complexes have been described previously: with $CHCl_3$ (Zhang *et al.*, 2001), C_6H_6 (Butcher & Sinn, 1976) and CH_2Cl_2 (Healy & Sinn, 1975) as solvating molecules. Recently, we have devoted our interest to complexes with dtc ligands and we present here the structure of unsolvated $[Co(S_2CNC_4H_8O)_3]$ complex, (I) (Fig. 1).

Monoclinic crystals of this mononuclear complex are built of $[Co(S_2CN(C_4H_8O)_3]$ units with cobalt octahedrally co-ordinated by three bidentate dithiocarbamate ligands. The title compound possess D_3 pseudosymmetry. The deformation of the coordination geometry is undoubtedly caused by the presence of three chelating agents and thus imposed S—Co—S bite angles. It is noteworthy that (**I**) which was recrystallized from chloroform did not retain the solvent within its crystal structure, unlike related tris(1-pyrrolidinylcarbodithioato-S,*S'*)-cobalt(III) chloroform disolvate (Kropidłowska *et al.*, 2007) reported by us earlier. Molecules of (**I**) are instead tightly packed (Fig. 2) forming layers (Fig. 3). Many short C—H···S contacts (with C···S distance of *ca*. 3.5 – 3.9 Å) are present between the adjacent layers. Some C—H···S interactions in the dithicarbamate cases have been observed and discussed previously (Healy *et al.*, 1990). Several C—H···O short contacts (with C···O distance of *ca*. 3.1 – 3.5 Å) are present as well.

Experimental

The complexing agent was obtained by conventional method from the reaction between carbon disulfide (Merck), morpholine (Merck) and potassium hydroxide (POCh) at 0°C, under constant stirring. The product was filtered, washed with cold methanol and recrystallized from the same solvent. Cobalt chloride, $CoCl_2\times6H_2O$ (0.58 g, 0.0025 mol) purchased from POCh) was dissolved in 50 ml of methanol/water (10/1, *v*/*v*) and this solution was added dropwise to the potassium salt of morpholinecarbodithioic acid $OC_4H_8NCS_2K$ (0.98 g, 0.005 mol, Fluka) dissolved in methanol/water (10/1, *v*/*v*). The mixture was stirred vigorously in an inert gas (Ar) atmosphere for 25 minutes. The solution was then filtered and filtrate left for crystallization at 5°C. After a week green crystals were collected.

Refinement

All H atoms were placed in calculated positions (0.99 Å) and refined as riding with $U_{iso}(H) = 1.3U_{eq}$ (methylene carrier).

The highest peak in the difference map is 0.05 Å from Co1 and the largest hole is 1.56 Å from S5.

Figures

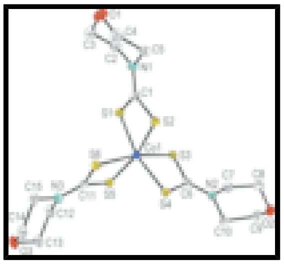

Fig. 1. Molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

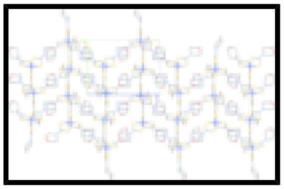

Fig. 2. Schematic drawing of the crystal packing of **I** viewed along *a* axis.

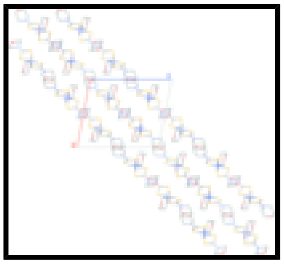

Fig. 3. Schematic drawing of the crystal packing of **I** viewed along *b* axis.

Tris(4-morpholinecarbodithioato-κ^2*S*,*S*')cobalt(III)

Crystal data

$[Co(C_5H_8NOS_2)_3]$	$Z = 4$
$M_r = 545.66$	$F_{000} = 1128$
Monoclinic, $P2_1/c$	$D_x = 1.552$ Mg m^{-3}
Hall symbol: -P 2ybc	Mo *K*α radiation λ = 0.71073 Å
$a = 13.1952$ (6) Å	θ = 2.4–32.5°
$b = 11.4668$ (5) Å	μ = 1.29 mm^{-1}
$c = 15.7281$ (9) Å	$T = 120$ (2) K
β = 101.006 (5)°	Prism, dark green
$V = 2336.0$ (2) Å^3	0.19 × 0.10 × 0.02 mm

Data collection

Oxford Diffraction KM4 CCD area-detector diffractometer	4538 independent reflections
Monochromator: graphite	4094 reflections with $I > 2\sigma(I)$
Detector resolution: 8.1883 pixels mm^{-1}	$R_{\text{int}} = 0.039$
$T = 120(2)$ K	$\theta_{\text{max}} = 26°$
ω scans, 0.75 deg width	$\theta_{\text{min}} = 2.4°$
Absorption correction: analytical [CrysAlis RED (Oxford Diffraction, 2006); analytical numerical absorption correction using a multifaceted crystal model (Clark & Reid, 1995)]	$h = -16 \rightarrow 15$
$T_{\text{min}} = 0.74$, $T_{\text{max}} = 0.9$	$k = -13 \rightarrow 14$
12971 measured reflections	$l = -19 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 4.281P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{\text{max}} < 0.001$
4538 reflections	$\Delta\rho_{\text{max}} = 1.11$ e Å^{-3}
253 parameters	$\Delta\rho_{\text{min}} = -0.82$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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 (Å^2)

	x	y	z	$U_{\text{iso}}*/U_{\text{eq}}$
Co1	0.26983 (3)	0.01485 (4)	0.26399 (3)	0.01532 (14)
S1	0.42699 (6)	0.10412 (7)	0.28576 (5)	0.0203 (2)
S2	0.30882 (6)	0.03786 (7)	0.40951 (5)	0.01715 (19)

S3	0.33634 (6)	−0.16687 (7)	0.25782 (5)	0.01816 (19)
S4	0.13436 (6)	−0.10359 (7)	0.27236 (5)	0.01796 (19)
S5	0.23133 (6)	0.03742 (7)	0.11798 (5)	0.01843 (19)
S6	0.17989 (6)	0.18432 (7)	0.24632 (5)	0.01834 (19)
N1	0.4846 (2)	0.1614 (3)	0.45449 (17)	0.0203 (6)
N2	0.1923 (2)	−0.3293 (2)	0.27148 (19)	0.0216 (6)
N3	0.1270 (2)	0.2387 (2)	0.07649 (17)	0.0221 (6)
O1	0.5547 (2)	0.3653 (2)	0.54704 (17)	0.0362 (6)
O2	0.1546 (2)	−0.5539 (2)	0.33120 (16)	0.0276 (5)
O3	−0.0211 (2)	0.3479 (2)	−0.05188 (15)	0.0292 (6)
C1	0.4184 (2)	0.1095 (3)	0.3928 (2)	0.0171 (6)
C2	0.5761 (3)	0.2238 (3)	0.4379 (2)	0.0246 (7)
H2A	0.5812	0.2157	0.3762	0.032*
H2B	0.6392	0.1902	0.4737	0.032*
C3	0.5668 (3)	0.3514 (3)	0.4601 (2)	0.0333 (9)
H3A	0.6294	0.3936	0.4513	0.043*
H3B	0.5066	0.3859	0.4209	0.043*
C4	0.4636 (3)	0.3081 (3)	0.5611 (2)	0.0305 (8)
H4A	0.4028	0.3427	0.5228	0.04*
H4B	0.4558	0.3202	0.6218	0.04*
C5	0.4676 (3)	0.1783 (3)	0.5430 (2)	0.0231 (7)
H5A	0.5243	0.1417	0.5847	0.03*
H5B	0.4018	0.1411	0.5496	0.03*
C6	0.2173 (2)	−0.2175 (3)	0.2675 (2)	0.0186 (6)
C7	0.2634 (3)	−0.4253 (3)	0.2633 (2)	0.0267 (8)
H7A	0.3347	−0.3949	0.2702	0.035*
H7B	0.2445	−0.4606	0.2049	0.035*
C8	0.2581 (3)	−0.5172 (3)	0.3318 (3)	0.0291 (8)
H8A	0.3	−0.5855	0.3215	0.038*
H8B	0.2881	−0.4851	0.3896	0.038*
C9	0.0937 (3)	−0.4574 (3)	0.3478 (2)	0.0243 (7)
H9A	0.1245	−0.4219	0.4042	0.032*
H9B	0.0233	−0.4844	0.351	0.032*
C10	0.0878 (2)	−0.3671 (3)	0.2769 (2)	0.0215 (7)
H10A	0.0534	−0.4008	0.2209	0.028*
H10B	0.0466	−0.2994	0.2898	0.028*
C11	0.1718 (2)	0.1661 (3)	0.1371 (2)	0.0179 (6)
C12	0.1283 (3)	0.2207 (3)	−0.0155 (2)	0.0251 (7)
H12A	0.1536	0.1412	−0.0245	0.033*
H12B	0.1755	0.2776	−0.0349	0.033*
C13	0.0202 (3)	0.2361 (3)	−0.0674 (2)	0.0263 (7)
H13A	0.0216	0.2282	−0.1299	0.034*
H13B	−0.025	0.1742	−0.0516	0.034*
C14	−0.0276 (3)	0.3579 (3)	0.0376 (2)	0.0256 (7)
H14A	−0.0726	0.2953	0.0529	0.033*
H14B	−0.059	0.4338	0.0476	0.033*
C15	0.0785 (3)	0.3487 (3)	0.0951 (2)	0.0243 (7)
H15A	0.1219	0.4154	0.0839	0.032*
H15B	0.072	0.351	0.1567	0.032*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0159 (2)	0.0152 (2)	0.0145 (2)	−0.00138 (15)	0.00206 (17)	−0.00065 (15)
S1	0.0214 (4)	0.0249 (4)	0.0148 (4)	−0.0058 (3)	0.0039 (3)	−0.0013 (3)
S2	0.0173 (4)	0.0193 (4)	0.0149 (4)	−0.0030 (3)	0.0032 (3)	0.0000 (3)
S3	0.0166 (4)	0.0175 (4)	0.0203 (4)	0.0001 (3)	0.0032 (3)	−0.0012 (3)
S4	0.0163 (4)	0.0153 (4)	0.0218 (4)	0.0001 (3)	0.0026 (3)	0.0004 (3)
S5	0.0214 (4)	0.0182 (4)	0.0153 (4)	0.0012 (3)	0.0024 (3)	−0.0020 (3)
S6	0.0236 (4)	0.0159 (4)	0.0152 (4)	−0.0001 (3)	0.0027 (3)	−0.0018 (3)
N1	0.0189 (13)	0.0256 (15)	0.0168 (13)	−0.0025 (11)	0.0044 (10)	−0.0021 (11)
N2	0.0187 (13)	0.0153 (13)	0.0299 (15)	0.0016 (10)	0.0023 (11)	0.0022 (11)
N3	0.0326 (15)	0.0181 (14)	0.0151 (13)	0.0033 (12)	0.0031 (11)	−0.0010 (11)
O1	0.0446 (16)	0.0303 (14)	0.0331 (14)	−0.0102 (12)	0.0056 (12)	−0.0115 (11)
O2	0.0325 (13)	0.0148 (11)	0.0334 (13)	−0.0013 (10)	0.0011 (11)	0.0023 (10)
O3	0.0423 (15)	0.0227 (13)	0.0207 (12)	0.0092 (11)	0.0016 (10)	0.0036 (10)
C1	0.0196 (15)	0.0152 (15)	0.0169 (14)	−0.0011 (12)	0.0038 (12)	0.0013 (11)
C2	0.0202 (16)	0.0305 (19)	0.0224 (16)	−0.0080 (14)	0.0027 (13)	−0.0028 (14)
C3	0.039 (2)	0.028 (2)	0.0315 (19)	−0.0114 (16)	0.0025 (16)	−0.0012 (15)
C4	0.0333 (19)	0.0291 (19)	0.0284 (18)	0.0018 (15)	0.0041 (15)	−0.0087 (15)
C5	0.0224 (16)	0.0314 (19)	0.0155 (15)	−0.0025 (14)	0.0034 (12)	−0.0023 (13)
C6	0.0178 (14)	0.0214 (16)	0.0153 (14)	−0.0011 (12)	−0.0001 (11)	0.0002 (12)
C7	0.0234 (17)	0.0186 (17)	0.038 (2)	0.0017 (13)	0.0050 (15)	−0.0023 (14)
C8	0.0283 (18)	0.0166 (17)	0.038 (2)	0.0009 (13)	−0.0057 (15)	0.0010 (14)
C9	0.0294 (18)	0.0181 (16)	0.0246 (17)	−0.0039 (13)	0.0030 (14)	0.0008 (13)
C10	0.0182 (15)	0.0179 (16)	0.0266 (17)	−0.0031 (12)	−0.0003 (13)	0.0002 (13)
C11	0.0194 (15)	0.0173 (15)	0.0171 (15)	−0.0051 (12)	0.0038 (12)	−0.0018 (12)
C12	0.0342 (19)	0.0245 (17)	0.0171 (16)	0.0064 (14)	0.0060 (13)	0.0020 (13)
C13	0.0367 (19)	0.0225 (17)	0.0179 (16)	0.0038 (14)	0.0001 (14)	0.0001 (13)
C14	0.0351 (19)	0.0213 (17)	0.0210 (16)	0.0033 (14)	0.0068 (14)	0.0040 (13)
C15	0.0382 (19)	0.0146 (16)	0.0191 (16)	0.0020 (14)	0.0032 (14)	−0.0008 (12)

Geometric parameters (Å, °)

Co1—S2	2.2634 (8)	C2—H2B	0.99
Co1—S6	2.2663 (9)	C3—H3A	0.99
Co1—S4	2.2688 (9)	C3—H3B	0.99
Co1—S5	2.2702 (8)	C4—C5	1.518 (5)
Co1—S3	2.2703 (9)	C4—H4A	0.99
Co1—S1	2.2790 (9)	C4—H4B	0.99
S1—C1	1.710 (3)	C5—H5A	0.99
S2—C1	1.726 (3)	C5—H5B	0.99
S3—C6	1.708 (3)	C7—C8	1.519 (5)
S4—C6	1.715 (3)	C7—H7A	0.99
S5—C11	1.725 (3)	C7—H7B	0.99
S6—C11	1.713 (3)	C8—H8A	0.99
N1—C1	1.317 (4)	C8—H8B	0.99
N1—C5	1.465 (4)	C9—C10	1.512 (5)

N1—C2	1.468 (4)	C9—H9A	0.99
N2—C6	1.329 (4)	C9—H9B	0.99
N2—C10	1.464 (4)	C10—H10A	0.99
N2—C7	1.468 (4)	C10—H10B	0.99
N3—C11	1.318 (4)	C12—C13	1.513 (5)
N3—C12	1.465 (4)	C12—H12A	0.99
N3—C15	1.469 (4)	C12—H12B	0.99
O1—C3	1.415 (5)	C13—H13A	0.99
O1—C4	1.423 (5)	C13—H13B	0.99
O2—C9	1.420 (4)	C14—C15	1.518 (5)
O2—C8	1.428 (4)	C14—H14A	0.99
O3—C14	1.430 (4)	C14—H14B	0.99
O3—C13	1.432 (4)	C15—H15A	0.99
C2—C3	1.516 (5)	C15—H15B	0.99
C2—H2A	0.99		

S2—Co1—S6	92.10 (3)	N1—C5—H5B	109.9
S2—Co1—S4	92.33 (3)	C4—C5—H5B	109.9
S6—Co1—S4	96.91 (3)	H5A—C5—H5B	108.3
S2—Co1—S5	166.76 (4)	N2—C6—S3	124.9 (3)
S6—Co1—S5	76.55 (3)	N2—C6—S4	124.5 (3)
S4—Co1—S5	95.75 (3)	S3—C6—S4	110.5 (2)
S2—Co1—S3	97.76 (3)	N2—C7—C8	110.0 (3)
S6—Co1—S3	168.36 (3)	N2—C7—H7A	109.7
S4—Co1—S3	76.61 (3)	C8—C7—H7A	109.7
S5—Co1—S3	94.31 (3)	N2—C7—H7B	109.7
S2—Co1—S1	76.77 (3)	C8—C7—H7B	109.7
S6—Co1—S1	94.22 (3)	H7A—C7—H7B	108.2
S4—Co1—S1	164.70 (3)	O2—C8—C7	111.9 (3)
S5—Co1—S1	97.02 (3)	O2—C8—H8A	109.2
S3—Co1—S1	94.05 (3)	C7—C8—H8A	109.2
C1—S1—Co1	86.3 (1)	O2—C8—H8B	109.2
C1—S2—Co1	86.4 (1)	C7—C8—H8B	109.2
C6—S3—Co1	86.5 (1)	H8A—C8—H8B	107.9
C6—S4—Co1	86.4 (1)	O2—C9—C10	110.5 (3)
C11—S5—Co1	86.7 (1)	O2—C9—H9A	109.6
C11—S6—Co1	87.1 (1)	C10—C9—H9A	109.6
C1—N1—C5	124.0 (3)	O2—C9—H9B	109.6
C1—N1—C2	122.8 (3)	C10—C9—H9B	109.6
C5—N1—C2	112.6 (3)	H9A—C9—H9B	108.1
C6—N2—C10	122.2 (3)	N2—C10—C9	109.2 (3)
C6—N2—C7	123.4 (3)	N2—C10—H10A	109.8
C10—N2—C7	114.1 (3)	C9—C10—H10A	109.8
C11—N3—C12	122.5 (3)	N2—C10—H10B	109.8
C11—N3—C15	123.4 (3)	C9—C10—H10B	109.8
C12—N3—C15	113.9 (3)	H10A—C10—H10B	108.3
C3—O1—C4	110.6 (3)	N3—C11—S6	125.6 (3)
C9—O2—C8	110.1 (3)	N3—C11—S5	124.8 (2)
C14—O3—C13	109.6 (2)	S6—C11—S5	109.6 (2)
N1—C1—S1	125.6 (2)	N3—C12—C13	109.2 (3)

N1—C1—S2	124.1 (2)	N3—C12—H12A	109.8
S1—C1—S2	110.33 (17)	C13—C12—H12A	109.8
N1—C2—C3	108.9 (3)	N3—C12—H12B	109.8
N1—C2—H2A	109.9	C13—C12—H12B	109.8
C3—C2—H2A	109.9	H12A—C12—H12B	108.3
N1—C2—H2B	109.9	O3—C13—C12	111.3 (3)
C3—C2—H2B	109.9	O3—C13—H13A	109.4
H2A—C2—H2B	108.3	C12—C13—H13A	109.4
O1—C3—C2	111.2 (3)	O3—C13—H13B	109.4
O1—C3—H3A	109.4	C12—C13—H13B	109.4
C2—C3—H3A	109.4	H13A—C13—H13B	108
O1—C3—H3B	109.4	O3—C14—C15	111.0 (3)
C2—C3—H3B	109.4	O3—C14—H14A	109.4
H3A—C3—H3B	108	C15—C14—H14A	109.4
O1—C4—C5	111.3 (3)	O3—C14—H14B	109.4
O1—C4—H4A	109.4	C15—C14—H14B	109.4
C5—C4—H4A	109.4	H14A—C14—H14B	108
O1—C4—H4B	109.4	N3—C15—C14	109.1 (3)
C5—C4—H4B	109.4	N3—C15—H15A	109.9
H4A—C4—H4B	108	C14—C15—H15A	109.9
N1—C5—C4	109.0 (3)	N3—C15—H15B	109.9
N1—C5—H5A	109.9	C14—C15—H15B	109.9
C4—C5—H5A	109.9	H15A—C15—H15B	108.3

S2—Co1—S1—C1	−3.29 (11)	C5—N1—C2—C3	−54.6 (4)
S6—Co1—S1—C1	87.88 (11)	C4—O1—C3—C2	−60.6 (4)
S4—Co1—S1—C1	−48.75 (18)	N1—C2—C3—O1	56.9 (4)
S5—Co1—S1—C1	164.83 (11)	C3—O1—C4—C5	60.2 (4)
S3—Co1—S1—C1	−100.32 (11)	C1—N1—C5—C4	−117.1 (3)
S6—Co1—S2—C1	−90.58 (11)	C2—N1—C5—C4	54.2 (4)
S4—Co1—S2—C1	172.41 (11)	O1—C4—C5—N1	−56.1 (4)
S5—Co1—S2—C1	−59.94 (18)	C10—N2—C6—S3	−178.0 (2)
S3—Co1—S2—C1	95.61 (11)	C7—N2—C6—S3	−3.5 (5)
S1—Co1—S2—C1	3.26 (11)	C10—N2—C6—S4	2.7 (5)
S2—Co1—S3—C6	89.61 (11)	C7—N2—C6—S4	177.2 (2)
S6—Co1—S3—C6	−58.1 (2)	Co1—S3—C6—N2	−178.1 (3)
S4—Co1—S3—C6	−0.94 (10)	Co1—S3—C6—S4	1.30 (14)
S5—Co1—S3—C6	−95.84 (11)	Co1—S4—C6—N2	178.1 (3)
S1—Co1—S3—C6	166.79 (11)	Co1—S4—C6—S3	−1.30 (14)
S2—Co1—S4—C6	−96.49 (11)	C6—N2—C7—C8	135.6 (3)
S6—Co1—S4—C6	171.11 (10)	C10—N2—C7—C8	−49.5 (4)
S5—Co1—S4—C6	94.01 (11)	C9—O2—C8—C7	−60.1 (4)
S3—Co1—S4—C6	0.94 (10)	N2—C7—C8—O2	52.4 (4)
S1—Co1—S4—C6	−52.51 (17)	C8—O2—C9—C10	62.8 (3)
S2—Co1—S5—C11	−30.55 (18)	C6—N2—C10—C9	−132.7 (3)
S6—Co1—S5—C11	1.03 (10)	C7—N2—C10—C9	52.3 (4)
S4—Co1—S5—C11	96.79 (11)	O2—C9—C10—N2	−58.1 (3)
S3—Co1—S5—C11	173.73 (11)	C12—N3—C11—S6	176.3 (3)
S1—Co1—S5—C11	−91.64 (11)	C15—N3—C11—S6	1.2 (5)
S2—Co1—S6—C11	172.07 (11)	C12—N3—C11—S5	−3.8 (5)

S4—Co1—S6—C11	−95.33 (11)	C15—N3—C11—S5	−178.9 (3)
S5—Co1—S6—C11	−1.04 (11)	Co1—S6—C11—N3	−178.7 (3)
S3—Co1—S6—C11	−39.9 (2)	Co1—S6—C11—S5	1.41 (14)
S1—Co1—S6—C11	95.19 (11)	Co1—S5—C11—N3	178.7 (3)
C5—N1—C1—S1	171.1 (3)	Co1—S5—C11—S6	−1.41 (14)
C2—N1—C1—S1	0.6 (5)	C11—N3—C12—C13	132.2 (3)
C5—N1—C1—S2	−8.2 (5)	C15—N3—C12—C13	−52.3 (4)
C2—N1—C1—S2	−178.7 (3)	C14—O3—C13—C12	−61.6 (4)
Co1—S1—C1—N1	−174.9 (3)	N3—C12—C13—O3	56.1 (4)
Co1—S1—C1—S2	4.48 (15)	C13—O3—C14—C15	61.6 (4)
Co1—S2—C1—N1	174.9 (3)	C11—N3—C15—C14	−132.2 (3)
Co1—S2—C1—S1	−4.51 (15)	C12—N3—C15—C14	52.3 (4)
C1—N1—C2—C3	116.9 (3)	O3—C14—C15—N3	−56.1 (4)

Fig. 1

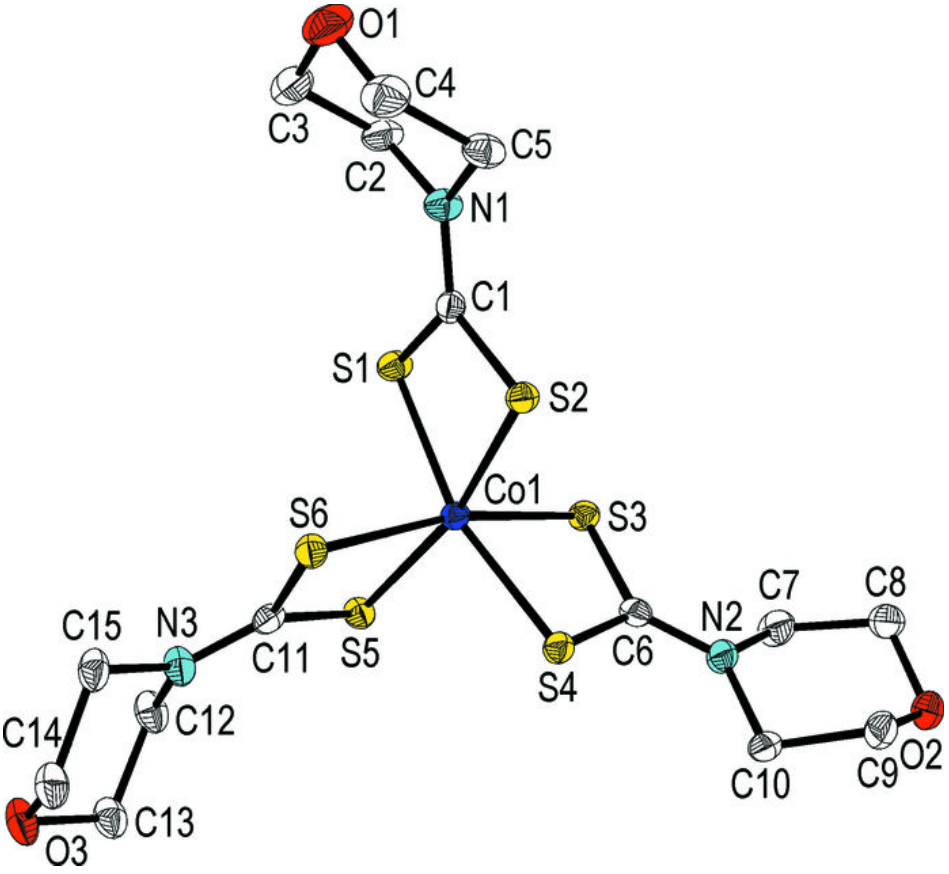
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Fig. 2

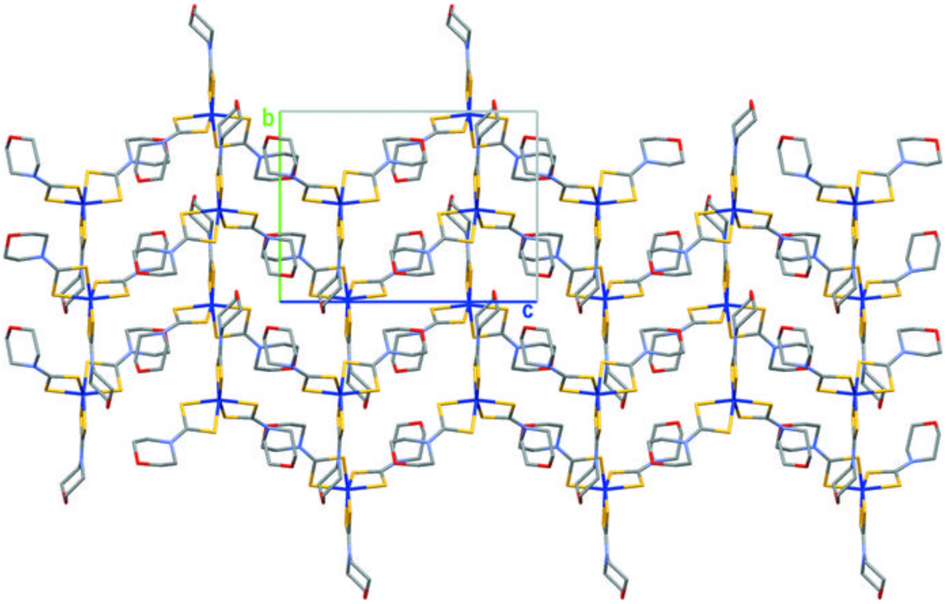

Fig. 3