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trans-Bis[2-(piperazin-1-yl)ethanamine]-bis(saccharinato)cobalt(II)

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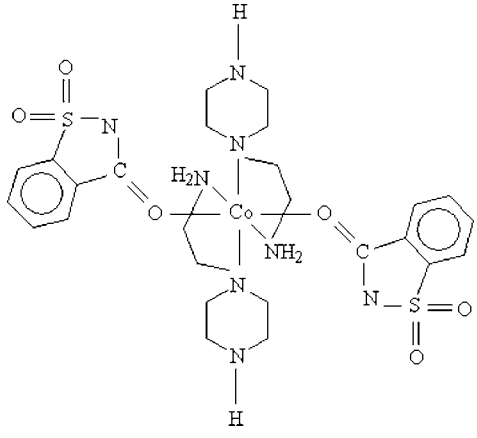
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.094; data-to-parameter ratio = 14.0.

In the centrosymmetric title complex, $[Co(C_7H_4NO_3S)_2(C_6H_{15}N_3)_2]$, the Co^{II} ion is coordinated by two saccharinate (sac) anions and two neutral 2-piperazin-1-ylethanamine (ppzea) ligands, showing a distorted octahedral coordination. Sac is O-bonded *via* the carbonyl group, while ppzea acts as an *N*,*N*′-bidentate chelating ligand. The molecules are connected by N—H···N and N—H···O hydrogen bonds, forming a linear chain running parallel to the crystallographic *a* axis. The compound is isostructural with the reported Ni, Zn, and Cd analogues.

Related literature

For the structures of the analogous Ni, Zn, and Cd complexes, see: Guney *et al.* (2005); Yilmaz *et al.* (2005). For a review of saccharinate complexes, see: Baran & Yilmaz (2006).



Experimental

Crystal data

$[Co(C_7H_4NO_3S)_2(C_6H_{15}N_3)_2]$
M_r = 681.69
Triclinic, $P\overline{1}$
a = 8.4294 (7) Å
b = 9.3742 (10) Å
c = 11.5618 (10) Å
α = 93.651 (8)°
β = 110.473 (6)°
γ = 116.486 (13)°
V = 739.31 (17) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.78 mm^{-1}
T = 293 (2) K
0.58 × 0.41 × 0.25 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED*; Stoe & Cie, 2002)
T_{min} = 0.721, T_{max} = 0.865
9652 measured reflections
2913 independent reflections
2635 reflections with $I > 2\sigma(I)$
R_{int} = 0.103

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.094
S = 1.07
2913 reflections
208 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.0897 (13)	Co1—N3	2.3589 (16)
Co1—N2	2.1101 (16)		
O1—Co1—N2^{i}	91.53 (6)	N2—Co1—N3	80.62 (6)
O1—Co1—N2	88.47 (6)	O1—Co1—N3^{i}	92.94 (6)
O1—Co1—N3	87.06 (6)	N2—Co1—N3^{i}	99.38 (6)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N4^{ii}	0.85 (3)	2.38 (3)	3.172 (3)	154 (2)
N2—H2A···N1^{i}	0.91 (3)	2.25 (3)	2.982 (2)	137 (2)
N4—H4A···O3^{iii}	0.838 (17)	2.221 (18)	3.054 (3)	173 (3)

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SQ2006).

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supplementary materials

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trans-Bis[2-(piperazin-1-yl)ethanamine]bis(saccharinato)cobalt(II)

V. T. Yilmaz, S. Guney and C. Kazak

Comment

The saccharinate (sac) anion is formed by the deprotonation of saccharin and coordinates to various metal ions rather easily (Baran & Yilmaz 2006). In the course of the synthesis and structural characterization of mixed ligand–metal complexes of sac, recently we reported nickel(II), zinc(II) and cadmium(II) complexes of sac with 2-piperazin-1-ylethanamine (ppzea) (Guney *et al.*, 2005; Yilmaz *et al.*, 2005). In this paper, the crystal and molecular structure of the isomorphous sac complex of cobalt(II) with ppzea (I) is reported.

The title complex (I) is isostructural with the nickel(II), zinc(II) and cadmium(II) complexes of the same ligands (Guney *et al.*, 2005; Yilmaz *et al.*, 2005) and shows similar structural characteristics. In these isostructural complexes, the M^{II} ions show an elongated octahedral geometry, possibly due to a poor overlap of the sp^3 lone pair on the N atom of ppz with the valence orbitals of the metal ions. As shown in Fig. 1, (I) is a mononuclear Co^{II} complex, in which the Co^{II} ion lies on a centre of inversion and also exhibits an elongated distorted octahedral geometry with two neutral bidendate (N,*N*') ppzea ligands and two anionic sac ligands. In spite of the common N-coordination mode, sac coordinates to Co^{II} through the carbonyl O atom. The puckering parameters of the ppz ring system in (I) are q = 0.538 (2)Å and Θ = 5.4 (2)°, suggesting that the ppz rings exhibit a typical (*e.g.*, cyclohexane-like) chair conformation.

The amine hydrogen atoms of ppzea form intramolecular hydrogen bonds with the negatively charged N atom of sac. The individual molecules are linked by N—H···N and N—H···O hydrogen bonds, involving the amine H atoms of ppzea and the ring N atom of ppzea and the sulfonyl O atoms of sac, forming a linear chain running paralel to the crystallographic *a* axis.

Experimental

A 20 ml e thanol solution containing ppzea (0.26 g, 2 mmol) and sacH (0.36 g, 2 mmol) was mixed with a 20 ml e thanol solution of $Co(OAc)_2{\cdot}4H_2O$ (0.25 g, 1 mmol). The reaction solution was stirred for 1 h at room temperature. Red-brown prisms were obtained after 5 days by slow evaporation of the solution at room temperature.

Refinement

All N-bonded H atoms were refined freely, while C-bonded H atoms were placed in idealized locations (C—H = 0.95 Å) and included as riding atoms with $U_{iso}(H) = 1.2*U_{eq}(C)$. The instruction *DFIX* was applied to the N4—H4A bond to increase its length to a reasonable value.

Figures

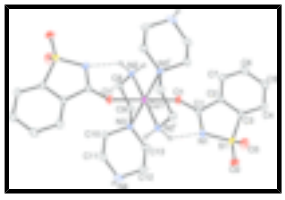

Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). Symmetry code: (i) −*x* + 1, −*y* + 1, −*z* + 1. The intramolecular N—H···N hydrogen bonds are indicated by dashed lines.

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Crystal data

$[Co(C_7H_4NO_3S)_2(C_6H_{15}N_3)_2]$	$Z = 1$
$M_r = 681.69$	$F_{000} = 357$
Triclinic, $P\overline{1}$	$D_x = 1.531$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.4294$ (7) Å	Cell parameters from 16784 reflections
$b = 9.3742$ (10) Å	$\theta = 2.0$–28.0º
$c = 11.5618$ (10) Å	$\mu = 0.78$ mm^{-1}
$\alpha = 93.651$ (8)º	$T = 293$ (2) K
$\beta = 110.473$ (6)º	Prism, light brown
$\gamma = 116.486$ (13)º	0.58 × 0.41 × 0.25 mm
$V = 739.31$ (17) Å^3	

Data collection

Stoe IPDS 2 diffractometer	2913 independent reflections
Radiation source: fine-focus sealed tube	2635 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.103$
Detector resolution: 6.67 pixels mm^{-1}	$\theta_{max} = 26.0$º
$T = 293(2)$ K	$\theta_{min} = 2.0$º
rotation method scans	$h = -10 \rightarrow 10$
Absorption correction: integration (X-RED; Stoe & Cie, 2002)	$k = -10 \rightarrow 11$
$T_{min} = 0.721$, $T_{max} = 0.865$	$l = -14 \rightarrow 14$
9652 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.094$	$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 0.1493P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
2913 reflections	$\Delta\rho_{max} = 0.47$ e Å^{-3}
208 parameters	$\Delta\rho_{min} = -0.64$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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_{iso}*/U_{eq}
Co1	0.5000	0.5000	0.5000	0.02842 (12)
S1	0.60105 (7)	0.20581 (6)	0.86106 (4)	0.03467 (14)
O1	0.4721 (2)	0.46565 (17)	0.67018 (13)	0.0386 (3)
O2	0.7830 (2)	0.2754 (2)	0.97136 (15)	0.0540 (4)
O3	0.5203 (3)	0.03573 (19)	0.79884 (17)	0.0557 (4)
N1	0.6138 (2)	0.3163 (2)	0.75875 (16)	0.0379 (4)
N2	0.4126 (2)	0.6783 (2)	0.50483 (16)	0.0324 (3)
N3	0.8077 (2)	0.73527 (18)	0.62659 (14)	0.0312 (3)
N4	1.1486 (2)	0.7105 (2)	0.6325 (2)	0.0498 (5)
C1	0.4967 (3)	0.3785 (2)	0.74533 (16)	0.0313 (4)
C2	0.3873 (3)	0.3351 (2)	0.82672 (17)	0.0311 (4)
C3	0.4282 (3)	0.2328 (2)	0.89749 (17)	0.0332 (4)
C4	0.3404 (3)	0.1714 (3)	0.9774 (2)	0.0441 (5)
H4	0.3693	0.1030	1.0251	0.053*
C5	0.2076 (3)	0.2162 (3)	0.9835 (2)	0.0501 (5)
H5	0.1437	0.1752	1.0352	0.060*
C6	0.1672 (3)	0.3207 (3)	0.9146 (2)	0.0508 (5)
H6	0.0790	0.3508	0.9219	0.061*
C7	0.2570 (3)	0.3805 (3)	0.8352 (2)	0.0436 (5)
H7	0.2298	0.4502	0.7884	0.052*
C8	0.5815 (3)	0.8468 (2)	0.5672 (2)	0.0379 (4)
H8A	0.5428	0.9166	0.6017	0.046*
H8B	0.6277	0.8934	0.5052	0.046*
C9	0.7420 (3)	0.8403 (2)	0.67326 (19)	0.0381 (4)
H9A	0.8524	0.9514	0.7150	0.046*

H9B	0.6957	0.7976	0.7363	0.046*
C10	0.9221 (3)	0.8211 (2)	0.5561 (2)	0.0405 (4)
H10A	1.0226	0.9321	0.6082	0.049*
H10B	0.8365	0.8297	0.4785	0.049*
C11	1.0174 (3)	0.7314 (3)	0.5215 (2)	0.0475 (5)
H11A	0.9159	0.6234	0.4642	0.057*
H11B	1.0910	0.7925	0.4759	0.057*
C12	1.0468 (3)	0.6362 (3)	0.7102 (2)	0.0448 (5)
H12A	1.1410	0.6398	0.7898	0.054*
H12B	0.9525	0.5210	0.6657	0.054*
C13	0.9411 (3)	0.7169 (3)	0.74108 (18)	0.0390 (4)
H13A	0.8658	0.6515	0.7842	0.047*
H13B	1.0371	0.8253	0.7997	0.047*
H2A	0.348 (3)	0.681 (3)	0.424 (2)	0.043 (6)*
H2B	0.337 (3)	0.655 (3)	0.543 (2)	0.040 (6)*
H4A	1.244 (3)	0.804 (2)	0.677 (3)	0.064 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0362 (2)	0.03155 (19)	0.02755 (19)	0.02107 (15)	0.01746 (14)	0.01371 (14)
S1	0.0412 (3)	0.0402 (3)	0.0304 (2)	0.0253 (2)	0.0159 (2)	0.01366 (19)
O1	0.0519 (8)	0.0450 (7)	0.0335 (7)	0.0294 (6)	0.0246 (6)	0.0217 (6)
O2	0.0454 (8)	0.0778 (11)	0.0397 (8)	0.0367 (8)	0.0107 (7)	0.0189 (8)
O3	0.0727 (10)	0.0430 (8)	0.0596 (10)	0.0346 (8)	0.0296 (8)	0.0114 (7)
N1	0.0430 (8)	0.0491 (9)	0.0348 (8)	0.0276 (7)	0.0228 (7)	0.0197 (7)
N2	0.0360 (8)	0.0385 (8)	0.0332 (8)	0.0238 (7)	0.0178 (7)	0.0141 (7)
N3	0.0333 (7)	0.0337 (7)	0.0310 (7)	0.0190 (6)	0.0150 (6)	0.0102 (6)
N4	0.0321 (9)	0.0534 (11)	0.0560 (12)	0.0198 (8)	0.0152 (8)	−0.0008 (9)
C1	0.0357 (9)	0.0347 (8)	0.0249 (8)	0.0176 (7)	0.0141 (7)	0.0094 (7)
C2	0.0333 (8)	0.0336 (8)	0.0267 (8)	0.0158 (7)	0.0139 (7)	0.0096 (7)
C3	0.0369 (9)	0.0344 (9)	0.0288 (9)	0.0169 (7)	0.0154 (7)	0.0104 (7)
C4	0.0558 (12)	0.0434 (10)	0.0360 (10)	0.0218 (10)	0.0251 (9)	0.0181 (9)
C5	0.0530 (12)	0.0553 (12)	0.0423 (11)	0.0178 (10)	0.0330 (10)	0.0128 (10)
C6	0.0481 (12)	0.0639 (14)	0.0501 (13)	0.0302 (11)	0.0289 (10)	0.0108 (11)
C7	0.0504 (11)	0.0519 (11)	0.0425 (11)	0.0327 (10)	0.0239 (9)	0.0181 (9)
C8	0.0467 (10)	0.0328 (9)	0.0447 (11)	0.0256 (8)	0.0222 (9)	0.0134 (8)
C9	0.0427 (10)	0.0347 (9)	0.0366 (10)	0.0208 (8)	0.0155 (8)	0.0037 (8)
C10	0.0393 (10)	0.0368 (9)	0.0458 (11)	0.0156 (8)	0.0226 (8)	0.0144 (8)
C11	0.0425 (11)	0.0496 (12)	0.0512 (12)	0.0181 (9)	0.0280 (9)	0.0087 (10)
C12	0.0377 (10)	0.0491 (11)	0.0437 (11)	0.0267 (9)	0.0077 (8)	0.0057 (9)
C13	0.0378 (10)	0.0454 (10)	0.0320 (9)	0.0229 (8)	0.0104 (8)	0.0086 (8)

Geometric parameters (Å, °)

Co1—O1^{i}	2.0897 (13)	C3—C4	1.378 (3)
Co1—O1	2.0897 (13)	C4—C5	1.380 (3)
Co1—N2^{i}	2.1101 (16)	C4—H4	0.9300

Co1—N2	2.1101 (16)	C5—C6	1.385 (4)
Co1—N3	2.3589 (16)	C5—H5	0.9300
Co1—N3^{i}	2.3589 (16)	C6—C7	1.379 (3)
S1—O2	1.4274 (15)	C6—H6	0.9300
S1—O3	1.4376 (16)	C7—H7	0.9300
S1—N1	1.6214 (16)	C8—C9	1.504 (3)
S1—C3	1.763 (2)	C8—H8A	0.9700
O1—C1	1.257 (2)	C8—H8B	0.9700
N1—C1	1.326 (3)	C9—H9A	0.9700
N2—C8	1.474 (2)	C9—H9B	0.9700
N2—H2A	0.91 (3)	C10—C11	1.515 (3)
N2—H2B	0.85 (3)	C10—H10A	0.9700
N3—C10	1.478 (3)	C10—H10B	0.9700
N3—C9	1.482 (2)	C11—H11A	0.9700
N3—C13	1.485 (2)	C11—H11B	0.9700
N4—C12	1.454 (3)	C12—C13	1.512 (3)
N4—C11	1.463 (3)	C12—H12A	0.9700
N4—H4A	0.838 (17)	C12—H12B	0.9700
C1—C2	1.490 (3)	C13—H13A	0.9700
C2—C7	1.373 (3)	C13—H13B	0.9700
C2—C3	1.380 (2)		
O1^{i}—Co1—O1	180.000 (1)	C3—C4—H4	121.5
O1^{i}—Co1—N2^{i}	88.47 (6)	C5—C4—H4	121.5
O1—Co1—N2^{i}	91.53 (6)	C4—C5—C6	121.7 (2)
O1^{i}—Co1—N2	91.53 (6)	C4—C5—H5	119.2
O1—Co1—N2	88.47 (6)	C6—C5—H5	119.2
N2^{i}—Co1—N2	180.000 (1)	C7—C6—C5	120.3 (2)
O1^{i}—Co1—N3	92.94 (6)	C7—C6—H6	119.9
O1—Co1—N3	87.06 (6)	C5—C6—H6	119.9
N2^{i}—Co1—N3	99.38 (6)	C2—C7—C6	118.75 (19)
N2—Co1—N3	80.62 (6)	C2—C7—H7	120.6
O1^{i}—Co1—N3^{i}	87.06 (5)	C6—C7—H7	120.6
O1—Co1—N3^{i}	92.94 (6)	N2—C8—C9	109.12 (15)
N2^{i}—Co1—N3^{i}	80.62 (6)	N2—C8—H8A	109.9
N2—Co1—N3^{i}	99.38 (6)	C9—C8—H8A	109.9
N3—Co1—N3^{i}	180.0	N2—C8—H8B	109.9
O2—S1—O3	114.88 (11)	C9—C8—H8B	109.9
O2—S1—N1	111.71 (10)	H8A—C8—H8B	108.3
O3—S1—N1	110.32 (10)	N3—C9—C8	112.44 (16)
O2—S1—C3	110.86 (10)	N3—C9—H9A	109.1
O3—S1—C3	110.47 (10)	C8—C9—H9A	109.1
N1—S1—C3	97.23 (9)	N3—C9—H9B	109.1
C1—O1—Co1	136.88 (13)	C8—C9—H9B	109.1
C1—N1—S1	110.72 (14)	H9A—C9—H9B	107.8
C8—N2—Co1	112.04 (11)	N3—C10—C11	111.99 (17)
C8—N2—H2A	105.0 (14)	N3—C10—H10A	109.2

Co1—N2—H2A	110.7 (16)	C11—C10—H10A	109.2
C8—N2—H2B	110.3 (16)	N3—C10—H10B	109.2
Co1—N2—H2B	110.0 (16)	C11—C10—H10B	109.2
H2A—N2—H2B	109 (2)	H10A—C10—H10B	107.9
C10—N3—C9	109.30 (15)	N4—C11—C10	113.47 (19)
C10—N3—C13	107.64 (15)	N4—C11—H11A	108.9
C9—N3—C13	107.08 (15)	C10—C11—H11A	108.9
C10—N3—Co1	115.28 (12)	N4—C11—H11B	108.9
C9—N3—Co1	99.17 (11)	C10—C11—H11B	108.9
C13—N3—Co1	117.56 (11)	H11A—C11—H11B	107.7
C12—N4—C11	109.61 (16)	N4—C12—C13	115.08 (18)
C12—N4—H4A	108 (2)	N4—C12—H12A	108.5
C11—N4—H4A	109 (2)	C13—C12—H12A	108.5
O1—C1—N1	125.08 (18)	N4—C12—H12B	108.5
O1—C1—C2	120.27 (17)	C13—C12—H12B	108.5
N1—C1—C2	114.64 (15)	H12A—C12—H12B	107.5
C7—C2—C3	120.25 (19)	N3—C13—C12	113.48 (17)
C7—C2—C1	128.66 (17)	N3—C13—H13A	108.9
C3—C2—C1	111.08 (17)	C12—C13—H13A	108.9
C4—C3—C2	122.14 (19)	N3—C13—H13B	108.9
C4—C3—S1	131.55 (16)	C12—C13—H13B	108.9
C2—C3—S1	106.31 (14)	H13A—C13—H13B	107.7
C3—C4—C5	116.93 (19)		
$N2^{i}$—Co1—O1—C1	0.70 (18)	C1—C2—C3—C4	−178.03 (17)
N2—Co1—O1—C1	−179.30 (18)	C7—C2—C3—S1	−179.55 (15)
N3—Co1—O1—C1	−98.62 (18)	C1—C2—C3—S1	1.80 (18)
$N3^{i}$—Co1—O1—C1	81.38 (18)	O2—S1—C3—C4	−64.8 (2)
O2—S1—N1—C1	−115.72 (15)	O3—S1—C3—C4	63.7 (2)
O3—S1—N1—C1	115.20 (15)	N1—S1—C3—C4	178.58 (19)
C3—S1—N1—C1	0.18 (15)	O2—S1—C3—C2	115.35 (14)
$O1^{i}$—Co1—N2—C8	−86.23 (13)	O3—S1—C3—C2	−116.12 (14)
O1—Co1—N2—C8	93.77 (13)	N1—S1—C3—C2	−1.22 (14)
N3—Co1—N2—C8	6.49 (13)	C2—C3—C4—C5	0.3 (3)
$N3^{i}$—Co1—N2—C8	−173.51 (13)	S1—C3—C4—C5	−179.46 (17)
$O1^{i}$—Co1—N3—C10	−3.65 (13)	C3—C4—C5—C6	−1.3 (3)
O1—Co1—N3—C10	176.35 (13)	C4—C5—C6—C7	1.3 (4)
$N2^{i}$—Co1—N3—C10	85.29 (13)	C3—C2—C7—C6	−0.6 (3)
N2—Co1—N3—C10	−94.71 (13)	C1—C2—C7—C6	177.80 (19)
$O1^{i}$—Co1—N3—C9	112.87 (11)	C5—C6—C7—C2	−0.4 (3)
O1—Co1—N3—C9	−67.13 (11)	Co1—N2—C8—C9	−34.5 (2)
$N2^{i}$—Co1—N3—C9	−158.19 (11)	C10—N3—C9—C8	72.7 (2)
N2—Co1—N3—C9	21.81 (11)	C13—N3—C9—C8	−170.98 (16)
$O1^{i}$—Co1—N3—C13	−132.30 (13)	Co1—N3—C9—C8	−48.30 (17)
O1—Co1—N3—C13	47.70 (13)	N2—C8—C9—N3	59.5 (2)
$N2^{i}$—Co1—N3—C13	−43.36 (14)	C9—N3—C10—C11	172.09 (16)
N2—Co1—N3—C13	136.64 (14)	C13—N3—C10—C11	56.1 (2)
Co1—O1—C1—N1	24.4 (3)	Co1—N3—C10—C11	−77.30 (18)

Co1—O1—C1—C2	−154.52 (14)	C12—N4—C11—C10	52.0 (2)
S1—N1—C1—O1	−178.10 (15)	N3—C10—C11—N4	−58.3 (2)
S1—N1—C1—C2	0.9 (2)	C11—N4—C12—C13	−49.1 (2)
O1—C1—C2—C7	−1.3 (3)	C10—N3—C13—C12	−53.1 (2)
N1—C1—C2—C7	179.63 (19)	C9—N3—C13—C12	−170.55 (17)
O1—C1—C2—C3	177.19 (16)	Co1—N3—C13—C12	79.06 (19)
N1—C1—C2—C3	−1.9 (2)	N4—C12—C13—N3	52.0 (2)
C7—C2—C3—C4	0.6 (3)		

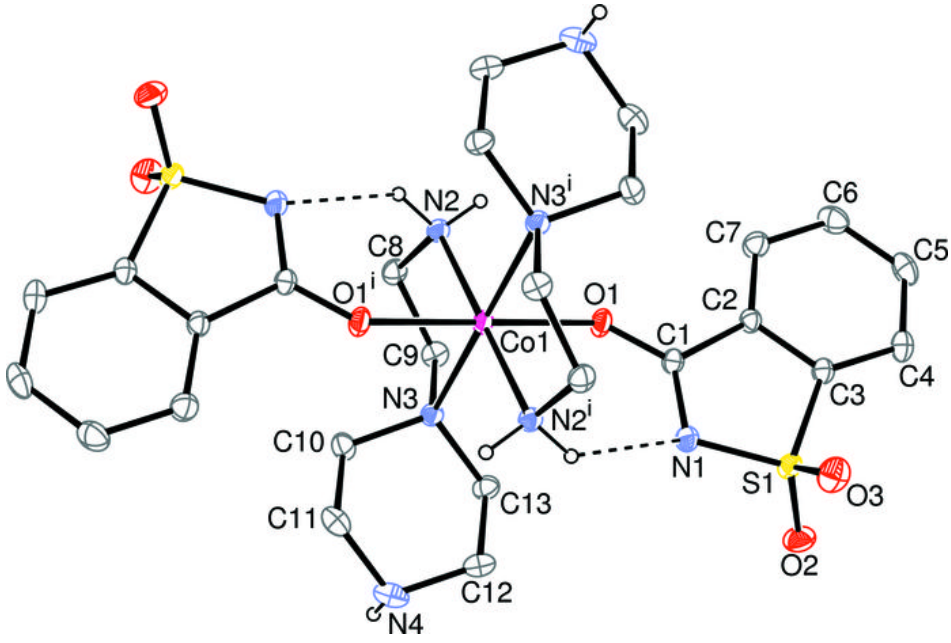
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···N4^{ii}	0.85 (3)	2.38 (3)	3.172 (3)	154 (2)
N2—H2A···N1^{i}	0.91 (3)	2.25 (3)	2.982 (2)	137 (2)
N4—H4A···O3^{iii}	0.838 (17)	2.221 (18)	3.054 (3)	173 (3)

Symmetry codes: (ii) *x*−1, *y*, *z*; (i) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1, *y*+1, *z*.

Fig. 1


N2
N3i
C6
C7
C5
C8
O1i
O1
C2
Co1
C1
C9
C4
C3
N3
N2i
C10
N1
S1
O3
C13
C11
O2
C12
N4