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Triaqua[(4-nitrophenylsulfonyl)acetato-κO](1,10-phenanthroline-κ²N,N′)-cobalt(II) (4-nitrophenylsulfonyl)acetate monohydrate

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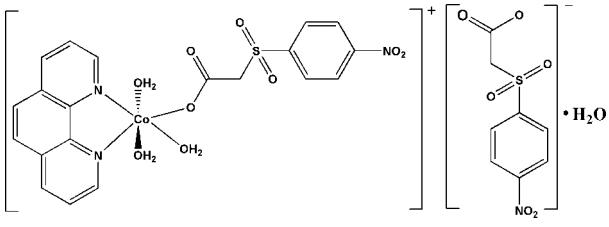
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.091; data-to-parameter ratio = 16.1.

In the title compound, $[Co(C_8H_6NO_6S)(C_{12}H_8N_2)(H_2O)_3]\cdot(C_8H_6NO_6S)\cdot H_2O$, the Co^{II} atom shows an octahedral coordination, the geometry being defined by a carboxylate O atom from a 4-nitrophenylsulfonylacetate anion, two N atoms from the phenanthroline ligand and three water molecules. The molecules of the complex are linked by O—H···O hydrogen bonds, which also involve the solvent water molecule, to form a linear chain structure.

Related literature

For related literature on metal arylsulfonylacetates, see: Gao *et al.* (2006); Hou *et al.* (2007); Shi *et al.* (2007). For related literature on the synthesis of 4-nitrophenylsulfonylacetic acid, see: Nobles & Thompson (1965).



Experimental

Crystal data

$[Co(C_8H_6NO_6S)(C_{12}H_8N_2)(H_2O)_3]\cdot(C_8H_6NO_6S)\cdot H_2O$
M_r = 799.59
Monoclinic, $P2_1/c$
a = 7.5710 (12) Å
b = 15.750 (4) Å
c = 27.403 (5) Å
β = 96.76 (2)°
V = 3244.8 (11) Å³
Z = 4
Mo $K\alpha$ radiation
μ = 0.74 mm⁻¹
T = 293 (2) K
0.22 × 0.21 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.852, T_{max} = 0.873
29459 measured reflections
7420 independent reflections
5686 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.091
S = 1.07
7420 reflections
460 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 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
O13—H21···O10^{i}	0.85	1.89	2.732 (2)	171
O13—H22···O3^{ii}	0.85	1.91	2.750 (2)	170
O14—H23···O9^{iii}	0.85	1.96	2.805 (2)	179
O14—H24···O16	0.85	1.85	2.693 (2)	173
O15—H25···O3	0.85	1.90	2.698 (2)	155
O15—H26···O7^{iii}	0.85	2.25	3.026 (2)	152
O15—H26···O9^{iii}	0.85	2.61	3.049 (2)	114
O16—H28···O10^{iv}	0.85	1.89	2.724 (2)	166
O16—H27···O9^{i}	0.85	2.08	2.848 (2)	150

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2278).

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Shi, A.-E., Zhang, S., Li, B.-Y., Hou, Y.-J. & Hou, G.-F. (2007). *Acta Cryst.* E**63**, m265–m266.

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supplementary materials

Acta Cryst. (2007). E**63**, m1884 [**doi:10.1107/S160053680702819X**]

Triaqua[(4-nitrophenylsulfonyl)acetato-κO](1,10-phenanthroline-$\kappa^2 N,N'$)cobalt(II) (4-nitrophenylsulfonyl)acetate monohydrate

Y.-J. Hou, Y.-H. Yu, Z.-Z. Sun, B.-Y. Li and G.-F. Hou

Comment

Recently, we reported the crystal structures of metal complexes of 4-nitrophenylsulfanylacetic acid (Gao *et al.*, 2006; Shi *et al.*, 2007) and 4-nitrophenylsulfinylacetic acid (Hou *et al.*, 2007); following this study, we report the cobalt complex of 4-nitrophenylsulfonylacetic acid.

The Co atom exists in an octahedral geometry that is defined by a carboxyl O-atom from a 4-nitrophenylsulfonylacetate, two N-atom donorss from the 1,10-phenanthroline ligand, and three water molecules. The other 4-nitrophenylsulfonylacetate exists as a counterion. The cations and anions are linked by O—H···O hydrogen bonds that also involve the free water molecule into a linear chain (Table 1), (Fig. 2).

Experimental

(4-Nitrophenylsulfanyl)acetic acid was prepared by the nucleophilic reaction of chloroacetic acid and 4-nitrothiophenol under basic conditions. (4-Nitrophenylsulfanyl)acetic acid was then oxidized by using 30% hydrogen peroxide at 323 K in acetic anhydride to form 4-nitrophenylsulfonylacetic acid (Nobles & Thompson, 1965). Cobalt nitrate hexahydrate (0.582 g, 2 mmol), 4-nitrophenylsulfonylacetic acid (0.490 g, 2 mmol) and 1,10-phenanthroline (0.360 g, 2 mmol) were dissolved in water, and the pH was adjusted to 6 with 0.01 *M* sodium hydroxide. Pink crystals separated from the filtered solution after several days.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C) or C—H = 0.97 Å (methylene C), and with U_{iso}(H) = 1.2Ueq(C). Water H atoms were initially located in a difference Fourier map but they were treated as riding on their parent atoms with O—H = 0.85 Å and with U_{iso}(H) = 1.5Ueq(O).

Figures

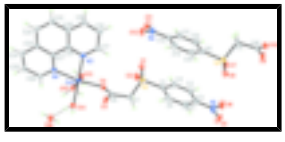

Fig. 1. The molecular structure of (I), with the atomlabelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii.

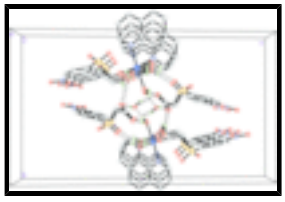

Fig. 2. A partial packing plot of (I). Dashed lines indicate the hydrogen-bonding interactions. H atoms not involved in hydrogen bonds have been omitted.

3-[2-(1,3-Dioxo-2,3-dihydro-1*H*-isoindol-2-yl)ethyl] 5-methyl 2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate

Crystal data

$[Co(C_8H_6NO_6S)(C_{12}H_8N_2)(H_2O)_3](C_8H_6NO_6S)\cdot H_2O$	F_{000} = 1644
M_r = 799.59	D_x = 1.637 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 24616 reflections
a = 7.5710 (12) Å	θ = 6.0–55.1º
b = 15.750 (4) Å	μ = 0.74 mm^{-1}
c = 27.403 (5) Å	T = 293 (2) K
β = 96.76 (2)º	Block, brown
V = 3244.8 (11) Å^3	0.22 × 0.21 × 0.19 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	7420 independent reflections
Radiation source: fine-focus sealed tube	5686 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.0º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −9→8
T_{min} = 0.852, T_{max} = 0.873	k = −20→19
29459 measured reflections	l = −34→35

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H-atom parameters constrained
$wR(F^2)$ = 0.091	$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.7882P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
7420 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}

460 parameters

Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -0.28$ e Å^{-3}

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_{iso}*/U_{eq}
C14	0.2081 (3)	0.05732 (18)	0.23292 (8)	0.0410 (6)
H10	0.0961	0.0618	0.2434	0.049*
C1	0.3901 (3)	0.25583 (14)	0.29159 (8)	0.0316 (5)
C2	0.4135 (3)	0.27113 (16)	0.24320 (8)	0.0371 (5)
H1	0.5255	0.2660	0.2327	0.045*
C3	0.2672 (3)	0.29429 (16)	0.21037 (9)	0.0401 (6)
H2	0.2790	0.3044	0.1775	0.048*
C4	0.1064 (3)	0.30176 (15)	0.22747 (9)	0.0383 (5)
C5	0.0805 (3)	0.28633 (19)	0.27527 (10)	0.0486 (7)
H3	−0.0319	0.2915	0.2855	0.058*
C6	0.2254 (3)	0.26278 (19)	0.30816 (9)	0.0461 (6)
H4	0.2119	0.2518	0.3409	0.055*
C7	0.6451 (3)	0.32177 (14)	0.36356 (8)	0.0308 (5)
H5	0.7163	0.3536	0.3427	0.037*
H6	0.5425	0.3559	0.3689	0.037*
C8	0.7563 (3)	0.30262 (13)	0.41335 (8)	0.0278 (4)
C9	0.2321 (3)	0.07507 (15)	0.18470 (8)	0.0318 (5)
C10	0.3966 (3)	0.06930 (18)	0.16834 (8)	0.0426 (6)
H7	0.4100	0.0817	0.1358	0.051*
C11	0.5421 (3)	0.04481 (18)	0.20070 (9)	0.0434 (6)
H8	0.6544	0.0402	0.1903	0.052*
C12	0.5164 (3)	0.02755 (15)	0.24841 (8)	0.0331 (5)
C13	0.3533 (3)	0.03286 (17)	0.26532 (8)	0.0416 (6)
H9	0.3406	0.0203	0.2979	0.050*
C15	−0.0254 (3)	0.01360 (14)	0.11237 (8)	0.0325 (5)
H12	0.0634	−0.0056	0.0921	0.039*
H11	−0.0410	−0.0303	0.1363	0.039*
C16	−0.2025 (3)	0.02950 (14)	0.08012 (8)	0.0292 (5)
C17	1.0355 (3)	0.10297 (15)	0.41274 (8)	0.0340 (5)
H13	0.9735	0.1357	0.3881	0.041*

C18	1.0324 (3)	0.01502 (15)	0.40761 (9)	0.0386 (5)
H14	0.9718	−0.0100	0.3798	0.046*
C19	1.1190 (3)	−0.03400 (15)	0.44369 (9)	0.0350 (5)
H15	1.1150	−0.0929	0.4411	0.042*
C20	1.2146 (3)	0.00456 (14)	0.48507 (8)	0.0293 (4)
C21	1.3122 (3)	−0.04159 (15)	0.52464 (8)	0.0343 (5)
H16	1.3081	−0.1006	0.5247	0.041*
C22	1.4098 (3)	−0.00060 (15)	0.56172 (8)	0.0350 (5)
H17	1.4718	−0.0320	0.5869	0.042*
C23	1.4200 (3)	0.08987 (14)	0.56315 (7)	0.0295 (5)
C24	1.5307 (3)	0.13657 (16)	0.59854 (8)	0.0358 (5)
H18	1.5987	0.1085	0.6240	0.043*
C25	1.5379 (3)	0.22245 (16)	0.59538 (8)	0.0379 (5)
H19	1.6148	0.2533	0.6177	0.045*
C26	1.4279 (3)	0.26418 (15)	0.55802 (8)	0.0337 (5)
H20	1.4315	0.3231	0.5567	0.040*
C27	1.3185 (2)	0.13685 (13)	0.52623 (7)	0.0250 (4)
C28	1.2143 (2)	0.09319 (13)	0.48656 (7)	0.0252 (4)
Co1	1.11759 (3)	0.271690 (18)	0.470528 (10)	0.02375 (8)
N1	−0.0495 (3)	0.32900 (15)	0.19281 (9)	0.0538 (6)
N2	0.6722 (3)	0.00193 (13)	0.28317 (7)	0.0398 (5)
N3	1.1231 (2)	0.14254 (11)	0.45124 (6)	0.0268 (4)
N4	1.3195 (2)	0.22337 (11)	0.52474 (6)	0.0269 (4)
O1	0.7125 (2)	0.19468 (13)	0.30757 (7)	0.0535 (5)
O2	0.5068 (2)	0.17049 (11)	0.36949 (6)	0.0498 (5)
O3	0.67295 (19)	0.29140 (11)	0.44933 (6)	0.0402 (4)
O4	0.92091 (18)	0.29871 (10)	0.41255 (5)	0.0324 (3)
O5	−0.1903 (3)	0.33969 (18)	0.20932 (9)	0.0833 (8)
O6	−0.0263 (3)	0.33942 (14)	0.14991 (8)	0.0677 (6)
O7	0.1129 (2)	0.16613 (11)	0.10874 (6)	0.0405 (4)
O8	−0.0901 (2)	0.13696 (11)	0.17102 (6)	0.0415 (4)
O9	−0.20498 (19)	0.08437 (10)	0.04747 (6)	0.0380 (4)
O10	−0.33081 (19)	−0.01520 (10)	0.08976 (6)	0.0372 (4)
O11	0.8171 (2)	−0.00010 (14)	0.26820 (7)	0.0592 (5)
O12	0.6470 (2)	−0.01711 (13)	0.32480 (7)	0.0548 (5)
O13	1.31159 (18)	0.31532 (10)	0.43023 (6)	0.0339 (3)
H21	1.3075	0.3674	0.4220	0.051*
H22	1.4205	0.3025	0.4376	0.051*
O14	1.09095 (18)	0.39623 (9)	0.49578 (5)	0.0320 (3)
H23	1.0024	0.4019	0.5119	0.048*
H24	1.1726	0.4263	0.5111	0.048*
O15	0.92631 (19)	0.24054 (10)	0.52086 (5)	0.0322 (3)
H25	0.8316	0.2613	0.5058	0.048*
H26	0.9415	0.2656	0.5485	0.048*
S2	0.57385 (7)	0.22492 (4)	0.33429 (2)	0.03431 (13)
S3	0.04701 (7)	0.10854 (4)	0.142977 (19)	0.03007 (13)
O16	1.3329 (2)	0.50265 (11)	0.54252 (6)	0.0461 (4)
H28	1.4396	0.4976	0.5558	0.069*
H27	1.3203	0.5411	0.5206	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C14	0.0270 (11)	0.0615 (17)	0.0346 (13)	−0.0072 (11)	0.0037 (9)	0.0063 (11)
C1	0.0273 (11)	0.0343 (13)	0.0302 (11)	−0.0017 (9)	−0.0085 (8)	−0.0005 (9)
C2	0.0320 (11)	0.0443 (15)	0.0342 (12)	−0.0059 (10)	−0.0002 (9)	0.0008 (10)
C3	0.0455 (14)	0.0423 (15)	0.0297 (12)	−0.0090 (11)	−0.0070 (9)	0.0072 (10)
C4	0.0337 (12)	0.0328 (13)	0.0437 (14)	−0.0005 (10)	−0.0153 (10)	0.0020 (10)
C5	0.0277 (12)	0.071 (2)	0.0459 (15)	0.0034 (11)	−0.0022 (10)	0.0002 (13)
C6	0.0348 (13)	0.071 (2)	0.0309 (13)	−0.0012 (12)	−0.0007 (9)	0.0052 (12)
C7	0.0252 (10)	0.0322 (12)	0.0332 (11)	0.0013 (8)	−0.0046 (8)	0.0034 (9)
C8	0.0245 (10)	0.0230 (11)	0.0335 (12)	0.0019 (8)	−0.0068 (8)	−0.0026 (8)
C9	0.0278 (11)	0.0386 (13)	0.0271 (11)	−0.0068 (9)	−0.0049 (8)	−0.0003 (9)
C10	0.0338 (12)	0.0664 (18)	0.0275 (12)	0.0003 (11)	0.0039 (9)	0.0043 (11)
C11	0.0288 (12)	0.0646 (18)	0.0371 (13)	0.0014 (11)	0.0055 (9)	0.0041 (12)
C12	0.0309 (11)	0.0337 (13)	0.0329 (12)	−0.0033 (9)	−0.0037 (8)	0.0019 (9)
C13	0.0383 (12)	0.0588 (17)	0.0274 (12)	−0.0043 (11)	0.0024 (9)	0.0106 (11)
C15	0.0294 (11)	0.0298 (12)	0.0362 (12)	−0.0035 (9)	−0.0052 (8)	0.0009 (9)
C16	0.0263 (10)	0.0272 (12)	0.0328 (12)	−0.0013 (8)	−0.0023 (8)	−0.0078 (9)
C17	0.0294 (11)	0.0358 (13)	0.0345 (12)	0.0033 (9)	−0.0060 (9)	−0.0060 (9)
C18	0.0320 (11)	0.0387 (14)	0.0431 (14)	−0.0025 (10)	−0.0038 (9)	−0.0160 (11)
C19	0.0303 (11)	0.0265 (12)	0.0492 (14)	−0.0020 (9)	0.0085 (9)	−0.0084 (10)
C20	0.0248 (10)	0.0260 (12)	0.0384 (12)	0.0003 (8)	0.0085 (8)	−0.0011 (9)
C21	0.0352 (12)	0.0250 (12)	0.0443 (13)	0.0040 (9)	0.0117 (9)	0.0077 (10)
C22	0.0332 (11)	0.0365 (14)	0.0358 (12)	0.0089 (9)	0.0067 (9)	0.0137 (10)
C23	0.0251 (10)	0.0355 (13)	0.0282 (11)	0.0055 (9)	0.0047 (8)	0.0053 (9)
C24	0.0293 (11)	0.0502 (15)	0.0260 (11)	0.0065 (10)	−0.0043 (8)	0.0041 (10)
C25	0.0334 (12)	0.0465 (15)	0.0310 (12)	0.0009 (10)	−0.0079 (9)	−0.0061 (10)
C26	0.0309 (11)	0.0336 (13)	0.0350 (12)	0.0002 (9)	−0.0035 (9)	−0.0050 (10)
C27	0.0202 (9)	0.0283 (11)	0.0267 (10)	0.0030 (8)	0.0030 (7)	0.0002 (8)
C28	0.0199 (9)	0.0248 (11)	0.0309 (11)	0.0024 (8)	0.0030 (7)	−0.0009 (8)
Co1	0.01967 (13)	0.02391 (15)	0.02642 (15)	0.00178 (11)	−0.00259 (9)	−0.00077 (11)
N1	0.0501 (14)	0.0426 (14)	0.0609 (16)	−0.0023 (11)	−0.0258 (11)	0.0066 (11)
N2	0.0383 (11)	0.0382 (12)	0.0404 (12)	−0.0016 (9)	−0.0059 (9)	0.0042 (9)
N3	0.0242 (8)	0.0264 (10)	0.0288 (9)	0.0027 (7)	−0.0015 (6)	−0.0015 (7)
N4	0.0250 (8)	0.0274 (10)	0.0275 (9)	0.0033 (7)	−0.0008 (6)	−0.0018 (7)
O1	0.0402 (10)	0.0624 (13)	0.0550 (11)	0.0171 (9)	−0.0069 (8)	−0.0185 (9)
O2	0.0603 (11)	0.0365 (10)	0.0477 (10)	−0.0079 (8)	−0.0139 (8)	0.0116 (8)
O3	0.0280 (8)	0.0594 (12)	0.0319 (9)	0.0062 (7)	−0.0016 (6)	0.0002 (7)
O4	0.0231 (7)	0.0390 (9)	0.0332 (8)	0.0031 (6)	−0.0050 (6)	0.0005 (7)
O5	0.0416 (12)	0.107 (2)	0.0948 (18)	0.0209 (12)	−0.0180 (11)	0.0114 (15)
O6	0.0770 (14)	0.0620 (14)	0.0550 (13)	−0.0044 (11)	−0.0296 (10)	0.0210 (10)
O7	0.0414 (9)	0.0398 (10)	0.0383 (9)	−0.0109 (7)	−0.0042 (7)	0.0075 (7)
O8	0.0356 (8)	0.0478 (11)	0.0402 (9)	0.0020 (7)	0.0005 (7)	−0.0064 (8)
O9	0.0343 (8)	0.0371 (10)	0.0399 (9)	−0.0021 (7)	−0.0070 (7)	0.0066 (7)
O10	0.0269 (8)	0.0430 (10)	0.0408 (9)	−0.0037 (7)	0.0007 (6)	−0.0022 (7)
O11	0.0307 (9)	0.0784 (15)	0.0677 (13)	0.0071 (9)	0.0019 (8)	0.0212 (11)

O12	0.0539 (11)	0.0711 (14)	0.0369 (10)	0.0089 (9)	−0.0049 (8)	0.0110 (9)
O13	0.0229 (7)	0.0354 (9)	0.0441 (9)	0.0062 (6)	0.0069 (6)	0.0067 (7)
O14	0.0291 (8)	0.0277 (8)	0.0395 (9)	−0.0026 (6)	0.0048 (6)	−0.0063 (6)
O15	0.0328 (8)	0.0296 (9)	0.0337 (8)	0.0015 (6)	0.0016 (6)	−0.0009 (6)
S2	0.0318 (3)	0.0335 (3)	0.0344 (3)	0.0033 (2)	−0.0101 (2)	−0.0016 (2)
S3	0.0272 (3)	0.0326 (3)	0.0287 (3)	−0.0044 (2)	−0.00373 (19)	0.0005 (2)
O16	0.0339 (9)	0.0479 (11)	0.0530 (11)	−0.0098 (7)	−0.0101 (7)	0.0091 (8)

Geometric parameters (Å, °)

C14—C9	1.383 (3)	C19—C20	1.409 (3)
C14—C13	1.384 (3)	C19—H15	0.9300
C14—H10	0.9300	C20—C28	1.396 (3)
C1—C2	1.380 (3)	C20—C21	1.436 (3)
C1—C6	1.381 (3)	C21—C22	1.348 (3)
C1—S2	1.777 (2)	C21—H16	0.9300
C2—C3	1.391 (3)	C22—C23	1.427 (3)
C2—H1	0.9300	C22—H17	0.9300
C3—C4	1.360 (3)	C23—C27	1.407 (3)
C3—H2	0.9300	C23—C24	1.411 (3)
C4—C5	1.369 (4)	C24—C25	1.357 (3)
C4—N1	1.488 (3)	C24—H18	0.9300
C5—C6	1.386 (3)	C25—C26	1.405 (3)
C5—H3	0.9300	C25—H19	0.9300
C6—H4	0.9300	C26—N4	1.320 (3)
C7—C8	1.546 (3)	C26—H20	0.9300
C7—S2	1.778 (2)	C27—N4	1.363 (3)
C7—H5	0.9700	C27—C28	1.440 (3)
C7—H6	0.9700	C28—N3	1.364 (3)
C8—O3	1.244 (3)	Co1—O13	2.0570 (15)
C8—O4	1.250 (2)	Co1—O4	2.0894 (15)
C9—C10	1.376 (3)	Co1—O14	2.0975 (16)
C9—S3	1.781 (2)	Co1—N3	2.1033 (18)
C10—C11	1.385 (3)	Co1—N4	2.1419 (17)
C10—H7	0.9300	Co1—O15	2.1705 (16)
C11—C12	1.371 (3)	N1—O5	1.218 (3)
C11—H8	0.9300	N1—O6	1.220 (3)
C12—C13	1.371 (3)	N2—O11	1.216 (3)
C12—N2	1.482 (3)	N2—O12	1.216 (3)
C13—H9	0.9300	O1—S2	1.4302 (18)
C15—C16	1.537 (3)	O2—S2	1.4277 (18)
C15—S3	1.770 (2)	O7—S3	1.4361 (16)
C15—H12	0.9700	O8—S3	1.4338 (17)
C15—H11	0.9700	O13—H21	0.8500
C16—O9	1.242 (3)	O13—H22	0.8500
C16—O10	1.253 (3)	O14—H23	0.8499
C17—N3	1.333 (3)	O14—H24	0.8500
C17—C18	1.392 (3)	O15—H25	0.8500
C17—H13	0.9300	O15—H26	0.8500

C18—C19	1.360 (3)	O16—H28	0.8500
C18—H14	0.9300	O16—H27	0.8500
C9—C14—C13	119.0 (2)	C21—C22—H17	119.3
C9—C14—H10	120.5	C23—C22—H17	119.3
C13—C14—H10	120.5	C27—C23—C24	116.7 (2)
C2—C1—C6	121.7 (2)	C27—C23—C22	118.8 (2)
C2—C1—S2	120.09 (17)	C24—C23—C22	124.4 (2)
C6—C1—S2	118.20 (17)	C25—C24—C23	120.1 (2)
C1—C2—C3	119.0 (2)	C25—C24—H18	120.0
C1—C2—H1	120.5	C23—C24—H18	120.0
C3—C2—H1	120.5	C24—C25—C26	119.2 (2)
C4—C3—C2	118.5 (2)	C24—C25—H19	120.4
C4—C3—H2	120.8	C26—C25—H19	120.4
C2—C3—H2	120.8	N4—C26—C25	122.9 (2)
C3—C4—C5	123.3 (2)	N4—C26—H20	118.6
C3—C4—N1	118.7 (2)	C25—C26—H20	118.6
C5—C4—N1	118.0 (2)	N4—C27—C23	122.86 (19)
C4—C5—C6	118.6 (2)	N4—C27—C28	117.34 (18)
C4—C5—H3	120.7	C23—C27—C28	119.7 (2)
C6—C5—H3	120.7	N3—C28—C20	123.47 (19)
C1—C6—C5	118.9 (2)	N3—C28—C27	116.73 (19)
C1—C6—H4	120.5	C20—C28—C27	119.77 (18)
C5—C6—H4	120.5	O13—Co1—O4	90.79 (6)
C8—C7—S2	109.61 (15)	O13—Co1—O14	88.12 (6)
C8—C7—H5	109.7	O4—Co1—O14	88.44 (6)
S2—C7—H5	109.7	O13—Co1—N3	98.71 (7)
C8—C7—H6	109.7	O4—Co1—N3	92.26 (6)
S2—C7—H6	109.7	O14—Co1—N3	173.12 (6)
H5—C7—H6	108.2	O13—Co1—N4	89.70 (6)
O3—C8—O4	127.34 (19)	O4—Co1—N4	170.49 (6)
O3—C8—C7	116.90 (18)	O14—Co1—N4	101.07 (6)
O4—C8—C7	115.75 (19)	N3—Co1—N4	78.29 (6)
C10—C9—C14	121.6 (2)	O13—Co1—O15	171.40 (6)
C10—C9—S3	118.98 (17)	O4—Co1—O15	93.45 (6)
C14—C9—S3	119.42 (17)	O14—Co1—O15	84.52 (6)
C9—C10—C11	119.5 (2)	N3—Co1—O15	88.61 (6)
C9—C10—H7	120.3	N4—Co1—O15	87.36 (6)
C11—C10—H7	120.3	O5—N1—O6	124.8 (2)
C12—C11—C10	118.3 (2)	O5—N1—C4	117.8 (2)
C12—C11—H8	120.9	O6—N1—C4	117.4 (2)
C10—C11—H8	120.9	O11—N2—O12	123.9 (2)
C13—C12—C11	123.0 (2)	O11—N2—C12	118.1 (2)
C13—C12—N2	118.7 (2)	O12—N2—C12	117.95 (19)
C11—C12—N2	118.4 (2)	C17—N3—C28	117.27 (19)
C12—C13—C14	118.6 (2)	C17—N3—Co1	128.93 (15)
C12—C13—H9	120.7	C28—N3—Co1	113.34 (13)
C14—C13—H9	120.7	C26—N4—C27	118.13 (18)
C16—C15—S3	109.61 (15)	C26—N4—Co1	129.87 (16)
C16—C15—H12	109.7	C27—N4—Co1	111.70 (12)

S3—C15—H12	109.7	C8—O4—Co1	128.25 (14)
C16—C15—H11	109.7	Co1—O13—H21	117.3
S3—C15—H11	109.7	Co1—O13—H22	121.8
H12—C15—H11	108.2	H21—O13—H22	107.3
O9—C16—O10	126.59 (19)	Co1—O14—H23	112.5
O9—C16—C15	117.77 (18)	Co1—O14—H24	126.3
O10—C16—C15	115.64 (19)	H23—O14—H24	104.8
N3—C17—C18	123.1 (2)	Co1—O15—H25	101.0
N3—C17—H13	118.4	Co1—O15—H26	115.5
C18—C17—H13	118.4	H25—O15—H26	105.8
C19—C18—C17	119.4 (2)	O2—S2—O1	119.12 (12)
C19—C18—H14	120.3	O2—S2—C1	107.23 (10)
C17—C18—H14	120.3	O1—S2—C1	108.60 (11)
C18—C19—C20	119.9 (2)	O2—S2—C7	108.88 (11)
C18—C19—H15	120.1	O1—S2—C7	108.35 (11)
C20—C19—H15	120.1	C1—S2—C7	103.56 (10)
C28—C20—C19	116.9 (2)	O8—S3—O7	118.82 (11)
C28—C20—C21	119.1 (2)	O8—S3—C15	108.32 (11)
C19—C20—C21	124.0 (2)	O7—S3—C15	109.65 (11)
C22—C21—C20	120.9 (2)	O8—S3—C9	108.23 (10)
C22—C21—H16	119.5	O7—S3—C9	107.38 (10)
C20—C21—H16	119.5	C15—S3—C9	103.34 (11)
C21—C22—C23	121.5 (2)	H28—O16—H27	113.0

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O13—H21···O10^{i}	0.85	1.89	2.732 (2)	171
O13—H22···O3^{ii}	0.85	1.91	2.750 (2)	170
O14—H23···O9^{iii}	0.85	1.96	2.805 (2)	179
O14—H24···O16	0.85	1.85	2.693 (2)	173
O15—H25···O3	0.85	1.90	2.698 (2)	155
O15—H26···O7^{iii}	0.85	2.25	3.026 (2)	152
O15—H26···O9^{iii}	0.85	2.61	3.049 (2)	114
O16—H28···O10^{iv}	0.85	1.89	2.724 (2)	166
O16—H27···O9^{i}	0.85	2.08	2.848 (2)	150

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) *x*+1, *y*, *z*; (iii) *x*+1, −*y*+1/2, *z*+1/2; (iv) *x*+2, −*y*+1/2, *z*+1/2.

Fig. 1

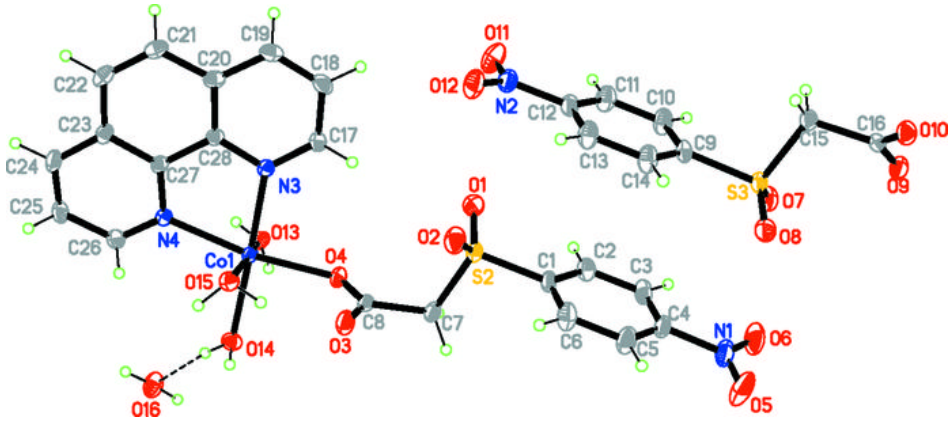
C21
C19
C20
C18
C22
C23
C17
C24
C28
N3
C27
C25
N4
C26
Co1
O13
O15
O4
O14
C8
O3
C7
O16
O11
O12
N2
C12
C11
C10
C13
C9
C14
C15
C16
O10
O9
S3
O7
O8
O1
O2
S2
C1
C2
C3
C4
C6
C5
N1
O6
O5

Fig. 2