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Tetraaquabis(1,3-di-4-pyridylpropane-κN)cobalt(II) bis(4-aminonaphthalene-1-sulfonate)

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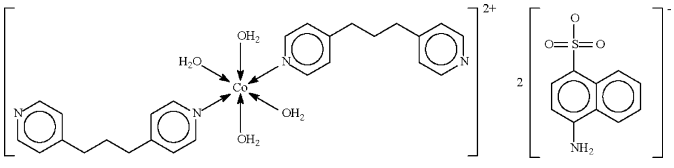
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.089; data-to-parameter ratio = 16.9.

The Co^{II} atom in the crystal structure of the title compound, $[Co(C_{13}H_{14}N_2)_2(H_2O)_4](C_{10}H_8NO_3S)_2$, lies on a center of inversion in an N_2O_4 octahedron. The sulfonate anion interacts with the cation through hydrogen bonds, giving rise to a three-dimensional network.

Related literature

For a crystallographic review of metal arenesulfonates, see Cai (2004). For examples of metal 4-amino-naphthalenesulfonates in which the anion is not directly bonded to the metal, see Li *et al.* (2006) and Zhou *et al.* (2005) for the cadmium salts, and Li *et al.* (2005) for the copper salt.



Experimental

Crystal data

$[Co(C_{13}H_{14}N_2)_2(H_2O)_4](C_{10}H_8NO_3S)_2$
M_r = 971.99
Monoclinic, $P2_1/c$
a = 9.7790 (6) Å
b = 16.261 (1) Å
c = 15.375 (1) Å
β = 104.625 (1)°
V = 2365.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.51 mm^{-1}
T = 295 (2) K
0.42 × 0.31 × 0.26 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.759, T_{max} = 0.878
16557 measured reflections
5383 independent reflections
4524 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.089
S = 1.03
5383 reflections
319 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H12···O1	0.84 (1)	1.99 (1)	2.809 (1)	164 (2)
O1W—H11···N3^{i}	0.84 (1)	1.98 (1)	2.807 (2)	167 (2)
O2W—H21···O3^{ii}	0.84 (1)	2.00 (1)	2.790 (2)	157 (2)
O2W—H22···N2^{iii}	0.84 (1)	1.96 (1)	2.802 (2)	175 (2)
N3—H31···O2^{iv}	0.85 (1)	2.01 (1)	2.858 (2)	170 (2)
N3—H32···O3^{v}	0.86 (1)	2.13 (1)	2.942 (2)	159 (2)

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2475).

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supplementary materials

Acta Cryst. (2007). E**63**, m2353 [**doi:10.1107/S1600536807039633**]

Tetraaquabis(1,3-di-4-pyridylpropane-*κN*)cobalt(II) bis(4-aminonaphthalene-1-sulfonate)

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Comment

Among metal sulfonates, some have the sulfonate anion directly bonded to the metal center whereas other have the anion in an outer-sphere type of coordination, the anion interacting indirectly through hydrogen bonds (Cai, 2004). The few metal 4-amino-naphthalenesulfonates that have been identified by crystallography show this feature (Li *et al.*, 2005; Li *et al.*, 2006; Zhou *et al.*, 2005). The cobalt(II) atom in the title compound lies on a center-of-inversion in an N_2O_4 octahedron (see Table 1). The sulfonate anion interacts with the cation through hydrogen bonds (see Table 2), these giving rise to a three-dimensional network,

Experimental

To cobalt(II) nitrate (1 mmol) dissolved in water was sodium 4-amino-naphthalene sulfonate (1 mmol) dissolved in methanol. 1,3-Bis(4-pyridyl)propane (1 mmol) dissolved in methanol was then added. Large red crystals separated from the solution after several days (in 80% yield).

Refinement

The water and amino H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H = N–H = 0.85±0.01 Å; their displacement parameters were freely refined. The carbon-bound H-atoms were generated geometrically (C–H 0.93 to 0.97 Å); they were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

Figures

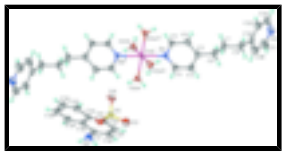


Fig. 1. Thermal ellipsoid plot depicting the coordination geometry of cobalt; displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radius·[Symmetry code (i): 1 – x, 1 – y, 1 − z.]

Tetraaquabis(1,3-di-4-pyridylpropane-κ*N*)cobalt(II) bis(4-aminonaphthalene-1-sulfonate)

Crystal data

$[Co(C_{13}H_{14}N_2)_2(H_2O)_4](C_{10}H_8NO_3S)_2$	F_{000} = 1018
M_r = 971.99	D_x = 1.365 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 743 reflections

a = 9.7790 (6) Å	θ = 2.5–28.2º
b = 16.261 (1) Å	μ = 0.51 mm^{-1}
c = 15.375 (1) Å	T = 295 (2) K
β = 104.625 (1)º	Block, red
V = 2365.6 (3) Å^3	0.42 × 0.31 × 0.26 mm
Z = 2	

Data collection

Bruker APEX II area-detector diffractometer	5383 independent reflections
Radiation source: fine-focus sealed tube	4524 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 295(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −8→12
T_{min} = 0.759, T_{max} = 0.878	k = −21→21
16557 measured reflections	l = −18→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.031	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.089	$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.4354P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
5383 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
319 parameters	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.03216 (9)
S1	0.04035 (4)	0.59566 (2)	0.64502 (2)	0.04044 (11)
O1	0.17834 (13)	0.56048 (8)	0.64976 (8)	0.0567 (3)
O2	−0.02305 (14)	0.63540 (8)	0.55948 (8)	0.0586 (3)
O3	−0.05603 (13)	0.53643 (8)	0.66932 (8)	0.0535 (3)
O1W	0.35327 (13)	0.58214 (8)	0.53205 (8)	0.0472 (3)
H11	0.2855 (17)	0.5976 (12)	0.4894 (11)	0.067 (6)*
H12	0.315 (2)	0.5725 (13)	0.5741 (11)	0.067 (6)*
O2W	0.65302 (13)	0.55626 (8)	0.60223 (7)	0.0481 (3)

H21	0.7406 (11)	0.5579 (13)	0.6092 (14)	0.063 (6)*
H22	0.640 (2)	0.5608 (14)	0.6540 (8)	0.077 (7)*
N1	0.53869 (13)	0.58325 (8)	0.39844 (8)	0.0360 (3)
N2	0.62516 (18)	0.57641 (11)	−0.22209 (10)	0.0620 (4)
N3	0.10056 (15)	0.87085 (8)	0.90985 (9)	0.0418 (3)
H31	0.0643 (17)	0.8627 (10)	0.9540 (9)	0.042 (5)*
H32	0.0650 (18)	0.9146 (8)	0.8821 (11)	0.046 (5)*
C1	0.43213 (18)	0.61539 (11)	0.33443 (11)	0.0466 (4)
H1	0.3400	0.6053	0.3379	0.056*
C2	0.45187 (19)	0.66237 (11)	0.26416 (11)	0.0498 (4)
H2	0.3744	0.6838	0.2222	0.060*
C3	0.58785 (19)	0.67768 (10)	0.25596 (10)	0.0440 (4)
C4	0.69713 (18)	0.64612 (10)	0.32255 (11)	0.0473 (4)
H4	0.7901	0.6556	0.3207	0.057*
C5	0.66959 (17)	0.60054 (10)	0.39194 (10)	0.0412 (3)
H5	0.7457	0.5809	0.4363	0.049*
C6	0.6135 (2)	0.72465 (11)	0.17690 (11)	0.0547 (4)
H6A	0.7018	0.7546	0.1959	0.066*
H6B	0.5383	0.7645	0.1568	0.066*
C7	0.6199 (2)	0.66793 (10)	0.09830 (10)	0.0502 (4)
H7A	0.6977	0.6296	0.1174	0.060*
H7B	0.5331	0.6364	0.0805	0.060*
C8	0.6399 (2)	0.71753 (11)	0.01797 (11)	0.0559 (4)
H8A	0.5661	0.7588	0.0026	0.067*
H8B	0.7298	0.7460	0.0352	0.067*
C9	0.5088 (2)	0.59422 (16)	−0.19520 (14)	0.0721 (6)
H9	0.4222	0.5763	−0.2304	0.086*
C10	0.5104 (2)	0.63766 (15)	−0.11825 (13)	0.0639 (5)
H10	0.4261	0.6482	−0.1027	0.077*
C11	0.63622 (19)	0.66574 (11)	−0.06400 (10)	0.0473 (4)
C12	0.75670 (19)	0.64531 (13)	−0.09045 (11)	0.0563 (5)
H121	0.8449	0.6610	−0.0554	0.068*
C13	0.7465 (2)	0.60173 (13)	−0.16871 (13)	0.0609 (5)
H13	0.8295	0.5894	−0.1850	0.073*
C14	0.06477 (15)	0.67457 (9)	0.72696 (9)	0.0347 (3)
C15	0.03967 (16)	0.75405 (9)	0.69763 (10)	0.0402 (3)
H15	0.0136	0.7648	0.6362	0.048*
C16	0.05262 (17)	0.81950 (9)	0.75851 (10)	0.0408 (3)
H16	0.0368	0.8730	0.7370	0.049*
C17	0.08839 (15)	0.80554 (8)	0.84941 (9)	0.0342 (3)
C18	0.11955 (15)	0.72344 (8)	0.88304 (9)	0.0338 (3)
C19	0.16225 (18)	0.70681 (10)	0.97662 (10)	0.0454 (4)
H19	0.1718	0.7500	1.0174	0.054*
C20	0.1896 (2)	0.62808 (11)	1.00766 (12)	0.0574 (5)
H20	0.2157	0.6180	1.0692	0.069*
C21	0.1782 (2)	0.56277 (11)	0.94689 (13)	0.0579 (5)
H211	0.1973	0.5095	0.9685	0.069*
C22	0.13945 (18)	0.57630 (10)	0.85632 (11)	0.0465 (4)
H221	0.1335	0.5322	0.8171	0.056*

C23	0.10801 (15)	0.65683 (9)	0.82121 (9)	0.0343 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02968 (15)	0.04245 (16)	0.02514 (13)	0.00390 (11)	0.00836 (10)	0.00034 (10)
S1	0.0375 (2)	0.0465 (2)	0.0397 (2)	−0.00494 (16)	0.01423 (16)	−0.01240 (15)
O1	0.0469 (7)	0.0694 (8)	0.0596 (7)	0.0074 (6)	0.0247 (6)	−0.0138 (6)
O2	0.0647 (8)	0.0700 (8)	0.0381 (6)	−0.0011 (7)	0.0075 (6)	−0.0122 (5)
O3	0.0531 (7)	0.0504 (7)	0.0613 (7)	−0.0169 (6)	0.0224 (6)	−0.0178 (6)
O1W	0.0430 (7)	0.0627 (7)	0.0386 (6)	0.0179 (5)	0.0151 (5)	0.0059 (5)
O2W	0.0384 (7)	0.0732 (8)	0.0326 (6)	−0.0061 (6)	0.0085 (5)	−0.0093 (5)
N1	0.0342 (6)	0.0458 (7)	0.0290 (6)	0.0041 (5)	0.0096 (5)	0.0005 (5)
N2	0.0634 (10)	0.0840 (11)	0.0420 (8)	−0.0129 (9)	0.0198 (7)	−0.0087 (7)
N3	0.0493 (8)	0.0349 (7)	0.0418 (7)	−0.0032 (6)	0.0127 (6)	−0.0047 (5)
C1	0.0368 (8)	0.0635 (10)	0.0404 (8)	0.0056 (7)	0.0116 (7)	0.0089 (7)
C2	0.0489 (10)	0.0612 (10)	0.0375 (8)	0.0078 (8)	0.0074 (7)	0.0107 (7)
C3	0.0601 (10)	0.0413 (8)	0.0349 (7)	−0.0015 (7)	0.0199 (7)	−0.0023 (6)
C4	0.0429 (9)	0.0555 (9)	0.0479 (9)	−0.0028 (7)	0.0198 (7)	0.0008 (7)
C5	0.0358 (8)	0.0499 (9)	0.0382 (8)	0.0022 (7)	0.0098 (6)	0.0014 (6)
C6	0.0803 (13)	0.0478 (9)	0.0426 (9)	−0.0027 (9)	0.0276 (9)	0.0034 (7)
C7	0.0684 (12)	0.0492 (9)	0.0370 (8)	−0.0014 (8)	0.0209 (8)	0.0042 (6)
C8	0.0754 (13)	0.0560 (10)	0.0405 (8)	−0.0084 (9)	0.0228 (8)	0.0040 (7)
C9	0.0514 (12)	0.1150 (18)	0.0483 (11)	−0.0213 (12)	0.0099 (9)	−0.0140 (11)
C10	0.0437 (10)	0.1006 (16)	0.0516 (10)	−0.0075 (10)	0.0195 (8)	−0.0068 (10)
C11	0.0537 (10)	0.0561 (9)	0.0335 (7)	−0.0064 (8)	0.0137 (7)	0.0089 (6)
C12	0.0427 (9)	0.0831 (13)	0.0414 (9)	−0.0087 (9)	0.0075 (7)	0.0015 (8)
C13	0.0491 (11)	0.0883 (14)	0.0495 (10)	−0.0010 (10)	0.0206 (8)	−0.0010 (9)
C14	0.0304 (7)	0.0391 (7)	0.0359 (7)	−0.0036 (6)	0.0106 (6)	−0.0053 (5)
C15	0.0420 (8)	0.0457 (8)	0.0326 (7)	−0.0018 (7)	0.0086 (6)	0.0006 (6)
C16	0.0460 (9)	0.0348 (7)	0.0410 (8)	0.0015 (6)	0.0099 (7)	0.0035 (6)
C17	0.0297 (7)	0.0347 (7)	0.0386 (7)	−0.0042 (5)	0.0093 (6)	−0.0039 (5)
C18	0.0292 (7)	0.0371 (7)	0.0348 (7)	−0.0027 (6)	0.0078 (6)	−0.0006 (5)
C19	0.0495 (9)	0.0483 (9)	0.0367 (8)	−0.0007 (7)	0.0078 (7)	−0.0017 (6)
C20	0.0719 (13)	0.0576 (10)	0.0395 (9)	0.0064 (9)	0.0083 (8)	0.0104 (7)
C21	0.0728 (13)	0.0425 (9)	0.0567 (10)	0.0083 (9)	0.0134 (9)	0.0134 (7)
C22	0.0519 (10)	0.0356 (8)	0.0518 (9)	0.0014 (7)	0.0129 (8)	−0.0008 (6)
C23	0.0294 (7)	0.0362 (7)	0.0378 (7)	−0.0021 (6)	0.0095 (6)	−0.0015 (5)

Geometric parameters (Å, °)

Co1—O1w	2.108 (1)	C6—H6B	0.9700
Co1—O2w	2.088 (1)	C7—C8	1.528 (2)
Co1—N1	2.171 (1)	C7—H7A	0.9700
Co1—O2w^{i}	2.088 (1)	C7—H7B	0.9700
Co1—O1w^{i}	2.108 (1)	C8—C11	1.509 (2)
Co1—N1^{i}	2.171 (1)	C8—H8A	0.9700
S1—O1	1.4504 (12)	C8—H8B	0.9700

S1—O2	1.4560 (13)	C9—C10	1.375 (3)
S1—O3	1.4606 (12)	C9—H9	0.9300
S1—C14	1.7717 (14)	C10—C11	1.378 (3)
O1W—H11	0.84 (1)	C10—H10	0.9300
O1W—H12	0.84 (1)	C11—C12	1.380 (2)
O2W—H21	0.84 (1)	C12—C13	1.378 (3)
O2W—H22	0.84 (1)	C12—H121	0.9300
N1—C5	1.339 (2)	C13—H13	0.9300
N1—C1	1.345 (2)	C14—C15	1.370 (2)
N2—C13	1.326 (3)	C14—C23	1.4327 (19)
N2—C9	1.337 (3)	C15—C16	1.402 (2)
N3—C17	1.3962 (18)	C15—H15	0.9300
N3—H31	0.85 (1)	C16—C17	1.371 (2)
N3—H32	0.86 (1)	C16—H16	0.9300
C1—C2	1.376 (2)	C17—C18	1.4363 (19)
C1—H1	0.9300	C18—C19	1.419 (2)
C2—C3	1.390 (2)	C18—C23	1.4266 (19)
C2—H2	0.9300	C19—C20	1.369 (2)
C3—C4	1.379 (2)	C19—H19	0.9300
C3—C6	1.509 (2)	C20—C21	1.400 (3)
C4—C5	1.380 (2)	C20—H20	0.9300
C4—H4	0.9300	C21—C22	1.365 (2)
C5—H5	0.9300	C21—H211	0.9300
C6—C7	1.534 (2)	C22—C23	1.420 (2)
C6—H6A	0.9700	C22—H221	0.9300
$O2W^{i}$—Co1—O2W	180.0	C8—C7—H7A	109.4
$O2W^{i}$—Co1—O1W	93.03 (5)	C6—C7—H7A	109.4
O2W—Co1—O1W	86.97 (5)	C8—C7—H7B	109.4
$O2W^{i}$—Co1—$O1W^{i}$	86.97 (5)	C6—C7—H7B	109.4
O2W—Co1—$O1W^{i}$	93.03 (5)	H7A—C7—H7B	108.0
O1W—Co1—$O1W^{i}$	180.0	C11—C8—C7	113.56 (14)
$O2W^{i}$—Co1—N1	87.34 (5)	C11—C8—H8A	108.9
O2W—Co1—N1	92.66 (5)	C7—C8—H8A	108.9
O1W—Co1—N1	91.47 (5)	C11—C8—H8B	108.9
$O1W^{i}$—Co1—N1	88.53 (5)	C7—C8—H8B	108.9
$O2W^{i}$—Co1—$N1^{i}$	92.66 (5)	H8A—C8—H8B	107.7
O2W—Co1—$N1^{i}$	87.34 (5)	N2—C9—C10	123.52 (19)
O1W—Co1—$N1^{i}$	88.53 (5)	N2—C9—H9	118.2
$O1W^{i}$—Co1—$N1^{i}$	91.47 (5)	C10—C9—H9	118.2
N1—Co1—$N1^{i}$	180.00 (5)	C9—C10—C11	120.34 (18)
O1—S1—O2	113.51 (8)	C9—C10—H10	119.8
O1—S1—O3	112.29 (8)	C11—C10—H10	119.8
O2—S1—O3	111.63 (8)	C10—C11—C12	116.10 (16)
O1—S1—C14	107.05 (7)	C10—C11—C8	121.30 (17)
O2—S1—C14	105.73 (7)	C12—C11—C8	122.58 (16)
O3—S1—C14	105.99 (7)	C13—C12—C11	120.13 (17)

Co1—O1W—H11	117.0 (15)	C13—C12—H121	119.9
Co1—O1W—H12	121.5 (15)	C11—C12—H121	119.9
H11—O1W—H12	104 (2)	N2—C13—C12	123.77 (18)
Co1—O2W—H21	128.8 (14)	N2—C13—H13	118.1
Co1—O2W—H22	120.1 (16)	C12—C13—H13	118.1
H21—O2W—H22	106 (2)	C15—C14—C23	120.35 (13)
C5—N1—C1	116.26 (13)	C15—C14—S1	117.93 (11)
C5—N1—Co1	121.89 (10)	C23—C14—S1	121.72 (11)
C1—N1—Co1	121.67 (11)	C14—C15—C16	121.19 (13)
C13—N2—C9	116.09 (17)	C14—C15—H15	119.4
C17—N3—H31	115.5 (12)	C16—C15—H15	119.4
C17—N3—H32	110.1 (12)	C17—C16—C15	120.77 (14)
H31—N3—H32	109 (2)	C17—C16—H16	119.6
N1—C1—C2	123.62 (16)	C15—C16—H16	119.6
N1—C1—H1	118.2	C16—C17—N3	120.62 (13)
C2—C1—H1	118.2	C16—C17—C18	119.81 (13)
C1—C2—C3	119.86 (15)	N3—C17—C18	119.52 (13)
C1—C2—H2	120.1	C19—C18—C23	118.97 (13)
C3—C2—H2	120.1	C19—C18—C17	121.56 (13)
C4—C3—C2	116.49 (14)	C23—C18—C17	119.47 (12)
C4—C3—C6	122.09 (16)	C20—C19—C18	120.87 (15)
C2—C3—C6	121.40 (16)	C20—C19—H19	119.6
C3—C4—C5	120.52 (15)	C18—C19—H19	119.6
C3—C4—H4	119.7	C19—C20—C21	120.07 (16)
C5—C4—H4	119.7	C19—C20—H20	120.0
N1—C5—C4	123.18 (14)	C21—C20—H20	120.0
N1—C5—H5	118.4	C22—C21—C20	120.87 (16)
C4—C5—H5	118.4	C22—C21—H211	119.6
C3—C6—C7	112.23 (13)	C20—C21—H211	119.6
C3—C6—H6A	109.2	C21—C22—C23	120.91 (15)
C7—C6—H6A	109.2	C21—C22—H221	119.5
C3—C6—H6B	109.2	C23—C22—H221	119.5
C7—C6—H6B	109.2	C22—C23—C18	118.28 (13)
H6A—C6—H6B	107.9	C22—C23—C14	123.39 (13)
C8—C7—C6	110.99 (14)	C18—C23—C14	118.33 (12)
O2W^{i}—Co1—N1—C5	−132.91 (12)	C11—C12—C13—N2	−0.6 (3)
O2W—Co1—N1—C5	47.09 (12)	O1—S1—C14—C15	113.60 (13)
O1W—Co1—N1—C5	134.13 (12)	O2—S1—C14—C15	−7.73 (14)
O1W^{i}—Co1—N1—C5	−45.87 (12)	O3—S1—C14—C15	−126.36 (13)
O2W^{i}—Co1—N1—C1	42.01 (12)	O1—S1—C14—C23	−67.00 (13)
O2W—Co1—N1—C1	−137.99 (12)	O2—S1—C14—C23	171.67 (12)
O1W—Co1—N1—C1	−50.96 (13)	O3—S1—C14—C23	53.04 (14)
O1W^{i}—Co1—N1—C1	129.04 (13)	C23—C14—C15—C16	−1.3 (2)
C5—N1—C1—C2	1.2 (2)	S1—C14—C15—C16	178.07 (12)
Co1—N1—C1—C2	−173.96 (13)	C14—C15—C16—C17	−1.2 (2)
N1—C1—C2—C3	1.0 (3)	C15—C16—C17—N3	−179.70 (14)
C1—C2—C3—C4	−2.2 (2)	C15—C16—C17—C18	3.0 (2)
C1—C2—C3—C6	176.33 (16)	C16—C17—C18—C19	177.55 (15)

C2—C3—C4—C5	1.2 (2)	N3—C17—C18—C19	0.2 (2)
C6—C3—C4—C5	−177.29 (15)	C16—C17—C18—C23	−2.2 (2)
C1—N1—C5—C4	−2.3 (2)	N3—C17—C18—C23	−179.58 (13)
Co1—N1—C5—C4	172.91 (12)	C23—C18—C19—C20	−1.2 (2)
C3—C4—C5—N1	1.1 (2)	C17—C18—C19—C20	179.03 (16)
C4—C3—C6—C7	88.7 (2)	C18—C19—C20—C21	1.2 (3)
C2—C3—C6—C7	−89.8 (2)	C19—C20—C21—C22	−0.3 (3)
C3—C6—C7—C8	177.69 (17)	C20—C21—C22—C23	−0.7 (3)
C6—C7—C8—C11	−175.75 (17)	C21—C22—C23—C18	0.7 (2)
C13—N2—C9—C10	1.4 (3)	C21—C22—C23—C14	−179.02 (16)
N2—C9—C10—C11	0.2 (4)	C19—C18—C23—C22	0.2 (2)
C9—C10—C11—C12	−1.9 (3)	C17—C18—C23—C22	180.00 (14)
C9—C10—C11—C8	176.58 (19)	C19—C18—C23—C14	179.99 (14)
C7—C8—C11—C10	77.4 (2)	C17—C18—C23—C14	−0.3 (2)
C7—C8—C11—C12	−104.1 (2)	C15—C14—C23—C22	−178.26 (15)
C10—C11—C12—C13	2.1 (3)	S1—C14—C23—C22	2.4 (2)
C8—C11—C12—C13	−176.35 (17)	C15—C14—C23—C18	2.0 (2)
C9—N2—C13—C12	−1.2 (3)	S1—C14—C23—C18	−177.38 (10)

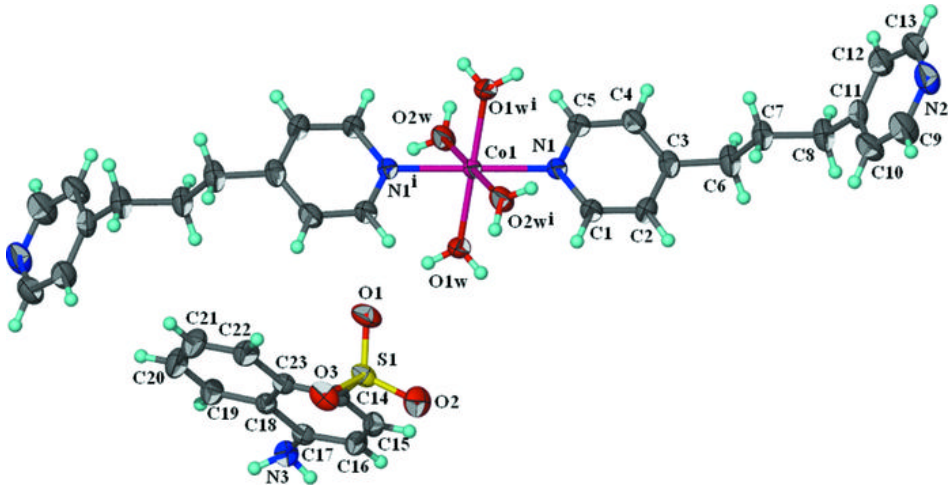
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H12···O1	0.84 (1)	1.99 (1)	2.809 (1)	164 (2)
O1W—H11···N3^{ii}	0.84 (1)	1.98 (1)	2.807 (2)	167 (2)
O2W—H21···O3^{iii}	0.84 (1)	2.00 (1)	2.790 (2)	157 (2)
O2W—H22···N2^{iv}	0.84 (1)	1.96 (1)	2.802 (2)	175 (2)
N3—H31···O2^{v}	0.85 (1)	2.01 (1)	2.858 (2)	170 (2)
N3—H32···O3^{vi}	0.86 (1)	2.13 (1)	2.942 (2)	159 (2)

Symmetry codes: (ii) *x*, −*y*+3/2, *z*−1/2; (iii) *x*+1, *y*, *z*; (iv) *x*, *y*, *z*+1; (v) *x*, −*y*+3/2, *z*+1/2; (vi) −*x*, *y*+1/2, −*z*+3/2.

Fig. 1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C14
O2
C19
C18
C15
C17
C16
N3