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trans-Tetraaquabis(1,3-di-4-pyridylpropane-κ*N*)cobalt(II) naphthalene-1,5-disulfonate monohydrate

Ke-Fei Han, He-Yan Chen and Zhong-Ming Wang*

Department of Chemistry, Beijing University of Chemical Technology, Beijing 100029, People's Republic of China
Correspondence e-mail: wangzm@mail.buct.edu.cn

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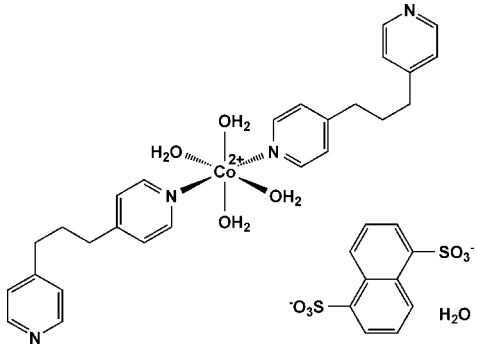
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.001 Å; disorder in main residue; R factor = 0.038; wR factor = 0.108; data-to-parameter ratio = 15.6.

In the title compound, $[Co(C_{13}H_{14}N_2)_2(H_2O)_4](C_{10}H_6O_6S_2)\cdot H_2O$, the Co^{II} ion, which lies on a centre of symmetry, is coordinated by two N atoms from two 1,3-di-4-pyridylpropane (dpp) ligands and four aqua O atoms in a distorted octahedral geometry. Two C atoms of the flexible $-CH_2CH_2CH_2-$ spacer in the dpp ligand are disordered over two positions. The 1,5-naphthalenedisulfonate dianion, which lies about an inversion centre, does not coordinate to the Co^{II} ion but balances the charge. The cations, anions and water molecules are connected by a three-dimensional hydrogen-bonding network.

Related literature

For related literature, see: Biradha *et al.* (2002); Côté & Shimizu (2003); Cai (2004); Cai *et al.* (2001); Carlucci *et al.* (2000, 2002); Chandrasekhar *et al.* (2003); Fu *et al.* (2003); Gao *et al.* (2005); Luan *et al.* (2005); Pan *et al.* (2001); Plater *et al.* (2000); Voogt & Blanch (2005); Wu *et al.* (2005).



Experimental

Crystal data

$[Co(C_{13}H_{14}N_2)_2(H_2O)_4](C_{10}H_6O_6S_2)\cdot H_2O$
M_r = 849.82
Monoclinic, $P2_1/c$
a = 11.844 (2) Å
b = 8.3912 (17) Å
c = 20.035 (4) Å
β = 97.56 (3)°
V = 1973.9 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.61 mm^{-1}
T = 298 (2) K
0.51 × 0.44 × 0.37 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.747, T_{max} = 0.807
17625 measured reflections
4418 independent reflections
3259 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.108
S = 1.02
4418 reflections
283 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O6	0.947 (15)	1.792 (14)	2.7176 (11)	164.8 (13)
O3—H3A···O1^{i}	0.599 (14)	2.436 (14)	2.9013 (12)	136.6 (16)
O2—H2A···O4^{ii}	0.823 (10)	1.916 (10)	2.7363 (11)	174.6 (10)
O1—H1B···O5^{iii}	0.735 (10)	1.979 (10)	2.7096 (10)	173.1 (10)
O1—H1A···N2^{iv}	0.884 (10)	1.872 (10)	2.7495 (12)	171.3 (11)
O2—H2B···O3^{v}	0.771 (11)	1.940 (11)	2.6959 (11)	166.8 (11)

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

Data collection: *RAPID-AUTO* (Rigaku 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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*) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97* and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2023).

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supplementary materials

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trans-Tetraaquabis(1,3-di-4-pyridylpropane-*κN*)cobalt(II) naphthalene-1,5-disulfonate monohydrate

K.-F. Han, H.-Y. Chen and Z.-M. Wang

Comment

As a bipyridine-type ligand with a flexible –$CH_2CH_2CH_2$– spacer, 1,3-di-4-pyridylpropane (dpp) has been employed to construct novel metal-organic coordination polymers with intriguing structural topologies (Plater *et al.*, 2000; Pan *et al.*, 2001; Biradha *et al.*, 2002; Fu *et al.*, 2003; Wu *et al.*, 2005; Carlucci *et al.*, 2000, 2002; Luan *et al.*, 2005). The 1,5-naphthalenedisulfonate dianion (NDS^{2-}), which possesses six O atoms, has been also employed either as a ligand with multiple binding sites available to construct coordination polymers with varying dimensionalities, or as a counter ion, forming extensive hydrogen-bonding interaction with the water molecules (Cai *et al.*, 2001; Chandrasekhar *et al.*, 2003; Côté & Shimizu, 2003; Cai, 2004; Gao *et al.*, 2005; Voogt & Blanch, 2005). In the present work, we report a cobalt(II) complex, $[Co(C_{13}H_{14}N_2)_2(H_2O)_4]\cdot(C_{10}H_6O_6S_2)\cdot H_2O$, (I), with a three-dimensional H-bonding network structure created by the sulfonate dianions acting as hydrogen-bond acceptors.

As shown in Fig. 1, four water molecules coordinate to Co(II) ion in the equatorial positions with Co—O bonds (2.1022 (8)–2.1230 (7) Å), while the two dpp ligands coordinate to Co(II) through N atoms [Co—N = 2.1294 (8) Å] in the long axial direction to complete a distorted octahedral coordination (Table 1). The dihedral angle is 58.76 (5)° between the two pyridyl planes, and the N···N distance is 9.121 (5) Å in the same dpp ligand. The NDS dianion, which lies about an inversion site, does not coordinate to the Co(II) ion, but balances the charge.

Hydrogen bonds play an important role for enhancing the stability of the solid-state structure (Table 2). Two intermolecular hydrogen bonds are formed between O atoms of the two coordinated water molecules and two O atoms of sulfonate groups, respectively. An additional intermolecular hydrogen bond is formed between atom O3 of the uncoordinated water molecule and the sulfonate atom O6. All these intermolecular hydrogen bonds result in a two-dimensional structure (Fig. 2). The two-dimensional structures are further linked *via* another hydrogen bond between uncoordinated N atom of dpp and coordinated O1 atom to give rise to a three-dimensional network (Fig. 3).

Experimental

An aqueous solution (10 ml) of $CoCl_2\cdot 6H_2O$ (0.0238 g, 1 mmol) and a mixture of disodium 1,5-naphthalenedisulfonate (0.0332 g, 1 mmol) and dpp (0.0398 g, 2 mmol) in distilled water (10 ml) were placed in two tubes of an H-tube. Slow diffusion of the two solutions into joint aqueous solution produced deep purple crystals after 1 month (*ca* 10% yield based on Co).

Refinement

The atoms C7 and C8 are disordered over two positions. H atoms attached to C atoms were placed in geometrically idealized positions, with C_{sp3}—H = 0.97 Å and C_{sp2}—H= 0.93 Å, and constrained to ride on their parent atoms, with U_{iso}(H) =

1.2Ueq(C). H atoms attached to O atoms were located in difference Fourier maps and refined with a global U_{iso}(H) value. The O—H distances are in the range 0.599 (14)–0.947 (15) Å.

Figures

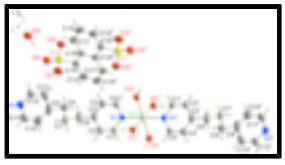


Fig. 1. View of a fragment of the title compound, showing 50% probability displacement ellipsoids for non-H atoms. For the sake of clarity, only the major component of the disordered atoms C7 and C8 is shown. [Symmetry codes: (i). −*x*, −*y*, −*z*; (ii). 1 − *x*, 1 − *y*, −*z*].

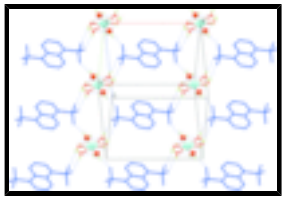


Fig. 2. The two-dimensional network formed by hydrogen-bonding interactions (blue dotted lines). For clarity, the dpp ligands and H atoms attached to C atoms have been omitted.

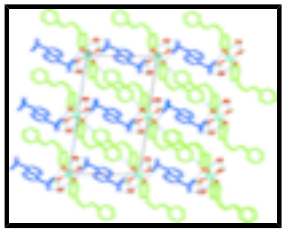


Fig. 3. The three-dimensional network of the title complex (I). Hydrogen bonds are shown as blue dotted lines, and H atoms attached to C atoms have been omitted.

trans-Tetraaquabis(1,3-di-4-pyridylpropane-κ*N*)cobalt(II) naphthalene-1,5-disulfonate monohydrate

Crystal data

$[Co(C_{13}H_{14}N_2)_2(H_2O)_4](C_{10}H_6O_6S_2)\cdot H_2O$	F_{000} = 890
M_r = 849.82	D_x = 1.43 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 17625 reflections
a = 11.844 (2) Å	θ = 1.7–27.5º
b = 8.3912 (17) Å	μ = 0.61 mm^{-1}
c = 20.035 (4) Å	T = 298 (2) K
β = 97.56 (3)º	Block, pink
V = 1973.9 (7) Å^3	0.51 × 0.44 × 0.37 mm
Z = 2	

Data collection

Rigaku R-axis Rapid IP area-detector diffractometer	R_{int} = 0.041
ω Oscillation scans	θ_{max} = 27.5º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	θ_{min} = 1.7º
T_{min} = 0.747, T_{max} = 0.807	h = 0→15

17625 measured reflections
4418 independent reflections
3259 reflections with $I > 2\sigma(I)$

$k = 0 \rightarrow 10$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.108$
$S = 1.02$
4418 reflections
283 parameters
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0	0	0	0.03243 (4)	
S1	0.747491 (16)	0.35189 (3)	0.086588 (11)	0.04424 (6)	
N1	0.05768 (5)	0.16358 (9)	0.07838 (3)	0.03629 (17)	
N2	0.71693 (6)	0.35709 (11)	0.35647 (4)	0.0559 (2)	
O1	0.09129 (4)	−0.18980 (7)	0.05235 (3)	0.04155 (16)	
O2	−0.14437 (5)	−0.05367 (8)	0.04662 (3)	0.04633 (17)	
O6	0.76383 (6)	0.47271 (9)	0.13864 (3)	0.0592 (2)	
O4	0.76400 (5)	0.19127 (8)	0.11191 (4)	0.0585 (2)	
O5	0.81263 (5)	0.38569 (8)	0.03177 (3)	0.05015 (18)	
C1	0.04884 (7)	0.12998 (12)	0.14243 (4)	0.0447 (2)	
H1	0.0158	0.0337	0.1523	0.054*	
C2	0.08631 (7)	0.23099 (13)	0.19450 (5)	0.0498 (3)	
H2	0.0775	0.203	0.2384	0.06*	
C3	0.13715 (6)	0.37430 (12)	0.18186 (4)	0.0434 (2)	
C4	0.14654 (7)	0.40891 (12)	0.11582 (5)	0.0459 (2)	
H4	0.1805	0.5036	0.1048	0.055*	
C5	0.10545 (7)	0.30265 (11)	0.06603 (4)	0.0423 (2)	
H5	0.1113	0.3292	0.0216	0.051*	
C6	0.18164 (8)	0.48559 (13)	0.23797 (5)	0.0579 (3)	0.5
H6A	0.1227	0.5047	0.2664	0.069*	0.5

H6B	0.2013	0.5869	0.2192	0.069*	0.5
C7	0.28932 (14)	0.4136 (3)	0.28140 (9)	0.0529 (5)	0.5103 (12)
H7A	0.3116	0.4813	0.3201	0.063*	0.5103 (12)
H7B	0.2712	0.309	0.2976	0.063*	0.5103 (12)
C8	0.38620 (15)	0.4003 (2)	0.24030 (10)	0.0507 (4)*	0.5103 (12)
H8A	0.3953	0.4995	0.2168	0.061*	0.5103 (12)
H8B	0.3711	0.3159	0.2072	0.061*	0.5103 (12)
C6'	0.18164 (8)	0.48559 (13)	0.23797 (5)	0.0579 (3)	0.5
H6'A	0.1556	0.449	0.2793	0.069*	0.5
H6'B	0.1496	0.5907	0.228	0.069*	0.5
C7'	0.31428 (14)	0.4992 (2)	0.24959 (10)	0.0461 (5)	0.4897 (12)
H7'A	0.3413	0.5425	0.2097	0.055*	0.4897 (12)
H7'B	0.3376	0.5707	0.2869	0.055*	0.4897 (12)
C8'	0.36579 (16)	0.3346 (3)	0.26491 (11)	0.0546 (5)*	0.4897 (12)
H8'A	0.3555	0.2683	0.2249	0.066*	0.4897 (12)
H8'B	0.3299	0.2828	0.3	0.066*	0.4897 (12)
C9	0.49568 (8)	0.36248 (15)	0.28889 (6)	0.0698 (3)	
C10	0.51811 (9)	0.31754 (17)	0.35430 (6)	0.0756 (4)	
H10	0.4588	0.2874	0.3777	0.091*	
C11	0.62792 (9)	0.31639 (16)	0.38596 (6)	0.0682 (4)	
H11	0.6405	0.2851	0.4309	0.082*	
C12	0.69455 (9)	0.39956 (14)	0.29287 (5)	0.0620 (3)	
H12	0.7553	0.4277	0.2703	0.074*	
C13	0.58737 (9)	0.40483 (16)	0.25804 (6)	0.0714 (4)	
H13	0.5769	0.4373	0.2133	0.086*	
C14	0.53333 (7)	0.23713 (12)	0.06039 (5)	0.0537 (3)	
H14	0.5629	0.1496	0.0853	0.064*	
C15	0.60165 (6)	0.36363 (11)	0.05135 (4)	0.0416 (2)	
C16	0.55874 (6)	0.50062 (10)	0.01431 (4)	0.0402 (2)	
C17	0.62546 (7)	0.63484 (12)	0.00435 (5)	0.0509 (3)	
H17	0.7014	0.6369	0.0233	0.061*	
C18	0.58165 (8)	0.76140 (13)	−0.03229 (6)	0.0604 (3)	
H18	0.6281	0.8479	−0.0389	0.072*	
O3	0.91963 (6)	0.70891 (10)	0.13413 (4)	0.0646 (2)	
H1B	0.1124 (8)	−0.2462 (12)	0.0288 (5)	0.056 (3)*	
H2B	−0.1361 (8)	−0.1205 (13)	0.0732 (5)	0.069 (3)*	
H1A	0.1499 (9)	−0.1651 (14)	0.0826 (6)	0.079 (4)*	
H3A	0.9564 (10)	0.6867 (17)	0.1185 (7)	0.091 (4)*	
H2A	−0.1742 (8)	0.0219 (12)	0.0639 (5)	0.054 (3)*	
H3B	0.8764 (11)	0.6151 (19)	0.1378 (7)	0.105 (5)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02614 (5)	0.04243 (8)	0.02745 (6)	−0.00126 (6)	−0.00123 (5)	−0.00051 (7)
S1	0.03892 (9)	0.05174 (12)	0.04334 (11)	0.00923 (9)	0.01024 (8)	0.00641 (10)
N1	0.0296 (3)	0.0474 (4)	0.0306 (3)	−0.0017 (3)	−0.0007 (2)	−0.0010 (3)
N2	0.0445 (3)	0.0709 (5)	0.0487 (4)	−0.0011 (4)	−0.0072 (3)	0.0056 (4)

O1	0.0343 (2)	0.0515 (3)	0.0367 (3)	0.0046 (3)	−0.0036 (2)	−0.0015 (3)
O2	0.0389 (3)	0.0546 (3)	0.0462 (3)	−0.0026 (3)	0.0083 (2)	0.0012 (3)
O6	0.0601 (3)	0.0717 (5)	0.0471 (3)	−0.0018 (3)	0.0124 (3)	−0.0068 (3)
O4	0.0535 (3)	0.0603 (4)	0.0631 (4)	0.0170 (3)	0.0132 (3)	0.0197 (3)
O5	0.0426 (3)	0.0606 (4)	0.0503 (3)	0.0114 (3)	0.0171 (2)	0.0075 (3)
C1	0.0445 (4)	0.0541 (5)	0.0346 (4)	−0.0113 (4)	0.0022 (3)	0.0006 (4)
C2	0.0483 (4)	0.0692 (6)	0.0309 (4)	−0.0042 (5)	0.0019 (3)	−0.0018 (4)
C3	0.0302 (3)	0.0571 (5)	0.0413 (4)	0.0078 (4)	−0.0007 (3)	−0.0121 (4)
C4	0.0426 (4)	0.0447 (5)	0.0486 (5)	−0.0033 (4)	−0.0013 (4)	−0.0019 (4)
C5	0.0408 (4)	0.0521 (5)	0.0330 (4)	−0.0034 (4)	0.0014 (3)	0.0012 (4)
C6	0.0428 (4)	0.0712 (6)	0.0564 (5)	0.0090 (5)	−0.0057 (4)	−0.0288 (5)
C7	0.0462 (8)	0.0649 (11)	0.0454 (9)	−0.0040 (9)	−0.0018 (7)	−0.0238 (9)
C6'	0.0428 (4)	0.0712 (6)	0.0564 (5)	0.0090 (5)	−0.0057 (4)	−0.0288 (5)
C7'	0.0417 (8)	0.0449 (9)	0.0483 (9)	−0.0019 (8)	−0.0071 (7)	−0.0075 (9)
C9	0.0473 (4)	0.0830 (7)	0.0721 (6)	0.0170 (5)	−0.0184 (4)	−0.0303 (6)
C10	0.0463 (5)	0.1014 (9)	0.0795 (7)	−0.0036 (6)	0.0099 (5)	−0.0072 (7)
C11	0.0552 (5)	0.0993 (9)	0.0486 (5)	0.0038 (6)	0.0013 (4)	0.0113 (6)
C12	0.0591 (5)	0.0731 (7)	0.0515 (6)	−0.0039 (6)	−0.0013 (5)	0.0091 (5)
C13	0.0754 (6)	0.0836 (8)	0.0482 (6)	0.0172 (6)	−0.0180 (5)	−0.0014 (6)
C14	0.0490 (4)	0.0438 (5)	0.0695 (6)	0.0063 (4)	0.0123 (4)	0.0179 (5)
C15	0.0371 (3)	0.0437 (5)	0.0460 (4)	0.0070 (4)	0.0131 (3)	0.0044 (4)
C16	0.0373 (3)	0.0387 (4)	0.0473 (4)	0.0053 (4)	0.0151 (3)	0.0029 (4)
C17	0.0368 (4)	0.0489 (5)	0.0680 (6)	0.0003 (4)	0.0106 (4)	0.0100 (5)
C18	0.0460 (4)	0.0468 (5)	0.0892 (7)	−0.0055 (4)	0.0122 (5)	0.0173 (5)
O3	0.0722 (4)	0.0668 (5)	0.0584 (4)	−0.0010 (4)	0.0218 (3)	0.0022 (4)

Geometric parameters (Å, °)

Co1—O2^{i}	2.1022 (8)	C7—H7A	0.97
Co1—O2	2.1022 (8)	C7—H7B	0.97
Co1—O1	2.1230 (7)	C8—C9	1.548 (2)
Co1—O1^{i}	2.1230 (7)	C8—H8A	0.97
Co1—N1^{i}	2.1294 (8)	C8—H8B	0.97
Co1—N1	2.1294 (8)	C7'—C8'	1.525 (3)
S1—O4	1.4444 (8)	C7'—H7'A	0.97
S1—O6	1.4491 (8)	C7'—H7'B	0.97
S1—O5	1.4508 (8)	C8'—C9	1.568 (2)
S1—C15	1.7807 (9)	C8'—H8'A	0.97
N1—C1	1.3314 (11)	C8'—H8'B	0.97
N1—C5	1.3341 (12)	C9—C10	1.3559 (17)
N2—C12	1.3161 (13)	C9—C13	1.3654 (17)
N2—C11	1.3193 (14)	C10—C11	1.3700 (15)
O1—H1B	0.735 (10)	C10—H10	0.93
O1—H1A	0.884 (10)	C11—H11	0.93
O2—H2B	0.771 (11)	C12—C13	1.3665 (15)
O2—H2A	0.823 (10)	C12—H12	0.93
C1—C2	1.3718 (13)	C13—H13	0.93
C1—H1	0.93	C14—C15	1.3612 (13)

C2—C3	1.3831 (14)	C14—C18^{ii}	1.4036 (13)
C2—H2	0.93	C14—H14	0.93
C3—C4	1.3732 (13)	C15—C16	1.4252 (12)
C3—C6	1.5026 (13)	C16—C17	1.4051 (13)
C4—C5	1.3782 (13)	C16—C16^{ii}	1.4336 (15)
C4—H4	0.93	C17—C18	1.3549 (14)
C5—H5	0.93	C17—H17	0.93
C6—C7	1.567 (2)	C18—C14^{ii}	1.4036 (13)
C6—H6A	0.97	C18—H18	0.93
C6—H6B	0.97	O3—H3A	0.599 (14)
C7—C8	1.502 (3)	O3—H3B	0.947 (15)
O2^{i}—Co1—O2	180.00 (3)	C8—C7—H7A	109.6
O2^{i}—Co1—O1	89.37 (3)	C6—C7—H7A	109.6
O2—Co1—O1	90.63 (3)	C8—C7—H7B	109.6
O2^{i}—Co1—O1^{i}	90.63 (3)	C6—C7—H7B	109.6
O2—Co1—O1^{i}	89.37 (3)	H7A—C7—H7B	108.1
O1—Co1—O1^{i}	180.00 (4)	C7—C8—C9	107.91 (14)
O2^{i}—Co1—N1^{i}	90.64 (3)	C7—C8—H8A	110.1
O2—Co1—N1^{i}	89.36 (3)	C9—C8—H8A	110.1
O1—Co1—N1^{i}	88.50 (3)	C7—C8—H8B	110.1
O1^{i}—Co1—N1^{i}	91.50 (3)	C9—C8—H8B	110.1
O2^{i}—Co1—N1	89.36 (3)	H8A—C8—H8B	108.4
O2—Co1—N1	90.64 (3)	C8'—C7'—H7'A	109.8
O1—Co1—N1	91.50 (3)	C8'—C7'—H7'B	109.8
O1^{i}—Co1—N1	88.50 (3)	H7'A—C7'—H7'B	108.3
N1^{i}—Co1—N1	180.00 (4)	C7'—C8'—C9	106.09 (15)
O4—S1—O6	113.64 (5)	C7'—C8'—H8'A	110.5
O4—S1—O5	112.80 (4)	C9—C8'—H8'A	110.5
O6—S1—O5	111.97 (4)	C7'—C8'—H8'B	110.5
O4—S1—C15	105.68 (4)	C9—C8'—H8'B	110.5
O6—S1—C15	106.11 (5)	H8'A—C8'—H8'B	108.7
O5—S1—C15	105.89 (4)	C10—C9—C13	116.33 (10)
C1—N1—C5	116.94 (7)	C10—C9—C8	134.91 (12)
C1—N1—Co1	121.07 (6)	C13—C9—C8	108.20 (12)
C5—N1—Co1	121.99 (6)	C10—C9—C8'	108.32 (12)
C12—N2—C11	115.63 (9)	C13—C9—C8'	134.99 (13)
Co1—O1—H1B	111.1 (7)	C9—C10—C11	120.18 (11)
Co1—O1—H1A	117.8 (7)	C9—C10—H10	119.9
H1B—O1—H1A	106.7 (10)	C11—C10—H10	119.9
Co1—O2—H2B	115.2 (8)	N2—C11—C10	123.83 (11)
Co1—O2—H2A	116.1 (7)	N2—C11—H11	118.1
H2B—O2—H2A	107.0 (11)	C10—C11—H11	118.1
N1—C1—C2	122.92 (9)	N2—C12—C13	123.95 (11)
N1—C1—H1	118.5	N2—C12—H12	118
C2—C1—H1	118.5	C13—C12—H12	118
C1—C2—C3	120.20 (9)	C9—C13—C12	120.08 (11)

C1—C2—H2	119.9	C9—C13—H13	120
C3—C2—H2	119.9	C12—C13—H13	120
C4—C3—C2	116.92 (8)	C15—C14—C18^{ii}	120.14 (9)
C4—C3—C6	121.64 (9)	C15—C14—H14	119.9
C2—C3—C6	121.44 (8)	C18^{ii}—C14—H14	119.9
C3—C4—C5	119.66 (9)	C14—C15—C16	121.39 (7)
C3—C4—H4	120.2	C14—C15—S1	117.82 (7)
C5—C4—H4	120.2	C16—C15—S1	120.79 (6)
N1—C5—C4	123.34 (8)	C17—C16—C15	123.49 (7)
N1—C5—H5	118.3	C17—C16—C16^{ii}	118.91 (10)
C4—C5—H5	118.3	C15—C16—C16^{ii}	117.60 (10)
C3—C6—C7	110.84 (11)	C18—C17—C16	121.52 (8)
C3—C6—H6A	109.5	C18—C17—H17	119.2
C7—C6—H6A	109.5	C16—C17—H17	119.2
C3—C6—H6B	109.5	C17—C18—C14^{ii}	120.42 (9)
C7—C6—H6B	109.5	C17—C18—H18	119.8
H6A—C6—H6B	108.1	C14^{ii}—C18—H18	119.8
C8—C7—C6	110.43 (14)	H3A—O3—H3B	102.7 (16)

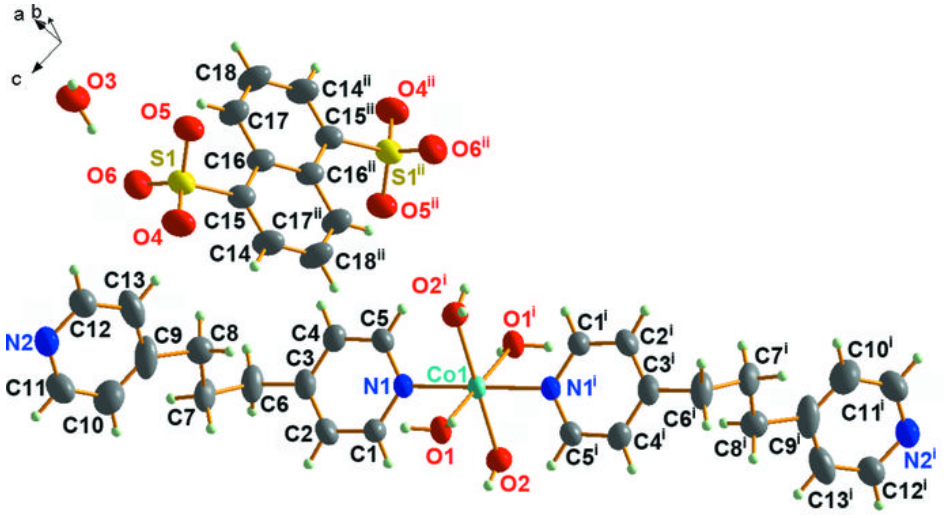
Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3B···O6	0.947 (15)	1.792 (14)	2.7176 (11)	164.8 (13)
O3—H3A···O1^{iii}	0.599 (14)	2.436 (14)	2.9013 (12)	136.6 (16)
O2—H2A···O4^{iv}	0.823 (10)	1.916 (10)	2.7363 (11)	174.6 (10)
O1—H1B···O5^{v}	0.735 (10)	1.979 (10)	2.7096 (10)	173.1 (10)
O1—H1A···N2^{vi}	0.884 (10)	1.872 (10)	2.7495 (12)	171.3 (11)
O2—H2B···O3^{vii}	0.771 (11)	1.940 (11)	2.6959 (11)	166.8 (11)

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

Fig. 1


a
b
c
O3
C18
C14ii
O4ii
O5
C17
C15ii
O6ii
S1
C16
C16ii
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O6
O5ii
C15
C17ii
O4
C14
C18ii
C13
O2i
O1i
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C2i
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C9
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C5
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C11i
C6
C10
C7
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N2i
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O1
C5i
C12i
O2
C13i

Fig. 2

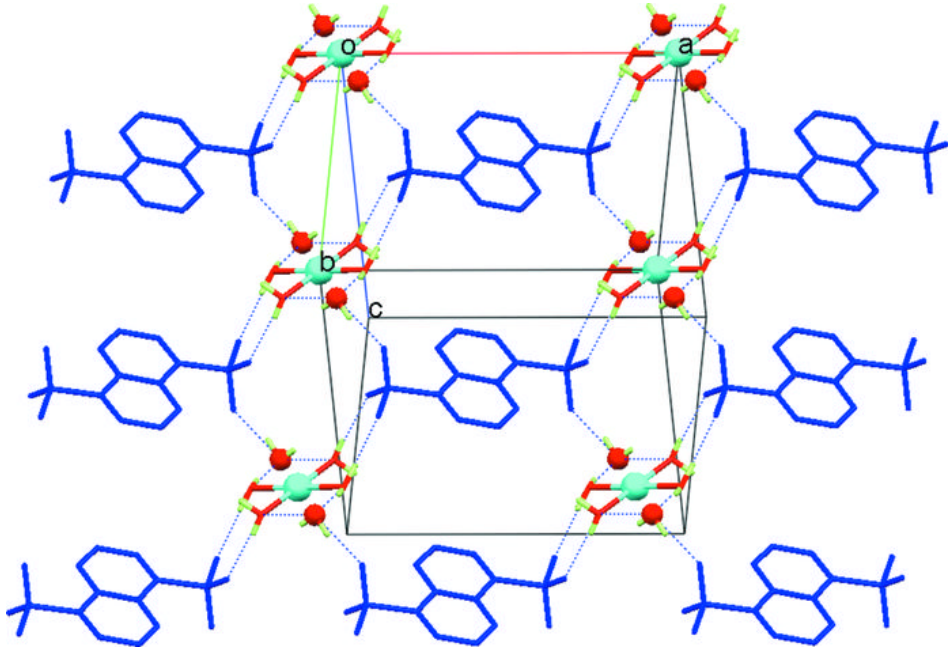

Fig. 3