Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaqua(1,10-phenanthroline)cobalt(II) naphthalene-1,5-disulfonate dihydrate

Yin-Qiu Liu,[a]* Yuan-Xiang Wu,[a] Xi-Rui Zeng[a] and He-Rui Wen[b]

[a]College of Chemistry and Chemical Engineering, JiangXi Province Key Laboratory of Coordination Chemistry, JingGangShan University, 343009 Ji'an, JiangXi, People's Republic of China, and [b]Chemistry Department of GanNan Teachers' College, 343009 GanZhou, JiangXi, People's Republic of China
Correspondence e-mail: liuyiqja@163.com

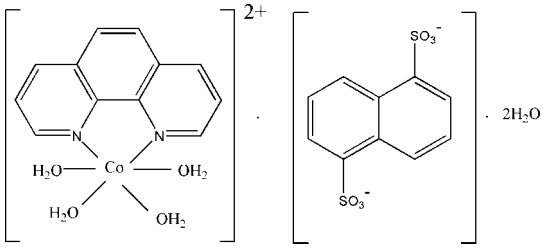
Received 15 November 2007; accepted 16 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.097; data-to-parameter ratio = 14.6.

The title complex, $[Co(C_{12}H_8N_2)(H_2O)_4](C_{10}H_6O_6S_2)\cdot 2H_2O$, was synthesized hydrothermally. The Co^{2+} cation, which lies on a twofold rotation axis, is six-coordinate. The anion is located on a centre of inversion. An extensive network of O—H···O hydrogen bonds links the components into a three-dimensional network.

Related literature

For a related copper(II) structure, see: Liu & Zeng (2007).



Experimental

Crystal data

$[Co(C_{12}H_8N_2)(H_2O)_4](C_{10}H_6O_6S_2)\cdot 2H_2O$
M_r = 633.52
Monoclinic, $C2/c$
a = 20.578 (4) Å
b = 12.431 (3) Å
c = 12.462 (3) Å
β = 123.867 (2)°
V = 2647.0 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 293 (2) K
0.40 × 0.35 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
8365 measured reflections
2590 independent reflections
2353 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.098
S = 1.07
2590 reflections
177 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5B···O2^{i}	0.82	1.98	2.7953 (17)	176
O5—H5A···O3^{ii}	0.82	1.91	2.7255 (17)	178
O4—H4B···O1^{i}	0.82	1.95	2.7660 (19)	174
O4—H4A···O6^{iii}	0.82	1.86	2.663 (3)	166
O6—H6B···O2^{iv}	0.85	2.05	2.896 (2)	179
O6—H6A···O1^{v}	0.85	1.97	2.821 (3)	179

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Key Laboratory of Coordination Chemistry, JingGangShan University, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2626).

References

Bruker (1997). *SMART*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT*. Version 7.06A. Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, Y.-Q. & Zeng, X.-R. (2007). *Acta Cryst.* E**63**, m2414.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

  doi:10.1107/S160053680705982X

supplementary materials

Acta Cryst. (2007). E**63**, m3120 [**doi:10.1107/S160053680705982X**]

Tetraaqua(1,10-phenanthroline)cobalt(II) naphthalene-1,5-disulfonate dihydrate

Y.-Q. Liu, Y.-X. Wu, X.-R. Zeng and H.-R. Wen

Comment

The title compound is consisted of Cobalt(II) coordination cations, naphthalene-1,5-disulfonic acid anions and latice water molecules. In the complex there exists an extensive network of O—H···O hydrogen bonds which form among the coordinated water molecules, the sulfonate groups of the anions and the latice water molecules (Fig. 2).

Experimental

A mixture of naphthalene-1,5-disulfonic acid (0.2810 g, 0.001 mol), 1,10-phenanthroline(0.1780 g, 0.001 mol) and $CoNO_3{\cdot}6H_2O$ (0.2310,0.001 mol) was added to 20 ml water, The mixture was closed in a steel tomb and heated at 418 K for 4 days. Single crystals suitable for X-ray diffraction analysis formed after it cooled down to room temperature.

Refinement

All H atoms bonded to C atoms were set to calculated positions and refined as riding on their parent C atoms with the C—H bond length fixed to 0.93Å with U_{iso}(H) = 1.2 times U_{eq}(C). The H atoms of the water molecules were taken from an electron density map and refined as riding on their parent O atoms with the O—H bond length fixed to 0.82Å with U_{iso}(H) = 1.5 times U_{eq}(O).

Figures

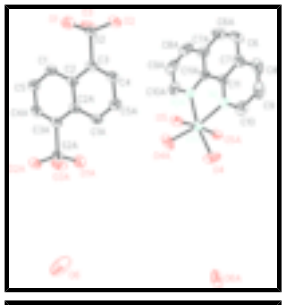


Fig.1. Perspective view of the title compound showing 50% probability displacement ellipsoids.

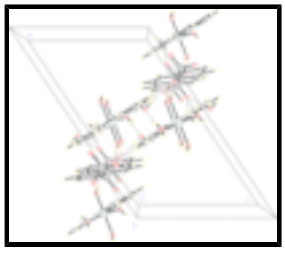


Fig.2. The packing diagram, viewed along the *b* axis; hydrogen bonds are shown as dashed lines.

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

Tetraaqua(1,10-phenanthroline)cobalt(II) naphthalene-1,5-disulfonate dihydrate

Crystal data

$[Co(C_{12}H_8N_2)(H_2O)_4](C_{10}H_6O_6S_2)\cdot 2H_2O$	$F_{000} = 1308$
$M_r = 633.52$	$D_x = 1.590$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 7881 reflections
$a = 20.578$ (4) Å	$\theta = 1.0$–28.3º
$b = 12.431$ (3) Å	$\mu = 0.87$ mm^{-1}
$c = 12.462$ (3) Å	$T = 293$ (2) K
$\beta = 123.867$ (2)º	Block, brown
$V = 2647.0$ (10) Å^3	0.40 × 0.35 × 0.32 mm
$Z = 4$	

Data collection

CCD area-detector diffractometer	2353 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.018$
Monochromator: graphite	$\theta_{max} = 26.0$º
$T = 293(2)$ K	$\theta_{min} = 2.0$º
φ and ω scans	$h = -25\rightarrow25$
Absorption correction: none	$k = -15\rightarrow15$
8365 measured reflections	$l = -15\rightarrow15$
2590 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.098$	$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 2.5933P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.004$
2590 reflections	$\Delta\rho_{max} = 0.77$ e Å^{-3}
177 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
6 restraints	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}
O6	0.92197 (10)	0.91248 (19)	0.91351 (19)	0.1020 (7)
H6A	0.9014	0.9461	0.9470	0.153*
H6B	0.8862	0.9122	0.8332	0.153*
C1	0.74393 (8)	0.18231 (13)	0.36018 (14)	0.0350 (4)
H1	0.7508	0.1143	0.3369	0.042*
C2	0.75484 (8)	0.19727 (11)	0.48239 (14)	0.0296 (3)
C3	0.77564 (8)	0.11167 (12)	0.57272 (14)	0.0315 (4)
C4	0.78621 (9)	0.12984 (13)	0.68961 (14)	0.0369 (4)
H4	0.7996	0.0731	0.7470	0.044*
C5	0.72373 (9)	0.26630 (14)	0.27639 (15)	0.0392 (4)
H5	0.7162	0.2547	0.1965	0.047*
C6	0.52159 (13)	−0.21659 (15)	0.8154 (2)	0.0628 (6)
H6	0.5368	−0.2817	0.8596	0.075*
C7	0.54443 (9)	−0.11799 (15)	0.88668 (16)	0.0437 (4)
C8	0.58766 (10)	−0.11283 (18)	1.02151 (17)	0.0522 (5)
H8	0.6036	−0.1756	1.0704	0.063*
C9	0.60609 (10)	−0.01630 (19)	1.08079 (16)	0.0522 (5)
H9	0.6356	−0.0123	1.1705	0.063*
C10	0.58099 (9)	0.07835 (17)	1.00709 (15)	0.0429 (4)
H10	0.5936	0.1443	1.0494	0.052*
C11	0.52200 (8)	−0.01967 (12)	0.81936 (13)	0.0312 (4)
Co1	0.5000	0.21031 (2)	0.7500	0.03305 (8)
N1	0.53944 (7)	0.07706 (11)	0.87848 (11)	0.0322 (3)
O1	0.85225 (7)	−0.02251 (10)	0.52277 (13)	0.0548 (3)
O2	0.79931 (7)	−0.08974 (9)	0.64024 (11)	0.0466 (3)
O3	0.71259 (8)	−0.04810 (10)	0.41253 (12)	0.0523 (4)
O4	0.53359 (7)	0.32180 (12)	0.89771 (15)	0.0656 (4)
H4A	0.5049	0.3500	0.9159	0.098*
H4B	0.5648	0.3713	0.9178	0.098*
O5	0.61506 (6)	0.21906 (9)	0.79332 (11)	0.0394 (3)
H5A	0.6446	0.1682	0.8308	0.059*
H5B	0.6405	0.2750	0.8162	0.059*
S2	0.78554 (2)	−0.02258 (3)	0.53385 (4)	0.03427 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O6	0.0932 (9)	0.1232 (16)	0.1006 (10)	0.0290 (11)	0.0608 (8)	−0.0182 (10)
C1	0.0407 (6)	0.0264 (7)	0.0379 (6)	−0.0013 (6)	0.0219 (5)	−0.0038 (5)
C2	0.0274 (5)	0.0232 (7)	0.0344 (6)	−0.0021 (5)	0.0150 (5)	−0.0014 (5)
C3	0.0305 (5)	0.0231 (7)	0.0378 (6)	0.0004 (5)	0.0170 (5)	0.0008 (5)
C4	0.0415 (6)	0.0289 (7)	0.0371 (6)	0.0010 (6)	0.0199 (5)	0.0050 (6)
C5	0.0478 (7)	0.0348 (8)	0.0335 (6)	−0.0003 (7)	0.0217 (5)	−0.0011 (6)
C6	0.0847 (11)	0.0287 (9)	0.0812 (11)	0.0067 (8)	0.0501 (9)	0.0116 (8)
C7	0.0441 (6)	0.0397 (9)	0.0520 (7)	0.0062 (7)	0.0296 (5)	0.0121 (7)
C8	0.0451 (7)	0.0611 (11)	0.0501 (8)	0.0106 (8)	0.0263 (6)	0.0253 (8)
C9	0.0348 (7)	0.0840 (14)	0.0320 (7)	0.0016 (8)	0.0150 (5)	0.0156 (8)
C10	0.0342 (6)	0.0587 (11)	0.0322 (6)	−0.0082 (7)	0.0162 (5)	−0.0057 (7)
C11	0.0297 (5)	0.0316 (8)	0.0340 (6)	0.0010 (5)	0.0188 (4)	0.0032 (5)
Co1	0.03179 (11)	0.02513 (14)	0.04219 (13)	0.000	0.02060 (9)	0.000
N1	0.0302 (5)	0.0354 (7)	0.0302 (5)	−0.0037 (5)	0.0163 (4)	−0.0014 (5)
O1	0.0607 (5)	0.0418 (7)	0.0830 (6)	0.0173 (5)	0.0530 (5)	0.0175 (5)
O2	0.0643 (6)	0.0266 (6)	0.0546 (5)	0.0084 (5)	0.0368 (4)	0.0107 (4)
O3	0.0597 (7)	0.0294 (6)	0.0514 (6)	−0.0095 (5)	0.0208 (5)	−0.0068 (5)
O4	0.0556 (5)	0.0521 (7)	0.1043 (8)	−0.0211 (6)	0.0539 (5)	−0.0404 (6)
O5	0.0339 (4)	0.0262 (5)	0.0552 (6)	0.0003 (4)	0.0230 (4)	0.0014 (4)
S2	0.04075 (15)	0.02087 (17)	0.04330 (16)	0.00339 (13)	0.02474 (13)	0.00308 (12)

Geometric parameters (Å, °)

O6—H6A	0.8504	C9—C10	1.402 (3)
O6—H6B	0.8501	C9—H9	0.9301
C1—C5	1.367 (2)	C10—N1	1.331 (2)
C1—C2	1.422 (2)	C10—H10	0.9300
C1—H1	0.9300	C11—N1	1.350 (2)
C2—C3	1.430 (2)	C11—C11^{ii}	1.437 (3)
C2—C2^{i}	1.431 (3)	Co1—O4	2.0902 (15)
C3—C4	1.366 (2)	Co1—O4^{ii}	2.0902 (15)
C3—S2	1.7808 (16)	Co1—O5^{ii}	2.1177 (13)
C4—C5^{i}	1.409 (2)	Co1—O5	2.1177 (13)
C4—H4	0.9300	Co1—N1^{ii}	2.1255 (14)
C5—C4^{i}	1.409 (2)	Co1—N1	2.1255 (14)
C5—H5	0.9301	O1—S2	1.4543 (15)
C6—C6^{ii}	1.354 (4)	O2—S2	1.4548 (13)
C6—C7	1.431 (3)	O3—S2	1.4528 (12)
C6—H6	0.9300	O4—H4A	0.8206
C7—C8	1.397 (3)	O4—H4B	0.8203
C7—C11	1.407 (2)	O5—H5A	0.8190
C8—C9	1.348 (3)	O5—H5B	0.8196
C8—H8	0.9300		

H6A—O6—H6B	103.9	N1—C11—C11^{ii}	117.02 (8)
C5—C1—C2	121.16 (15)	C7—C11—C11^{ii}	119.67 (10)
C5—C1—H1	119.4	O4—Co1—O4^{ii}	96.93 (9)
C2—C1—H1	119.5	O4—Co1—O5^{ii}	87.97 (5)
C1—C2—C3	123.01 (14)	O4^{ii}—Co1—O5^{ii}	88.13 (5)
C1—C2—C2^{i}	118.83 (17)	O4—Co1—O5	88.13 (5)
C3—C2—C2^{i}	118.16 (18)	O4^{ii}—Co1—O5	87.97 (5)
C4—C3—C2	121.07 (14)	O5^{ii}—Co1—O5	174.11 (6)
C4—C3—S2	118.07 (12)	O4—Co1—N1^{ii}	168.58 (6)
C2—C3—S2	120.84 (12)	O4^{ii}—Co1—N1^{ii}	93.06 (6)
C3—C4—C5^{i}	120.57 (15)	O5^{ii}—Co1—N1^{ii}	86.83 (5)
C3—C4—H4	119.8	O5—Co1—N1^{ii}	97.78 (5)
C5^{i}—C4—H4	119.6	O4—Co1—N1	93.06 (6)
C1—C5—C4^{i}	120.22 (16)	O4^{ii}—Co1—N1	168.58 (6)
C1—C5—H5	119.8	O5^{ii}—Co1—N1	97.78 (5)
C4^{i}—C5—H5	119.9	O5—Co1—N1	86.83 (5)
C6^{ii}—C6—C7	121.03 (11)	N1^{ii}—Co1—N1	77.60 (7)
C6^{ii}—C6—H6	119.4	C10—N1—C11	117.69 (14)
C7—C6—H6	119.5	C10—N1—Co1	128.09 (12)
C8—C7—C11	117.04 (17)	C11—N1—Co1	114.16 (9)
C8—C7—C6	123.68 (18)	Co1—O4—H4A	126.2
C11—C7—C6	119.28 (16)	Co1—O4—H4B	125.7
C9—C8—C7	119.74 (18)	H4A—O4—H4B	99.0
C9—C8—H8	119.9	Co1—O5—H5A	118.4
C7—C8—H8	120.3	Co1—O5—H5B	122.6
C8—C9—C10	119.96 (16)	H5A—O5—H5B	109.2
C8—C9—H9	120.1	O3—S2—O1	112.58 (9)
C10—C9—H9	119.9	O3—S2—O2	112.74 (8)
N1—C10—C9	122.24 (18)	O1—S2—O2	111.85 (8)
N1—C10—H10	118.8	O3—S2—C3	106.21 (7)
C9—C10—H10	118.9	O1—S2—C3	106.41 (8)
N1—C11—C7	123.32 (14)	O2—S2—C3	106.48 (8)

Symmetry codes: (i) −*x*+3/2, −*y*+1/2, −*z*+1; (ii) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5B···O2^{iii}	0.82	1.98	2.7953 (17)	176
O5—H5A···O3^{iv}	0.82	1.91	2.7255 (17)	178
O4—H4B···O1^{iii}	0.82	1.95	2.7660 (19)	174
O4—H4A···O6^{v}	0.82	1.86	2.663 (3)	166
O6—H6B···O2^{vi}	0.85	2.05	2.896 (2)	179
O6—H6A···O1^{vii}	0.85	1.97	2.821 (3)	179

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

Fig. 1

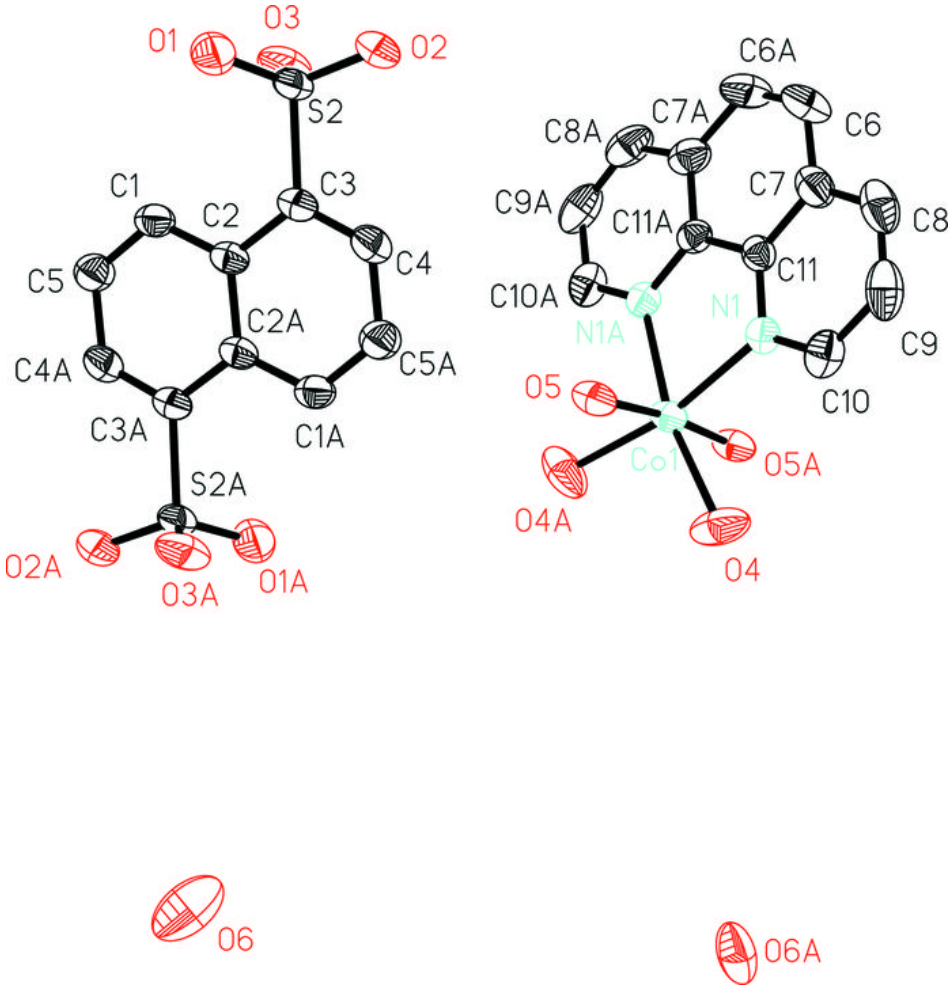

O1
O3
O2
S2
C1
C2
C3
C4
C5
C2A
C4A
C5A
C3A
C1A
S2A
O2A
O3A
O1A
C6A
C7A
C6
C8A
C7
C8
C9A
C11A
C11
C10A
N1A
N1
C9
O5
C10
Co1
O5A
O4A
O4
O6
O6A

Fig. 2