

Hexaaquacobalt(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

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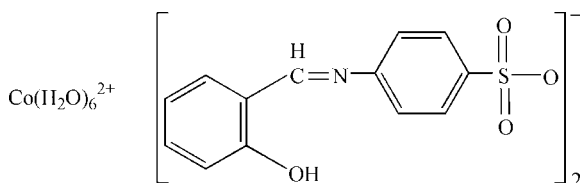
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.071; wR factor = 0.141; data-to-parameter ratio = 13.4.

In the cation of the title compound, $[\text{Co}(\text{H}_2\text{O})_6](\text{C}_{13}\text{H}_{10}\text{NO}_4\text{S})_2$, the Co atom lies on a centre of symmetry and its coordination geometry is octahedral. The crystal structure is stabilized by water-anion $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds. An intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond occurs in the anion.

Related literature

For related literature, see: Allen *et al.* (1987); Tai & Feng (2008); Tai *et al.* (2003); Tai *et al.* (2008); Tai, Yin & Feng (2007); Tai, Yin & Hao (2007); Tai, Yin, Feng & Kong (2007); Wang *et al.* (2007).



Experimental

Crystal data

$[\text{Co}(\text{H}_2\text{O})_6](\text{C}_{13}\text{H}_{10}\text{NO}_4\text{S})_2$
 $M_r = 719.59$
 Monoclinic, $P2_1/n$
 $a = 6.3216$ (13) Å
 $b = 35.211$ (3) Å
 $c = 6.9924$ (15) Å
 $\beta = 90.186$ (2)°

$V = 1556.4$ (5) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.76$ mm⁻¹
 $T = 298$ (2) K
 $0.40 \times 0.35 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.752$, $T_{\max} = 0.895$

7328 measured reflections
 2749 independent reflections
 2171 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.070$
 $wR(F^2) = 0.141$
 $S = 1.17$
 2749 reflections

205 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.69$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O4}-\text{H4}\cdots\text{N1}$	0.82	1.88	2.588 (7)	143
$\text{O5}-\text{H5A}\cdots\text{O2}^{\text{i}}$	0.85	1.96	2.736 (6)	151
$\text{O5}-\text{H5B}\cdots\text{O1}$	0.85	1.97	2.744 (6)	151
$\text{O6}-\text{H6A}\cdots\text{O1}^{\text{ii}}$	0.85	1.99	2.757 (5)	150
$\text{O6}-\text{H6B}\cdots\text{O3}$	0.85	2.03	2.768 (5)	144
$\text{O7}-\text{H7A}\cdots\text{O3}^{\text{i}}$	0.85	1.96	2.759 (5)	157
$\text{O7}-\text{H7B}\cdots\text{O2}^{\text{iii}}$	0.85	1.98	2.761 (5)	152
$\text{C6}-\text{H6}\cdots\text{O3}$	0.93	2.56	2.918 (7)	104

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

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2558).

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supplementary materials

Acta Cryst. (2008). E64, m645 [doi:10.1107/S1600536808009422]

Hexaaquacobalt(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

X.-S. Tai, Y.-M. Feng and F.-Y. Kong

Comment

As part of our ongoing studies of the coordination chemistry of Schiff base ligands (Xi-Shi & Yi-Min, 2008; Tai, Feng & Zhang, 2008; Tai, Yin & Feng, 2007; Tai, Yin, Feng & Kong, 2007; Tai, Yin & Hao, 2007; Wang *et al.*, 2007; Tai *et al.*, 2003), we now report the synthesis and structure of the title compound, (I), (Fig. 1).

In the molecule of (I), the Co (II) centre is six-coordinate with six O donors of the water molecules. The C7—N1 bond length of 1.281 (8) Å is close to double-bond. Otherwise, the geometrical parameters for (I) are in normal range (Allen *et al.*, 1987). The dihedral angle between the two benzene ring is 33.5°, indicating that the molecule is non-planar, which perhaps correlates with the intramolecular and intermolecular hydrogen bonds (Table 1).

Experimental

1 mmol of Cobalt acetate was added to a solution of salicylaldehyde-4-aminobenzene sulfonic acid (1 mmol) in 10 ml of 95% ethanol. The mixture was stirred for 2 h at refluxing temperature. Evaporating some ethanol, clear blocks of (I) were obtained after one weeks.

Refinement

The H atoms were placed geometrically [C—H = 0.93 Å, O—H = 0.82 for hydroxy group and O—H = 0.85 Å for water molecules] and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

Figures

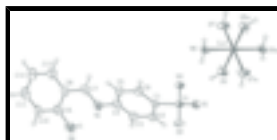


Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids. [Symmetry code: (a) $-x + 2, -y, -z$].

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Crystal data

$[\text{Co}(\text{H}_2\text{O})_6](\text{C}_{13}\text{H}_{10}\text{NO}_4\text{S})_2$

$M_r = 719.59$

Monoclinic, $P2_1/n$

Hall symbol: $-P 2_1n$

$a = 6.3216 (13) \text{ \AA}$

$F_{000} = 746$

$D_x = 1.535 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2380 reflections

$\theta = 2.4\text{--}25.3^\circ$

supplementary materials

$b = 35.211 (3) \text{ \AA}$
 $c = 6.9924 (15) \text{ \AA}$
 $\beta = 90.186 (2)^\circ$
 $V = 1556.4 (5) \text{ \AA}^3$
 $Z = 2$

$\mu = 0.76 \text{ mm}^{-1}$
 $T = 298 (2) \text{ K}$
Block, light purple
 $0.40 \times 0.35 \times 0.15 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	2749 independent reflections
Radiation source: fine-focus sealed tube	2171 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.040$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -5 \rightarrow 7$
$T_{\text{min}} = 0.752$, $T_{\text{max}} = 0.895$	$k = -41 \rightarrow 37$
7328 measured reflections	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.071$	H-atom parameters constrained
$wR(F^2) = 0.141$	$w = 1/[\sigma^2(F_o^2) + (0.0118P)^2 + 5.6103P]$
$S = 1.17$	where $P = (F_o^2 + 2F_c^2)/3$
2749 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
205 parameters	$\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.69 \text{ e \AA}^{-3}$
	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 (\AA^2)

x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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Co1	1.0000	0.0000	0.0000	0.0332 (3)
N1	0.4234 (9)	0.23121 (15)	0.5063 (8)	0.0585 (14)
O1	0.5135 (6)	0.05103 (11)	0.3289 (6)	0.0480 (10)
O2	0.5140 (6)	0.05158 (12)	0.6754 (6)	0.0504 (11)
O3	0.8400 (5)	0.06145 (11)	0.5055 (5)	0.0418 (9)
O4	0.1496 (8)	0.28449 (14)	0.5667 (7)	0.0772 (15)
H4	0.1993	0.2632	0.5809	0.116*
O5	0.7065 (5)	0.02585 (12)	0.0016 (6)	0.0496 (10)
H5A	0.6839	0.0392	-0.0978	0.060*
H5B	0.6850	0.0389	0.1020	0.060*
O6	1.1038 (6)	0.03462 (13)	0.2207 (6)	0.0571 (12)
H6A	1.2332	0.0310	0.2484	0.069*
H6B	1.0279	0.0325	0.3203	0.069*
O7	1.1055 (6)	0.03864 (12)	-0.2024 (6)	0.0575 (12)
H7A	1.0260	0.0392	-0.3007	0.069*
H7B	1.2326	0.0344	-0.2355	0.069*
S1	0.61081 (19)	0.06622 (4)	0.50249 (19)	0.0345 (3)
C1	0.5625 (8)	0.11545 (15)	0.4991 (7)	0.0349 (12)
C2	0.3648 (9)	0.12848 (17)	0.4446 (9)	0.0471 (15)
H2	0.2605	0.1115	0.4059	0.056*
C3	0.3241 (10)	0.16694 (17)	0.4483 (10)	0.0542 (17)
H3	0.1907	0.1758	0.4140	0.065*
C4	0.4787 (10)	0.19236 (17)	0.5021 (10)	0.0522 (15)
C5	0.6758 (10)	0.17953 (18)	0.5569 (9)	0.0545 (17)
H5	0.7794	0.1967	0.5950	0.065*
C6	0.7197 (9)	0.14085 (17)	0.5552 (8)	0.0471 (15)
H6	0.8527	0.1320	0.5911	0.056*
C7	0.5616 (11)	0.25709 (18)	0.4752 (10)	0.0571 (17)
H7	0.6992	0.2500	0.4448	0.069*
C8	0.5093 (11)	0.29731 (17)	0.4862 (10)	0.0542 (16)
C9	0.3064 (12)	0.3093 (2)	0.5366 (10)	0.0624 (19)
C10	0.2661 (13)	0.34768 (19)	0.5538 (10)	0.067 (2)
H10	0.1313	0.3557	0.5881	0.080*
C11	0.4190 (14)	0.3740 (2)	0.5216 (10)	0.071 (2)
H11	0.3882	0.3997	0.5362	0.085*
C12	0.6230 (15)	0.3628 (2)	0.4664 (12)	0.080 (2)
H12	0.7268	0.3808	0.4399	0.095*
C13	0.6654 (12)	0.32435 (19)	0.4525 (10)	0.0661 (19)
H13	0.8009	0.3164	0.4199	0.079*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0218 (5)	0.0452 (6)	0.0327 (5)	-0.0015 (5)	-0.0018 (4)	-0.0005 (5)
N1	0.063 (4)	0.047 (3)	0.066 (4)	0.009 (3)	-0.001 (3)	-0.008 (3)
O1	0.032 (2)	0.060 (3)	0.051 (3)	0.0021 (18)	-0.0070 (18)	-0.011 (2)
O2	0.035 (2)	0.065 (3)	0.051 (3)	0.0022 (19)	0.0071 (18)	0.018 (2)
O3	0.0233 (18)	0.057 (2)	0.045 (2)	0.0035 (17)	0.0008 (16)	0.0017 (19)

supplementary materials

O4	0.081 (4)	0.063 (3)	0.087 (4)	0.014 (3)	0.020 (3)	0.006 (3)
O5	0.037 (2)	0.075 (3)	0.037 (2)	0.013 (2)	-0.0008 (17)	0.001 (2)
O6	0.028 (2)	0.095 (3)	0.048 (3)	-0.002 (2)	-0.0009 (18)	-0.023 (2)
O7	0.028 (2)	0.090 (3)	0.055 (3)	-0.002 (2)	-0.0028 (18)	0.026 (2)
S1	0.0233 (6)	0.0456 (8)	0.0348 (7)	0.0022 (6)	-0.0004 (5)	0.0012 (6)
C1	0.028 (3)	0.047 (3)	0.030 (3)	0.002 (2)	-0.002 (2)	-0.001 (2)
C2	0.033 (3)	0.051 (4)	0.058 (4)	0.002 (3)	-0.016 (3)	-0.002 (3)
C3	0.041 (3)	0.049 (4)	0.072 (5)	0.011 (3)	-0.005 (3)	-0.001 (3)
C4	0.053 (4)	0.048 (3)	0.056 (4)	0.012 (3)	0.001 (3)	-0.003 (3)
C5	0.061 (4)	0.045 (4)	0.057 (4)	-0.004 (3)	-0.014 (3)	-0.009 (3)
C6	0.038 (3)	0.057 (4)	0.046 (4)	-0.001 (3)	-0.014 (3)	-0.003 (3)
C7	0.061 (4)	0.053 (4)	0.057 (4)	0.012 (3)	-0.001 (3)	-0.007 (3)
C8	0.065 (4)	0.049 (4)	0.049 (4)	0.002 (3)	-0.003 (3)	-0.013 (3)
C9	0.084 (5)	0.057 (4)	0.047 (4)	0.007 (4)	0.008 (4)	-0.002 (3)
C10	0.104 (6)	0.045 (4)	0.051 (4)	0.017 (4)	0.008 (4)	-0.003 (3)
C11	0.107 (6)	0.046 (4)	0.059 (5)	0.019 (4)	-0.010 (4)	-0.002 (4)
C12	0.105 (7)	0.045 (4)	0.089 (6)	0.000 (4)	-0.009 (5)	0.001 (4)
C13	0.067 (5)	0.057 (4)	0.075 (5)	0.003 (4)	-0.005 (4)	-0.007 (4)

Geometric parameters (\AA , $^\circ$)

Co1—O5	2.067 (3)	C1—C6	1.392 (7)
Co1—O5 ⁱ	2.067 (3)	C2—C3	1.379 (8)
Co1—O6	2.072 (4)	C2—H2	0.9300
Co1—O6 ⁱ	2.072 (4)	C3—C4	1.377 (8)
Co1—O7 ⁱ	2.075 (4)	C3—H3	0.9300
Co1—O7	2.075 (4)	C4—C5	1.379 (8)
N1—C7	1.281 (8)	C5—C6	1.390 (8)
N1—C4	1.412 (7)	C5—H5	0.9300
O1—S1	1.460 (4)	C6—H6	0.9300
O2—S1	1.452 (4)	C7—C8	1.456 (8)
O3—S1	1.458 (3)	C7—H7	0.9300
O4—C9	1.338 (8)	C8—C13	1.392 (9)
O4—H4	0.8200	C8—C9	1.397 (9)
O5—H5A	0.8501	C9—C10	1.381 (9)
O5—H5B	0.8500	C10—C11	1.359 (10)
O6—H6A	0.8500	C10—H10	0.9300
O6—H6B	0.8500	C11—C12	1.404 (10)
O7—H7A	0.8500	C11—H11	0.9300
O7—H7B	0.8500	C12—C13	1.384 (9)
S1—C1	1.760 (5)	C12—H12	0.9300
C1—C2	1.384 (7)	C13—H13	0.9300
O5—Co1—O5 ⁱ	180.0 (2)	C3—C2—H2	120.4
O5—Co1—O6	91.09 (15)	C1—C2—H2	120.4
O5 ⁱ —Co1—O6	88.91 (15)	C4—C3—C2	120.8 (6)
O5—Co1—O6 ⁱ	88.91 (15)	C4—C3—H3	119.6
O5 ⁱ —Co1—O6 ⁱ	91.09 (15)	C2—C3—H3	119.6

O6—Co1—O6 ⁱ	180.0 (2)	C3—C4—C5	120.2 (6)
O5—Co1—O7 ⁱ	89.69 (15)	C3—C4—N1	117.4 (6)
O5 ⁱ —Co1—O7 ⁱ	90.31 (15)	C5—C4—N1	122.4 (6)
O6—Co1—O7 ⁱ	88.81 (17)	C4—C5—C6	119.9 (6)
O6 ⁱ —Co1—O7 ⁱ	91.19 (17)	C4—C5—H5	120.0
O5—Co1—O7	90.31 (15)	C6—C5—H5	120.0
O5 ⁱ —Co1—O7	89.69 (15)	C5—C6—C1	119.3 (5)
O6—Co1—O7	91.19 (17)	C5—C6—H6	120.3
O6 ⁱ —Co1—O7	88.81 (17)	C1—C6—H6	120.3
O7 ⁱ —Co1—O7	180.0 (3)	N1—C7—C8	121.8 (6)
C7—N1—C4	121.1 (6)	N1—C7—H7	119.1
C9—O4—H4	109.5	C8—C7—H7	119.1
Co1—O5—H5A	112.8	C13—C8—C9	119.2 (6)
Co1—O5—H5B	112.9	C13—C8—C7	119.7 (6)
H5A—O5—H5B	110.4	C9—C8—C7	121.1 (6)
Co1—O6—H6A	112.5	O4—C9—C10	119.2 (7)
Co1—O6—H6B	112.4	O4—C9—C8	121.6 (6)
H6A—O6—H6B	110.2	C10—C9—C8	119.2 (7)
Co1—O7—H7A	112.2	C11—C10—C9	121.5 (7)
Co1—O7—H7B	112.2	C11—C10—H10	119.3
H7A—O7—H7B	110.0	C9—C10—H10	119.3
O2—S1—O3	111.6 (2)	C10—C11—C12	120.5 (7)
O2—S1—O1	112.6 (2)	C10—C11—H11	119.7
O3—S1—O1	112.7 (2)	C12—C11—H11	119.7
O2—S1—C1	106.7 (2)	C13—C12—C11	118.2 (8)
O3—S1—C1	106.6 (2)	C13—C12—H12	120.9
O1—S1—C1	106.1 (2)	C11—C12—H12	120.9
C2—C1—C6	120.5 (5)	C12—C13—C8	121.3 (7)
C2—C1—S1	119.1 (4)	C12—C13—H13	119.3
C6—C1—S1	120.4 (4)	C8—C13—H13	119.3
C3—C2—C1	119.3 (5)		
O2—S1—C1—C2	-77.9 (5)	C2—C1—C6—C5	0.4 (9)
O3—S1—C1—C2	162.7 (4)	S1—C1—C6—C5	-178.0 (5)
O1—S1—C1—C2	42.4 (5)	C4—N1—C7—C8	-177.6 (6)
O2—S1—C1—C6	100.5 (5)	N1—C7—C8—C13	179.6 (7)
O3—S1—C1—C6	-18.9 (5)	N1—C7—C8—C9	1.8 (11)
O1—S1—C1—C6	-139.2 (5)	C13—C8—C9—O4	178.6 (6)
C6—C1—C2—C3	-0.7 (9)	C7—C8—C9—O4	-3.6 (11)
S1—C1—C2—C3	177.7 (5)	C13—C8—C9—C10	-0.7 (10)
C1—C2—C3—C4	1.2 (10)	C7—C8—C9—C10	177.1 (6)
C2—C3—C4—C5	-1.3 (11)	O4—C9—C10—C11	-178.9 (7)
C2—C3—C4—N1	-178.6 (6)	C8—C9—C10—C11	0.4 (11)
C7—N1—C4—C3	-150.6 (7)	C9—C10—C11—C12	1.1 (11)
C7—N1—C4—C5	32.2 (10)	C10—C11—C12—C13	-2.2 (11)
C3—C4—C5—C6	0.9 (11)	C11—C12—C13—C8	2.0 (11)
N1—C4—C5—C6	178.2 (6)	C9—C8—C13—C12	-0.5 (11)
C4—C5—C6—C1	-0.5 (10)	C7—C8—C13—C12	-178.3 (7)

supplementary materials

Symmetry codes: (i) $-x+2, -y, -z$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4 \cdots N1	0.82	1.88	2.588 (7)	143
O5—H5A \cdots O2 ⁱⁱ	0.85	1.96	2.736 (6)	151
O5—H5B \cdots O1	0.85	1.97	2.744 (6)	151
O6—H6A \cdots O1 ⁱⁱⁱ	0.85	1.99	2.757 (5)	150
O6—H6B \cdots O3	0.85	2.03	2.768 (5)	144
O7—H7A \cdots O3 ⁱⁱ	0.85	1.96	2.759 (5)	157
O7—H7B \cdots O2 ^{iv}	0.85	1.98	2.761 (5)	152
C6—H6 \cdots O3	0.93	2.56	2.918 (7)	104

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

Fig. 1

