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4,4′-Bipyridinium hexaaquacobalt(II) disulfate

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The title compound, $(C_{10}H_{10}N_2)[Co(H_2O)_6](SO_4)_2$, consists of 4,4′-bipyridinium dications, hexaaquacobalt(II) cations and sulfate anions that are linked by hydrogen bonds into a network structure. Six water molecules are coordinated to the Co atom and the geometry is octahedral. The bipyridinium cation has site symmetry 2 and the Co atom lies on a position of site symmetry 2/*m*.

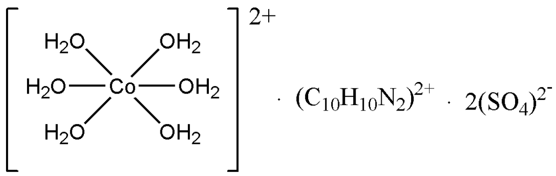
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.090
Data-to-parameter ratio = 11.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

4,4′-Bipyridine acts as a bridging ligand in metal complexes (Tong *et al.*, 2000), as a host molecule in inclusion compounds (Lu *et al.*, 2001), and as a proton acceptor in charge-transfer complexes (Zhu, 2003). The heterocycle is, however, not involved in such interactions but is protonated in the title compound, (I), which consists of the diprotonated 4,4′-bipyridinium cation (which has site symmetry 2), $[Co(H_2O)_6]^{2+}$ cations and sulfate anions. The Co atom lies on a position of site symmetry 2/*m* and its geometry is octahedral, arising from coordination by six water molecules (Fig. 1). The dications and anions interact through hydrogen bonds (Fig. 2) to generate a three-dimensional network.



(I)

Experimental

Cobalt sulfate heptahydrate (0.06 g, 0.2 mmol) was dissolved in water (10 ml) and the solution was mixed with a dimethylformamide solution (10 ml) of sodium 5-sulfoisophthalate (0.11 g, 0.4 mmol) and 4,4′-bipyridine (0.03 g, 0.2 mmol). The reaction mixture was filtered; pink plate-shaped crystals separated from the solution after about three months.

Crystal data

$(C_{10}H_{10}N_2)[Co(H_2O)_6](SO_4)_2$
M_r = 517.35
Monoclinic, *C*2/*m*
a = 11.9210 (11) Å
b = 6.6042 (6) Å
c = 12.9122 (12) Å
β = 108.951 (1)°
V = 961.46 (15) Å^3
Z = 2

D_x = 1.787 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 937 reflections
θ = 2.6–21.4°
μ = 1.19 mm^{-1}
T = 298 (2) K
Plate, pink
0.26 × 0.22 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.74$, $T_{\max} = 0.94$
2551 measured reflections
937 independent reflections
905 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\max} = 25.1°$
$h = -14 \rightarrow 14$
$k = -7 \rightarrow 7$
$l = -15 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.090$
$S = 1.19$
937 reflections
85 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 1.0311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.30$ e Å^{-3}
$\Delta\rho_{\min} = -0.57$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O1	2.0695 (18)	Co1—O2	2.078 (2)
O1$^{\rm i}$—Co1—O1$^{\rm ii}$	180	O1—Co1—O2	86.80 (8)
O1$^{\rm i}$—Co1—O1	91.99 (12)	O1$^{\rm ii}$—Co1—O2	93.20 (8)
O1$^{\rm ii}$—Co1—O1	88.01 (12)	O2—Co1—O2$^{\rm iii}$	180

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1N$\cdots$O4	0.86	1.79	2.634 (3)	166
N1—H1N$\cdots$O4	0.86	1.79	2.634 (3)	166
O2—H2$A\cdots$O3$^{\rm iv}$	0.82	1.98	2.759 (2)	158
O1—H1$A\cdots$O5$^{\rm v}$	0.82	1.97	2.750 (2)	159
O1—H1$B\cdots$O3	0.82	1.95	2.741 (2)	161
N1—H1N$\cdots$O4	0.86	1.79	2.634 (3)	166

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

The water H atoms were refined subject to the restraint O—H = 0.82 (1) Å. The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.86 (N—H) and 0.93 Å (C—H), with $U_{\rm iso} = 1.2U_{\rm eq}$(C,N).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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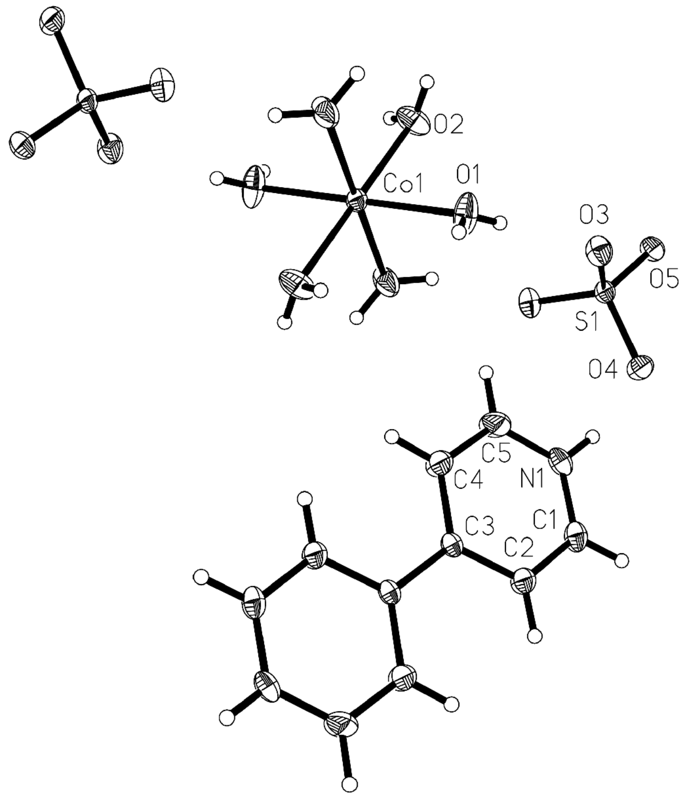

Figure 1
The structure of (I), with the atom numbering, showing displacement ellipsoids at the 50% probability level.

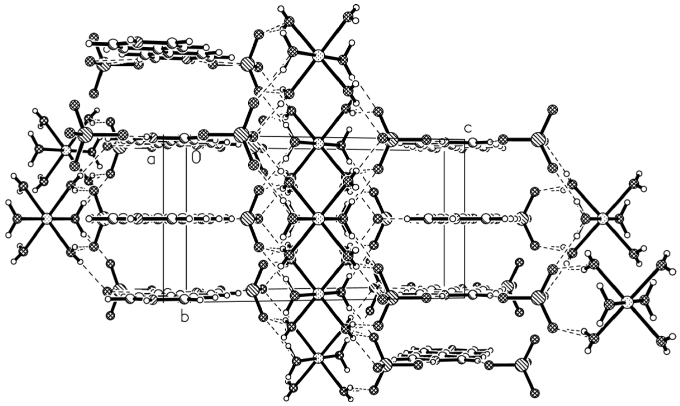

Figure 2
The three-dimensional network formed by hydrogen-bonding interactions in (I), which are shown as dashed lines.

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