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Hexaaquacobalt(II) bis[(4-nitrophenylsulfanyl)-acetate]

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In the title compound, $[Co(H_2O)_6](C_8H_6NO_4S)_2$, the Co^{II} atom lies on a centre of inversion and is six-coordinate in an octahedral environment. Cations and anions are linked by O—H···O hydrogen bonds into a three-dimensional network.

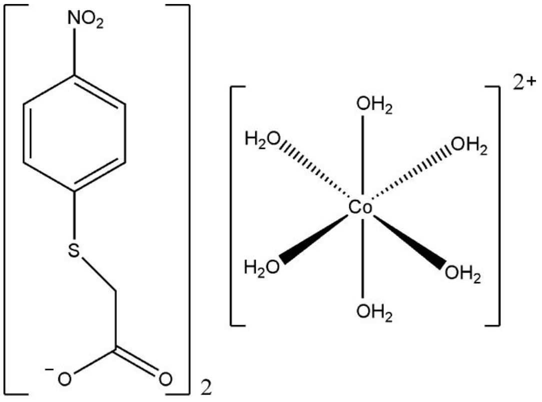
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.027
wR factor = 0.092
Data-to-parameter ratio = 16.9

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

Comment

Recently, we reported a complex of (4-nitrophenylsulfanyl)acetate with hexaaquanickel(II) (Gao *et al.*, 2006). We report here a related complex, (I), synthesized by reaction of (4-nitrophenylsulfanyl)acetic acid and cobalt(II) dinitrate hexahydrate in aqueous solution.



(I)

In (I), the Co^{II} atom lies on a centre of inversion and is coordinated by six water molecules in an octahedral geometry (Fig. 1). The (4-nitrophenylsulfanyl)acetate anion is close to planar, the largest deviation being 0.396 (2) Å for atom O2. This reflects a twist of the acetate group from the molecular plane [torsion angle S1/C7/C8/O1 = 24.1 (1)°].

The structure of compound (I) is similar to its Ni^{II} analogue (Gao *et al.*, 2006), but the two are not isostructural. In (I), the anions adopt a parallel arrangement, and cations and anions are linked through O—H···O hydrogen bonds (Table 1) to form a three-dimensional network.

Experimental

(4-Nitrophenylsulfanyl)acetic acid was prepared by nucleophilic reaction of chloroacetic acid and 4-nitrothiophenol under basic conditions (Nobles & Thompson, 1965). Cobalt(II) dinitrate hexahydrate (0.582 g, 2 mmol) and (4-nitrophenylsulfanyl)acetic acid (0.394 g, 2 mmol) were dissolved in hot water (10 ml) and the pH was adjusted to 6 with 0.01M sodium hydroxide. Brown crystals separated from the filtered solution after several days.

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Crystal data

$[Co(H_2O)_6](C_8H_6NO_4S)_2$
$M_r = 591.42$
Triclinic, $P\overline{1}$
$a = 7.164$ (6) Å
$b = 7.639$ (5) Å
$c = 12.011$ (8) Å
$\alpha = 102.07$ (2)°
$\beta = 102.23$ (3)°
$\gamma = 105.32$ (3)°
$V = 594.6$ (8) Å^3
$Z = 1$
$D_x = 1.652$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.97$ mm^{-1}
$T = 291$ (2) K
Block, brown
0.24 × 0.22 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.803$, $T_{max} = 0.903$
5922 measured reflections
2700 independent reflections
2379 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.092$
$S = 0.98$
2700 reflections
160 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.4155P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O5—H7$\cdots$O2^{ii}	0.84	1.89	2.720 (3)	169
O5—H8$\cdots$O2	0.84	1.93	2.749 (3)	164
O6—H9$\cdots$O1^{iii}	0.85	1.98	2.813 (3)	165
O6—H10$\cdots$O1	0.86	1.96	2.802 (3)	165
O7—H11$\cdots$O1^{iv}	0.85	1.93	2.773 (3)	170
O7—H12$\cdots$O3^{v}	0.84	2.27	3.053 (3)	155

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

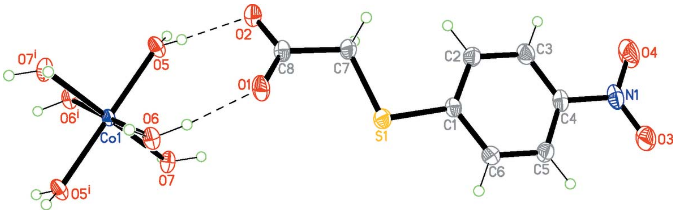

Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level for non-H atoms. Dashed lines indicate O—H$\cdots$O hydrogen bonds. [Symmetry code: (i) $-x, 1-y, -z$.]

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C) or 0.97 Å (methylene C), and with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of the water molecules were located in difference Fourier maps and their positions were refined with the restraints O—H = 0.85 (1) Å and H$\cdots$H = 1.39 (1) Å applied. In the final cycles of refinement, these H atoms were constrained to ride on their parent O atoms, with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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