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# *cis*-Acetato(diethylenetriamine)bis(5,5-diphenylhydantoinato-$\kappa N^3$)cobalt(III)

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**Key indicators**

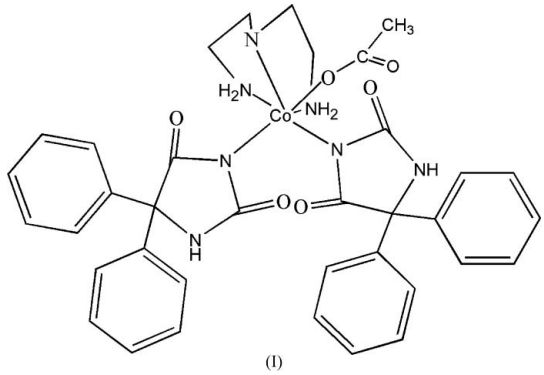
Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.007 Å
$R$ factor = 0.050
$wR$ factor = 0.122
Data-to-parameter ratio = 13.4

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

In the title compound, $[Co(C_{15}H_{11}N_2O_2)_2(C_2H_4O_2(C_4H_{12}N_3)]$, the $Co^{III}$ atom exhibits a distorted octahedral coordination geometry. There are intermolecular N—H···O hydrogen bonds, forming a three-dimensional network.

## Comment

As part of an ongoing investigation of transition metal complexes, we have recently synthesized a series of copper(II) (Hu, Xu, Wang & Xu, 2006; Hu *et al.*, 2006*a*; Hu, Xu, Liu *et al.*, 2006) and cobalt(II) (Hu *et al.*, 2006*b*) complexes with 5,5-diphenylimidazoline-2,4-dione (phenytoin, PHT). In this paper, we report the crystal structure of the title compound, (I).




(I)

The cobalt(III) metal centre is coordinated in a distorted octahedral geometry (Fig. 1) by two N atoms of two PHT anions, one O atom of an acetate anion and three N atoms of a *mer*-arranged diethylenetriamine ligand. The dihedral angles formed by the hydantoin ring N1/C1/N2/C2/C3 with phenyl rings C4–C9 and C10–C15 of the PHT ligand are 71.66 (17) and 82.37 (13)°, respectively; the dihedral angles between the hydantoin ring N3/C16/N4/C17/C18 and phenyl rings C19–C24 and C25–C30 are 66.87 (15) and 79.93 (16)°, respectively. In the crystal structure, there are intra- and intermolecular N—H···O hydrogen bonds (Table 1), forming a three-dimensional network.

## Experimental

Cobalt(II) was oxidized by oxygen in the air during the synthesis. To a solution of 5,5-diphenylhydantoin (1.00 mmol) in methanol (10 ml) was added cobalt(II) acetate tetrahydrate (0.5 mmol) and a solution of diethylenetriamine (1 mmol) in methanol (10 ml). The mixture was sealed in a 25 ml stainless steel vessel with a Teflon liner and heated to 393 K for 50 h. After cooling to room temperature, red single crystals were obtained by slow evaporation of the filtrate (m.p. 528 K).

*Crystal data*

| | |
|---|---|
| $[Co(C_{15}H_{11}N_2O_2)_2(C_2H_4O_2)(C_4H_{12}N_3)]$ | $V$ = 6871.3 (9) Å$^3$ |
| $M_r$ = 723.66 | $Z$ = 8 |
| Monoclinic, $C2/c$ | $D_x$ = 1.399 Mg m$^{-3}$ |
| $a$ = 24.389 (3) Å | Mo $K\alpha$ radiation |
| $b$ = 12.6330 (2) Å | $\mu$ = 0.56 mm$^{-1}$ |
| $c$ = 24.6320 (3) Å | $T$ = 298 (2) K |
| $\beta$ = 115.123 (2)° | Block, red |
| | 0.28 × 0.20 × 0.13 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 17534 measured reflections |
| $\varphi$ and $\omega$ scans | 6062 independent reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 3621 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.860, $T_{max}$ = 0.931 | $R_{int}$ = 0.064 |
| | $\theta_{max}$ = 25.0° |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 15.0091P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.050 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $wR(F^2)$ = 0.122 | $\Delta\rho_{max}$ = 0.45 e Å$^{-3}$ |
| $S$ = 1.05 | $\Delta\rho_{min}$ = −0.39 e Å$^{-3}$ |
| 6062 reflections | |
| 451 parameters | |
| H-atom parameters constrained | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.86 | 2.33 | 3.062 (4) | 144 |
| N3—H3···O3$^{ii}$ | 0.86 | 2.05 | 2.865 (4) | 158 |
| N5—H5*A*···O2 | 0.90 | 1.97 | 2.758 (4) | 145 |
| N5—H5*B*···O4 | 0.90 | 2.44 | 2.889 (4) | 111 |
| N6—H6···O1 | 0.91 | 2.45 | 3.111 (4) | 130 |
| N7—H7*A*···O6 | 0.90 | 2.04 | 2.789 (5) | 139 |
| N7—H7*B*···O3 | 0.90 | 2.19 | 2.768 (4) | 122 |

Symmetry codes: (i) $-x+\frac{3}{2}, -y+\frac{5}{2}, -z+1$; (ii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$.

All H atoms were positioned geometrically calculated position and refined using a riding model, with C—H = 0.93–0.97 Å, N—H = 0.86–0.91 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C,N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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*); software used to prepare material for publication: *SHELXTL*.

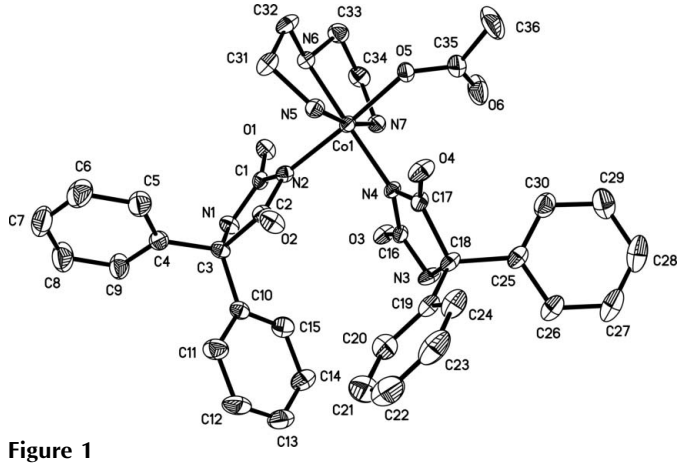



**Figure 1**
The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted.

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