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(μ-*p*-Phenylenediaminetetraacetato)bis[aqua-(2,2′-bipyridine)cobalt(II)] tetrahydrate

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In the crystal structure of the title compound, $[Co_2(C_{14}H_{12}N_2O_8)(C_{10}H_8N_2)_2(H_2O)_2]\cdot 4H_2O$, *p*-phenylenediaminetetraacetate (PhDTA) is located across an inversion center and bridges two Co^{II} atoms to form the dinuclear molecule. The Co^{II} atom has a distorted octahedral coordination geometry. Extensive intermolecular hydrogen bonding helps to stabilize the crystal structure.

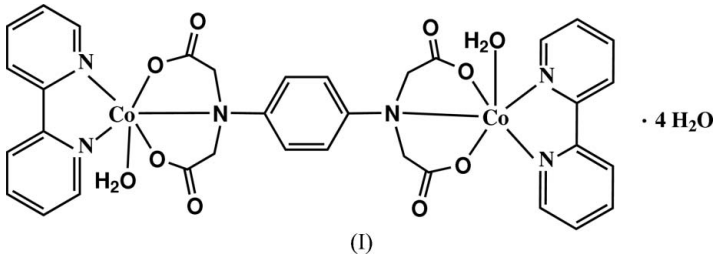
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.031
wR factor = 0.078
Data-to-parameter ratio = 11.5

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

Comment

p-Phenylenediaminetetraacetic acid (H_4PhDTA) is structurally similar to edta and plays a multidentate ligand role in metal complexes. In contrast to the flexible edta, there is a rigid aromatic ring in the PhDTA molecule. Thus, it may show different behavior in complex formation. We report here the structure of the title complex, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. PhDTA is located across an inversion center and bridges two Co^{II} atoms to form a dinuclear complex. The Co^{II} atom has a distorted octahedral coordination geometry. The Co1—N1 bond distance is much longer than Co1—N2 and Co1—N3 distances (Table 1).

Extensive intermolecular hydrogen bonding occurs (Table 2), which helps to stabilize the crystal structure.

Experimental

H_4PhDTA was prepared according to the literature procedure (Gonzalez *et al.*, 1997). H_4PhDTA (0.3 mmol) and 2,2-bipyridine (0.3 mmol) were dissolved in an aqueous solution (20 ml) of $Co(NO_3)_2$ (0.3 mmol). The solution was adjusted with an aqueous solution of NaOH to pH 5 and then refluxed for 1 h and filtered. Single crystals of (I) were obtained from the filtrate after 5 d.

Crystal data

$[Co_2(C_{14}H_{12}N_2O_8)(C_{10}H_8N_2)_2(H_2O)_2]\cdot 4H_2O$
M_r = 874.58
Triclinic, $P\overline{1}$
a = 9.8813 (9) Å
b = 9.9042 (9) Å
c = 10.824 (1) Å
α = 66.108 (2)°
β = 75.257 (2)°
γ = 86.508 (2)°
V = 935.59 (15) Å^3
Z = 1
D_x = 1.552 Mg m^{-3}
Mo *Kα* radiation
μ = 0.96 mm^{-1}
T = 295 (2) K
Block, red
0.26 × 0.22 × 0.20 mm

Data collection

Bruker APEX area-dectector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.737, T_{max} = 0.820
6768 measured reflections
3278 independent reflections
2976 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.078
S = 1.06
3278 reflections
285 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.2519P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N1	2.2828 (17)	Co1—O1	2.0366 (15)
Co1—N2	2.1345 (17)	Co1—O4	2.0642 (14)
Co1—N3	2.1268 (17)	Co1—O5*W*	2.0752 (16)
O1—Co1—O4	97.82 (6)	O5*W*—Co1—N2	89.20 (7)
O1—Co1—O5*W*	91.47 (6)	N3—Co1—N2	76.44 (7)
O4—Co1—O5*W*	95.18 (6)	O1—Co1—N1	78.75 (6)
O1—Co1—N3	165.84 (6)	O4—Co1—N1	75.90 (6)
O4—Co1—N3	93.84 (6)	O5*W*—Co1—N1	165.56 (6)
O5*W*—Co1—N3	95.47 (7)	N3—Co1—N1	96.44 (6)
O1—Co1—N2	91.37 (6)	N2—Co1—N1	101.52 (6)
O4—Co1—N2	169.70 (6)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O5*W*—H5*WA*···O6^{i}	0.84 (3)	2.06 (3)	2.879 (4)	166 (3)
O5*W*—H5*WB*···O4^{ii}	0.85 (2)	1.87 (2)	2.699 (2)	165 (3)
O6—H6*WA*···O7^{iii}	0.84 (2)	1.88 (3)	2.701 (3)	165 (3)
O6—H6*WB*···O2^{iv}	0.85 (2)	2.07 (2)	2.862 (3)	155 (3)
O7—H7*WA*···O1^{v}	0.84 (2)	2.06 (2)	2.871 (3)	161 (3)
O7—H7*WB*···O3^{vi}	0.83 (3)	1.93 (3)	2.757 (3)	172 (3)

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+2, -y+2, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+2, -y+1, -z+1$; (v) $-x+1, -y+2, -z+1$; (vi) $x-1, y, z-1$.

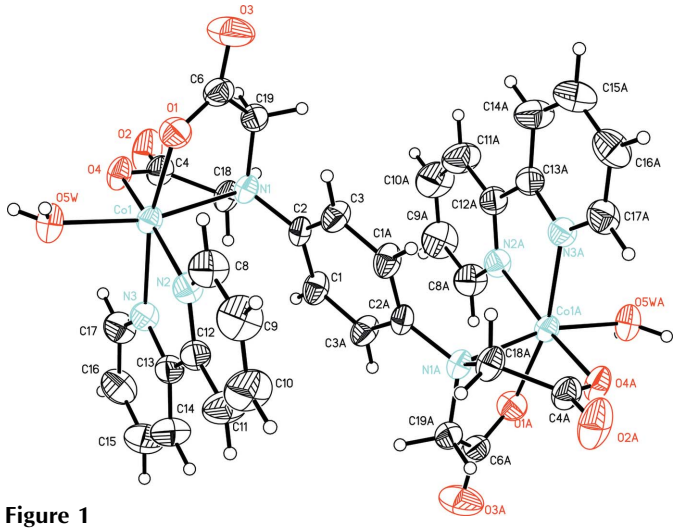


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry code: (A) $1-x$, $1-y$, $2-z$]. The uncoordinated water molecules have been omitted.

H atoms of water molecules were located in a difference Fourier map and refined isotropically. Other H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 Å (methylene), and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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