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Di-μ_2-acetato-tetrakis(4-aminopyridine)-diaquabis(μ_3-biphenyl-2,2′-dicarboxylato)-tricobalt(II) *N*,*N*′-dimethylformamide tetrasolvate

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The title complex, $[Co_3(C_2H_3O_2)_2(C_{14}H_8O_4)_2(C_5H_6N_2)_4(H_2O)_2]\cdot 4C_3H_7NO$, is a linear trinuclear cobalt complex crystallizing with the central Co atom on a centre of symmetry and with with four dimethylformamide solvent molecules per complex. The crystal packing is stabilized by N—H···O and O—H···O hydrogen bonds.

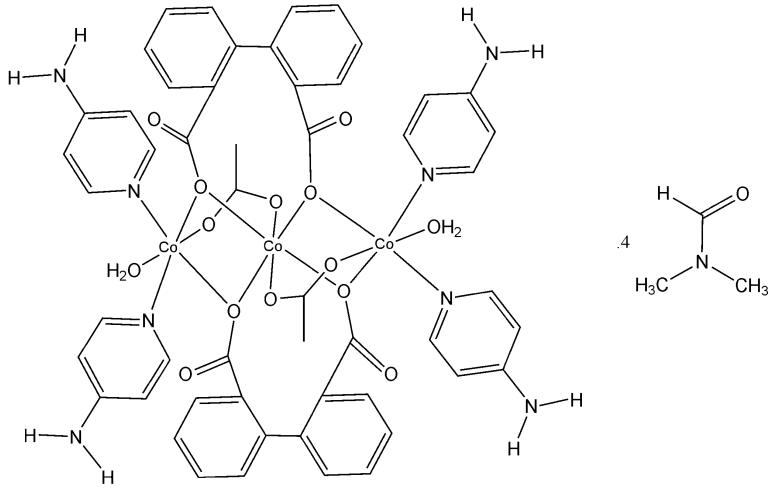
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.063
wR factor = 0.158
Data-to-parameter ratio = 13.8

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

Comment

Linear tricobalt complexes have been investigated extensively because of their potential application in molecular wires, as magnetic materials and as catalysts (Clerac *et al.*, 2000).



(I)

In the title complex, (I) (Fig. 1), the outer Co atoms are six-coordinate in a slightly distorted octahedral mode. Whereas the central Co atom is bonded to six O atoms, the terminal two Co atoms are each bonded to four O and two N atoms. The Co1···Co2 distance is 3.2141 (7) Å, which is slightly shorter than in the complex $[Co_3(C_{18}H_{18}N_2O_2)_2(C_2H_3O_2)_2]$ (You *et al.*, 2004). The crystal packing is stabilized by N—H···O and O—H···O hydrogen bonds (Table 1).

Experimental

When a mixture of $Co(CH_3COO)_2\cdot 2H_2O$ (0.0754 g, 0.032 mmol), diphenic acid (0.0772 g, 0.032 mmol) and 4-aminopyridine (0.0570 g, 0.060 mmol) was dissolved in CH_3OH (10 ml) and dimethylformamide (10 ml), a red solution was obtained, which was set aside at room temperature and allowed to evaporate slowly. After 10 d, pink block-shaped crystals were collected by filtration. Analysis calculated for $C_{64}H_{78}Co_3N_{12}O_{18}$: C 51.93, H 5.31, N 11.36%; found: C 51.98, H 5.36, N 11.41%.

Crystal data

$[Co_3(C_2H_3O_2)_2(C_{14}H_8O_4)_2(C_5H_6N_2)_4(H_2O)_2]\cdot 4C_3H_7NO$
M_r = 1480.17
Monoclinic, $P2_1/c$
a = 12.2379 (17) Å
b = 11.1660 (15) Å
c = 25.985 (4) Å
β = 96.571 (2)°
V = 3527.5 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 293 (2) K
0.11 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.920, T_{max} = 0.927
24864 measured reflections
6218 independent reflections
3850 reflections with $I > 2\sigma(I)$
R_{int} = 0.100

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.158
S = 1.02
6218 reflections
452 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O8	0.86	2.15	2.966 (8)	157
N2—H2B···O9	0.86	2.03	2.832 (7)	155
N4—H4A···O7^{i}	0.86	2.10	2.944 (6)	164
N4—H4B···O9^{ii}	0.86	2.13	2.983 (7)	170
O7—H7A···O2^{iii}	0.85 (4)	1.80 (4)	2.627 (5)	164 (4)
O7—H7B···O3	0.85 (2)	1.75 (2)	2.605 (6)	175 (4)

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

H atoms bonded to C and N were positioned geometrically and refined using a riding model, with aromatic C—H = 0.93 Å, methyl C—H = 0.96 Å and N—H = 0.86 Å. U_{iso}(H) values were set at $1.2U_{eq}$(C,N) or $1.5U_{eq}$(methyl C). The methyl groups were allowed to rotate but not to tip. Water H atoms were found in a difference Fourier map and refined with an O—H distance restraint of 0.89 (2) Å and with free U_{iso}(H) values.

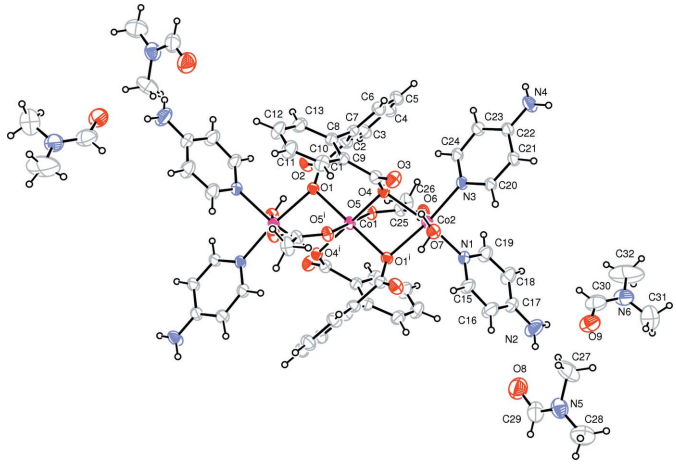


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. [Symmetry code: (i) $-x, 2-y, 2-z$.]

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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