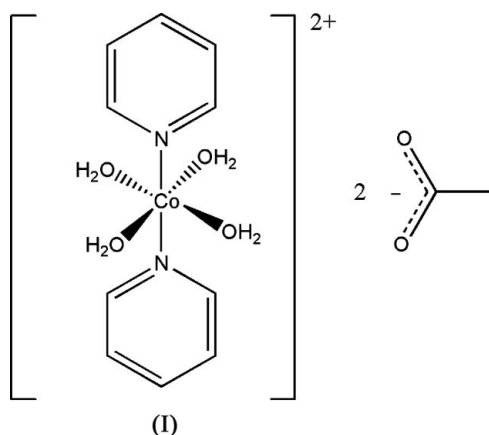


Tetraaquabis(pyridine- $\kappa$ N)cobalt(II) diacetateJack K. Clegg,<sup>a\*</sup> Michael J. Hayter,<sup>a</sup> Katrina A. Jolliffe<sup>b</sup> and Leonard F. Lindoy<sup>a</sup><sup>a</sup>Centre for Heavy Metals Research, School of Chemistry, F11, The University of Sydney, NSW, 2006, Australia, and <sup>b</sup>School of Chemistry, F11, The University of Sydney, NSW, 2006, AustraliaCorrespondence e-mail:  
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## Key indicators

Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
Disorder in solvent or counterion  
 $R$  factor = 0.023  
 $wR$  factor = 0.065  
Data-to-parameter ratio = 16.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.In the title complex,  $[\text{Co}(\text{C}_5\text{H}_5\text{N})_2(\text{H}_2\text{O})_4](\text{C}_2\text{H}_3\text{O}_2)_2$ , the octahedral cation is hydrogen bonded to the acetate anions *via* the coordinated water molecules. The cation and anions lie on a crystallographic mirror plane.Received 16 March 2006  
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## Comment

Our group has long been interested in the use of metal complexes as components for the construction of larger supramolecular architectures (Lindoy & Atkinson, 2000). In particular, we are interested in the behaviour of metallo-systems containing both N and O donor ligands (Clegg *et al.*, 2004, 2005, 2006). The title complex, (I), was obtained for use as a suitable precursor in such studies.As expected, the coordination geometry for the  $\text{Co}^{\text{II}}$  cation (Fig. 1) is close to the ideal octahedral (Table 1), with the O atoms of the coordinated water molecules occupying the equatorial positions and with the axial sites occupied by coordinated pyridine ligands. A mirror plane passes through Co, N1, N2, C1, H1, C6 and H6, and a second mirror plane passes through C7, C8, C9 and C10. The acetate anions are hydrogen bonded to the water ligands; see Table 2 for the geometric parameters describing these interactions.

## Experimental

The title complex was prepared from the stoichiometric addition of pyridine to an aqueous solution of hexaaquacobalt(II) acetate (2:1). Crystals suitable for the X-ray diffraction study were isolated from the resulting pink solution after several days of slow evaporation.

Crystal data

[Co(C<sub>5</sub>H<sub>5</sub>N)<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>](C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub>  
*M<sub>r</sub>* = 407.28  
 Monoclinic, *P*2<sub>1</sub>/*m*  
*a* = 8.3770 (13) Å  
*b* = 9.6030 (15) Å  
*c* = 11.6700 (18) Å  
 $\beta$  = 105.286 (2)°  
*V* = 905.6 (2) Å<sup>3</sup>  
*Z* = 2  
*D<sub>x</sub>* = 1.494 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 6128 reflections  
 $\theta$  = 2.5–28.2°  
 $\mu$  = 0.99 mm<sup>-1</sup>  
*T* = 150 (2) K  
 Prism, orange  
 0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART 1000 CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
*T<sub>min</sub>* = 0.668, *T<sub>max</sub>* = 0.820  
 8936 measured reflections  
 2304 independent reflections  
 2148 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.018  
 $\theta_{max}$  = 28.3°  
*h* = -11 → 11  
*k* = -12 → 12  
*l* = -15 → 14

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.023  
*wR* (*F*<sup>2</sup>) = 0.065  
*S* = 1.05  
 2304 reflections  
 141 parameters  
 H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.2088P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.41 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.20 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Co1—N1	2.1444 (13)	Co1—O1	2.0921 (8)
Co1—N2	2.1531 (13)	Co1—O2	2.0914 (8)
N1—Co1—N2	179.75 (4)	O2 <sup>ii</sup> —Co1—O1	90.03 (4)
O1—Co1—O1 <sup>ii</sup>	89.80 (5)	O2—Co1—O2 <sup>ii</sup>	90.13 (5)
O2—Co1—O1	179.80 (3)		

Symmetry code: (ii) *x*, -*y* +  $\frac{1}{2}$ , *z*.

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1O...O4 <sup>vi</sup>	0.83 (1)	1.96 (1)	2.7652 (12)	163 (1)
O1—H2O...O4 <sup>iii</sup>	0.88 (1)	1.79 (1)	2.6660 (12)	174 (2)
O2—H3O...O3 <sup>vii</sup>	0.85 (1)	1.88 (1)	2.7111 (12)	165 (1)
O2—H4O...O3 <sup>iv</sup>	0.87 (1)	1.83 (1)	2.6895 (12)	170 (1)

Symmetry codes: (iii) -*x* + 1, *y* -  $\frac{1}{2}$ , -*z* + 2; (iv) -*x* + 1, -*y* + 1, -*z* + 1; (vi) *x* + 1, -*y* +  $\frac{3}{2}$ , *z*; (vii) *x*, *y* - 1, *z*.

The C-bound H atoms were included in the riding-model approximation with aromatic and methyl C—H bond lengths fixed at 0.95 and 0.98 Å, respectively. Methyl H atoms were modelled in positions with idealized torsion angles from the electron density; they are disordered equally over 2 sites about the crystallographic mirror plane. The O-bound H atoms were located in a difference Fourier map and refined with bond-length restraints of 0.90 (2) Å. The *U*<sub>iso</sub>(H) values were fixed at 1.2*U*<sub>eq</sub> of the parent atoms.

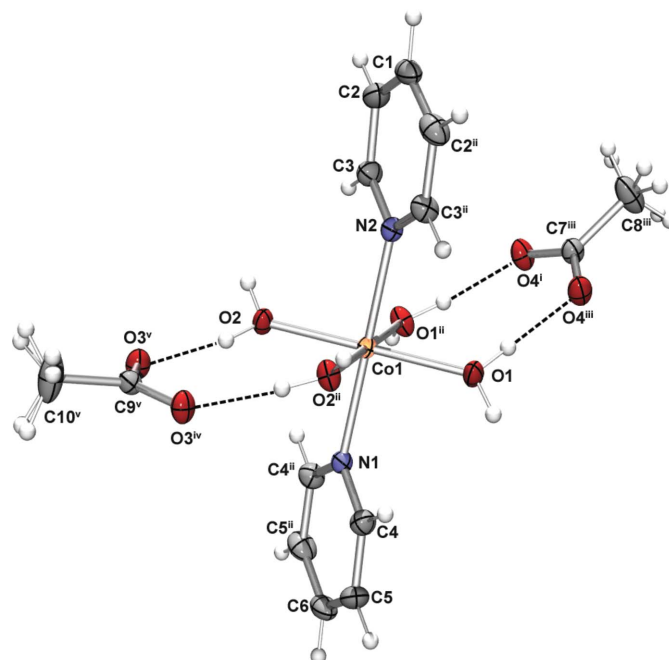


Figure 1

An ORTEP-3 (Farrugia, 1997) representation of (I), shown with 50% probability displacement ellipsoids. Hydrogen bonds are indicated with dashed lines. Methyl H atoms are equally disordered about the crystallographic mirror plane. [Symmetry codes: (i) 1 - *x*, 1 - *y*, 2 - *z*; (ii) *x*,  $\frac{1}{2}$  - *y*, *z*; (iii) 1 - *x*, - $\frac{1}{2}$  + *y*, 2 - *z*; (iv) 1 - *x*, 1 - *y*, 1 - *z*; (v) 1 - *x*, - $\frac{1}{2}$  + *y*, 1 - *z*.]

Data collection: SMART (Siemens, 1995); cell refinement: SAINT (Siemens, 1995); data reduction: SAINT and XPREP (Siemens, 1995); program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997) and WinGX32 (Farrugia, 1999); software used to prepare material for publication: enCIFer (Version 1.0; Allen *et al.*, 2004).

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