

Shi-Fan Wang,<sup>a</sup> Ban-Feng Ruan,<sup>a</sup>  
 Huang-Qiu Li,<sup>a</sup> Hai-Liang Zhu<sup>a</sup>  
 and Seik Weng Ng<sup>b\*</sup>

<sup>a</sup>Institute of Functional Biomolecules, State Key Laboratory of Pharmaceutical Biotechnology, Nanjing University, Nanjing 210093, People's Republic of China, and <sup>b</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

**Key indicators**

Single-crystal X-ray study  
 T = 295 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$   
 R factor = 0.062  
 wR factor = 0.148  
 Data-to-parameter ratio = 19.4

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

(5,5,7,12,12,14-Hexamethyl-1,4,8,11-tetraaza-cyclotetradecane-1,8-diacetato)cobalt(II) tetrahydrate

The Co atom in the title compound,  $[\text{Co}(\text{C}_{20}\text{H}_{38}\text{N}_4\text{O}_4)] \cdot 4\text{H}_2\text{O}$ , is chelated by the four N atoms of the macrocycle and also covalently bonded to two carboxylate O atoms in a *cis*- $\text{N}_4\text{O}_2\text{Co}$  octahedral environment. The mononuclear molecule interacts with the non-coordinated water molecules by way of  $\text{O}-\text{H} \cdots \text{O}$  interactions to form a three-dimensional network.

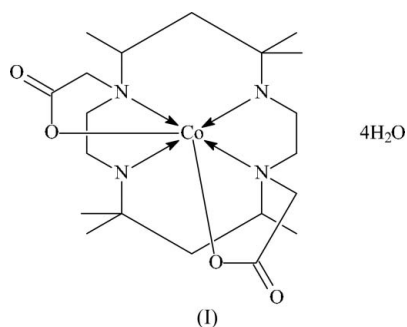
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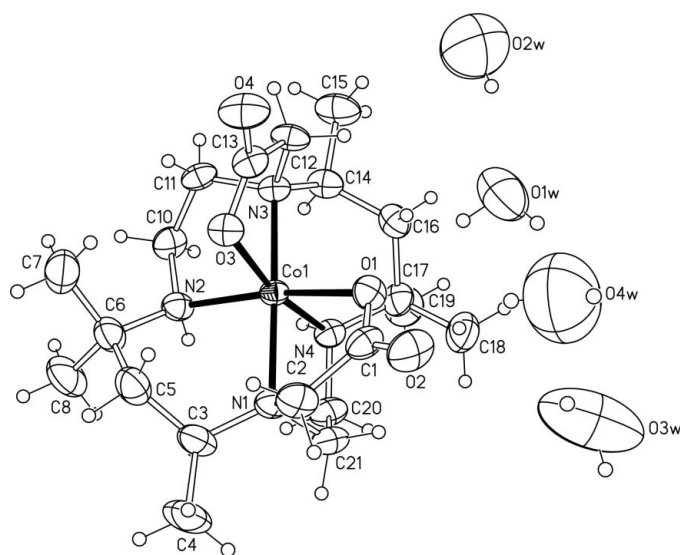
**Comment**

The title compound, (I) (Fig. 1), is isostructural with the nickel(II) derivative, which is described in the preceding report (Wang *et al.*, 2005). Selected geometrical data for (I) are listed in Tables 1 and 2.



**Experimental**

5,5,7,12,12,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane (0.28 g, 1 mmol) and ethyl bromoacetate (0.34 g, 2.05 mmol) were refluxed in



**Figure 1**  
 View of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

1 M aqueous sodium hydroxide for an hour. Hydrochloric acid (1 M) was added to give a pH of about 1, at which point cobalt sulfate hexahydrate (0.26 g, 1 mmol) was added to give a purple solution. Red prisms of (I) formed after several days. Chemical analysis found: C 45.3, H 8.5, N 10.5%; calculated: C 45.36, H 8.76, N 10.58%.

#### Crystal data

[Co(C <sub>20</sub> H <sub>38</sub> N <sub>4</sub> O <sub>4</sub> )]·4H <sub>2</sub> O	$D_x = 1.382 \text{ Mg m}^{-3}$
$M_r = 529.54$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 7719 reflections
$a = 9.1896 (6) \text{ \AA}$	$\theta = 2.4\text{--}28.3^\circ$
$b = 13.8731 (9) \text{ \AA}$	$\mu = 0.72 \text{ mm}^{-1}$
$c = 20.001 (1) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\beta = 93.641 (1)^\circ$	Prism, red
$V = 2544.7 (3) \text{ \AA}^3$	$0.28 \times 0.15 \times 0.15 \text{ mm}$
$Z = 4$	

#### Data collection

Bruker APEX CCD diffractometer	5057 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.039$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$\theta_{\text{max}} = 27.5^\circ$
$T_{\text{min}} = 0.673$ , $T_{\text{max}} = 0.899$	$h = -11 \rightarrow 11$
20921 measured reflections	$k = -17 \rightarrow 18$
5778 independent reflections	$l = -25 \rightarrow 25$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 3.0855P]$
$R[F^2 > 2\sigma(F^2)] = 0.062$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.149$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.18$	$\Delta\rho_{\text{max}} = 0.67 \text{ e \AA}^{-3}$
5778 reflections	$\Delta\rho_{\text{min}} = -0.68 \text{ e \AA}^{-3}$
298 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Co1—N1	2.104 (3)	Co1—N4	2.099 (3)
Co1—N2	2.105 (3)	Co1—O1	2.114 (2)
Co1—N3	2.088 (3)	Co1—O3	2.116 (2)
N1—Co1—N2	91.8 (1)	N2—Co1—O3	95.6 (1)
N1—Co1—N3	177.0 (1)	N3—Co1—N4	92.6 (1)
N1—Co1—N4	85.7 (1)	N3—Co1—O1	103.5 (1)
N1—Co1—O1	79.2 (1)	N3—Co1—O3	79.0 (1)
N1—Co1—O3	103.1 (1)	N4—Co1—O1	94.8 (1)
N2—Co1—N3	85.7 (1)	N4—Co1—O3	169.5 (1)
N2—Co1—N4	89.9 (1)	O1—Co1—O3	81.3 (1)
N2—Co1—O1	169.4 (1)		

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
N2—H2 $n$ ···O4 <sup>i</sup>	0.86	2.44	3.164 (4)	143
N4—H4 $n$ ···O4 <sup>i</sup>	0.86	2.22	2.993 (4)	150
O1 $w$ —H1 $w$ 1···O1	0.85	2.06	2.901 (4)	169
O1 $w$ —H1 $w$ 2···O4 $w$	0.85	2.30	2.95 (1)	133
O2 $w$ —H2 $w$ 1···O1 $w$	0.85	2.00	2.827 (8)	164
O2 $w$ —H2 $w$ 2···O3 $w$ <sup>ii</sup>	0.86	1.87	2.57 (1)	138
O3 $w$ —H3 $w$ 1···O4 <sup>iii</sup>	0.86	2.17	2.817 (7)	132
O3 $w$ —H3 $w$ 2···O4 $w$	0.88	1.75	2.40 (1)	128
O4 $w$ —H4 $w$ 2···O2	0.88	2.06	2.704 (9)	129

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

The carbon- and nitrogen-bound H atoms were positioned geometrically and refined as riding [C—H = 0.97  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for the methylene H atoms; C—H = 0.98  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for the methyl H atoms; N—H = 0.86  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ ]. The methyl groups were rotated to fit the electron density. The water H atoms were placed at chemically plausible positions on the basis of likely hydrogen bonds; this scheme has one water molecule forming only one hydrogen bond. All distances between H atoms exceed 2  $\text{\AA}$ .

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: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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