

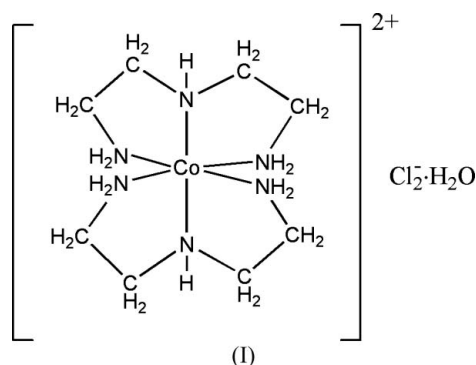
Hong-Juan Li, Li-Mei Sun and
Zhi-Hong Liu*School of Chemistry and Materials Science,
ShaanXi Normal University, Xi'an 710062,
People's Republic of China

Correspondence e-mail: liuzh@snnu.edu.cn

Key indicators

Single-crystal X-ray study
 $T = 298 \text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
 R factor = 0.035
 wR factor = 0.098
Data-to-parameter ratio = 16.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis(diethylenetriamine- κ^3N)cobalt(II) dichloride
monohydrateThe ions and water molecules of the title compound, $[\text{Co}(\text{C}_4\text{H}_{13}\text{N}_3)_2]\text{Cl}_2\cdot\text{H}_2\text{O}$, are held together through both electrostatic interactions and $\text{N}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds.Received 28 June 2006
Accepted 5 September 2006

Comment

The synthesis of new organic-inorganic hybrid compounds is a relatively new research area that has developed rapidly over the last several years owing to the structural diversity of these compounds associated with their potential applications in areas such as catalysis (Yu *et al.*, 2004), gas sorption and storage (Rosi *et al.*, 2003), pharmaceuticals (Caruso *et al.*, 1998), and emerging nanotechnologies (Julian *et al.*, 2004). Recently, our research interests have been focused on the synthesis of organic-inorganic hybrid borates templated by transition metal complexes. In the course of the research, we obtained an organic-inorganic hybrid compound, *viz.* (I).The structure of (I) consists of a discrete bis(diethylenetriamine- κ^3N)cobalt(II) dication, two Cl^- anions and a water molecule (Fig. 1). The Co atom is bonded to six N atoms from two diethylenetriamine ligands in a distorted octahedral geometry (Table 1). The cations, anions and water molecules are held together through both electrostatic interactions and $\text{N}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds (Table 2).

Experimental

A mixture of $\text{CoCl}_2\cdot 6\text{H}_2\text{O}$ (0.7145 g), $\text{KB}_5\text{O}_8\cdot 5\text{H}_2\text{O}$ (0.8437 g), diethylenetriamine (2 ml), pyridine (3.2 ml) and H_2O (0.5 ml) was sealed in a 40 ml Teflon-lined stainless steel vessel and heated at 463 K for about 7 d under autogenous pressure, then cooled to room temperature. The resulting emerald columnar crystals of (I) were collected and dried in air. Analysis calculated: C 27.10, H 7.90, N 23.71%; found: C 26.76, H 7.66, N 22.61%.

Crystal data

$[\text{Co}(\text{C}_4\text{H}_{13}\text{N}_3)_2]\text{Cl}_2 \cdot \text{H}_2\text{O}$
 $M_r = 354.19$
 Monoclinic, $P2_1/c$
 $a = 13.459$ (4) Å
 $b = 8.817$ (3) Å
 $c = 13.951$ (4) Å
 $\beta = 102.097$ (4)°
 $V = 1618.8$ (8) Å³

$Z = 4$
 $D_x = 1.453$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 1.39$ mm⁻¹
 $T = 298$ (2) K
 Block, amaranth
 $0.55 \times 0.52 \times 0.44$ mm

Data collection

Bruker SMART APEX area-
 detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 1999)
 $T_{\min} = 0.461$, $T_{\max} = 0.552$

8122 measured reflections
 2863 independent reflections
 2167 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.053$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.098$
 $S = 1.07$
 2863 reflections
 171 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.5627P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.48$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.35$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—N2	2.128 (3)	Co1—N3	2.193 (3)
Co1—N5	2.133 (3)	Co1—N6	2.199 (3)
Co1—N4	2.164 (3)	Co1—N1	2.215 (2)
N2—Co1—N5	176.58 (10)	N4—Co1—N6	159.25 (11)
N2—Co1—N4	97.69 (10)	N3—Co1—N6	90.09 (11)
N5—Co1—N4	80.29 (10)	N2—Co1—N1	80.11 (9)
N2—Co1—N3	79.96 (10)	N5—Co1—N1	102.61 (9)
N5—Co1—N3	97.57 (10)	N4—Co1—N1	90.84 (10)
N4—Co1—N3	98.50 (11)	N3—Co1—N1	158.94 (11)
N2—Co1—N6	102.41 (10)	N6—Co1—N1	87.59 (10)
N5—Co1—N6	79.87 (10)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H3 \cdots Cl1	0.83 (6)	2.38 (6)	3.186 (3)	164 (5)
O1—H1 \cdots Cl1 ⁱ	0.75 (4)	2.48 (4)	3.201 (4)	164 (4)
N6—H6B \cdots Cl2 ⁱⁱ	0.90	2.56	3.461 (3)	178
N6—H6A \cdots Cl2	0.90	2.45	3.341 (3)	172
N5—H5 \cdots Cl2 ⁱⁱⁱ	0.91	2.42	3.323 (3)	172
N4—H4B \cdots Cl1 ^{iv}	0.90	2.56	3.399 (3)	155
N4—H4A \cdots O1 ^v	0.90	2.38	3.189 (4)	150
N2—H2 \cdots Cl1	0.91	2.46	3.354 (3)	169

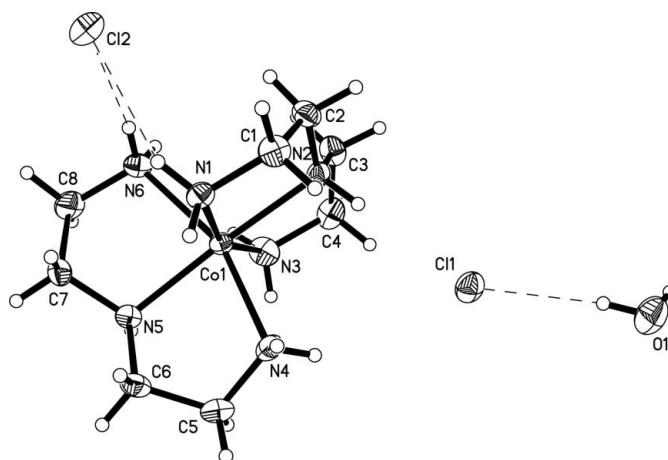


Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate hydrogen bonds.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1B \cdots Cl1 ^{iv}	0.90	2.58	3.411 (3)	154
N1—H1A \cdots Cl2	0.90	2.56	3.401 (3)	155

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

H atoms bonded to C and N atoms were positioned geometrically and refined as riding atoms, with C—H = 0.97 Å, N—H = 0.91 (NH) and 0.90 Å (NH₂), and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$. The H atoms bonded to O1 (water molecule) were located in a difference map and refined isotropically.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

Acknowledgement is expressed to the Postgraduate-innovated Foundation of ShaanXi Normal University.

References

- Bruker (1999). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2001). *SAINTE, SMART and SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Caruso, F., Caruso, R. A. & Mohwald, H. (1998). *Science*, **282**, 1111–1114.
 Julian, B., Corberan, R., Cordoncillo, E., Escribano, P., Viana, B. & Sanchez, C. (2004). *J. Mater. Chem.* **14**, 3337–3343.
 Rosi, N. L., Eckert, J., Eddaoudi, M., Vodak, D. T., Kim, J., O'Keeffe, M. & Yaghi, O. M. (2003). *Science*, **300**, 1127–1129.
 Sheldrick, G. M. (1997). *SHELXS97 and SHELXL97*. University of Göttingen, Germany.
 Yu, Z.-T., Liao, Z.-L., Jiang, Y.-S., Li, G.-H., Li, G.-D. & Chen, J.-S. (2004). *Chem. Commun.* pp. 1814–1815.