

Guo-Chen Dong* and
Rong-Chang ZhangDepartment of Chemistry, Beihua University,
Jilin City 132013, People's Republic of China

Correspondence e-mail: jlsgcd@126.com

Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.052
 wR factor = 0.139
Data-to-parameter ratio = 18.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[[μ_2 -1,1'-(butane-1,4-diyl)bis(imidazole)- $\kappa^2\text{N}^3:\text{N}^{3'}$]dichlorocobalt(II)]

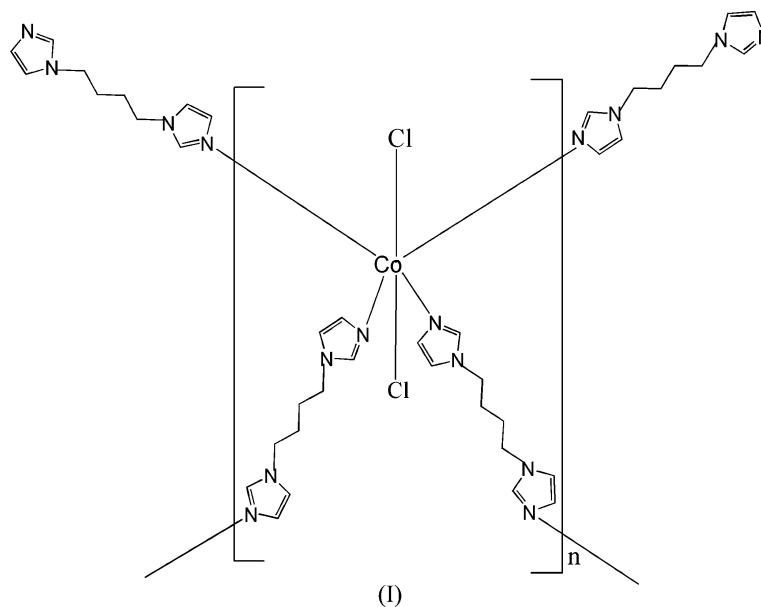
In the title compound, $[\text{CoCl}_2(\text{C}_{10}\text{H}_{14}\text{N}_4)_2]_n$ or $[\text{CoCl}_2(L)_2]_n$, where L is 1,1'-(1,4-butanediyl)bis(imidazole), the Co^{II} atom is located on a centre of inversion and is six-coordinated by four N atoms from four different L molecules and two Cl^- ions. The Co^{II} atoms are bridged by L molecules, generating a two-dimensional network.

Received 7 July 2006

Accepted 12 July 2006

Comment

The design and synthesis of coordination polymers with infinite two- and three-dimensional networks has been an area of rapid growth in recent years because of their potential applications (Eddaoudi *et al.*, 2001). 4,4'-Bipyridine is well known as a good candidate for rigid rod-like spacers in the construction of metal-organic polymers, and has shown hundreds of interesting supramolecular architectures (Batten & Robson, 1998). However, flexible ligands such as 1,1'-(1,4-butanediyl)bis(imidazole) (L) have not been well explored until now (Ma *et al.*, 2003). In this work, the assembly of L with a Co^{II} atom resulted in an interesting two-dimensional coordination polymer $[\text{CoCl}_2(L)_2]_n$.



In (I), each Co^{II} atom is located on a centre of inversion and is six-coordinated by four N atoms from four different L molecules, and two Cl^- ions, resulting in a slightly distorted octahedral geometry (Fig. 1). The $\text{Co}-\text{N}$ and $\text{Co}-\text{Cl}$ distances are normal (Table 1). The Co^{II} atoms are bridged by L molecules, generating a two-dimensional network (Fig. 2). The structure of (I) is entirely different from the related

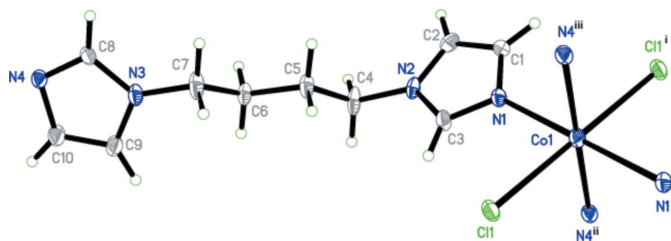


Figure 1
View of the local coordination of compound (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. [Symmetry codes: (i) $-x, -y, -z$; (ii) $1.5 + x, 1 - y, \frac{1}{2} + z$; (iii) $-1.5 - x, y - \frac{1}{2}, -z - \frac{1}{2}$]

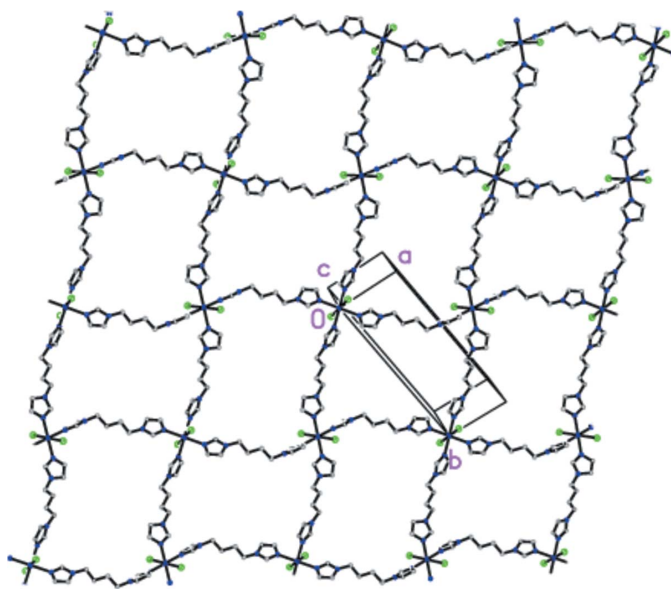


Figure 2
View of the two-dimensional (4,4)-network of (I).

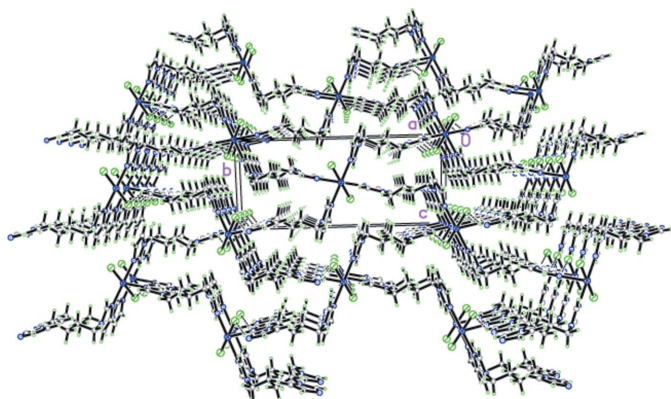


Figure 3
The packing of (I).

structure of $[\text{Ni}(\text{SCN})_2(\text{L})_2]$, for which a one-dimensional double-strand chain structure was described (Che *et al.*, 2006).

In addition, in compound (I) there are no supramolecular interactions such as hydrogen bonds or π - π interactions. A packing diagram of compound (I) is shown in Fig. 3.

Experimental

Ligand *L* was synthesized according to the literature (Ma *et al.*, 2000). Compound (I) was self-assembled by *L* and $\text{CoCl}_2 \cdot \text{H}_2\text{O}$. A methanol solution (12 ml) of *L* (0.5 mmol) was added slowly to an aqueous solution (15 ml) of $\text{CoCl}_2 \cdot \text{H}_2\text{O}$ (0.5 mmol) with stirring. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature for several days, yielding red crystals of (I) in 47% yield (based on Co).

Crystal data

$[\text{CoCl}_2(\text{C}_{10}\text{H}_{14}\text{N}_4)_2]$
 $M_r = 510.33$
Monoclinic, $P2_1/n$
 $a = 7.5731$ (15) Å
 $b = 18.615$ (4) Å
 $c = 8.6622$ (17) Å
 $\beta = 112.36$ (3)°
 $V = 1129.3$ (5) Å³

$Z = 2$
 $D_x = 1.501$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 1.02$ mm⁻¹
 $T = 292$ (2) K
Block, red
0.29 × 0.25 × 0.22 mm

Data collection

Rigaku R-Axis RAPID
diffractometer
 ω scans
Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)
 $T_{\text{min}} = 0.732, T_{\text{max}} = 0.791$

10911 measured reflections
2566 independent reflections
1920 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.056$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.139$
 $S = 1.06$
2566 reflections
142 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 1.1873P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.48$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.59$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—N1	2.260 (3)	Co1—N4 ^I	2.274 (3)
Co1—Cl1	2.5824 (10)		
N1 ^{III} —Co1—N4 ^I	89.82 (10)	N1—Co1—Cl1	88.83 (7)
N1 ^{III} —Co1—N4 ^{II}	90.18 (10)	N4 ^I —Co1—Cl1	90.28 (7)
N1 ^{III} —Co1—Cl1	91.17 (7)	N4 ^{II} —Co1—Cl1	89.72 (7)

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

All H atoms were positioned geometrically and refined as riding atoms, with aromatic C—H = 0.93 Å, methylene C—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The authors thank Beihua University for supporting this work.

References

- Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed.* **37**, 1460–1494.
Che, G.-B., Liu, H., Liu, C.-B. & Liu, B. (2006). *Acta Cryst.* **E62**, m286–m288.
Eddaoudi, E., Moler, D. B., Li, H., Chen, B., Reineke, T. M., O’Keeffe, M. & Yaghi, O. M. (2001). *Acc. Chem. Res.* **34**, 319–330.

- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Ma, J.-F., Liu, J.-F., Xing, Y., Jia, H.-Q. & Lin, Y. H. (2000). *J. Chem. Soc. Dalton Trans.* pp. 2403–2407.
- Ma, J.-F., Yang, J., Zheng, G.-L., Li, L. & Liu, J.-F. (2003). *Inorg. Chem.* **42**, 7531–7534.
- Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instrument Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.