

Hai-Liang Zhu,<sup>a,b\*</sup> Song Yang,<sup>a</sup>  
Xiao-Yang Qiu,<sup>a</sup> Zhong-Duo  
Xiong,<sup>b</sup> Zhong-Lu You<sup>b</sup> and  
Da-Qi Wang<sup>c</sup>

<sup>a</sup>Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, <sup>b</sup>Department of Chemistry, Wuhan University of Science and Engineering, Wuhan 430073, People's Republic of China, and <sup>c</sup>Department of Chemistry, Liaocheng University, Liaocheng 252059, People's Republic of China

Correspondence e-mail: hlzhu@wist.edu.cn

#### Key indicators

Single-crystal X-ray study

$T = 298\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$

$R$  factor = 0.044

w $R$  factor = 0.131

Data-to-parameter ratio = 14.8

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

## Hexakis(1*H*-imidazole- $\kappa N^3$ )cobalt(II) dichloride tetrahydrate

In the title compound,  $[\text{Co}(\text{C}_3\text{H}_4\text{N}_2)_6]\text{Cl}_2 \cdot 4\text{H}_2\text{O}$ , the  $\text{Co}^{\text{II}}$  atom is situated on an inversion center. It is coordinated by six N atoms of six imidazole ligands and has a slightly distorted octahedral geometry. In the crystal structure, the Cl atoms, the water molecules of crystallization and the imidazole NH groups contribute to the formation of a three-dimensional hydrogen-bonded network.

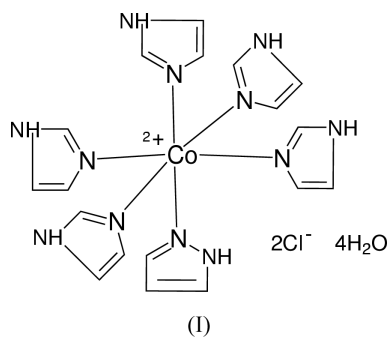
Received 7 August 2003

Accepted 27 October 2003

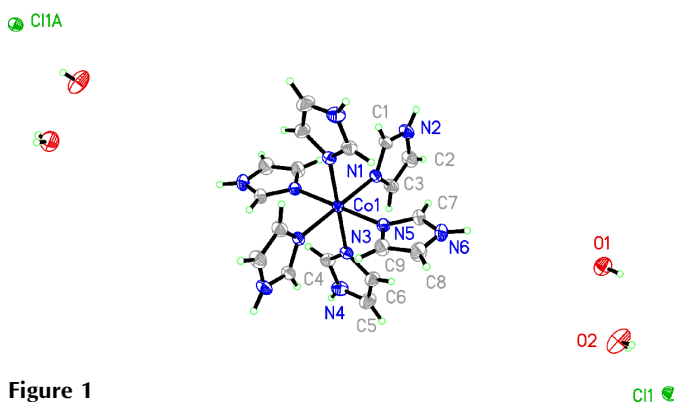
Online 8 November 2003

#### Comment

Metal complexes with imidazole ligands have been of interest for decades due to the importance of the imidazole group in biological systems. We report here the crystal structure of a new complex, hexakis(1*H*-imidazole- $\kappa N^3$ )cobalt(II) dichloride tetrahydrate, (I).

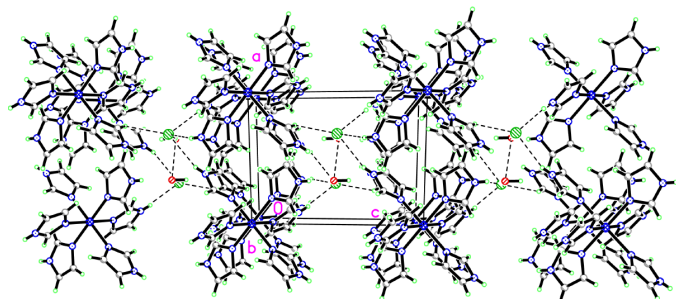


The title compound, (I), consists of a centrosymmetric hexakis(imidazole)cobalt(II) dication, two chloride counterions, and four uncoordinated water molecules in the chemical structural unit, as shown in Fig. 1. Atom Co1 has an octahedral geometry and is coordinated by six N atoms from six imidazole



**Figure 1**

The structure of the title compound, (I) (twice the asymmetric unit), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The suffix *A* denotes atoms related by the center of symmetry at the Co atom.



**Figure 2**  
The crystal packing of (I), showing the hydrogen-bonding interactions as dashed lines.

molecules. The three *trans* angles of the Co1 octahedron are 180° by symmetry, and the other angles vary from 89.39 (9) to 90.61 (9)°. The average Co—N bond length of 2.166 (2) Å is in the normal range for cobalt(II) complexes with imine N atoms. All the imidazole rings are planar, with a mean deviation of 0.0013 (2) Å. Opposing imidazole rings are parallel to one another, as required by the centrosymmetry. Neighboring imidazole rings are nearly perpendicular to one another, with dihedral angles of 84.4 (4), 85.2 (4) and 90.7 (4)°, thereby minimizing the steric effects between these rings.

In the crystal structure, the water molecules, involving atoms O1 and O2, the chloride anion Cl1, and all of the imidazole NH groups contribute to the formation of hydrogen bonds, as shown in Fig. 2. A number of intermolecular hydrogen-bond contacts involving NH groups and Cl<sup>−</sup> anions link the cations into layers in the *ab* plane (see Table 1). These, in turn, are linked *via* the water molecules and Cl<sup>−</sup> anions to form a three-dimensional network.

## Experimental

CoCl<sub>2</sub>·6H<sub>2</sub>O (1.0 mmol, 238 mg) and imidazole (6.0 mmol, 408 mg) were dissolved in water (20 ml). The mixture was stirred for a few minutes to obtain a clear pink solution. After allowing the resulting solution to stand in air for 20 d, dark-purple crystals were formed. The crystals were isolated, washed with water three times and dried in a vacuum desiccator using CaCl<sub>2</sub> (yield 39%). Elemental analysis found: C 35.50, H 5.35, N 27.69%; calculated for C<sub>18</sub>H<sub>32</sub>Cl<sub>2</sub>CoN<sub>12</sub>O<sub>4</sub>: C 35.42, H 5.28, N 27.54%.

### Crystal data

[Co(C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ) <sub>6</sub> ]Cl <sub>2</sub> ·4H <sub>2</sub> O	Z = 1
<i>M<sub>r</sub></i> = 610.39	<i>D<sub>x</sub></i> = 1.412 Mg m <sup>−3</sup>
Triclinic, <i>P</i> $\bar{1}$	Mo <i>K</i> α radiation
<i>a</i> = 8.783 (4) Å	Cell parameters from 2655 reflections
<i>b</i> = 9.064 (4) Å	$\theta$ = 2.6–26.3°
<i>c</i> = 10.575 (5) Å	$\mu$ = 0.83 mm <sup>−1</sup>
$\alpha$ = 75.156 (5)°	<i>T</i> = 298 (2) K
$\beta$ = 83.105 (6)°	Prism, dark purple
$\gamma$ = 61.848 (5)°	0.42 × 0.35 × 0.21 mm
<i>V</i> = 717.6 (5) Å <sup>3</sup>	

### Data collection

Bruker SMART CCD area-detector diffractometer	2494 independent reflections
$\varphi$ and $\omega$ scans	2186 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R</i> <sub>int</sub> = 0.021
<i>T</i> <sub>min</sub> = 0.715, <i>T</i> <sub>max</sub> = 0.843	$\theta$ <sub>max</sub> = 25.0°
3747 measured reflections	<i>h</i> = −10 → 9
	<i>k</i> = −10 → 6
	<i>l</i> = −12 → 12

### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.1518P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.131$	$(\Delta/\sigma)_{\max} = 0.001$
<i>S</i> = 1.23	$\Delta\rho_{\max} = 0.51 \text{ e } \text{Å}^{-3}$
2494 reflections	$\Delta\rho_{\min} = -0.62 \text{ e } \text{Å}^{-3}$
169 parameters	H-atom parameters constrained

**Table 1**

Hydrogen-bonding 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>
N2—H2B...Cl1 <sup>i</sup>	0.90	2.46	3.322 (3)	161
N4—H4B...Cl1 <sup>ii</sup>	0.90	2.33	3.217 (3)	169
N6—H6B...Cl1 <sup>iii</sup>	0.90	2.54	3.380 (3)	155
O1—H1B...O2 <sup>iii</sup>	0.85	2.42	2.720 (4)	101
O1—H1C...O1 <sup>iv</sup>	0.85	2.23	2.815 (6)	126
O2—H2C...O1 <sup>iii</sup>	0.85	2.19	2.720 (4)	121
O2—H2D...Cl1	0.85	2.44	3.178 (3)	145

Symmetry codes: (i)  $-x, 1-y, 1-z$ ; (ii)  $x-1, y, z-1$ ; (iii)  $1-x, 1-y, 1-z$ ; (iv)  $-x, 2-y, 1-z$ .

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms; N—H = 0.90 Å, C—H = 0.96 Å and O—H = 0.85 Å, with *U*<sub>iso</sub>(H) values fixed at 0.08 Å<sup>2</sup>.

Data collection: SMART (Siemens, 1996); cell refinement: SMART; data reduction: SAINT (Siemens, 1996); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

The authors thank the Education Office of Hubei Province, People's Republic of China, for research grant No. 2002B29002, and the Natural Science Foundation of Hubei Province, People's Republic of China, for research grant No.2003ABB010.

## References

- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997a). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.