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Hexakis(imidazole-κN^3)cobalt(II) diformate

Jian-Li Lin, Song-Ting Fei, Ke-Wei Lei and Yue-Qing Zheng*

State Key Laboratory Base of Novel Functional Materials and Preparation Science, Institute of Solid Materials Chemistry, Faculty of Materials Science and Chemical Engineering, Ningbo University, Ningbo 315211, People's Republic of China

Correspondence e-mail: zhengyueqing@nbu.edu.cn

Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.101
Data-to-parameter ratio = 16.8

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

In the title compound, $[Co(C_3H_4N_2)_6](HCO_2)_2$, the Co^{II} atom lies on an inversion centre and is coordinated by six N atoms of the imidazole ligands in a distorted octahedral geometry. The complex cations and formate anions are connected *via* N—H···O hydrogen bonds, forming a two-dimensional layer structure parallel to (010).

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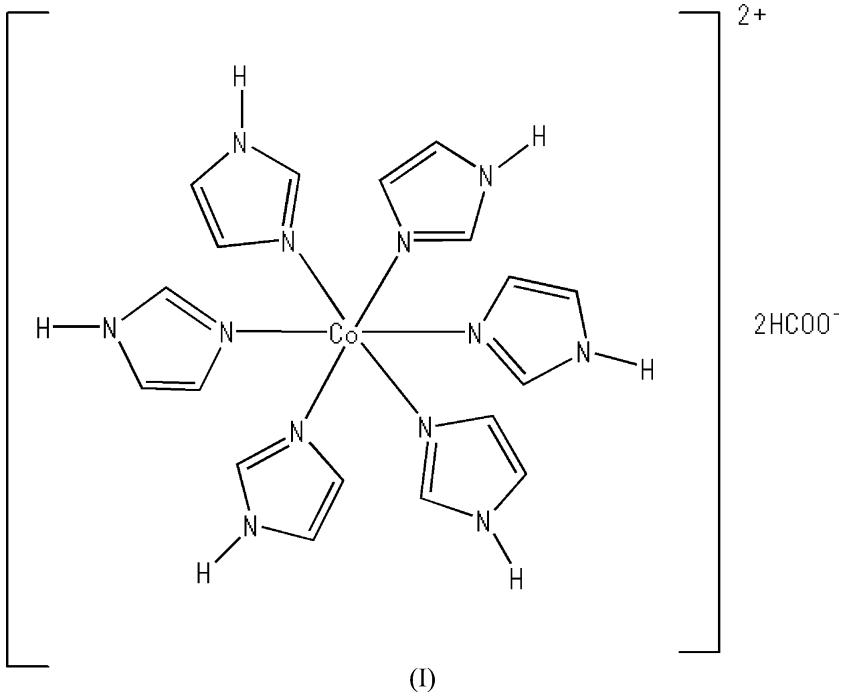
Comment

Cobalt(II) complexes with imidazole ligands have attracted much attention as models for metalloproteins, since they contain functionalities in the side chain (Strandbrerg & Lundberg, 1971). Imidazole has been used as a unidentate ligand to prepare the title Co^{II} complex, (I), in our laboratory.



(I)

The structure of (I) is illustrated in Fig. 1. Compound (I), which is isomorphous with $[Cu(imidazole)_6](HCO_2)_2$ (Server-Carrio *et al.*, 1996), consists of a centrosymmetric $[Co(imidazole)_6]^{2+}$ complex cation and formate anions. The Co atom, lying on an inversion centre, is coordinated by six N atoms in a distorted octahedral coordination geometry (Table 1). As shown in Fig. 2, the complex cations are connected to formate anions *via* N—H···O hydrogen bonds (Table 2), forming a two-dimensional layer structure parallel to (010). The two O atoms of the formate behave differently, O1 and O2 accepting one and two H atoms, respectively.

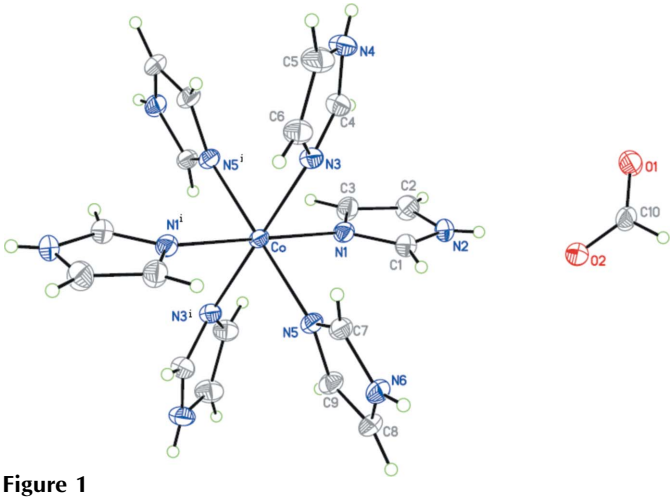


Figure 1
The complete cation and anion of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms and those with the superscript 'i' are at the symmetry position ($-x$, $-y$, $1-z$).

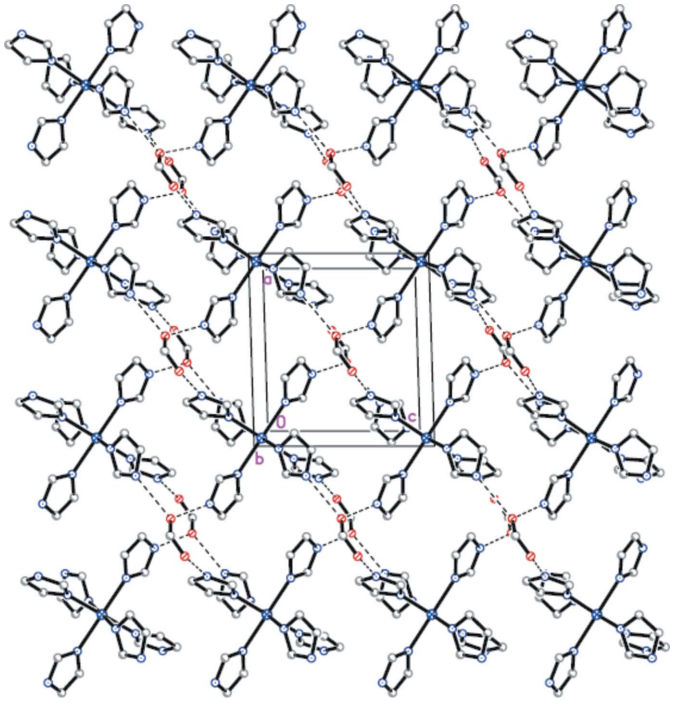


Figure 2
A view along the *b* axis, showing a single layer of (I), with the N—H···O hydrogen bonds indicated by dashed lines. H atoms have been omitted.

Experimental

1 *M* NaOH (6.0 ml) was added dropwise to a stirred aqueous solution of $CoCl_2{\cdot}6H_2O$ (0.700 g, 2.9 mmol) in H_2O (5.0 ml) to produce a blue precipitate, which was separated by centrifugation and washed with distilled water until no Cl^- anions were detected in the supernatant. The fresh precipitate was transferred to a solution of imidazole (0.200 g, 2.9 mmol) in CH_3OH–H_2O (1:1 *v*/*v*, 30 ml). The mixture was vigorously stirred and formic acid (1.0 *M*) was added dropwise until the precipitate had dissolved completely. The resulting brown solution (pH = 6.5) was allowed to stand at room temperature, and slow evaporation over several weeks afforded crystals of (I) (yield 75%).

Analytical data calculated for $C_{20}H_{26}CoN_{12}O_4$: C 43.09, H 4.70, N7 30.15%; found: C 43.18, H 4.52, N 30.22%.

Crystal data

$[Co(C_3H_4N_2)_6](HCO_2)_2$
M_r = 557.46
Monoclinic, $P2_1/c$
a = 8.9020 (18) Å
b = 16.916 (3) Å
c = 8.3250 (17) Å
β = 91.72 (3)°
V = 1253.1 (4) Å^3
Z = 2
D_x = 1.477 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.74 mm^{-1}
T = 296 (2) K
Block, red
0.47 × 0.27 × 0.24 mm

Data collection

Bruker *P*4 diffractometer
$\omega/2\theta$ scans
Absorption correction: multi-scan (*XSCANS*; Siemens, 1996)
T_{min} = 0.785, T_{max} = 0.840
3663 measured reflections
2864 independent reflections
2221 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 27.5°
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.101
S = 1.03
2864 reflections
170 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.3438P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—N5	2.1368 (17)	Co—N3	2.2077 (18)
Co—N1	2.1927 (19)		
N5—Co—N1	87.73 (7)	N1—Co—N3	87.52 (7)
N5—Co—N3	92.44 (7)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2	0.86	1.93	2.776 (3)	166
N4—H4A···O2^{i}	0.86	1.92	2.719 (3)	155
N6—H6B···O1^{ii}	0.86	1.87	2.725 (3)	172

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

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N).

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

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