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Key indicators

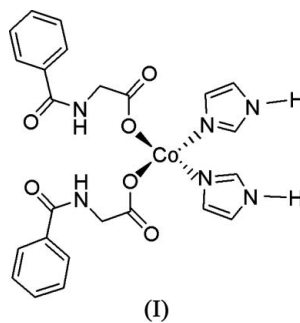
Single-crystal X-ray study
T = 100 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.039
wR factor = 0.060
Data-to-parameter ratio = 16.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis(*N*-benzoylglycinato)diimidazolecobalt(II)

In the title compound, $[\text{Co}(\text{C}_9\text{H}_8\text{NO}_3)_2(\text{C}_3\text{H}_4\text{N}_2)_2]$, the Co^{II} atom, located on a twofold rotation axis, is coordinated by two N atoms and two O atoms in a distorted tetrahedral geometry. The imine groups from the hippurate anion as well as the imidazole ligand act as donors in $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds; the two intermolecular $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds create a three-dimensional network.

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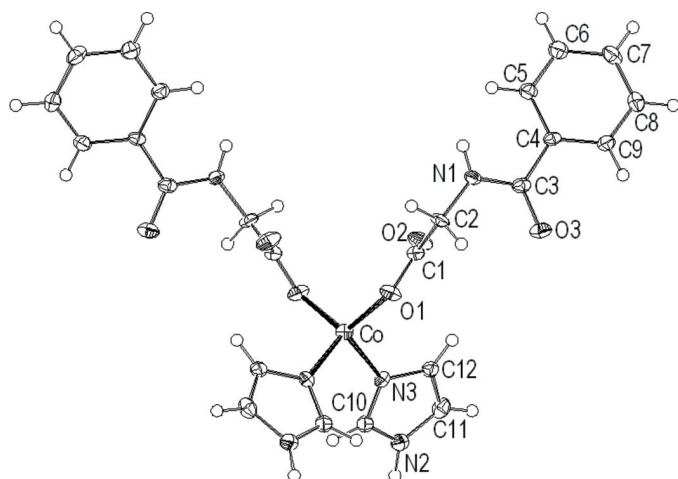
Comment

The great interest in amino acids and their derivatives is due to their diverse biological functions, including binding metals in metalloproteins (Fraústo da Silva & Williams, 1991). Hippuric acid (benzoylglycine) is a main metabolite of benzoic acid and toluene (Stryer, 1995). We are interested in the synthesis of heteroleptic complexes with the hippurate anion (hipp) and imidazole (Him) as ligands. Only one compound of this type has been reported to date, namely $[\text{Cu}(\text{hipp})_2(\text{Him})_2]$ (Antonini *et al.*, 1982). An X-ray crystal structure analysis of the title compound, (I), was undertaken, and the results are presented here.



In (I), the Co^{II} atom, located on a twofold rotation axis, is four-coordinated by two aromatic N atoms from two imidazole molecules and two O atoms from two monodentate hippurate anions, forming a distorted CoO_2N_2 tetrahedron. The bond angles around the Co^{II} atom range from $101.93(8)$ to $118.74(11)^\circ$ (Table 1). This type of structure contrasts with that observed in $[\text{Cu}(\text{hipp})_2(\text{Him})_2]$, where the Cu^{II} atom is four-coordinated in a square-planar geometry. The $\text{Co}-\text{N}$ bond length (Table 1) is slightly shorter than the mean value of those observed in the complexes with divalent cobalt and imidazole (2.022 \AA ; Orpen *et al.*, 1989). The $\text{Co}-\text{O}$ bond distance is shorter than that in $[\text{Co}(\text{hipp})_2(\text{H}_2\text{O})_3] \cdot 3\text{H}_2\text{O}$ (2.00 \AA ; Morelock *et al.*, 1982).

Bond distances and angles in the imidazole ligand correspond well with those in other metal complexes (Orpen *et al.*, 1989). The conformation of the hippurate ion is quite similar


Figure 1

View of the title compound, showing the atom-labelling scheme. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by $\frac{2}{3} - x, \frac{2}{3} - y, z$.

to that of hippuric acid (Ringertz, 1971) and that of the hipp ion in $[\text{Cu}(\text{hipp})_2(\text{Him})_2]$ (Antolini *et al.*, 1982); the dihedral angle between the phenyl ring and the peptide group in (I) $[18.5(3)^\circ]$ is close to the corresponding value of 14° in hippuric acid and 24° in the hippurate ion in $[\text{Cu}(\text{hipp})_2(\text{Him})_2]$.

The three-dimensional system of intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2) can be regarded as the superposition of two networks: one created by the hydrogen bond involving the peptide NH group and the peptide O atom (Fig. 2), and the other formed by the hydrogen bond between the imidazole NH group and the uncoordinated O atom from the hipp ion (Fig. 3).

Experimental

A solution of benzoylglycine (0.82 mmol, 0.147 g) in 2-propanol (20 ml) was added dropwise to a solution of $\text{Co}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ (0.41 mmol, 0.15 g) in 2-propanol (10 ml). The resulting solution was kept at room temperature. After several days, violet-blue crystals were obtained (yield 66.4%). Analysis calculated for $\text{C}_{24}\text{H}_{24}\text{CoN}_6\text{O}_6$: C 52.26, H 4.39, N 15.24%; found: C 52.64, H 4.00, N 15.65%.

Crystal data

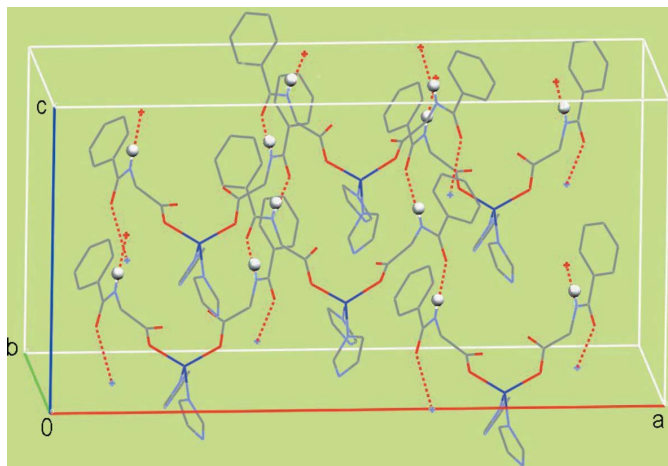
$[\text{Co}(\text{C}_9\text{H}_8\text{NO}_3)_2(\text{C}_3\text{H}_4\text{N}_2)_2]$
 $M_r = 551.42$
 Orthorhombic, $Fdd2$
 $a = 29.245(11) \text{ \AA}$
 $b = 11.540(5) \text{ \AA}$
 $c = 14.945(6) \text{ \AA}$
 $V = 5044(4) \text{ \AA}^3$

$Z = 8$
 $D_x = 1.452 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.73 \text{ mm}^{-1}$
 $T = 100(2) \text{ K}$
 Tetrahedron, violet-blue
 $0.15 \times 0.15 \times 0.14 \text{ mm}$

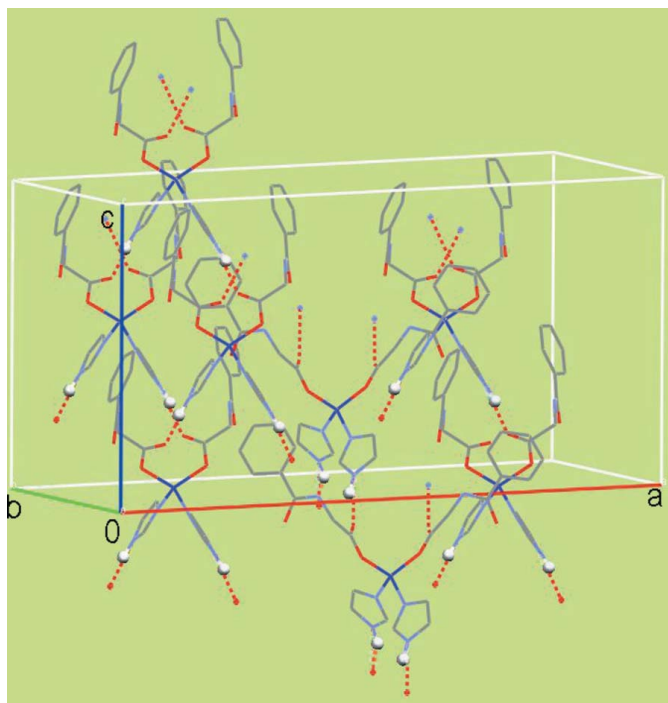
Data collection

Kuma KM-4-CCD κ -geometry
 diffractometer
 ω scans
 Absorption correction: analytical
 (CrysAlis RED; Oxford
 Diffraction, 2003)
 $T_{\min} = 0.890, T_{\max} = 0.927$

8319 measured reflections
 2899 independent reflections
 2212 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$
 $\theta_{\text{max}} = 28.5^\circ$


Figure 2

Two-dimensional structure created by amide-type $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, indicated by dashed lines. H atoms involved in the hydrogen bonds are marked as white spheres.


Figure 3

Two-dimensional structure created by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds between the imidazole and the uncoordinated carboxylate O atom. The hydrogen bonds are indicated by dashed lines and H atoms involved in the hydrogen bonds are marked as white spheres.

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.061$
 $S = 1.01$
 2899 reflections
 174 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.014P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.47 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.45 \text{ e \AA}^{-3}$
 Absolute structure: Flack (1983),
 1325 Friedel pairs
 Flack parameter: $-0.004(14)$

Table 1

Selected geometric parameters (Å, °).

Co—O1	1.950 (2)	Co—N3	2.012 (2)
O1 ⁱ —Co—O1	118.74 (11)	O1—Co—N3	113.96 (8)
O1 ⁱ —Co—N3	101.93 (8)	N3—Co—N3 ⁱ	106.04 (12)

Symmetry code: (i) $-x + \frac{3}{2}, -y + \frac{3}{2}, z$.

Table 2

Hydrogen-bond 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>
N1—H1...O3 ⁱⁱ	0.86 (3)	2.03 (3)	2.846 (3)	159 (3)
N2—H2...O2 ⁱⁱⁱ	0.98 (3)	1.77 (3)	2.713 (3)	160 (2)

Symmetry codes: (ii) $-x + \frac{5}{4}, y + \frac{1}{4}, z + \frac{1}{4}$; (iii) $-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}$.

The N atoms bonded to H atoms were found in a difference map and their coordinates were refined freely. Other H atoms were positioned geometrically and treated as riding, with C—H = 0.95–0.99 Å. $U_{iso}(H)$ values for all H atoms were set equal to $1.2U_{eq}$ of the parent atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97*

(Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *MERCURY* (Version 1.2.1; Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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