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# Aquapentakis(1*H*-imidazole-$\kappa N^3$)cobalt(II) dibromosuccinate

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The title compound, $[Co(C_3H_4N_2)_5(H_2O)](C_4H_2Br_2O_4)$, consists of Co$^{II}$ complex cations and dibromosuccinate anions. The Co atom, water O atom and one imidazole N atom of the complex cation occupy a twofold axis. The anion lies on an inversion centre. The crystal packing is reinforced by O—H···O and N—H···O hydrogen bonds, but there are no $\pi$–$\pi$ stacking interactions.

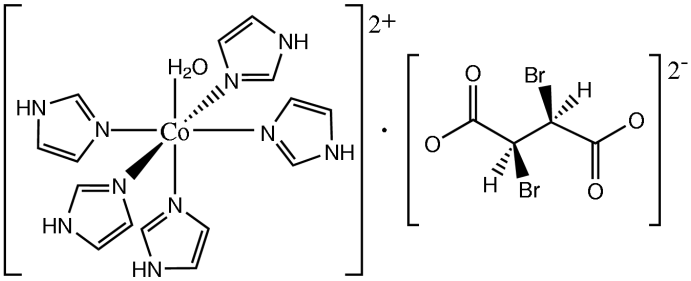
**Key indicators**

Single-crystal X-ray study
*T* = 295 K
Mean $\sigma$(C–C) = 0.007 Å
Disorder in main residue
*R* factor = 0.037
*wR* factor = 0.089
Data-to-parameter ratio = 13.2

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

## Comment

As $\pi$–$\pi$ stacking plays an important role in some biological processes (Deisenhofer & Michel, 1989), the nature of $\pi$–$\pi$ stacking has attracted our attention. A series of metal complexes incorporating different aromatic ligands has been prepared and their structures determined to compare the effect of the size of the aromatic ring on $\pi$–$\pi$ stacking (Liu *et al.*, 2004; Pan & Xu, 2004). The title Co$^{II}$ complex, (I), with imidazole ligands and dibromosuccinate anions, has been prepared but its crystal structure shows no $\pi$–$\pi$ stacking.



(I)

The crystal structure of (I) consists of Co$^{II}$ complex cations and dibromosuccinate anions (DBrS), as shown in Fig. 1. The Co$^{II}$ atom, located on a twofold axis, is coordinated by five imidazole ligands and one water molecule in octahedral geometry. The coordinated water O atom and the N5-containing imidazole ligand are also located on the twofold axis. Thus, the N5-imidazole is disordered, the atoms N6 and C8 occupying the same site with 0.5 occupancy each. The N5-imidazole species links with the carboxyl group of DBrS *via* the disordered N6—H6*a*···O3*a* or C8—H8···O3*a* hydrogen bond (Table 2).

The complete DBrS anion has inversion symmetry. The carboxyl groups display two different orientations (Fig. 1), the dihedral angle between the disordered components of the same carboxyl group being 46 (2)°. The disorder components *A* (O2*a* and O3*a*) and *B* (O2*b* and O3*b*) participate in similar

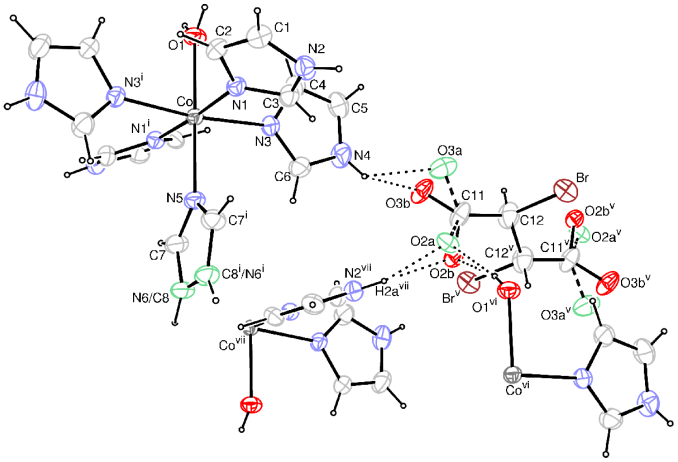


**Figure 1**
The molecular structure of (I), shown with 30% probability displacement ellipsoids. The atomic label of N6/C8 indicates two different elements occupying the same site within the N5-imidazole ligand. Dashed lines show one of the disordered carboxyl components. Dotted lines indicate hydrogen bonding [symmetry codes: (i) $1 - x, y, \frac{3}{2} - z$; (v) $-x, 1 - y, 2 - z$; (vi) $x - \frac{1}{2}, y - \frac{1}{2}, z$; (vii) $x, 1 - y, z + \frac{1}{2}$].

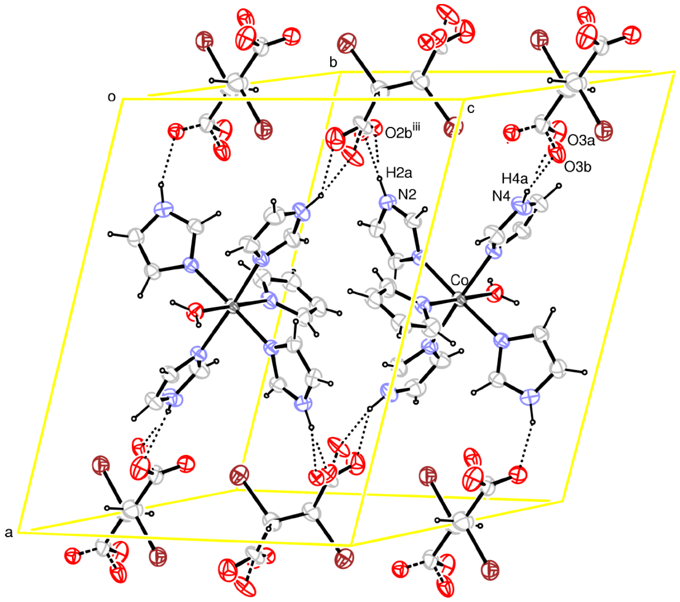


**Figure 2**
The crystal packing for (I). Dashed lines indicate the hydrogen bonding between imidazole ligands and disordered carboxyl groups [symmetry code: (iii) $x, 1 - y, z - \frac{1}{2}$].

hydrogen-bond linkages with the $N2^{vii}$-imidazole, N4-imidazole and $O1^{vi}$ water molecule, as shown in Fig. 1 [symmetry code: (vii) $x, 1 - y, z + \frac{1}{2}$]. No $\pi$–$\pi$ stacking is observed in (I). The nearest distance between imidazole rings of neighbouring complex cations is 3.257 (6) Å [$N2\cdots N2^{viii}$; symmetry code: (viii) $x - \frac{1}{2}, \frac{3}{2} - y, z - \frac{1}{2}$)] (Fig. 3).

## Experimental

An ethanol–water solution (5 ml, 1:1) of $CoCl_2 \cdot 6H_2O$ (0.24 g, 1 mmol) was mixed with an aqueous solution (4 ml) containing $DBrSH_2$ (0.55 g, 2 mmol) and $Na_2CO_3$ (0.21 g, 2 mmol). The mixture was refluxed for 4 h and filtered. After cooling to room temperature, imidazole (0.20 g, 3 mmol) was added to the filtrate and pink single crystals of (I) were obtained after 2 d.

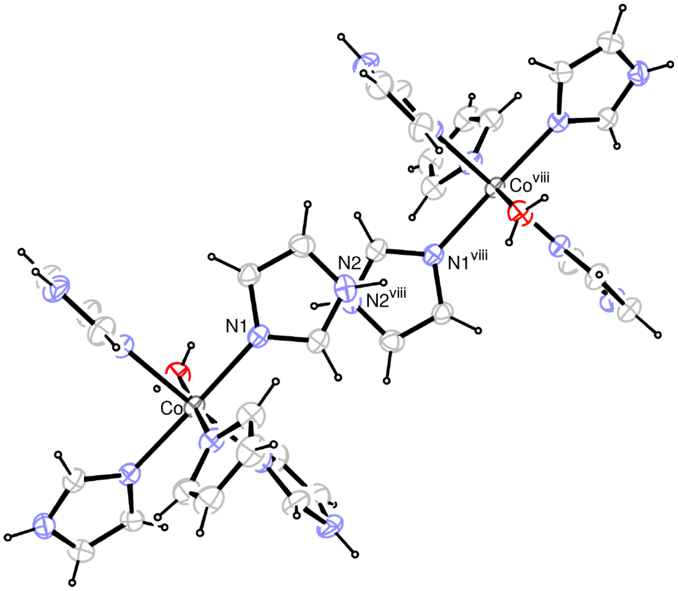


**Figure 3**
The nearest contact between imidazole rings of neighbouring complex cations [symmetry code: (viii) $x - \frac{1}{2}, \frac{3}{2} - y, z - \frac{1}{2}$].

### *Crystal data*

$[Co(C_3H_4N_2)_5(H_2O)](C_4H_2Br_2O_4)$
$M_r = 691.23$
Monoclinic, $C2/c$
$a = 15.713$ (3) Å
$b = 12.798$ (2) Å
$c = 13.806$ (3) Å
$\beta = 109.468$ (9)°
$V = 2617.6$ (9) Å$^3$
$Z = 4$

$D_x = 1.754$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2322 reflections
$\theta = 2.5$–25.0°
$\mu = 3.76$ mm$^{-1}$
$T = 295$ (2) K
Prism, pink
0.35 × 0.22 × 0.21 mm

### *Data collection*

Rigaku R-AXIS RAPID diffractometer
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.274$, $T_{max} = 0.450$
4637 measured reflections

2500 independent reflections
1880 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 25.7°$
$h = -19 \rightarrow 19$
$k = -15 \rightarrow 15$
$l = -16 \rightarrow 16$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.089$
$S = 1.05$
2500 reflections
189 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 2.2996P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.68$ e Å$^{-3}$
$\Delta\rho_{min} = -0.62$ e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Co—N1 | 2.133 (3) | Co—N3 | 2.164 (3) |
| Co—O1 | 2.157 (3) | Co—N5 | 2.190 (4) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D—H\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D—H\cdots A$ |
|---|---|---|---|---|
| $O1—H1a\cdots O2a^{ii}$ | 0.85 | 1.97 | 2.80 (2) | 166 |
| $O1—H1a\cdots O2b^{ii}$ | 0.85 | 1.84 | 2.67 (2) | 166 |
| $N2—H2a\cdots O2a^{iii}$ | 0.86 | 1.93 | 2.74 (3) | 157 |
| $N2—H2a\cdots O2b^{iii}$ | 0.86 | 1.91 | 2.73 (3) | 157 |
| $N4—H4a\cdots O3a$ | 0.86 | 2.23 | 2.903 (10) | 135 |
| $N4—H4a\cdots O3b$ | 0.86 | 1.88 | 2.670 (11) | 152 |
| $N6—H6a\cdots O3a^{iv}$ | 0.85 | 2.11 | 2.956 (8) | 171 |
| $C8—H8\cdots O3a^{iv}$ | 0.92 | 2.05 | 2.956 (8) | 170 |

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

Two different orientations for the carboxyl group were found in a difference Fourier map. Their occupancies were initially refined and then fixed as 0.53:0.47 in the final cycles of refinement. H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) and 0.98 Å (methine), and N—H = 0.86 Å. H atoms of water and the disordered imidazole were included with fixed positional parameters and isotropic displacement parameters of 0.08 Å$^2$. The other H atoms were refined as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$ of the carrier atom.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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