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# Tris({2-[(1-methylimidazol-2-yl)methylimino]ethyl}amine)cobalt(II) diperchlorate

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The $Co^{II}$ atom of the title complex, $[Co(C_{21}H_{30}N_{10})](ClO_4)_2$, located on a threefold rotation axis, is coordinated in an octahedral geometry by three imine N atoms and the three imidazole N atoms, with Co—N distance of 2.131 (3)–2.164 (3) Å, and *cis* and *trans* N—Co—N angles of 76.17 (12)–102.77 (10) and 163.66 (12)°, respectively. The perchlorate counter-anions are located on centers of symmetry.

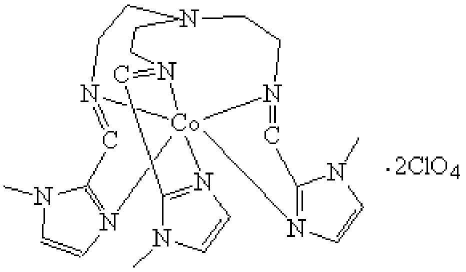
**Key indicators**

Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.007 Å
$R$ factor = 0.051
$wR$ factor = 0.137
Data-to-parameter ratio = 16.5

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

## Comment

Metal complexes of imidazole and its derivatives are of current interest in the investigation of model complexes relevant to metalloenzymes, since imidazole, a component of histidine, is frequently found to ligate metal ions in the active centers of metalloenzymes (Wilcox, 1997). A number of $Co^{II}$–imidazole complexes have been structurally characterized (Katsuki *et al.*, 2002). [A text search of the CSD for cobalt(II) and imidazole yielded 117 hits; please reword.] Recently, we have synthesized a series of imidazole-containing Schiff base compounds, which are used in the synthesis of transition metal complexes as structural models of some metalloenzymes and for crystal engineering (Chen et al., 2003; Yang et al., 1999, 2000, 2001, 2004). As a continuation of our studies, we have isolated the title compound, a new Schiff base cobalt(II) complex, (I). The structure consists of a $[CoL]^{2+}$ cation (L = tris{2-[(1-methylimidazol-2-yl)methylimino]ethyl}amine) and two perchlorate anions. The coordination environment around Co is shown in Fig. 1 and the molecular packing is shown in Fig. 2.



(I)

Although the ligand is potentially heptadentate, the tripodal N atoms are not bonded to the $Co^{II}$ atom, with a $Co\cdots N_{tripodal}$ distance of 2.946 (3) Å. The metal atom in the complex is coordinated octahedrally by the three imine groups and the three imidazole groups, with Co—N distances of 2.164 (3) and 2.131 (3) Å, and *cis* and *trans* N—Co—N angles of 76.17 (12)–102.77 (10) and 163.66 (12)°, respectively. The two equilateral triangles, one formed by the three $N_{imine}$ atoms

[N3, N3$^{i}$ and N3$^{ii}$; symmetry codes: (i) $1 - y$, $x - y$, $z$; (ii) $1 - x + y$, $1 - x$, $z$] and the other formed by the $N_{imidazole}$ atoms (N1, N1$^{i}$ and N1$^{ii}$) are parallel and are both perpendicular to the $C_3$ axis. The site symmetry of each complex cation is close to $C3$, with the $C3$ axis passing through the metal and the tripodal N atoms. This is similar to related complexes reported previously (Yang *et al.*, 2001; Kichner *et al.*, 1987; Sim & Sinn, 1978). Perchlorate counter-anions are located on two different sites and are also located on centers of symmetry.

## Experimental

1-Methylimidazole-2-carbaldehyde (3 mmol, 0.330 g) was added to a solution of tris(2-aminoethyl)amine (1 mmol, 0.146 g) in dry methanol. The mixture was refluxed for 5 h, then a solution of $CoCl_3 \cdot 6H_2O$ (1 mmol, 0.156 g) and an aqueous methanol (10 ml, 1:1 *v*/*v*) solution of $NaClO_4$ (2 mmol, 0.250 g) were added. After filtration, the solution was allowed to stand at room temperature in air for 15 d, after which time red crystals of the complex were collected and washed with methanol.

*Crystal data*

$[Co(C_{21}H_{30}N_{10})](ClO_4)_2$
$M_r = 680.38$
Trigonal, $P31c$
$a = 10.8349$ (7) Å
$c = 14.6028$ (13) Å
$V = 1484.62$ (19) Å$^3$
$Z = 2$
$D_x = 1.522$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3994 reflections
$\theta = 4.3$–$49.1°$
$\mu = 0.82$ mm$^{-1}$
$T = 298$ (2) K
Block, red
0.52 × 0.49 × 0.44 mm

*Data collection*

Bruker SMART 1K area-detector diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.646$, $T_{max} = 0.691$
8257 measured reflections
2115 independent reflections
1893 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.0°$
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 7$
$l = -18 \rightarrow 18$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.137$
$S = 1.04$
2115 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0959P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.015$
$\Delta\rho_{max} = 0.87$ e Å$^{-3}$
$\Delta\rho_{min} = -0.54$ e Å$^{-3}$
Absolute structure: (Flack, 1983), 1023 Friedel pairs
Flack parameter = 0.03 (3)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Co—N3 | 2.131 (3) | Co—N1 | 2.164 (3) |
| | | | |
| N3$^{i}$—Co—N3 | 102.77 (10) | N3—Co—N1 | 76.17 (12) |
| N3—Co—N1$^{i}$ | 93.29 (14) | N1$^{i}$—Co—N1 | 87.57 (13) |
| N3$^{i}$—Co—N1 | 163.66 (12) | | |

Symmetry code: (i) $1 - y$, $x - y$, $z$.

All H atoms were positioned geometrically (C—H = 0.96 and 0.97 Å) and refined using the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The highest peak and deepest hole in the difference Fourier map are located 1.42 and 0.46 Å, respectively, from atoms Cl2 and O1, respectively.

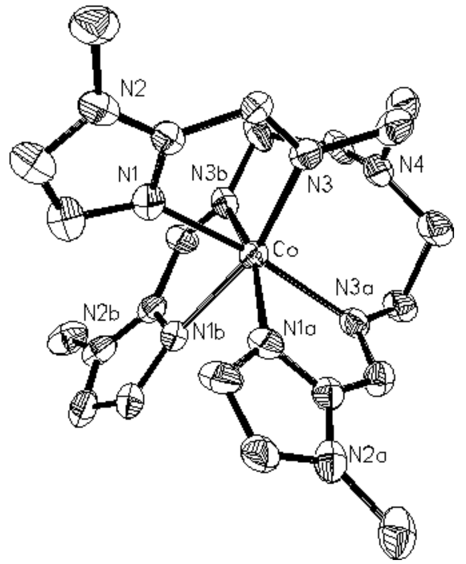


**Figure 1**
The structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 35% probability level. H atoms shown as small circles with arbitrary radius. The $ClO_4^-$ ions have been omitted for clarity. Suffixes a and b, respectively, correspond to symmetry codes (i) and (ii) in the text.

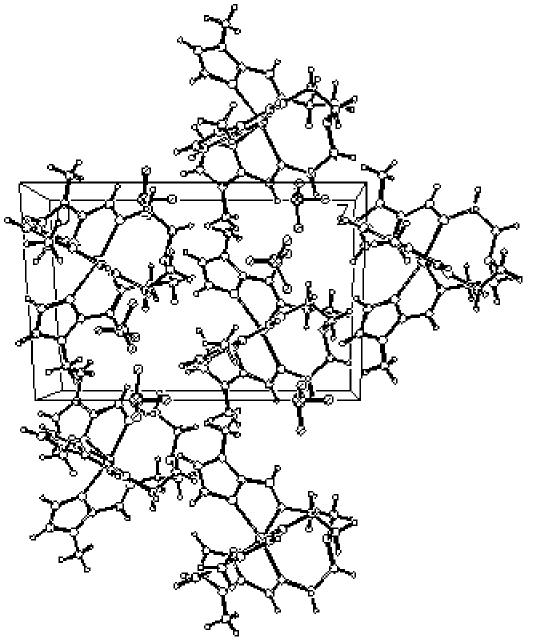


**Figure 2**
Perspective view (*ORTEP-3*; Farrugia, 1997) of the molecular packing of the title compound, viewed down the *a* axis

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

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