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Key indicators

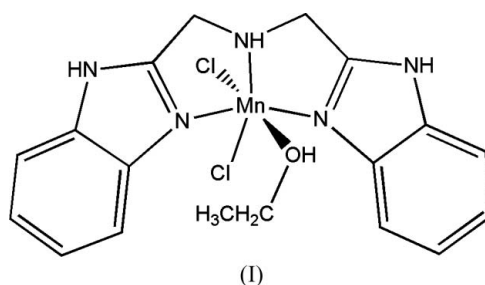
Single-crystal X-ray study
 $T = 292\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.038
 wR factor = 0.101
Data-to-parameter ratio = 16.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**[Bis(1*H*-benzimidazol-2-ylmethyl)amine]-
dichloro(ethanol)manganese(II)**

In the molecular structure of the title compound, $[\text{MnCl}_2(\text{C}_{16}\text{H}_{15}\text{N}_5)(\text{C}_2\text{H}_6\text{O})]$, the Mn cation is in a distorted octahedral configuration. A three-dimensional framework structure is formed by means of $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds.

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Comment

Histidine is an important ligand in iron, copper, zinc and manganese metalloproteins such as superoxide dismutases, lipoxygenases, tyrosinases, amine oxidases and hemocyanins (Que & Ho, 1996; Kaim & Rall, 1996). Bis(1*H*-benzimidazol-2-ylmethyl)amine (IDB) is a benzimidazole-rich ligand, which has the advantage that the basicity of the coordinating group approximates that of histidine ($\text{p}K_{\text{b}}$: histidine = 7.96 and benzimidazole = 8.47; Main, 1992). We obtained the title compound, (I), in the process of synthesizing an IDB–metal complex in 95% ethanol with 1% dilute hydrochloric acid.



In (I), the Mn atom displays a distorted octahedral coordination geometry provided by the tridentate IDB ligand, two chloride anions and the O atom of an ethanol molecule (Fig. 1). The IDB ligand is *mer*-coordinated, with the central N3 atom in the axial position and atoms N2 and N4 of the benzimidazolyl groups in the equatorial positions. The remaining two equatorial positions are occupied by atoms Cl2 and O1. The bond distance between the Mn^{II} ion and the axial N3 atom is about 0.21 Å longer than those between the Mn^{II} ion and the equatorial N atoms of the benzimidazolyl groups (mean value = 2.210 Å; Table 1). The Mn–Cl bond length involving the equatorial atom Cl2 is about 0.24 Å longer than that involving the axial atom Cl1.

In the crystal structure, the molecules are linked into a three-dimensional framework by intermolecular $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds (Table 2 and Fig. 2). In addition to these interactions, $\pi-\pi$ stacking interactions between centrosymmetrically related imidazole rings at (x, y, z) and $(-x, 1-y, 1-z)$ are observed, with an interplanar spacing of 3.379 Å and a centroid–centroid distance of 3.634 (1) Å.

Experimental

All reagents and solvents were used as obtained without further purification. Compound (I) was synthesized by refluxing stoichiometric quantities (1:1 molar ratio) of IDB (0.28 g, 1.0 mmol) and manganese(II) chloride tetrahydrate (0.20 g, 1 mmol) in 95% ethanol (30 ml) at 333 K for 4 h. The solution was cooled to room temperature, filtered and evaporated to obtain the product (yield 30%). Crystals of (I) were grown by slow evaporation of an ethanol solution.

Crystal data

[MnCl₂(C₁₆H₁₅N₅)(C₂H₆O)]
M_r = 449.24
 Monoclinic, *P*2₁/*c*
a = 7.2920 (5) Å
b = 13.8686 (10) Å
c = 19.6429 (14) Å
 β = 98.009 (1)°
V = 1967.1 (2) Å³
Z = 4
D_x = 1.517 Mg m⁻³
 Mo Kα radiation
 μ = 0.96 mm⁻¹
T = 292 (2) K
 Block, colourless
 0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2001)
T_{min} = 0.761, *T_{max}* = 0.910
 15190 measured reflections
 4278 independent reflections
 3433 reflections with *I* > 2σ(*I*)
R_{int} = 0.038
 θ_{max} = 27.0°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.038
wR (*F*²) = 0.101
S = 1.02
 4278 reflections
 261 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.0319P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.32 e Å⁻³
 Δρ_{min} = -0.26 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------|-------------|-------------|-------------|
| Mn1—N4 | 2.2027 (17) | Mn1—Cl1 | 2.4057 (7) |
| Mn1—N2 | 2.2159 (17) | Mn1—N3 | 2.4210 (19) |
| Mn1—O1 | 2.2512 (17) | Mn1—Cl2 | 2.6444 (7) |
| N4—Mn1—N2 | 143.31 (7) | O1—Mn1—N3 | 79.89 (7) |
| N4—Mn1—O1 | 89.40 (6) | Cl1—Mn1—N3 | 176.75 (5) |
| N2—Mn1—O1 | 87.21 (6) | N4—Mn1—Cl2 | 91.04 (5) |
| N4—Mn1—Cl1 | 107.75 (5) | N2—Mn1—Cl2 | 84.62 (5) |
| N2—Mn1—Cl1 | 108.93 (5) | O1—Mn1—Cl2 | 166.90 (5) |
| O1—Mn1—Cl1 | 96.94 (5) | Cl1—Mn1—Cl2 | 95.38 (2) |
| N4—Mn1—N3 | 71.62 (6) | N3—Mn1—Cl2 | 87.83 (5) |
| N2—Mn1—N3 | 71.82 (6) | | |

Table 2

Hydrogen-bond geometry (Å, °).

| <i>D</i> — <i>H</i> ··· <i>A</i> | <i>D</i> — <i>H</i> | <i>H</i> ··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> — <i>H</i> ··· <i>A</i> |
|----------------------------------|---------------------|-----------------------|-----------------------|----------------------------------|
| N5—H5A···Cl2 ⁱ | 0.86 (1) | 2.48 (2) | 3.215 (2) | 144 (2) |
| O1—H1A···Cl2 ⁱⁱ | 0.82 (3) | 2.34 (2) | 3.1265 (18) | 161 (3) |
| N1—H1···Cl2 ⁱⁱⁱ | 0.86 (1) | 2.41 (2) | 3.186 (2) | 150 (2) |

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

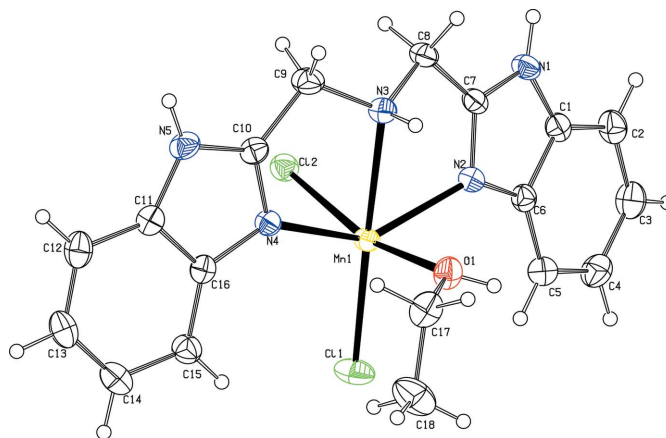


Figure 1

The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

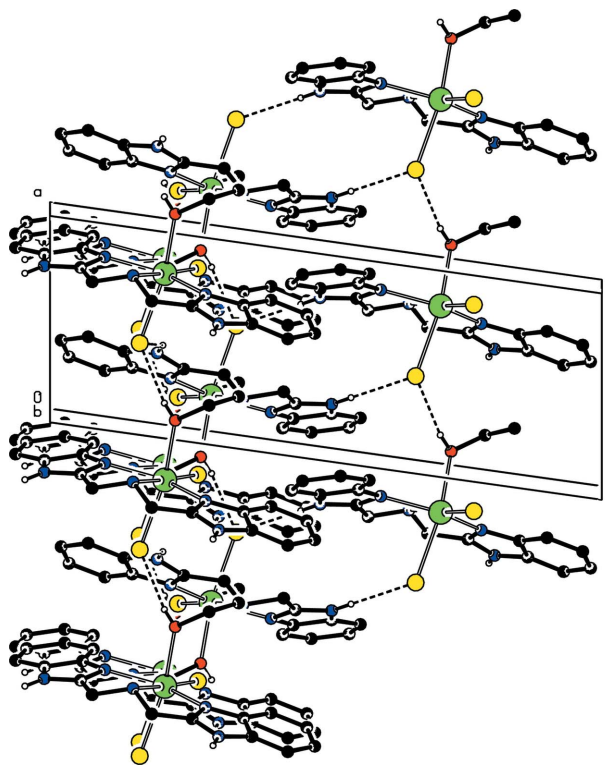


Figure 2

A partial packing diagram for (I), showing the intermolecular hydrogen bonds as dashed lines.

H atoms bonded to C atoms were placed in calculated positions, with C—H distances of 0.93–0.97 Å, and refined using a riding model, with *U_{iso}*(H) = 1.2*U_{eq}*(C). H atoms bonded to N and O atoms were located in difference density maps and isotropically refined with soft restraints, N—H = 0.86 (1) Å and O—H = 0.82 (1) Å.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

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