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Key indicators

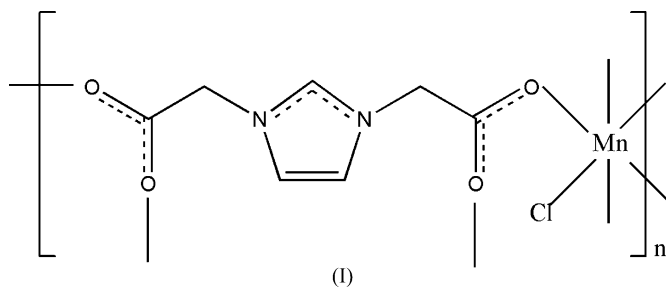
Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.035
 wR factor = 0.097
Data-to-parameter ratio = 15.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[[chloromanganese(II)]- μ_4 -imidazole-
1,3-diyl diacetato]

In the title coordination polymer, $[\text{Mn}(\text{C}_7\text{H}_7\text{N}_2\text{O}_4)\text{Cl}]_n$, each Mn^{2+} ion has a distorted octahedral geometry, defined by four acetate O atoms from four different imidazolyl-1,3-diyl diacetate (IDA^-) ligands and two Cl^- ions. The IDA^- groups serve as bridging ligands to link the Mn^{2+} ions into a two-dimensional layer structure.

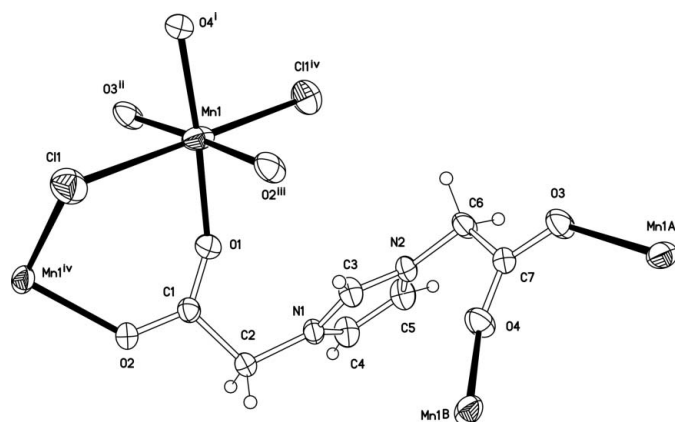
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Comment

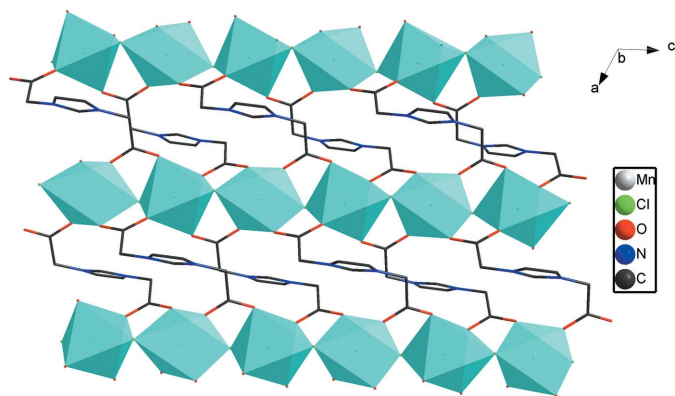
We are interested in the solid-state coordination chemistry of *N*-heterocyclic carboxylic acids, such as imidazolyl-1,3-diyl diacetic acid (IDA) (Zhang *et al.*, 2006). The deprotonated monoanion is, interestingly, a zwitterionic aminoacetate anion, having two $-\text{CH}_2\text{CO}_2^-$ arms which can each bind to a metal centre. Metal complexes of this ligand have been reported only very recently and are so far limited to the metals Ba, Cs, Ca, Sr, Co and Zn (Fei, Ang *et al.*, 2006; Fei, Geldbach *et al.*, 2005; Fei, Geldbach *et al.*, 2006; Fei, Zhao *et al.*, 2005), in which compounds the authors' principal interest arises from the incorporation of water aggregates into the coordination polymers. Recently, we reported the structure of a two-dimensional Cd^{II} polymer in this class, $[\text{Cd}(\text{IDA})_2]_n$ (Zhang *et al.*, 2006), in which each IDA^- ligand acts in a bis-bidentate chelating mode to connect the Cd^{II} atoms, forming a two-dimensional layer structure. In an extension of our investigation of the IDA^- ligand, we report here the synthesis and structure of a new Mn^{2+} polymer, $[\text{Mn}(\text{IDA})(\text{Cl})]_n$, (I).



The asymmetric unit of (I) comprises an Mn^{2+} ion, one IDA^- ligand and one coordinated Cl^- ion (Fig. 1). Each Mn^{2+} ion has a distorted octahedral coordination geometry, defined by four acetate O atoms $[\text{Mn}-\text{O} 2.1033(17)-2.1588(18)$ Å] from four IDA^- ligands and two Cl^- ions $[\text{Mn}-\text{Cl} = 2.6321(9)$ and $2.8081(9)$ Å]. The equatorial plane of the octahedron is defined by atoms O1, O2ⁱⁱ, O3ⁱⁱⁱ and O4ⁱ [symmetry codes: (i) $x + 1, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x + 1, y, z + 1$; (iii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$], with an r.m.s. deviation from the plane of 0.008 Å. Atoms Cl1 and Cl1^{iv} occupy the axial sites, with $\text{Cl}-\text{Mn}-\text{Cl} = 179.56(2)^\circ$.


Figure 1

Part of the structure of the title complex, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted. [Symmetry codes: (i) $x + 1, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x + 1, y, z + 1$; (iii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (iv) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (A) $x - 1, y, z - 1$; (B) $x - 1, -y + \frac{1}{2}, z - \frac{1}{2}$]


Figure 2

The crystal packing of (I). The octahedra represent the coordination environments of the MnO_4Cl_2 units. H atoms have been omitted for clarity.

The C—O bond lengths in the carboxylate groups range between 1.240 (2) and 1.249 (2) Å, indicating an even delocalization of charge over the CO_2^- unit. In addition, each Cl^- ion bridges two Mn^{2+} ions, forming a one-dimensional chain structure, and the IDA^- group acts as a tetradentate bridging ligand, linking the chains into a two-dimensional layer structure (Fig. 2).

Experimental

Imidazolyl-1,3-diyldiacetic acid was prepared following the literature method of Kratochvíl *et al.* (1988). $\text{MnCl}_2 \cdot 6\text{H}_2\text{O}$ (2.34 g, 10 mmol) and imidazolyl-1,3-diyldiacetic acid (1.84 g, 10 mmol) were dissolved in a 1:1 ethanol–water solution (25 ml). The mixture was sealed in a 50 ml Teflon-lined stainless steel bomb. The bomb was heated at 393 K for 3 d and then cooled to room temperature to yield colourless crystals of the title compound. CHN analysis, calculated for $\text{C}_7\text{H}_7\text{N}_2\text{O}_4\text{ClMn}$: C 30.74, H 2.58, N 10.24%; found: C 30.78, H 2.53, N 10.19%.

Crystal data

$[\text{Mn}(\text{C}_7\text{H}_7\text{N}_2\text{O}_4)\text{Cl}]$
 $M_r = 273.54$
 Monoclinic, $P2_1/c$
 $a = 7.7767$ (16) Å
 $b = 16.313$ (3) Å
 $c = 8.2196$ (16) Å
 $\beta = 115.26$ (3)°
 $V = 943.0$ (4) Å³

$Z = 4$
 $D_x = 1.927$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 1.68$ mm⁻¹
 $T = 295$ (2) K
 Prism, colourless [Pink?]
 $0.31 \times 0.23 \times 0.15$ mm

Data collection

Rigaku R-Axis RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.625, T_{\max} = 0.787$

8823 measured reflections
 2160 independent reflections
 1827 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
 $\theta_{\max} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.097$
 $S = 1.08$
 2160 reflections
 136 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.9372P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.10$ e Å⁻³
 $\Delta\rho_{\min} = -0.57$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Mn1—O1	2.1033 (17)	Mn1—Cl1 ^{iv}	2.8081 (9)
Mn1—O4 ⁱ	2.1066 (17)	O1—C1	1.240 (3)
Mn1—O3 ⁱⁱⁱ	2.1538 (18)	O2—C1	1.249 (3)
Mn1—O2 ⁱⁱⁱ	2.1588 (18)	O3—C7	1.249 (3)
Mn1—Cl1	2.6321 (9)	O4—C7	1.241 (3)

Cl1—Mn1—Cl1^{iv} 179.56 (2)

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

Carbon-bound H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, and were refined in the riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The highest peak is located 0.805 (2) Å from atom Cl1.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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References

- Fei, Z.-F., Ang, W. H., Geldbach, T. J., Scopelliti, R. & Dyson, P. J. (2006). *Chem. Eur. J.* **12**, 4014–4020.
 Fei, Z.-F., Geldbach, T. J., Scopelliti, R. & Dyson, P. J. (2006). *Inorg. Chem.* **45**, 6331–6337.
 Fei, Z.-F., Geldbach, T., Zhao, D.-B., Scopelliti, R. & Dyson, P. J. (2005). *Inorg. Chem.* **44**, 5200–5202.

- Fei, Z.-F., Zhao, D.-B., Geldbach, T. J., Scopelliti, R., Dyson, P. J., Antonijevic, S. & Bodenhausen, G. (2005). *Angew. Chem. Int. Ed.* **44**, 5720–5725.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Kratochvíl, B., Ondráček, J., Velíšek, J. & Hašek, J. (1988). *Acta Cryst.* **C44**, 1579–1582.
- Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MSK (2002). *CrystalStructure*. Rigaku/MSK Inc., The Woodlands, Texas, USA.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Zhang, X.-F., Gao, S., Huo, L.-H. & Ng, S. W. (2006). *Acta Cryst.* **E62**, m2910–m2912.