metal-organic papers

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.008 Å
R factor = 0.064
wR factor = 0.202
Data-to-parameter ratio = 13.6

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

{Tris[2-(2-pyridylmethyleneimino)ethyl]-amine}manganese(II) bis(perchlorate)

In the title complex, [Mn($C_{24}H_{27}N_7$)](ClO_4)$_2$, the Mn^{II} ion is chelated by a tris[2-(2-pyridylmethyleneimino)ethyl]amine ligand, in a distorted octahedral coordination geometry. Weak C—H···O interactions occur between the perchlorate anions and the Mn^{II} complex cation.

Comment

The chemistry of Mn complexes is of interest because of their functions in biological systems. We report here the structure of the title Mn^{II} complex, (I), which contains a Schiff base ligand.

(I)
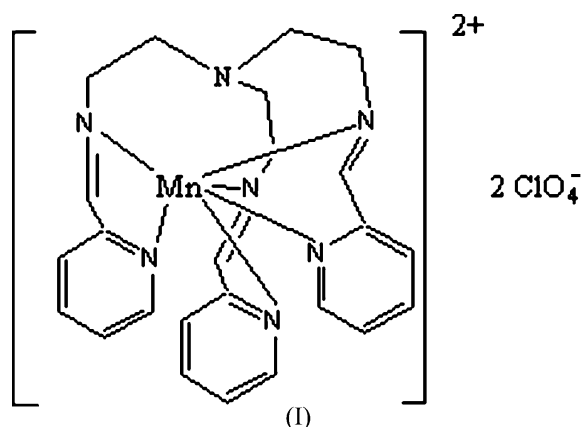
The structure of (I) is shown in Fig. 1. The crystal structure of (I) consists of discrete Mn^{II} complex cations and perchlorate anions. The Mn^{II} ion is chelated by a tris[2-(2-pyridylmethyleneimino)ethyl]amine ligand, in a distorted octahedral coordination geometry. The Mn—N(pyridine) bond distances are much longer than the Mn—N(imine) bond distances (Table 1). Weak C—H···O interactions occurs between the perchlorate anions and the Mn^{II} complex cation (Table 2).

Experimental

A methanol solution (10 ml) of tris(2-aminoethyl)amine (tren) (3 mmol) was mixed with a methanol solution (10 ml) of 2-pyridinecarboxaldehyde (9 mmol). After the mixture had been stirred at 323 K for 1 h, Mn(ClO_4)$_2$·6H_2O (3 mmol) was added to the orange solution and a yellow precipitate appeared. The precipitate was filtered off and dissolved in dimethylformamide (DMF). Yellow single crystals of (I) were obtained from the DMF solution after one month.
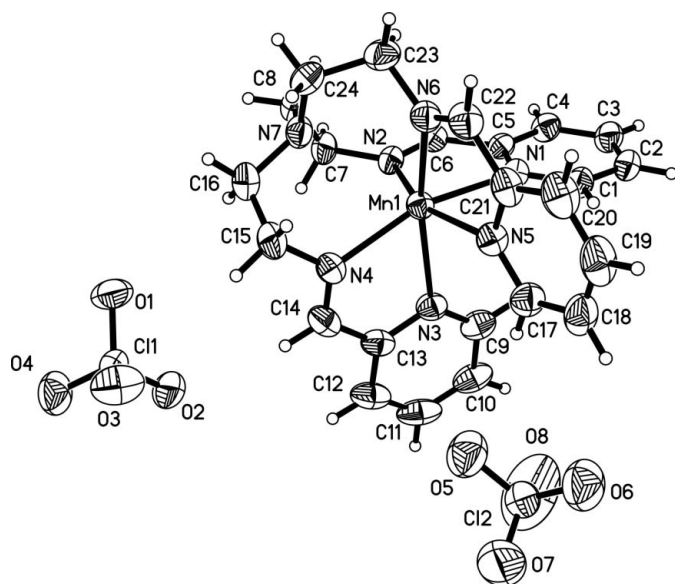
Figure 1
The asymmetric unit of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Crystal data

$[Mn(C_{24}H_{27}N_7)](ClO_4)_2$	$D_x = 1.519$ Mg m^{-3}
$M_r = 667.37$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 1930
$a = 28.3550 (13)$ Å	reflections
$b = 10.7721 (5)$ Å	$\theta = 2.8$–$19.8°$
$c = 19.4761 (8)$ Å	$\mu = 0.69$ mm^{-1}
$\beta = 101.070 (3)°$	$T = 296 (2)$ K
$V = 5838.1 (5)$ Å^3	Block, yellow
$Z = 8$	$0.40 \times 0.25 \times 0.21$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	5173 independent reflections
	3581 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.049$
Absorption correction: multi-scan ($SADABS$; Sheldrick, 2002)	$\theta_{max} = 25.1°$
	$h = -33 \rightarrow 33$
$T_{min} = 0.768$, $T_{max} = 0.869$	$k = -10 \rightarrow 12$
15092 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0889P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.064$	$+ 12.2245P]$
$wR(F^2) = 0.202$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
5173 reflections	$\Delta\rho_{max} = 0.89$ e Å^{-3}
379 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Mn1—N1	2.357 (4)	Mn1—N4	2.206 (4)
Mn1—N2	2.223 (4)	Mn1—N5	2.294 (4)
Mn1—N3	2.367 (4)	Mn1—N6	2.228 (4)
N4—Mn1—N2	101.62 (14)	N6—Mn1—N1	93.23 (14)
N4—Mn1—N6	109.41 (15)	N5—Mn1—N1	86.65 (13)
N2—Mn1—N6	104.12 (14)	N4—Mn1—N3	71.51 (15)
N4—Mn1—N5	99.32 (14)	N2—Mn1—N3	89.95 (13)
N2—Mn1—N5	158.56 (14)	N6—Mn1—N3	165.15 (15)
N6—Mn1—N5	72.80 (15)	N5—Mn1—N3	92.38 (14)
N4—Mn1—N1	157.35 (14)	N1—Mn1—N3	86.50 (13)
N2—Mn1—N1	72.22 (13)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots$O7^i	0.93	2.56	3.390 (13)	148
C11—H11$\cdots$O1^{ii}	0.93	2.58	3.326 (8)	138
C14—H14$\cdots$O2	0.93	2.57	3.466 (7)	163
C17—H17$\cdots$O5	0.93	2.57	3.362 (8)	144
C19—H19$\cdots$O3^{iii}	0.93	2.53	3.431 (8)	163
C22—H22$\cdots$O5^{iii}	0.93	2.57	3.464 (8)	163

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

H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 Å (methylene), and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

References

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