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Key indicators

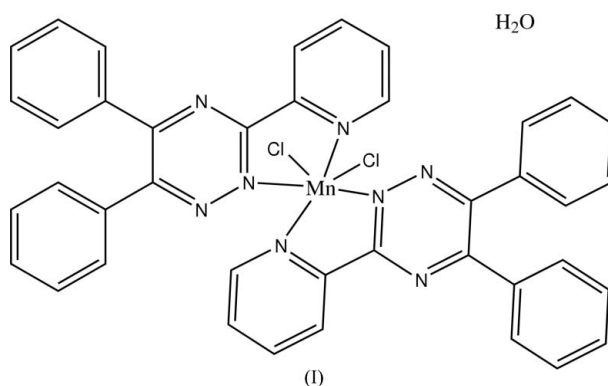
Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.036
 wR factor = 0.083
Data-to-parameter ratio = 14.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis[5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine- $\kappa^2\text{N},\text{N}'$]manganese(II) monohydrate

In the molecule of the title compound, $[\text{MnCl}_2(\text{C}_{20}\text{H}_{14}\text{N}_4)_2] \cdot \text{H}_2\text{O}$, the Mn atom is chelated by two 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine molecules in bidentate manner and bonded to two Cl atoms in a distorted octahedral environment. Intra- and intermolecular $\text{C}-\text{H} \cdots \text{Cl}$ and $\text{O}-\text{H} \cdots \text{Cl}$ hydrogen bonds, and also $\pi-\pi$ and $\text{C}-\text{H} \cdots \pi$ interactions may be effective in the stabilization of the crystal structure.

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Comment

There have been relatively fewer reports of 1,2,4-triazine derivatives and their metal complexes compared to the 1,3,5-analogues, although both compounds are well known for their pharmacological and medicinal properties, including anti-cancer and anti-HIV activities (Mashaly *et al.*, 1999; Soudi *et al.*, 2005). The title compound, (I), is an adduct consisting of a Mn atom chelated by two molecules of 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine, *viz.* both pyridyl N atoms and two Cl atoms (Fig. 1). The geometry of the Mn atom is distorted octahedral, with N8 and Cl2 atoms occupying the axial positions, with an angle about the Mn atom of $165.73(6)^\circ$. Atoms N1, N4, N5 and Cl1 occupy the equatorial positions. The bond lengths and angles are in normal ranges (Allen *et al.*, 1987; Orpen *et al.*, 1989) and are comparable with the corresponding ones in the 1,3,5-analogue $[\text{Mn}(\text{NCS})_2(\text{C}_{18}\text{H}_{12}\text{N}_6)_2(\text{CH}_4\text{O})_2]$ (Kim & Han, 2002). The chelated Mn1/N1/C5/C6/N4 and Mn1/N5/C25/C26/N8 fragments are both planar, with maximum deviations of 0.073 (2) (for N1) and 0.015 (2) Å (for C26), respectively, from the least-squares planes of the two fragments. The dihedral angle between the two planes is $85.93(10)^\circ$. Benzene rings *A* (C8–C13), *B* (C15–C20), *C* (C28–C33) and *D* (C35–C40) are, of course, planar; the dihedral angles between them are $A/B = 71.52(12)^\circ$ and $C/D = 56.20(5)^\circ$.



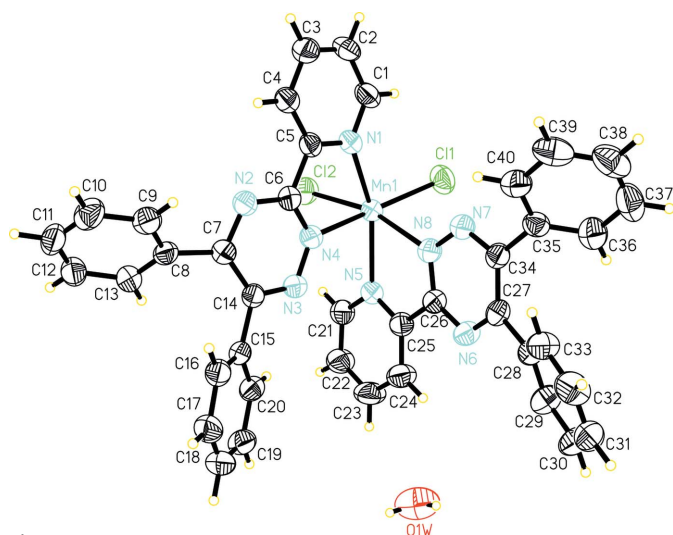


Figure 1
A drawing of the title molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

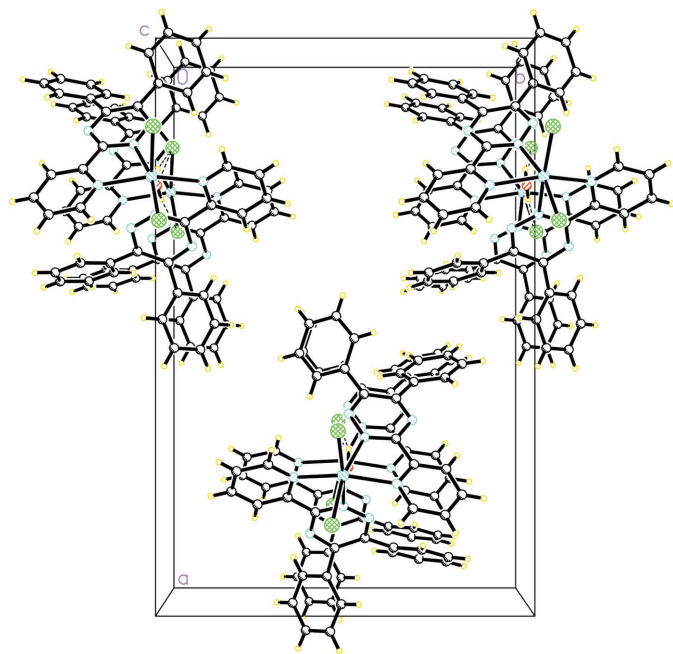


Figure 2
A packing diagram of (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines.

As can be seen from the packing diagram (Fig. 2), intra- and intermolecular C—H···Cl and O—H···Cl hydrogen bonds (Table 2) link the molecules along the *c* axis; they may be effective in the stabilization of the crystal structure. π – π Stacking interactions exist between (Mn1—N5—C25—C26—N8)ⁱⁱ and (Mn1—N1—C5—C6—N4)ⁱⁱ [symmetry code: (ii) *x*, *y*, *z*] chelated rings, with a distance between the two centroids of 3.176 Å; C—H··· π interactions, closest distance of 2.890 Å occurring between C13—H13A and (C8—C13)ⁱⁱⁱ [symmetry code: (iii) $\frac{3}{2} - x, \frac{1}{2} + y, -\frac{1}{2} + z$] centroid with an angle at H of 167°, may also contribute to the stabilization of the crystal structure.

Experimental

To a solution of 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine (0.31 g, 1 mmol) in ethanol (30 ml) was added manganese(II) chloride dihydrate (0.98 g, 0.5 mmol). The mixture was refluxed for 0.5 h. The resultant red–orange solution was filtered and left to slowly evaporate at room temperature. Red crystals were obtained after one week (yield 0.11 g, 31%; m.p. 540.5 K).

Crystal data

[MnCl₂(C₂₀H₁₄N₄)₂]·H₂O
M_r = 764.56
 Orthorhombic, *Pna*2₁
a = 24.610 (5) Å
b = 16.166 (3) Å
c = 8.9590 (17) Å
V = 3564.4 (11) Å³

Z = 4
D_x = 1.425 Mg m⁻³
 Mo *K*α radiation
 μ = 0.57 mm⁻¹
T = 298 (2) K
 Block, red
 0.42 × 0.29 × 0.28 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
T_{min} = 0.797, *T_{max}* = 0.857

19243 measured reflections
 6877 independent reflections
 5788 reflections with *I* > 2σ(*I*)
R_{int} = 0.026
 θ_{\max} = 26.0°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.036
wR (*F*²) = 0.083
S = 1.01
 6877 reflections
 475 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2 + 0.1974P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$
 Absolute structure: Flack (1983), with 3152 Friedel pairs
 Flack parameter: 0.00 (1)

Table 1

Selected geometric parameters (Å, °).

Mn1—N1	2.236 (2)	N2—C6	1.337 (3)
Mn1—N5	2.254 (2)	N3—N4	1.346 (3)
Mn1—N8	2.338 (2)	N4—C6	1.327 (3)
Mn1—N4	2.372 (2)	N6—C27	1.323 (3)
Mn1—Cl1	2.4313 (9)	N6—C26	1.334 (3)
Mn1—Cl2	2.4770 (9)	N7—C34	1.326 (3)
N2—C7	1.321 (3)	N7—N8	1.341 (3)
N1—Mn1—N5	152.48 (8)	N8—Mn1—Cl1	87.91 (6)
N1—Mn1—N8	98.75 (8)	N4—Mn1—Cl1	165.74 (6)
N5—Mn1—N8	71.85 (8)	N1—Mn1—Cl2	90.39 (6)
N1—Mn1—N4	70.86 (7)	N5—Mn1—Cl2	95.05 (6)
N5—Mn1—N4	82.03 (7)	N8—Mn1—Cl2	165.73 (6)
N8—Mn1—N4	81.38 (8)	N4—Mn1—Cl2	91.41 (6)
N1—Mn1—Cl1	101.77 (6)	Cl1—Mn1—Cl2	101.00 (4)
N5—Mn1—Cl1	103.61 (6)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C21—H21A···Cl2	0.93	2.83	3.486 (3)	129
O1W—H1WA···Cl2 ⁱ	0.83 (3)	2.44 (4)	3.264 (4)	171 (4)
O1W—H1WB···Cl1 ⁱ	0.84 (2)	2.54 (3)	3.249 (4)	143 (3)

Symmetry code: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, z - \frac{1}{2}$.

H atoms of the water molecule were located in difference syntheses, and refined with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. The remaining H atoms were positioned geometrically, with C–H = 0.93 Å, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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