Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis[5-(2-pyridylmethyl)-tetrazolato-κ^2N^1,N^5]manganese(II)

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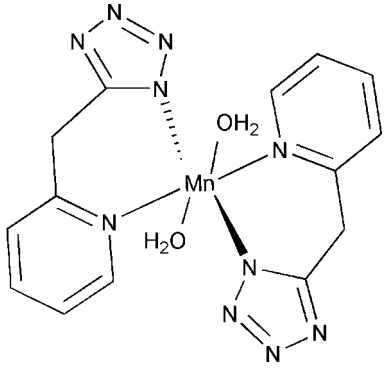
Received 20 June 2008; accepted 25 June 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.059; wR factor = 0.173; data-to-parameter ratio = 14.8.

The title complex, $[Mn(C_7H_6N_5)_2(H_2O)_2]$, was obtained by the *in situ* hydrothermal reaction of $MnCl_2$ with 2-(2-pyridyl)acetonitrile in the presence of NaN_3. The Mn^{II} atom, which is located on an inversion centre, has a distorted octahedral coordination geometry formed by two water molecules and two chelating ligands. Intermolecular hydrogen bonds and π–π interactions (3.452 Å) stabilize the crystal structure and lead to the formation of a three-dimensional network.

Related literature

For related literature, see: Demko & Sharpless (2001); Zhao *et al.* (2008). For the synthesis of similar complexes, see: Hu *et al.* (2007); Liu & Fan (2007).



Experimental

Crystal data

$[Mn(C_7H_6N_5)_2(H_2O)_2]$
M_r = 411.31
Monoclinic, $P2_1/n$
a = 6.638 (2) Å
b = 13.788 (5) Å
c = 8.771 (3) Å
β = 90.01 (5)°
V = 802.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.86 mm^{-1}
T = 293 (2) K
0.20 × 0.12 × 0.12 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.802, T_{max} = 1.000
(expected range = 0.723–0.902)
8070 measured reflections
1836 independent reflections
1550 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.172
S = 1.13
1836 reflections
124 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···N2^{i}	0.96	2.04	2.889 (8)	146
O1—H1B···N5^{i}	0.96	2.45	3.371 (8)	162
O1—H1C···N4^{ii}	0.96	1.96	2.786 (8)	142
C6—H6A···N5^{iii}	0.97	2.60	3.343 (5)	133

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Starter Fund of Southeast University for financial support to buy the CCD X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2418).

References

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supporting information

Acta Cryst. (2008). E**64**, m999 [doi:10.1107/S1600536808019272]

Diaquabis[5-(2-pyridylmethyl)tetrazolato-κ^2N^1,N^5]manganese(II)

Wei Wang

S1. Comment

Since Sharpless *et al.* reported the environmentally friendly process for the preparation of tetrazole (Demko & Sharpless, 2001), many novel tetrazole compounds have been reported through 2 + 3 cycloaddition reactions. Work in our group have found that single crystals of coordination polymers can often be generated under hydrothermal conditions through *in situ* synthesis. (Zhao *et al.*, 2008) The title complex was obtained by the *in situ* hydrothermal reaction of $MnCl_2$ with pyridin-2-yl-acetonitrile in the presence of NaN_3.

In the title compound, the central Mn(II) ion is located on an inversion center and coordinated by two water molecules and two 5-(pyridin-2-ylmethyl)tetrazolate ligands through the pyridine N and tetrazole N atoms with a distorted octahedral geometry (Fig. 1). Extensive intermolecular O—H···N and C—H···N hydrogen bonds and π-π interactions stabilize the crystal structure which leads to the formation of a three-dimensional network.

S2. Experimental

A mixture of pyridin-2-yl-acetonitrile (26 mg, 0.2 mmol), NaN_3 (26 mg, 0.4 mmol), $MnCl_2.4H_2O$(59.3 mg, 0.3 mmol), ethanol (1 ml) and a few drops of water sealed in a glass tube was maintained at 105°C. Colorless crystals suitable for X-ray analysis were obtained after a week.

S3. Refinement

The C-bound H atoms were placed in calculated positions (C—H 0.93 Å) and treated in the subsequent refinement as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C) while the water H atoms were located in Fourier difference map and refined with U_{iso}(H) = 1.5U_{eq}(O).

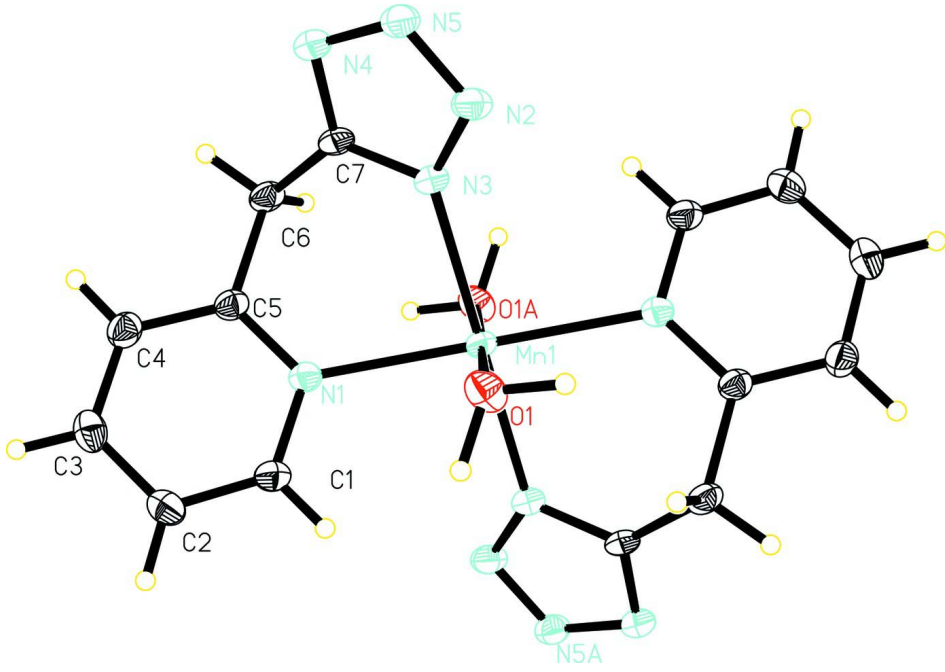

Figure 1

The molecular structure of the compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level. [symmetry code: -x, -y+2, -z+2]

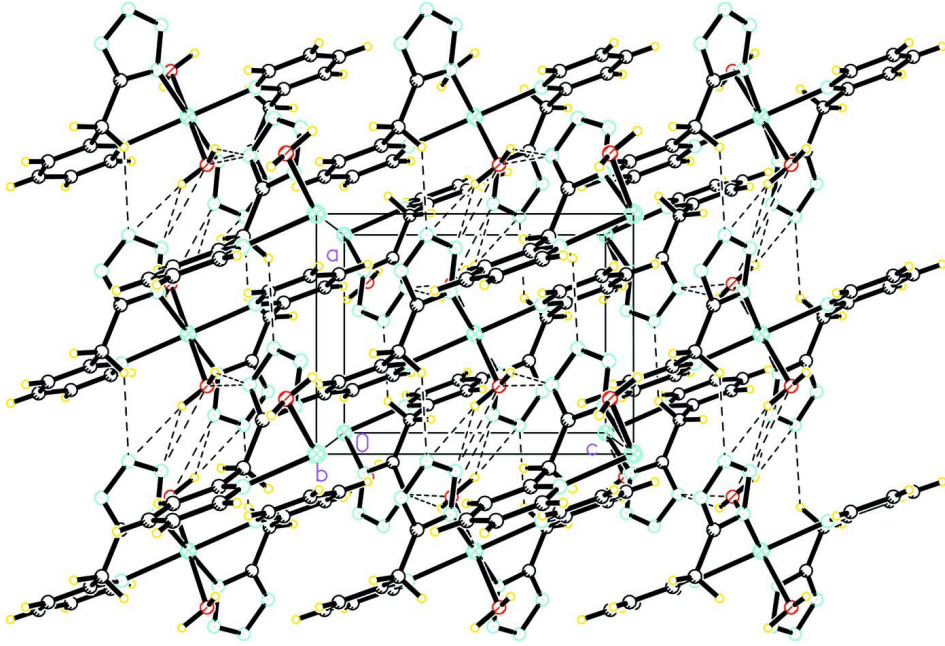

Figure 2

The packing view of title compound with $\pi\cdots\pi$ stacking along the *b* axis.

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Crystal data

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Hall symbol: -P 2yn
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$b = 13.788$ (5) Å
$c = 8.771$ (3) Å
$\beta = 90.01$ (5)°
$V = 802.9$ (4) Å^3
$Z = 2$
$F(000) = 422$
$D_x = 1.701$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2050 reflections
$\theta = 2.8$–$27.5°$
$\mu = 0.86$ mm^{-1}
$T = 293$ K
Prism, colorless
0.20 × 0.12 × 0.12 mm

Data collection

Rigaku Mercury2) diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.802$, $T_{max} = 1.000$
8070 measured reflections
1836 independent reflections
1550 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -8 \rightarrow 8$
$k = -17 \rightarrow 17$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.173$
$S = 1.13$
1836 reflections
124 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0834P)^2 + 0.8368P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.0000	1.0000	1.0000	0.0261 (3)
N5	0.4367 (4)	0.7962 (2)	0.8387 (3)	0.0354 (7)
O1	0.2353 (4)	1.10029 (18)	0.9172 (3)	0.0382 (6)
H1B	0.3241	1.1164	0.9997	0.057*

H1C	0.1730	1.1583	0.8792	0.057*
N3	0.1879 (4)	0.88112 (19)	0.9162 (3)	0.0299 (6)
C7	0.1284 (5)	0.8238 (2)	0.8048 (4)	0.0275 (7)
N2	0.3843 (4)	0.8625 (2)	0.9339 (3)	0.0346 (7)
N4	0.2778 (4)	0.7701 (2)	0.7545 (3)	0.0332 (6)
C6	−0.0793 (5)	0.8223 (2)	0.7415 (4)	0.0317 (7)
H6A	−0.1720	0.8028	0.8214	0.038*
H6B	−0.0860	0.7738	0.6614	0.038*
C5	−0.1465 (5)	0.9175 (2)	0.6782 (4)	0.0289 (7)
C4	−0.2173 (5)	0.9233 (3)	0.5316 (4)	0.0359 (8)
H4A	−0.2262	0.8677	0.4720	0.043*
C3	−0.2743 (6)	1.0105 (3)	0.4737 (4)	0.0371 (8)
H3A	−0.3202	1.0155	0.3738	0.045*
C2	−0.2628 (6)	1.0907 (3)	0.5649 (4)	0.0377 (8)
H2A	−0.3022	1.1513	0.5290	0.045*
C1	−0.1925 (5)	1.0797 (2)	0.7089 (4)	0.0340 (8)
H1A	−0.1832	1.1345	0.7704	0.041*
N1	−0.1363 (4)	0.99533 (17)	0.7671 (3)	0.0273 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0329 (4)	0.0185 (4)	0.0270 (4)	0.0025 (2)	−0.0001 (3)	−0.0016 (2)
N5	0.0353 (15)	0.0297 (15)	0.0413 (16)	0.0058 (12)	−0.0018 (12)	−0.0047 (12)
O1	0.0381 (13)	0.0326 (13)	0.0439 (14)	−0.0103 (10)	−0.0061 (11)	0.0116 (11)
N3	0.0341 (15)	0.0230 (13)	0.0326 (14)	0.0049 (11)	−0.0004 (11)	−0.0030 (11)
C7	0.0324 (16)	0.0155 (13)	0.0345 (16)	0.0003 (11)	0.0025 (13)	−0.0007 (12)
N2	0.0328 (15)	0.0265 (14)	0.0446 (16)	0.0041 (11)	−0.0027 (12)	−0.0019 (12)
N4	0.0371 (15)	0.0253 (13)	0.0371 (16)	0.0054 (11)	−0.0003 (12)	−0.0037 (12)
C6	0.0339 (17)	0.0217 (15)	0.0395 (17)	−0.0018 (12)	−0.0022 (14)	−0.0058 (13)
C5	0.0271 (15)	0.0245 (15)	0.0349 (17)	−0.0007 (12)	−0.0006 (13)	−0.0032 (13)
C4	0.0334 (17)	0.0372 (19)	0.0373 (18)	0.0010 (14)	−0.0045 (14)	−0.0081 (15)
C3	0.0299 (18)	0.051 (2)	0.0303 (17)	−0.0013 (14)	−0.0013 (14)	0.0029 (15)
C2	0.0399 (19)	0.0357 (18)	0.0376 (18)	0.0039 (15)	−0.0015 (15)	0.0079 (15)
C1	0.0417 (19)	0.0246 (16)	0.0357 (17)	0.0038 (13)	0.0001 (14)	0.0003 (13)
N1	0.0289 (14)	0.0239 (14)	0.0291 (14)	0.0009 (9)	0.0012 (11)	0.0003 (10)

Geometric parameters (Å, º)

Mn1—N3	2.187 (5)	C6—H6A	0.9700
Mn1—O1	2.209 (5)	C6—H6B	0.9700
Mn1—N1	2.235 (3)	C5—N1	1.328 (5)
N5—N2	1.286 (5)	C5—C4	1.371 (6)
N5—N4	1.337 (5)	C4—C3	1.359 (6)
O1—H1B	0.9600	C4—H4A	0.9300
O1—H1C	0.9600	C3—C2	1.367 (6)
N3—C7	1.317 (5)	C3—H3A	0.9300
N3—N2	1.338 (6)	C2—C1	1.355 (6)

C7—N4	1.314 (5)	C2—H2A	0.9300
C7—C6	1.487 (6)	C1—N1	1.324 (5)
C6—C5	1.494 (6)	C1—H1A	0.9300
N3—Mn1—O1	87.43 (11)	C7—C6—H6B	108.8
N3^{i}—Mn1—O1	92.57 (5)	C5—C6—H6B	108.8
N3—Mn1—N1	84.39 (17)	H6A—C6—H6B	107.7
N3^{i}—Mn1—N1	95.61 (17)	N1—C5—C4	121.4 (3)
O1^{i}—Mn1—N1	89.79 (18)	N1—C5—C6	118.5 (4)
O1—Mn1—N1	90.21 (18)	C4—C5—C6	120.1 (3)
N2—N5—N4	109.6 (3)	C3—C4—C5	119.9 (3)
Mn1—O1—H1B	109.3	C3—C4—H4A	120.1
Mn1—O1—H1C	109.3	C5—C4—H4A	120.1
H1B—O1—H1C	109.5	C4—C3—C2	118.8 (4)
C7—N3—N2	105.3 (3)	C4—C3—H3A	120.6
C7—N3—Mn1	121.9 (3)	C2—C3—H3A	120.6
N2—N3—Mn1	131.4 (2)	C1—C2—C3	118.3 (4)
N3—C7—N4	111.1 (3)	C1—C2—H2A	120.9
N3—C7—C6	124.3 (3)	C3—C2—H2A	120.9
N4—C7—C6	124.5 (3)	N1—C1—C2	123.7 (3)
N5—N2—N3	109.0 (3)	N1—C1—H1A	118.2
C7—N4—N5	105.0 (3)	C2—C1—H1A	118.2
C7—C6—C5	113.8 (3)	C1—N1—C5	118.0 (4)
C7—C6—H6A	108.8	C1—N1—Mn1	116.2 (2)
C5—C6—H6A	108.8	C5—N1—Mn1	125.5 (2)
O1^{i}—Mn1—N3—C7	64.4 (3)	C7—C6—C5—C4	125.9 (3)
O1—Mn1—N3—C7	−115.6 (3)	N1—C5—C4—C3	1.5 (5)
N1—Mn1—N3—C7	−25.2 (3)	C6—C5—C4—C3	−178.6 (3)
O1^{i}—Mn1—N3—N2	−131.9 (3)	C5—C4—C3—C2	−1.1 (6)
O1—Mn1—N3—N2	48.1 (3)	C4—C3—C2—C1	0.8 (6)
N1—Mn1—N3—N2	138.5 (3)	C3—C2—C1—N1	−0.8 (6)
N1^{i}—Mn1—N3—N2	−41.5 (3)	C2—C1—N1—C5	1.1 (5)
N2—N3—C7—N4	0.8 (4)	C2—C1—N1—Mn1	174.6 (3)
Mn1—N3—C7—N4	168.2 (2)	C4—C5—N1—C1	−1.5 (5)
N2—N3—C7—C6	−177.6 (3)	C6—C5—N1—C1	178.7 (3)
Mn1—N3—C7—C6	−10.2 (4)	C4—C5—N1—Mn1	−174.3 (2)
N4—N5—N2—N3	0.7 (4)	C6—C5—N1—Mn1	5.9 (4)
C7—N3—N2—N5	−0.9 (4)	N3—Mn1—N1—C1	−145.1 (3)
Mn1—N3—N2—N5	−166.6 (2)	N3^{i}—Mn1—N1—C1	34.9 (3)
N3—C7—N4—N5	−0.3 (4)	O1^{i}—Mn1—N1—C1	122.3 (3)
C6—C7—N4—N5	178.0 (3)	O1—Mn1—N1—C1	−57.7 (3)
N2—N5—N4—C7	−0.3 (4)	N3—Mn1—N1—C5	27.8 (3)
N3—C7—C6—C5	59.0 (5)	N3^{i}—Mn1—N1—C5	−152.2 (3)
N4—C7—C6—C5	−119.2 (4)	O1^{i}—Mn1—N1—C5	−64.8 (3)
C7—C6—C5—N1	−54.2 (4)	O1—Mn1—N1—C5	115.2 (3)

Symmetry code: (i) $-x$, $-y+2$, $-z+2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···N2^{ii}	0.96	2.04	2.889 (8)	146
O1—H1*B*···N5^{ii}	0.96	2.45	3.371 (8)	162
O1—H1*C*···N4^{iii}	0.96	1.96	2.786 (8)	142
C6—H6*A*···N5^{iv}	0.97	2.60	3.343 (5)	133

Symmetry codes: (ii) −*x*+1, −*y*+2, −*z*+2; (iii) −*x*+1/2, *y*+1/2, −*z*+3/2; (iv) *x*−1, *y*, *z*.