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Diazidobis[(1-methyl-1*H*-benzimidazol-2-yl)methanol-κ^2N^3,O]manganese(II)

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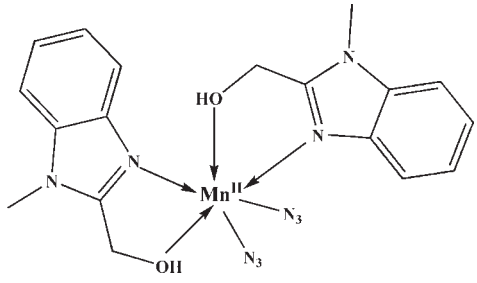
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.116; data-to-parameter ratio = 12.3.

The title complex, $[Mn(N_3)_2(C_9H_{10}N_2O)_2]$, possesses crystallographically imposed twofold symmetry. The Mn^{II} atom is coordinated by four N atoms and two O atoms in a distorted octahedral geometry. The crystal packing is stabilized by strong intermolecular O—H···N hydrogen bonds.

Related literature

For the synthesis of the ligand, see: van Albada *et al.* (1995) and literature cited therein. For the metal(II) complexes of a similar *N*-heterocycle, see: Zeng *et al.* (2006); Zhou *et al.* (2007); Alagna *et al.* (1984); Hamilton *et al.* (1979).



Experimental

Crystal data

$[Mn(N_3)_2(C_9H_{10}N_2O)_2]$
M_r = 463.38
Monoclinic, $C2/c$
a = 15.466 (3) Å
b = 7.5438 (16) Å
c = 18.095 (4) Å
β = 109.989 (4)°
V = 1984.0 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.71 mm^{-1}
T = 173 K
0.33 × 0.22 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
T_{min} = 0.801, T_{max} = 0.933
4125 measured reflections
1741 independent reflections
1345 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.116
S = 1.02
1741 reflections
142 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—Mn1	2.302 (2)	Mn1—N1	2.176 (2)
Mn1—N3	2.172 (3)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N5^{ii}	0.85	1.85	2.701 (4)	178

Symmetry code: (ii) $x, y-1, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2238).

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supporting information

Acta Cryst. (2010). E**66**, m188 [https://doi.org/10.1107/S1600536810002126]

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S1. Comment

The coordinated modes of (1-methyl-1*H*-benzimidazol-2-yl)methanol ligand are similar to our previously repored benzimidazol-2-yl methanol from the structural point, the latter has been shown to bind to cobalt(II) as a neutral chelate (Zeng *et al.*, 2006, Zhou *et al.*, 2007). This feature is also preserved in the present manganese(II) complex.

In the title compound, the ligand chelates through the hydroxyl O and imino N atoms, resulting in a N_4O_2Mn octahedral geometry at the metal center (Fig. 1, Table 1), like that observed in copper (Hamilton *et al.*, 1979) and nickel (Alagna *et al.*, 1984) adducts. In this structure, the azide anion as a terminal ligand coordinated to Mn^{II} atom, and N–N–N bond lengths and bond angle are close to compound $[Cu(tbz)(N_3)_2]_2(CH_3OH)_2$ (tbz = bis(2-benzimidazolyl)propane) (Albada *et al.*, 1995).The complex possesses crystallographically imposed twofold symmetry. The crystal packing is stabilized by strong intermolecular O—H···N hydrogen bonds which extend along the crystallographic twofold rotation axis (Fig. 2, Table 2).

S2. Experimental

(1-methyl-1*H*-benzimidazol-2-yl)methanol was purchased from a chemical supplier. This reagent (0.16 g, 1 mmol), manganese(II) nitrate hexahydrate (0.14 g, 0.5 mmol) and sodium azide (0.07 g, 1 mmol) were dissolved in water (10 ml) that was kept at about 333 K. Colorless blocks separated from the solution after one week.

S3. Refinement

The C-bound H atoms were placed in calculated positions (C—H = 0.93–0.98 Å) and included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2(1.5)U_{eq}(C, C_{methyl}). The hydroxy H atom has been located in a difference Fourier map and refined isotropically with a distance restraint of O—H = 0.85 (1) Å, and U_{iso}(H) = 1.2U_{eq}(O).

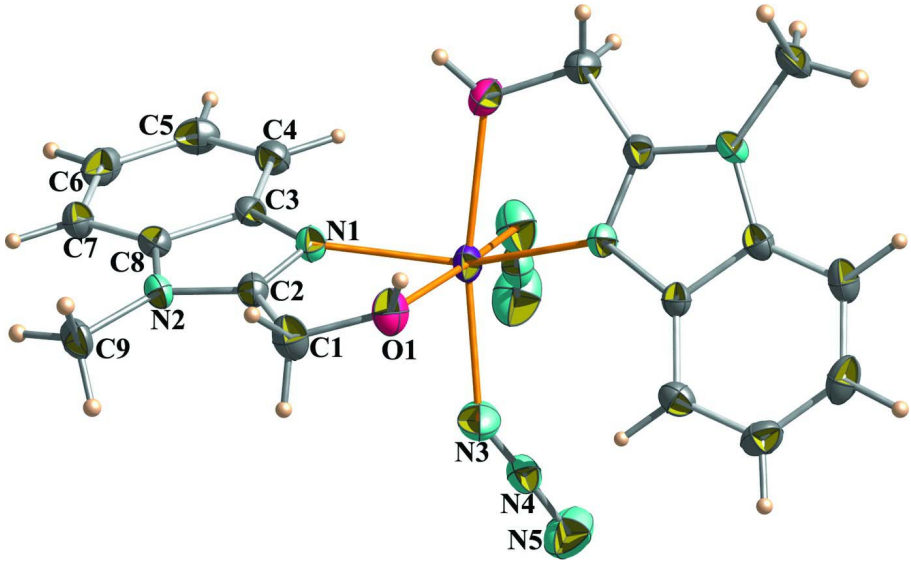

Figure 1

Anisotropic displacement ellipsoid plot of the $[Mn(II)(N_3)_2(C_9H_{10}N_2O)_2]$ molecule at the 50% probability level; hydrogen atoms are drawn as sphere of arbitrary radius. Symmetry codes: (i) -*x*, *y*, -*z* + 1/2, for the unlabelled atoms.

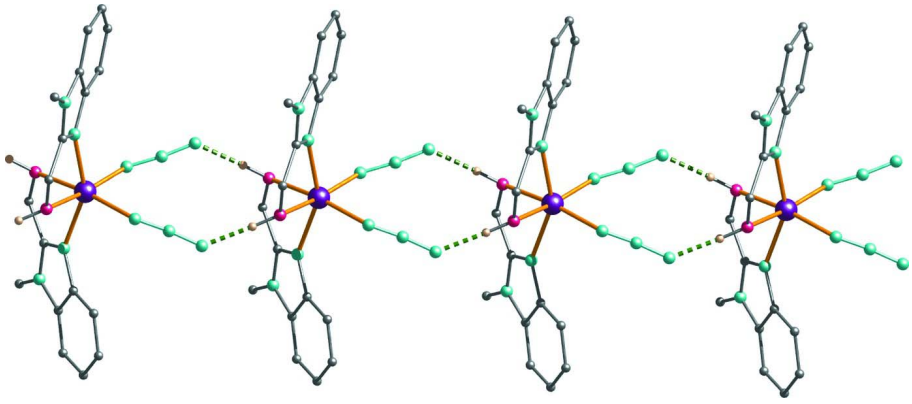

Figure 2

Part of the hydrogen bonded chain along [010] direction. Hydrogen bonds are shown as dashed lines. Symmetry codes: (i) *x*, *y* - 1, *z*.

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Crystal data

$[Mn(N_3)_2(C_9H_{10}N_2O)_2]$
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Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 15.466 (3) Å
b = 7.5438 (16) Å
c = 18.095 (4) Å
β = 109.989 (4)°
V = 1984.0 (7) Å^3
Z = 4
F(000) = 956
D_x = 1.551 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 1818 reflections
θ = 2.4–26.7°
μ = 0.71 mm^{-1}
T = 173 K
Block, colorless
0.33 × 0.22 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
T_{min} = 0.801, T_{max} = 0.933
4125 measured reflections
1741 independent reflections
1345 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.0°, θ_{min} = 2.8°
h = −16→18
k = −8→8
l = −15→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.116
S = 1.02
1741 reflections
142 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
$w = 1/[\sigma^2(F_o^2) + (0.0608P)^2 + 4.1072P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

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.
In Checkcif report, the following ALERTS were generated
PLAT230_ALERT_2_C Hirshfeld Test Diff for N3 – N4.. 5.98 su Author response: It is due to electron shift or resonance (N=N–N or N–N=N) bond lengths appear shorter than expected, see: Albada *et al.* (1995).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.12170 (15)	0.1356 (3)	0.26588 (12)	0.0324 (5)
H1	0.1264	0.0343	0.2875	0.049*
Mn1	0.0000	0.32504 (9)	0.2500	0.0247 (2)
N1	−0.00030 (17)	0.2562 (3)	0.13315 (13)	0.0228 (6)
N2	0.07803 (16)	0.1833 (3)	0.05480 (14)	0.0226 (5)
N3	0.1101 (2)	0.5198 (4)	0.28397 (17)	0.0405 (7)
N4	0.11891 (18)	0.6678 (4)	0.30523 (15)	0.0324 (7)
N5	0.1360 (3)	0.8099 (4)	0.3311 (2)	0.0545 (9)
C1	0.1524 (2)	0.1270 (5)	0.20037 (18)	0.0316 (8)
H1A	0.1698	0.0038	0.1928	0.038*
H1B	0.2070	0.2037	0.2096	0.038*
C2	0.0761 (2)	0.1879 (4)	0.12911 (17)	0.0226 (6)
C3	−0.05362 (19)	0.2995 (4)	0.05571 (17)	0.0208 (6)
C4	−0.1407 (2)	0.3733 (4)	0.02570 (18)	0.0257 (7)
H4A	−0.1745	0.4034	0.0590	0.031*
C5	−0.1764 (2)	0.4013 (4)	−0.05442 (18)	0.0307 (7)
H5A	−0.2359	0.4520	−0.0767	0.037*

C6	−0.1269 (2)	0.3569 (4)	−0.10337 (18)	0.0331 (8)
H6A	−0.1538	0.3782	−0.1583	0.040*
C7	−0.0403 (2)	0.2830 (4)	−0.07448 (18)	0.0289 (7)
H7B	−0.0068	0.2526	−0.1080	0.035*
C8	−0.0045 (2)	0.2554 (4)	0.00618 (17)	0.0230 (6)
C9	0.1533 (2)	0.1183 (5)	0.03086 (19)	0.0309 (7)
H9A	0.1617	−0.0089	0.0419	0.046*
H9B	0.2100	0.1814	0.0602	0.046*
H9C	0.1387	0.1388	−0.0256	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0388 (13)	0.0343 (13)	0.0242 (11)	0.0082 (10)	0.0111 (10)	0.0071 (9)
Mn1	0.0313 (4)	0.0266 (4)	0.0185 (3)	0.000	0.0116 (3)	0.000
N1	0.0244 (13)	0.0266 (14)	0.0183 (12)	0.0014 (11)	0.0087 (10)	−0.0004 (10)
N2	0.0221 (13)	0.0260 (13)	0.0238 (12)	0.0008 (10)	0.0129 (10)	−0.0026 (10)
N3	0.0522 (19)	0.0308 (18)	0.0451 (18)	−0.0144 (14)	0.0254 (15)	−0.0073 (14)
N4	0.0325 (15)	0.043 (2)	0.0243 (14)	−0.0057 (14)	0.0135 (12)	0.0027 (13)
N5	0.081 (3)	0.0340 (19)	0.048 (2)	−0.0135 (18)	0.0225 (19)	−0.0063 (16)
C1	0.0296 (17)	0.0375 (19)	0.0296 (17)	0.0092 (14)	0.0125 (14)	0.0043 (14)
C2	0.0248 (16)	0.0230 (16)	0.0214 (14)	−0.0001 (13)	0.0096 (12)	−0.0014 (12)
C3	0.0216 (15)	0.0198 (15)	0.0221 (14)	−0.0029 (12)	0.0088 (12)	0.0016 (11)
C4	0.0231 (16)	0.0266 (17)	0.0295 (16)	−0.0012 (13)	0.0117 (13)	−0.0016 (13)
C5	0.0238 (16)	0.0314 (18)	0.0314 (17)	0.0006 (14)	0.0023 (14)	0.0036 (14)
C6	0.0376 (19)	0.036 (2)	0.0205 (15)	−0.0087 (15)	0.0031 (14)	0.0024 (13)
C7	0.0333 (18)	0.0334 (19)	0.0235 (15)	−0.0070 (14)	0.0140 (14)	−0.0023 (13)
C8	0.0233 (15)	0.0240 (15)	0.0237 (15)	−0.0033 (12)	0.0106 (12)	−0.0022 (12)
C9	0.0273 (17)	0.0376 (19)	0.0330 (17)	0.0039 (14)	0.0170 (14)	−0.0043 (14)

Geometric parameters (Å, º)

O1—C1	1.421 (4)	C1—H1A	0.9900
O1—Mn1	2.302 (2)	C1—H1B	0.9900
O1—H1	0.8500	C3—C4	1.385 (4)
Mn1—N3	2.172 (3)	C3—C8	1.399 (4)
Mn1—N3^{i}	2.172 (3)	C4—C5	1.380 (4)
Mn1—N1	2.176 (2)	C4—H4A	0.9500
Mn1—N1^{i}	2.176 (2)	C5—C6	1.395 (5)
Mn1—O1^{i}	2.302 (2)	C5—H5A	0.9500
N1—C2	1.314 (4)	C6—C7	1.379 (5)
N1—C3	1.400 (4)	C6—H6A	0.9500
N2—C2	1.355 (4)	C7—C8	1.388 (4)
N2—C8	1.389 (4)	C7—H7B	0.9500
N2—C9	1.459 (4)	C9—H9A	0.9800
N3—N4	1.174 (4)	C9—H9B	0.9800
N4—N5	1.163 (4)	C9—H9C	0.9800
C1—C2	1.492 (4)		

C1—O1—Mn1	114.60 (17)	C2—C1—H1B	110.0
C1—O1—H1	110.0	H1A—C1—H1B	108.4
Mn1—O1—H1	123.6	N1—C2—N2	113.0 (3)
N3—Mn1—N3^{i}	94.89 (17)	N1—C2—C1	122.2 (3)
N3—Mn1—N1	100.23 (10)	N2—C2—C1	124.8 (3)
N3^{i}—Mn1—N1	98.36 (10)	C4—C3—C8	120.8 (3)
N3—Mn1—N1^{i}	98.36 (10)	C4—C3—N1	130.3 (3)
N3^{i}—Mn1—N1^{i}	100.23 (10)	C8—C3—N1	108.8 (3)
N1—Mn1—N1^{i}	152.37 (14)	C5—C4—C3	117.4 (3)
N3—Mn1—O1^{i}	169.59 (9)	C5—C4—H4A	121.3
N3^{i}—Mn1—O1^{i}	81.74 (10)	C3—C4—H4A	121.3
N1—Mn1—O1^{i}	90.02 (9)	C4—C5—C6	121.4 (3)
N1^{i}—Mn1—O1^{i}	72.72 (8)	C4—C5—H5A	119.3
N3—Mn1—O1	81.74 (10)	C6—C5—H5A	119.3
N3^{i}—Mn1—O1	169.59 (9)	C7—C6—C5	122.0 (3)
N1—Mn1—O1	72.72 (8)	C7—C6—H6A	119.0
N1^{i}—Mn1—O1	90.02 (9)	C5—C6—H6A	119.0
O1^{i}—Mn1—O1	103.23 (12)	C6—C7—C8	116.5 (3)
C2—N1—C3	105.6 (2)	C6—C7—H7B	121.8
C2—N1—Mn1	116.39 (19)	C8—C7—H7B	121.8
C3—N1—Mn1	136.2 (2)	C7—C8—N2	132.4 (3)
C2—N2—C8	106.9 (2)	C7—C8—C3	121.9 (3)
C2—N2—C9	126.4 (3)	N2—C8—C3	105.7 (2)
C8—N2—C9	126.6 (2)	N2—C9—H9A	109.5
N4—N3—Mn1	136.7 (3)	N2—C9—H9B	109.5
N5—N4—N3	173.4 (4)	H9A—C9—H9B	109.5
O1—C1—C2	108.4 (2)	N2—C9—H9C	109.5
O1—C1—H1A	110.0	H9A—C9—H9C	109.5
C2—C1—H1A	110.0	H9B—C9—H9C	109.5
O1—C1—H1B	110.0		

Symmetry code: (i) $-x, y, -z+1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N5^{ii}	0.85	1.85	2.701 (4)	178

Symmetry code: (ii) $x, y-1, z$.