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Retraction of articles

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This article reports the retraction of 11 articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), 11 additional articles are retracted by the authors or by the journal as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1
Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
[N,N′-Bis(2-hydroxynaphthylmethylene)-1,2-ethanediaminato]zinc(II)	Chen *et al.* (2005)	10.1107/S1600536805026796	YAWZOM
Diazidobis(2,2′-biimidazole)copper(II)	Liu *et al.* (2007)	10.1107/S1600536807047873	SILZIX
Dichlorido(1,10-phenanthroline)copper(II)	Liu (2007)	10.1107/S1600536807056735	MISSAJ
Diazidobis(2,2′-biimidazole)cobalt(II)	Li *et al.* (2008)	10.1107/S1600536807062873	MIRYAO
Diazidobis(2,2′-biimidazole)manganese(II)	Zhang *et al.* (2008)	10.1107/S1600536808017984	MODBUD
Diazidobis(2,2′-biimidazole)iron(II)	Hao *et al.* (2008*a*)	10.1107/S1600536808018539	MODFOB
Bis(pentane-2,4-dionato)bis[2-(4-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl 3-oxide]nickel(II)	Hao *et al.* (2008*b*)	10.1107/S1600536808018552	MODFUH
Bis(pentane-2,4-dionato-κ^2O,O')bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline-1-oxyl 3-oxide-κN^2]manganese(II)	Liu, Zhang *et al.* (2008)	10.1107/S1600536808022952	MODLUN
Bis[2,4-pentanedionato(1−)]bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline-1-oxyl 3-oxide]manganese(II)	Liu, He *et al.* (2008)	10.1107/S1600536808038440	MODLUN01
Di-μ-chlorido-bis[chlorido(1,10-phenanthroline-κ^2N,N')zinc(II)]	Yang *et al.* (2009)	10.1107/S1600536809014482	JOLBOC
Tris(ethylenediamine)manganese(II) sulfate	Lu (2009)	10.1107/S1600536809034874	YUCZEC

References

Chen, G., Zhao, B., Sun, M. & Qi, W. (2005). *Acta Cryst.* E**61**, m1869–m1870.
Hao, L., Mu, C. & Kong, B. (2008*a*). *Acta Cryst.* E**64**, m956.
Hao, L., Mu, C. & Kong, B. (2008*b*). *Acta Cryst.* E**64**, m957.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Li, S., Wang, S.-B., Zhang, F.-L. & Tang, K. (2008). *Acta Cryst.* E**64**, m76.
Liu, Y.-Q. (2007). *Acta Cryst.* E**63**, m2991.
Liu, Y., Dou, J., Li, D. & Zhang, X. (2007). *Acta Cryst.* E**63**, m2661.
Liu, Y., He, Q., Zhang, X., Xue, Z. & Lv, C. (2008). *Acta Cryst.* E**64**, m1604.
Liu, Y., Zhang, X., Xue, Z., He, Q. & Zhang, Y. (2008). *Acta Cryst.* E**64**, m1077.
Lu, J. (2009). *Acta Cryst.* E**65**, m1187.
Yang, X.-M., Leng, Q.-B., Chen, Y., He, Y.-G. & Luo, S.-W. (2009). *Acta Cryst.* E**65**, m567.
Zhang, X., Wei, P. & Li, B. (2008). *Acta Cryst.* E**64**, m934.

  doi:10.1107/S1600536810053882

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Diazidobis(2,2′-biimidazole)-manganese(II)

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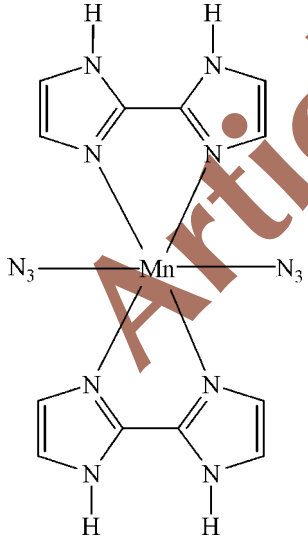
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.131; data-to-parameter ratio = 11.5.

In the title compound, $[Mn(N_3)_2(C_6H_6N_4)_2]$, the Mn atom (site symmetry $\bar{1}$) is bonded to two azide ions and two bidentate biimidizole ligands, resulting in a slightly distorted octahedral MnN_6 geometry for the metal ion. In the crystal structure, N—H···N hydrogen bonds help to consolidate the packing.

Related literature

For a related structure, see: Hester *et al.* (1997).



Experimental

Crystal data

$[Mn(N_3)_2(C_6H_6N_4)_2]$ M_r = 407.30
Monoclinic, $C2/c$
a = 12.5097 (10) Å
b = 8.9728 (5) Å
c = 14.1416 (10) Å
β = 91.883 (10)°
V = 1586.50 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 293 (2) K
0.40 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.723, T_{max} = 0.846
1966 measured reflections
1505 independent reflections
1250 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.131
S = 1.00
1505 reflections
131 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—N2	2.094 (3)	Mn1—N5	2.138 (3)
Mn1—N3	2.114 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N7^{i}	0.966 (18)	2.26 (3)	3.031 (4)	136 (3)
N1—H1A···N5^{ii}	0.966 (18)	2.33 (4)	3.021 (4)	127 (3)
N4—H4···N7^{i}	0.952 (19)	1.92 (2)	2.834 (4)	160 (4)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2744).

References

Bruker (2004). *APEX2*, *SADABS* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hester, C. A., Baughman, R. G. & Collier, H. L. (1997). *Polyhedron*, **16**, 2893–2895.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m934 [doi:10.1107/S1600536808017984]

Diazidobis(2,2′-biimidazole)manganese(II)

Xiutang Zhang, Peihai Wei and Bin Li

S1. Comment

The study of coordination compounds including one-, two- and three-dimensional infinite frameworks has been expanding rapidly because of their fascinating structural diversity and potential application as functional materials. To date, much of the work has been focused on coordination polymers with semi-rigid ligands, such as 4,4′-bipyridine, pyrazine and their analogues. In this paper, we report the structure of the molecular title compound, (I), with the use of the 2,2′-biimidazole bridging ligand (Hester *et al.*, 1997).

As shown in Fig. 1, the Mn ion in (I) occupies an inversion centre, and is hexacoordinated by six N atoms from two chelating ligands of H_2bim (biimidizole; $C_6H_6N_4$) and two azide ions, showing a slightly distorted MnN_6 octahedral geometry (Table 1).

In the crystal of (I), N—H···N hydrogen bonds, one of which is bifurcated (Table 2), help to consolidate the packing.

S2. Experimental

A mixture of manganese(II) perchlorate hexahydrate (1 mmol), 2,2′-biimidazoline (2 mmol) and Na_3N_3 (2 mmol) in 20 ml ethanol was reflued for several hours. The cooled solution was filtered and the filtrate was kept in an ice box for about one week. Yellow blocks of (I) were obtained with a yield of 10%. Anal. Calc. for $C_{12}H_{12}MnN_{14}$: C 35.35, H 2.95, N 48.12%; Found: C 35.31, H 2.92, N 48.06%.

S3. Refinement

The N-bound H atoms were located in a difference map and their positions were freely refined with U_{iso}(H) = 1.2U_{eq}(N). The C-bound H atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

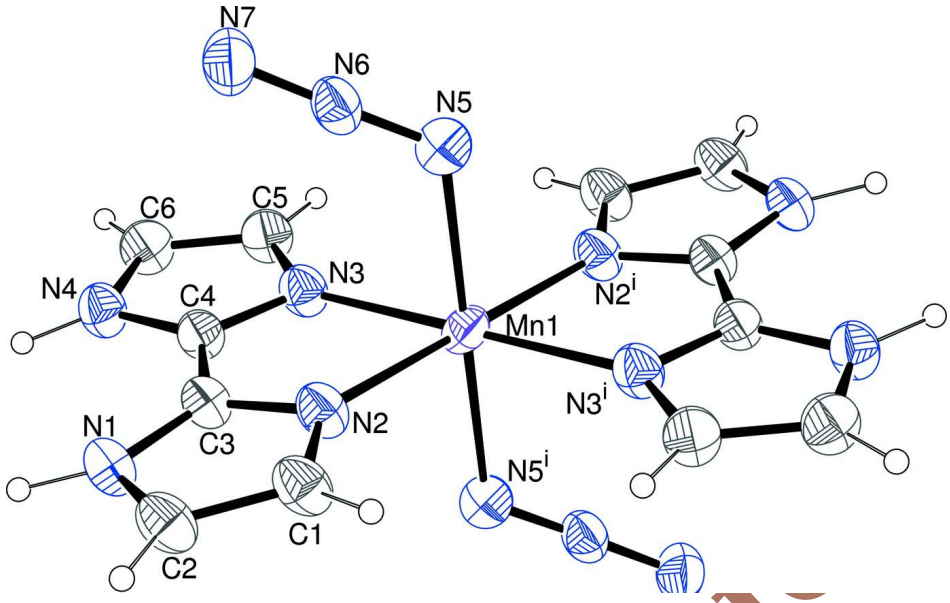

Figure 1

The molecular structure of (I), drawn with 30% probability displacement ellipsoids for the non-hydrogen atoms. Symmetry code: (i) 3/2-*x*, 3/2-*y*, 1-*z*.

Diazidobis(2,2′-biimidazole)manganese(II)

Crystal data

$[Mn(N_3)_2(C_6H_6N_4)_2]$
M_r = 407.30
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 12.5097 (10) Å
b = 8.9728 (5) Å
c = 14.1416 (10) Å
β = 91.883 (10)°
V = 1586.50 (19) Å^3
Z = 4
F(000) = 828
D_x = 1.705 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1505 reflections
θ = 2.8–25.9°
μ = 0.87 mm^{-1}
T = 293 K
Block, yellow
0.40 × 0.26 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.723, T_{max} = 0.846
1966 measured reflections
1505 independent reflections
1250 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.9°, θ_{min} = 2.8°
h = −1→15
k = −1→10
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.131
S = 1.00
1505 reflections
131 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites	$w = 1/[\sigma^2(F_o^2) + (0.081P)^2 + 1.7249P]$ where $P = (F_o^2 + 2F_c^2)/3$
H atoms treated by a mixture of independent and constrained refinement	$(\Delta/\sigma)_{max} = 0.024$
	$\Delta\rho_{max} = 0.49$ e Å^{-3}
	$\Delta\rho_{min} = -0.25$ 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	0.7500	0.7500	0.5000	0.0486 (5)
C1	0.5842 (3)	0.5617 (4)	0.3628 (2)	0.0572 (8)
H1	0.5711	0.6280	0.3132	0.069*
C2	0.5366 (3)	0.4245 (4)	0.3721 (2)	0.0585 (9)
H2	0.4865	0.3819	0.3303	0.070*
C3	0.6462 (2)	0.4631 (4)	0.4891 (2)	0.0482 (7)
C4	0.7106 (2)	0.4562 (4)	0.5744 (2)	0.0489 (7)
C5	0.8223 (3)	0.5322 (4)	0.6783 (2)	0.0580 (8)
H5	0.8713	0.5915	0.7118	0.070*
C6	0.7940 (3)	0.3903 (4)	0.7030 (2)	0.0610 (9)
H6	0.8195	0.3369	0.7554	0.073*
N1	0.5763 (2)	0.3633 (3)	0.45300 (18)	0.0534 (7)
H1A	0.546 (3)	0.270 (3)	0.474 (3)	0.064*
N2	0.6529 (2)	0.5851 (3)	0.43706 (17)	0.0520 (7)
N3	0.7688 (2)	0.5733 (3)	0.59802 (18)	0.0525 (7)
N4	0.7220 (2)	0.3432 (3)	0.63640 (19)	0.0551 (7)
H4	0.680 (3)	0.255 (3)	0.634 (3)	0.066*
N5	0.8833 (2)	0.6634 (3)	0.4268 (2)	0.0529 (7)
N6	0.8963 (2)	0.5320 (3)	0.4212 (2)	0.0552 (7)
N7	0.9109 (3)	0.4018 (3)	0.4143 (2)	0.0723 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0504 (12)	0.0400 (13)	0.0550 (13)	0.0096 (10)	−0.0016 (10)	−0.0034 (10)
C1	0.0542 (18)	0.069 (2)	0.0481 (17)	−0.0156 (16)	−0.0081 (14)	0.0038 (15)
C2	0.0551 (18)	0.070 (2)	0.0495 (17)	−0.0171 (16)	−0.0056 (14)	−0.0031 (15)
C3	0.0485 (16)	0.0500 (18)	0.0462 (15)	−0.0087 (13)	0.0012 (12)	−0.0003 (13)
C4	0.0481 (15)	0.0480 (17)	0.0503 (16)	−0.0051 (13)	0.0012 (13)	0.0026 (13)
C5	0.0598 (19)	0.061 (2)	0.0527 (17)	−0.0041 (16)	−0.0095 (14)	0.0033 (15)
C6	0.064 (2)	0.067 (2)	0.0510 (18)	−0.0005 (18)	−0.0087 (15)	0.0092 (16)

N1	0.0539 (15)	0.0539 (16)	0.0525 (15)	−0.0158 (13)	0.0020 (12)	−0.0012 (12)
N2	0.0512 (14)	0.0569 (17)	0.0477 (14)	−0.0117 (13)	−0.0035 (11)	0.0045 (12)
N3	0.0519 (15)	0.0543 (16)	0.0508 (14)	−0.0088 (13)	−0.0063 (11)	0.0042 (12)
N4	0.0600 (16)	0.0524 (16)	0.0524 (14)	−0.0079 (13)	−0.0021 (12)	0.0077 (12)
N5	0.0585 (16)	0.0552 (17)	0.0444 (14)	−0.0006 (14)	−0.0080 (12)	−0.0089 (12)
N6	0.0525 (15)	0.0540 (18)	0.0585 (16)	−0.0129 (13)	−0.0071 (12)	0.0069 (13)
N7	0.073 (2)	0.0512 (18)	0.092 (2)	−0.0078 (15)	−0.0108 (17)	0.0073 (16)

Geometric parameters (Å, º)

Mn1—N2	2.094 (3)	C3—C4	1.430 (4)
Mn1—N2^{i}	2.094 (3)	C4—N3	1.315 (4)
Mn1—N3^{i}	2.114 (3)	C4—N4	1.345 (4)
Mn1—N3	2.114 (3)	C5—N3	1.350 (4)
Mn1—N5	2.138 (3)	C5—C6	1.370 (5)
Mn1—N5^{i}	2.138 (3)	C5—H5	0.9300
C1—N2	1.351 (4)	C6—N4	1.350 (4)
C1—C2	1.375 (5)	C6—H6	0.9300
C1—H1	0.9300	N1—H1A	0.966 (18)
C2—N1	1.349 (4)	N4—H4	0.952 (19)
C2—H2	0.9300	N5—N6	1.193 (4)
C3—N2	1.323 (4)	N6—N7	1.187 (4)
C3—N1	1.340 (4)		
N2—Mn1—N2^{i}	180.0)	N3—C4—N4	113.0 (3)
N2—Mn1—N3^{i}	101.59 (10)	N3—C4—C3	118.2 (3)
N2^{i}—Mn1—N3^{i}	78.41 (10)	N4—C4—C3	128.8 (3)
N2—Mn1—N3	78.41 (10)	N3—C5—C6	110.1 (3)
N2^{i}—Mn1—N3	101.59 (10)	N3—C5—H5	125.0
N3^{i}—Mn1—N3	180.0	C6—C5—H5	125.0
N2—Mn1—N5	89.31 (11)	N4—C6—C5	106.5 (3)
N2^{i}—Mn1—N5	90.69 (11)	N4—C6—H6	126.7
N3^{i}—Mn1—N5	91.53 (11)	C5—C6—H6	126.7
N3—Mn1—N5	88.47 (11)	C3—N1—C2	105.6 (3)
N2—Mn1—N5^{i}	90.69 (11)	C3—N1—H1A	135 (3)
N2^{i}—Mn1—N5^{i}	89.31 (11)	C2—N1—H1A	119 (3)
N3^{i}—Mn1—N5^{i}	88.47 (11)	C3—N2—C1	104.7 (3)
N3—Mn1—N5^{i}	91.53 (11)	C3—N2—Mn1	113.26 (19)
N5—Mn1—N5^{i}	180.0	C1—N2—Mn1	141.7 (2)
N2—C1—C2	109.3 (3)	C4—N3—C5	104.5 (3)
N2—C1—H1	125.3	C4—N3—Mn1	112.6 (2)
C2—C1—H1	125.3	C5—N3—Mn1	142.9 (2)
N1—C2—C1	107.3 (3)	C4—N4—C6	105.8 (3)
N1—C2—H2	126.4	C4—N4—H4	124 (3)
C1—C2—H2	126.4	C6—N4—H4	130 (3)
N2—C3—N1	113.1 (3)	N6—N5—Mn1	120.1 (2)

N2—C3—C4	117.4 (3)	N7—N6—N5	178.6 (4)
N1—C3—C4	129.5 (3)		

Symmetry code: (i) −*x*+3/2, −*y*+3/2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N7^{ii}	0.97 (2)	2.26 (3)	3.031 (4)	136 (3)
N1—H1*A*···N5^{iii}	0.97 (2)	2.33 (4)	3.021 (4)	127 (3)
N4—H4···N7^{ii}	0.95 (2)	1.92 (2)	2.834 (4)	160 (4)

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