Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Retraction of articles

IUCr Editorial Office

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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

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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

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diazidobis(2,2′-biimidazole)iron(II)

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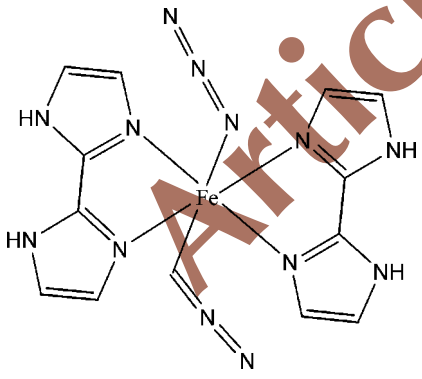
Received 16 June 2008; accepted 19 June 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.119; data-to-parameter ratio = 12.1.

In the title compound, $[Fe(N_3)_2(C_6H_6N_4)_2]$, the Fe atom is bonded to two azide ions located in axial positions and to two equatorially positioned bidentate biimidazole ligands, forming a slightly distorterd octahedron. The non-H atoms of the equatorial plane are coplanar, with a mean deviation of 0.0355 (2) Å. The Fe^{II} cation lies on an inversion centre. Thus, the asymmetric unit comprises one half-molecule.

Related literature

For related literature, see: Caneschi *et al.* (1989); Tsukuda *et al.* (2002); Vostrikova *et al.* (2000); Kuchar *et al.* (2003).



Experimental

Crystal data

$[Fe(N_3)_2(C_6H_6N_4)_2]$
M_r = 404.17
Monoclinic, $C2/c$
a = 12.487 (3) Å
b = 9.012 (2) Å
c = 14.222 (3) Å
β = 91.91 (3)°
V = 1599.6 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 293 (2) K
0.14 × 0.12 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.875, T_{max} = 0.909
1964 measured reflections
1504 independent reflections
1250 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.118
S = 1.00
1504 reflections
124 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—N5	2.100 (2)	Fe1—N2	2.134 (3)
Fe1—N4	2.123 (2)		
N5—Fe1—N5^{i}	180	N4—Fe1—N4^{i}	
N5—Fe1—N4	78.40 (9)	N4—Fe1—N2	88.71 (10)
N5—Fe1—N2	88.84 (10)	N2^{i}—Fe1—N2	180

Symmetry code: (i) $-x+\frac{3}{2}, -y+\frac{5}{2}, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); 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*.

The authors thank the National Ministry of Science and Technology of China for support (grant No. 2001CB6105–07).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2177).

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supporting information

Acta Cryst. (2008). E**64**, m956 [doi:10.1107/S1600536808018539]

Diazidobis(2,2′-biimidazole)iron(II)

Lujiang Hao, Chunhua Mu and Binbin Kong

S1. Comment

Different kinds of metal-radical coordination architectures with appropriate organic radicals and coligands have been an important subject during the last decade because of their potential use for molecule-based magnetic materials and optical devices (Caneschi *et al.*, 1989; Tsukuda *et al.*, 2002; Vostrikova *et al.*, 2000; Kuchar *et al.*, 2003). The organic species, such as tridentate nitronyl nitroxide radical, and bidentate nitroxide radical could result in a large number of building blocks with the potential applications. In this paper, we report the structure of the title compound, (I).

The Fe atom, located at the inversion centre, is bonded to two azide ions and the two bidentate biimidizole ligands, forming a slightly distorterd octahedron (Fig. 1). The four nitrogen atoms belonging to two biimidizole ligands lie in the equatorial plane and the two nitrogen atoms from azide groups lie at the axial coordination sites. In the equatorial plane the Fe—N(imidzole) bond lengths are in the range of 2.095 (2)–2.113 (2) /%A (Table 1).

S2. Experimental

A mixture of iron(II) dichloride anhydrous (1 mmoL), 2,2′-biimidazole(1 mmoL), and sodium azide (2 mmol) in 20 mL methanol was refluxed for several h. The above cooled solution was filterated and the filtrate was kept in the ice box. One week later, colourless blocks of (I) were obtained with the yield of *ca* 8%. Anal. Calc. for $C_{12}H_8FeN_{14}$: C 35.63, H 1.98, N 48.49%; Found: C 35.58, H 1.96, N 48.45%.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93Å and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

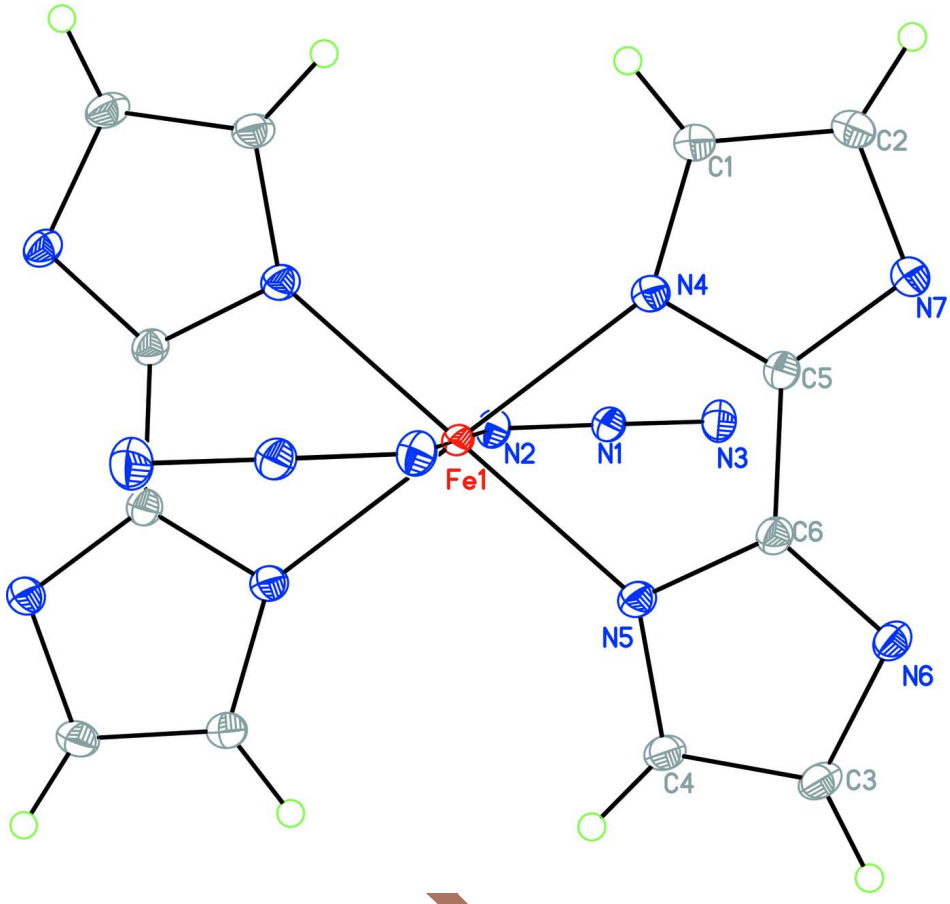

Figure 1

The molecular structure of (I) around Fe^{II} drawn with the 30% probability displacement ellipsoids for the non-hydrogen atoms.

Diazidobis(2,2′-biimidazole)iron(II)

Crystal data

$[Fe(N_3)_2(C_6H_6N_4)_2]$
$M_r = 404.17$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 12.487\ (3)$ Å
$b = 9.012\ (2)$ Å
$c = 14.222\ (3)$ Å
$\beta = 91.91\ (3)°$
$V = 1599.6\ (6)$ Å^3
$Z = 4$
$F(000) = 816$
$D_x = 1.678$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1504 reflections
$\theta = 2.8–25.7°$
$\mu = 0.98$ mm^{-1}
$T = 293$ K
Block, colourless
0.14 × 0.12 × 0.10 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, 2001)
$T_{min} = 0.875$, $T_{max} = 0.909$
1964 measured reflections
1504 independent reflections
1250 reflections with $I > 2\sigma(I)$

R_{int} = 0.022
θ_{max} = 25.7°, 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
$wR(F^2)$ = 0.118
S = 1.00
1504 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
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2 + 1.004P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Fe1	0.7500	1.2500	0.5000	0.0610 (9)
C1	0.6773 (3)	1.0317 (4)	0.3216 (2)	0.0554 (7)
H1	0.6279	1.0905	0.2883	0.067*
C2	0.7058 (3)	0.8903 (4)	0.2969 (2)	0.0583 (8)
H2	0.6805	0.8374	0.2446	0.070*
C3	0.9629 (2)	0.9250 (4)	0.6284 (2)	0.0555 (8)
H3	1.0126	0.8825	0.6704	0.067*
C4	0.9159 (2)	1.0612 (4)	0.63750 (19)	0.0543 (7)
H4	0.9290	1.1270	0.6869	0.065*
C5	0.7896 (2)	0.9564 (3)	0.42568 (19)	0.0456 (6)
C6	0.8539 (2)	0.9633 (3)	0.51069 (18)	0.0454 (6)
N1	0.60420 (19)	1.0322 (3)	0.57863 (17)	0.0519 (6)
N2	0.6173 (2)	1.1634 (3)	0.57318 (18)	0.0544 (6)
N3	0.5894 (2)	0.9020 (3)	0.5859 (2)	0.0697 (8)
N4	0.73154 (18)	1.0735 (3)	0.40187 (16)	0.0499 (6)
N5	0.84709 (18)	1.0851 (3)	0.56302 (15)	0.0491 (6)
N6	0.92402 (18)	0.8623 (3)	0.54644 (16)	0.0498 (6)
N7	0.7786 (2)	0.8422 (3)	0.36365 (16)	0.0517 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.064 (2)	0.067 (2)	0.0510 (18)	−0.0005 (18)	−0.0087 (15)	0.0092 (16)
C1	0.0573 (17)	0.0577 (18)	0.0505 (15)	0.0058 (14)	−0.0099 (13)	−0.0031 (14)
C2	0.0618 (18)	0.064 (2)	0.0489 (16)	−0.0009 (16)	−0.0092 (14)	−0.0094 (14)
C3	0.0499 (16)	0.069 (2)	0.0472 (15)	0.0174 (15)	−0.0050 (12)	0.0040 (14)
C4	0.0513 (16)	0.0661 (19)	0.0448 (14)	0.0160 (15)	−0.0081 (12)	−0.0049 (13)
C5	0.0440 (14)	0.0452 (15)	0.0473 (14)	0.0058 (12)	0.0004 (11)	−0.0026 (12)
C6	0.0454 (14)	0.0474 (16)	0.0435 (13)	0.0084 (12)	0.0018 (11)	−0.0004 (11)
N1	0.0492 (14)	0.0514 (16)	0.0547 (14)	0.0132 (11)	−0.0061 (11)	−0.0075 (11)
N2	0.0528 (14)	0.0487 (16)	0.0614 (15)	0.0104 (12)	−0.0006 (11)	−0.0037 (12)
N3	0.0706 (18)	0.0500 (17)	0.088 (2)	0.0088 (14)	−0.0093 (15)	−0.0077 (15)
N4	0.0497 (13)	0.0521 (15)	0.0474 (12)	0.0085 (11)	−0.0060 (10)	−0.0052 (11)
N5	0.0462 (13)	0.0545 (15)	0.0463 (12)	0.0117 (11)	−0.0042 (10)	−0.0045 (11)
N6	0.0476 (13)	0.0525 (14)	0.0491 (12)	0.0130 (11)	0.0005 (10)	0.0034 (11)
N7	0.0553 (14)	0.0513 (15)	0.0482 (12)	0.0048 (12)	−0.0012 (10)	−0.0068 (11)

Geometric parameters (Å, º)

Fe1—N5	2.100 (2)	C3—C4	1.368 (4)
Fe1—N5^{i}	2.100 (2)	C3—H3	0.9300
Fe1—N4^{i}	2.123 (2)	C4—N5	1.359 (3)
Fe1—N4	2.123 (2)	C4—H4	0.9300
Fe1—N2^{i}	2.134 (3)	C5—N4	1.318 (4)
Fe1—N2	2.134 (3)	C5—N7	1.360 (4)
C1—N4	1.361 (4)	C5—C6	1.430 (4)
C1—C2	1.373 (4)	C6—N5	1.330 (4)
C1—H1	0.9300	C6—N6	1.351 (4)
C2—N7	1.363 (4)	N1—N3	1.193 (4)
C2—H2	0.9300	N1—N2	1.197 (3)
C3—N6	1.369 (4)		
N5—Fe1—N5^{i}	180.000 (1)	N6—C3—H3	126.0
N5—Fe1—N4^{i}	101.60 (9)	C4—C3—H3	126.0
N5^{i}—Fe1—N4^{i}	78.40 (9)	N5—C4—C3	109.3 (3)
N5—Fe1—N4	78.40 (9)	N5—C4—H4	125.4
N5^{i}—Fe1—N4	101.60 (9)	C3—C4—H4	125.4
N4^{i}—Fe1—N4	180.000 (1)	N4—C5—N7	113.3 (2)
N5—Fe1—N2^{i}	91.16 (10)	N4—C5—C6	118.1 (2)
N5^{i}—Fe1—N2^{i}	88.84 (10)	N7—C5—C6	128.6 (3)
N4^{i}—Fe1—N2^{i}	88.71 (10)	N5—C6—N6	113.4 (2)
N4—Fe1—N2^{i}	91.29 (10)	N5—C6—C5	117.7 (2)
N5—Fe1—N2	88.84 (10)	N6—C6—C5	128.9 (3)
N5^{i}—Fe1—N2	91.16 (10)	N3—N1—N2	178.3 (3)
N4^{i}—Fe1—N2	91.29 (10)	N1—N2—Fe1	120.2 (2)
N4—Fe1—N2	88.71 (10)	C5—N4—C1	104.4 (2)
N2^{i}—Fe1—N2	180.0	C5—N4—Fe1	112.58 (18)

N4—C1—C2	110.2 (3)	C1—N4—Fe1	143.0 (2)
N4—C1—H1	124.9	C6—N5—C4	104.8 (2)
C2—C1—H1	124.9	C6—N5—Fe1	113.05 (17)
N7—C2—C1	106.8 (3)	C4—N5—Fe1	141.8 (2)
N7—C2—H2	126.6	C6—N6—C3	104.4 (2)
C1—C2—H2	126.6	C5—N7—C2	105.2 (2)
N6—C3—C4	108.0 (2)		

Symmetry code: (i) $-x+3/2, -y+5/2, -z+1$.