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Retraction of articles by T. Liu *et al.*

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A series of 29 papers by Liu *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 29 papers by Liu *et al.* are retracted. 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
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)	Liu & Xie (2007*a*)	10.1107/S1600536807026852	EDUMAS
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')copper(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*b*)	10.1107/S1600536807028255	EDUVAB
Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)	Liu & Xie (2007*b*)	10.1107/S1600536807028735	RIGQAA
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]	Liu, Wang, Wang & Xie (2007*c*)	10.1107/S1600536807030917	UDUMIQ
Polymeric $KNOF_2$	Liu Wang, Wang & Xie (2007*a*)	10.1107/S1600536807027195	ICSD 240891
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')cobalt(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*d*)	10.1107/S1600536807031224	WIHJED
Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]	Liu, Wang, Wang & Xie (2007*e*)	10.1107/S1600536807032679	WIHQEK
Tetrakis[μ-(2-pyridyloxy)acetato-$\kappa^2O:O'$]bis{(1,10-phenanthroline-κ^2N,N')-[(2-pyridyloxy)acetato-κO]neodymium(III)}	Liu, Wang, Wang & Xie (2007*f*)	10.1107/S1600536807035349	TIGDAP
(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')manganese(II) dinitrate dihydrate	Liu, Wang, Wang & Xie (2007*g*)	10.1107/S1600536807035076	TIGDET
2-Amino-3,5-dinitrobenzoic acid–ammonia (1/1)	Liu & Zhu (2007*j*)	10.1107/S1600536807040068	KIKQAX
2-Hydroxy-3,5-dinitrobenzamide monohydrate	Liu & Zhu (2007*k*)	10.1107/S1600536807039712	KIKQEB
2-(1-Hydroxy-2-pyridyl)acetamide monohydrate	Liu & Zhu (2007*l*)	10.1107/S1600536807040652	CIKQOD
Bis(2,2′-bipyridine-κN,N′)bis(thiocyanato-κN)iron(II)	Liu & Zhu (2007*a*)	10.1107/S1600536807043486	XIFXOA
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III]	Liu & Zhu (2007*b*)	10.1107/S1600536807045485	XILNAI
3-Hydroxy-2,4,6-trinitropyridine monohydrate	Liu & Zhu (2007*m*)	10.1107/S1600536807045230	PILNOO
catena-Poly[hexakis(μ_2-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]	Liu & Zhu (2007*c*)	10.1107/S1600536807047733	SILZET
catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]	Liu & Zhu (2007*d*)	10.1107/S1600536807050969	GIMZOS
Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)	Liu & Zhu (2007*e*)	10.1107/S1600536807051756	WINFAB
2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate	Liu & Zhu (2007*n*)	10.1107/S1600536807048477	GINFEP
2-(Benzoylhydrazinocarbonyl)benzoic acid	Liu & Zhu (2007*o*)	10.1107/S160053680705204X	TINZIA
Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)	Liu & Zhu (2007*f*)	10.1107/S1600536807054529	HIPZIQ
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')nickel(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*g*)	10.1107/S1600536807056504	XIRGIP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')copper(II)]-μ-acetamido-$\kappa^2O:N$]	Liu & Zhu (2007*h*)	10.1107/S1600536807059077	HIQROP
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')cobalt(II)]-μ-acetamidato-$\kappa^2O:N$]	Liu & Zhu (2007*i*)	10.1107/S1600536807060631	YIQMER
N′-Benzoyl-4-nitronicotinohydrazide	Liu & Zhu (2007*p*)	10.1107/S1600536807053068	CIPVON
N′-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide	Liu & Zhu (2007*q*)	10.1107/S1600536807054876	RIRWEV

 doi:10.1107/S1600536809049976

Table 1 (continued)

Title	Reference	DOI	Refcode
Ethylenediammonium sulfate	Liu & Zhu (2007*r*)	10.1107/S1600536807056280	ETDAMS03
Ethylenediammonium perchlorate	Liu & Zhu (2007*s*)	10.1107/S1600536807059909	HIRYEN
catena-Poly[[(nitrato-κO)(1,10-phenanthroline-κ^2N,N')manganese(II)]-μ-nitrato-$\kappa^2O:O'$]	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

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Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)

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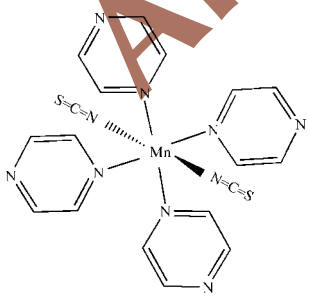
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.007 Å; R factor = 0.050; wR factor = 0.159; data-to-parameter ratio = 16.9.

In the molecule of the title complex, $[Mn(NCS)_2(C_4H_4N_2)_4]$, the Mn^{II} atom is coordinated in a distorted octahedral arrangement by two N atoms of two SCN^- and four N atoms of four pyrazine ligands. A crystallographic twofold rotation axis passes through the Mn atom, and the N and *para*-N atoms of two *trans* pyrazine rings. In the crystal structure, the non-classical hydrogen bonds and the weak π–π stacking interactions, involving the pyrazine rings of adjacent pyrazine ligands with a centroid–centroid distance of 3.3205 (4) Å, contribute to the formation of a supramolecular network structure.

Related literature

For related literature, see: Allen *et al.* (1987); Law *et al.* (1999); Li *et al.* (2005); Liu *et al.* (2004); Pan & Xu (2004); Pecoraro & Butler (1986); Wu *et al.* (2003).



Experimental

Crystal data

$[Mn(NCS)_2(C_4H_4N_2)_4]$
M_r = 491.47
Monoclinic, $C2/c$
a = 11.425 (5) Å
b = 14.543 (4) Å
c = 15.022 (3) Å
β = 90.759 (5)°
V = 2495.7 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 273 (2) K
0.26 × 0.16 × 0.07 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.836, T_{max} = 0.952
7912 measured reflections
2434 independent reflections
1675 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.159
S = 1.09
2434 reflections
144 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—N1	2.130 (4)	Mn1—N3	2.239 (3)
Mn1—N2	2.100 (4)	Mn1—N4	2.137 (4)
N1—Mn1—N2	91.29 (9)	N2—Mn1—N3	90.26 (8)
N1—Mn1—N3	90.98 (14)	N2—Mn1—N4	180
N1—Mn1—N4	88.71 (9)	N3—Mn1—N4	89.74 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···N1^{i}	0.93	2.55	3.109 (6)	119
C7—H7···N1	0.93	2.58	3.176 (6)	122

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

Data collection: *APEX2* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); 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: AT2309).

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supplementary materials

Acta Cryst. (2007). E**63**, m1820 [**doi:10.1107/S1600536807026852**]

Tetrakis(pyrazine-κ*N*)bis(thiocyanato-κ*N*)manganese(II)

T. Liu and Z.-P. Xie

Comment

There are three manganese enzymes containing a mononuclear manganese site, *viz*. superoxide dismutase, peroxidase and dioxygenase, which participate in redox changes in the respective areas of biology (Law *et al.*, 1999). Carboxylatobridged complexes, such as pyridine, phenanthroline, quinoline and benzimidazole, are often employed to mimic the function and structure of these active sites, based on the knowledge that Mn centres in these enzymes are predominately coordinated by N,*O* donors from available amino acid side chains (Pecoraro & Butler, 1986; Wu *et al.*, 2003; Pan & Xu, 2004; Liu *et al.*, 2004; Li *et al.*, 2005). We herein report the crystal structure of the title compound, (I).

In the molecule of (I), (Fig. 1) the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The two N atoms of two SCN^- and four N atoms of four pyrazine ligands are coordinated to the Mn atom, in a distorted octahedral arrangement (Table 1). A crystallographic twofold rotation axis passes through the Mn atom, and the N and *para*-N atoms of two *trans* pyrazine rings. The planar pyrazine rings I (N3/N6/C4—C7), II (N2/N7/C2A/C3A/C2—C3) and III (N4/N5/C8A/C9A/C8—C9) are nearly perpendicular to each other, with dihedral angles of I/II = 87.7 (2), I/III = 109.2 (6) and II/III = 85.9 (7)°.

In the crystal structure, the non-classical hydrogen bonds and the weak π-π stacking interactions, involving the pyrazine rings of adjacent pyrazine ligands with centroid-centroid distance of 3.3205 (4) Å [symmetry code: $1-x, 2-y, 1-z$], cause to the formation of a supramolecular network structure (Fig. 2).

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a Teflon-lined Parr bomb (23 ml), which was then sealed. Manganese(II) chloride tetrahydrate (39.6 mg, 0.2 mmol), potassium thiocyanate (38.9 mg, 0.4 mmol), pyrazine (1.5 ml), and distilled water (2 g) were placed into the bomb and sealed. The bomb was heated under autogenous pressure for 6 d at 413 K and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colourless solution was decanted from small yellow crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code (A): − *x*, *y*, 3/2 − *z*].

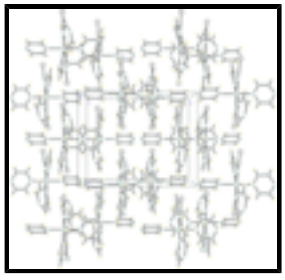

Fig. 2. A packing diagram for (I).

Tetrakis(pyrazine-κ*N*)bis(thiocyanato-κ*N*)manganese(II)

Crystal data

$[Mn(NCS)_2(C_4H_4N_2)_4]$	F_{000} = 1004
M_r = 491.47	D_x = 1.308 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2231 reflections
a = 11.425 (5) Å	θ = 2.3–23.8º
b = 14.543 (4) Å	μ = 0.72 mm^{-1}
c = 15.022 (3) Å	*T* = 273 (2) K
β = 90.759 (5)º	Block, yellow
V = 2495.7 (15) Å^3	0.26 × 0.16 × 0.07 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	2434 independent reflections
Radiation source: fine-focus sealed tube	1675 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 273(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −14→13
T_{min} = 0.836, T_{max} = 0.952	*k* = −17→17
7912 measured reflections	*l* = −18→18

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.159$

$S = 1.09$

2434 reflections

144 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.1074P)^2 + 0.9725P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.52$ e Å^{-3}

$\Delta\rho_{min} = -0.39$ e Å^{-3}

Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0113 (16)

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	0.35963 (4)	0.7500	0.0486 (3)
S1	−0.36253 (15)	0.36697 (11)	0.93412 (13)	0.1233 (6)
N1	−0.1575 (3)	0.3629 (2)	0.8242 (3)	0.0787 (10)
N2	0.0000	0.2153 (3)	0.7500	0.0686 (11)
N3	0.1076 (3)	0.3603 (2)	0.8756 (2)	0.0694 (8)
N4	0.0000	0.5066 (3)	0.7500	0.0700 (11)
N5	0.0000	0.6957 (5)	0.7500	0.150 (3)
N6	0.2516 (6)	0.3887 (4)	1.0292 (5)	0.142 (2)
N7	0.0000	0.0280 (5)	0.7500	0.131 (2)
C1	−0.2437 (3)	0.3646 (2)	0.8699 (3)	0.0663 (10)
C2	−0.0418 (4)	0.1680 (3)	0.8208 (3)	0.0785 (11)
H2	−0.0706	0.2007	0.8691	0.094*
C3	−0.0430 (5)	0.0761 (3)	0.8235 (3)	0.0957 (14)
H3	−0.0716	0.0449	0.8727	0.115*
C4	0.2251 (4)	0.3423 (3)	0.8760 (3)	0.0892 (13)
H4	0.2572	0.3205	0.8234	0.107*

C5	0.3009 (5)	0.3539 (4)	0.9491 (5)	0.1116 (19)
H5	0.3801	0.3396	0.9456	0.134*
C6	0.1327 (7)	0.4051 (5)	1.0275 (4)	0.140 (3)
H6	0.0974	0.4267	1.0788	0.168*
C7	0.0637 (5)	0.3904 (4)	0.9517 (3)	0.1084 (17)
H7	−0.0162	0.4022	0.9545	0.130*
C8	0.0981 (4)	0.5541 (3)	0.7764 (3)	0.0853 (12)
H8	0.1652	0.5214	0.7923	0.102*
C9	0.1006 (5)	0.6463 (3)	0.7802 (5)	0.112 (2)
H9	0.1663	0.6771	0.8020	0.134*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0436 (5)	0.0510 (5)	0.0515 (5)	0.000	0.0112 (3)	0.000
S1	0.0995 (11)	0.1354 (13)	0.1366 (14)	0.0019 (8)	0.0649 (10)	0.0009 (9)
N1	0.071 (2)	0.086 (3)	0.079 (2)	0.0017 (16)	0.0187 (17)	−0.0001 (17)
N2	0.074 (3)	0.065 (3)	0.067 (3)	0.000	0.005 (2)	0.000
N3	0.068 (2)	0.0669 (19)	0.074 (2)	0.0020 (15)	0.0040 (15)	−0.0021 (15)
N4	0.064 (3)	0.063 (3)	0.084 (3)	0.000	0.004 (2)	0.000
N5	0.142 (7)	0.086 (5)	0.220 (9)	0.000	−0.020 (6)	0.000
N6	0.148 (5)	0.141 (4)	0.134 (5)	0.002 (4)	−0.031 (4)	−0.020 (4)
N7	0.165 (7)	0.088 (4)	0.140 (6)	0.000	−0.015 (5)	0.000
C1	0.064 (2)	0.065 (2)	0.070 (2)	0.0039 (17)	0.0125 (17)	−0.0001 (17)
C2	0.087 (3)	0.070 (2)	0.078 (3)	−0.006 (2)	0.005 (2)	0.009 (2)
C3	0.127 (4)	0.071 (3)	0.089 (3)	−0.007 (3)	0.001 (3)	0.008 (2)
C4	0.071 (3)	0.107 (4)	0.090 (3)	0.012 (2)	0.001 (2)	0.015 (2)
C5	0.076 (3)	0.130 (5)	0.127 (5)	−0.001 (3)	−0.019 (3)	0.026 (4)
C6	0.129 (5)	0.188 (7)	0.101 (4)	0.048 (5)	−0.033 (4)	−0.042 (4)
C7	0.094 (3)	0.154 (5)	0.078 (3)	0.028 (3)	−0.008 (2)	−0.031 (3)
C8	0.074 (3)	0.071 (3)	0.111 (3)	−0.009 (2)	−0.003 (2)	0.005 (2)
C9	0.094 (4)	0.070 (3)	0.171 (6)	−0.010 (3)	−0.025 (4)	0.000 (3)

Geometric parameters (Å, °)

Mn1—N1	2.130 (4)	N6—C6	1.378 (8)
Mn1—N2	2.100 (4)	N6—C5	1.428 (9)
Mn1—N3	2.239 (3)	N7—C3^{i}	1.401 (6)
Mn1—N4	2.137 (4)	N7—C3	1.401 (6)
Mn1—N1^{i}	2.130 (4)	C2—C3	1.338 (6)
Mn1—N3^{i}	2.239 (3)	C2—H2	0.9300
S1—C1	1.676 (4)	C3—H3	0.9300
N1—C1	1.209 (6)	C4—C5	1.400 (7)
N2—C2^{i}	1.359 (5)	C4—H4	0.9300
N2—C2	1.359 (5)	C5—H5	0.9300
N3—C7	1.328 (6)	C6—C7	1.393 (7)
N3—C4	1.368 (5)	C6—H6	0.9300
N4—C8	1.371 (5)	C7—H7	0.9300

N4—C8^{i}	1.371 (5)	C8—C9	1.342 (6)
N5—C9	1.424 (6)	C8—H8	0.9300
N5—C9^{i}	1.424 (6)	C9—H9	0.9300
N1—Mn1—N2	91.29 (9)	C3^{i}—N7—C3	120.2 (6)
N1—Mn1—N3	90.98 (14)	N1—C1—S1	179.5 (4)
N1—Mn1—N4	88.71 (9)	C3—C2—N2	122.2 (4)
N2—Mn1—N3	90.26 (8)	C3—C2—H2	118.9
N2—Mn1—N4	180.000 (1)	N2—C2—H2	118.9
N3—Mn1—N4	89.74 (8)	C2—C3—N7	118.1 (5)
N2—Mn1—N1^{i}	91.29 (9)	C2—C3—H3	121.0
N1^{i}—Mn1—N1	177.42 (19)	N7—C3—H3	121.0
N1^{i}—Mn1—N4	88.71 (9)	N3—C4—C5	125.2 (5)
N1^{i}—Mn1—N3	89.01 (14)	N3—C4—H4	117.4
N2—Mn1—N3^{i}	90.26 (8)	C5—C4—H4	117.4
N1^{i}—Mn1—N3^{i}	90.98 (14)	C4—C5—N6	117.2 (5)
N1—Mn1—N3^{i}	89.01 (14)	C4—C5—H5	121.4
N4—Mn1—N3^{i}	89.74 (8)	N6—C5—H5	121.4
N3—Mn1—N3^{i}	179.48 (15)	N6—C6—C7	122.4 (6)
C1—N1—Mn1	176.9 (4)	N6—C6—H6	118.8
C2^{i}—N2—C2	119.2 (5)	C7—C6—H6	118.8
C2^{i}—N2—Mn1	120.4 (3)	N3—C7—C6	122.5 (5)
C2—N2—Mn1	120.4 (3)	N3—C7—H7	118.8
C7—N3—C4	116.3 (4)	C6—C7—H7	118.8
C7—N3—Mn1	121.1 (3)	C9—C8—N4	122.2 (5)
C4—N3—Mn1	122.0 (3)	C9—C8—H8	118.9
C8—N4—C8^{i}	119.4 (5)	N4—C8—H8	118.9
C8—N4—Mn1	120.3 (2)	C8—C9—N5	118.3 (5)
C8^{i}—N4—Mn1	120.3 (2)	C8—C9—H9	120.9
C9—N5—C9^{i}	119.4 (6)	N5—C9—H9	120.9
C6—N6—C5	116.5 (5)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···N1^{i}	0.93	2.55	3.109 (6)	119
C7—H7···N1	0.93	2.58	3.176 (6)	122

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

Fig. 1

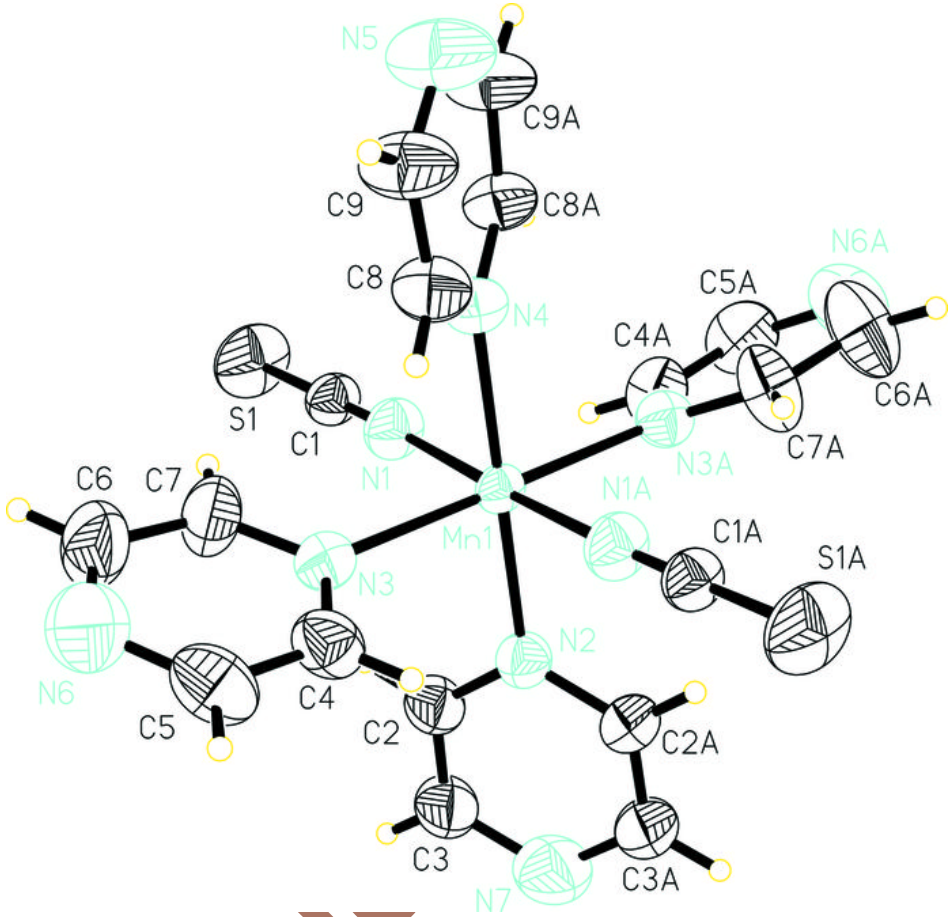
N5
C9A
C9
C8A
C8
N4
N6A
C5A
C4A
C6A
S1
C1
N1
N3A
C7A
C6
C7
N1A
Mn1
C1A
S1A
N3
N6
C4
N2
C5
C2
C2A
C3
N7
C3A

Fig. 2