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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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(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')manganese(II) dinitrate dihydrate

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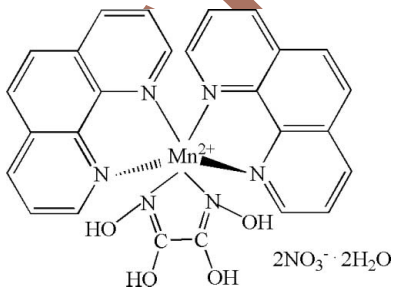
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.007 Å; R factor = 0.051; wR factor = 0.166; data-to-parameter ratio = 13.9.

In the cation of the title compound, $[Mn(C_{12}H_8N_2)_2(C_2H_4N_2O_4)](NO_3)_2\cdot 2H_2O$, the Mn atom has a distorted octahedral coordination formed by six N atoms from one dihydroxyglyoxime and two 1,10-phenanthroline ligands. In the crystal structure, the components are linked into a three-dimensional framework by O—H···O, C—H···O, C—H···N and O—H···N hydrogen bonds and π–π stacking interactions, with a centroid–centroid distance of 3.580 (2) Å (symmetry code: $1-x, 2-y, -z$).

Related literature

For a related structure, see: Liu *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Mn(C_{12}H_8N_2)_2(C_2H_4N_2O_4)](NO_3)_2\cdot 2H_2O$
M_r = 695.47
Monoclinic, $P2_1/c$
a = 13.913 (2) Å
b = 11.998 (5) Å
c = 18.131 (3) Å
β = 96.228 (4)°
V = 3008.6 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 273 (2) K
0.30 × 0.23 × 0.18 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.861, T_{max} = 0.912
20095 measured reflections
6179 independent reflections
3132 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.166
S = 0.99
6179 reflections
444 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—N1	1.933 (3)	Mn1—N4	1.949 (3)
Mn1—N2	1.966 (3)	Mn1—N5	1.881 (4)
Mn1—N3	1.955 (3)	Mn1—N6	1.877 (3)
N1—Mn1—N2	82.79 (15)	N2—Mn1—N6	95.16 (14)
N1—Mn1—N3	92.23 (14)	N3—Mn1—N4	84.17 (14)
N1—Mn1—N4	175.49 (14)	N3—Mn1—N5	93.32 (15)
N1—Mn1—N5	93.95 (15)	N3—Mn1—N6	174.40 (14)
N1—Mn1—N6	90.86 (14)	N4—Mn1—N5	88.99 (14)
N2—Mn1—N3	89.86 (13)	N4—Mn1—N6	92.95 (13)
N2—Mn1—N4	94.46 (14)	N5—Mn1—N6	81.81 (15)
N2—Mn1—N5	175.53 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N2	0.82	2.67	2.991 (4)	105
O2—H2A···O3	0.82	2.63	2.791 (7)	93
C1—H1···N5	0.93	2.53	3.009 (5)	112
C13—H13···N1	0.93	2.58	3.037 (6)	111
C22—H22···N6	0.93	2.58	3.030 (5)	110
O1—H1A···O5^{i}	0.82	2.33	2.958 (5)	134
O1—H1A···O6^{i}	0.82	1.96	2.674 (5)	145
C3—H3···O5^{ii}	0.93	2.54	3.385 (6)	151
C5—H5···O1^{iii}	0.93	2.54	3.344 (6)	145
C18—H18···O2^{iv}	0.93	2.37	3.225 (6)	152
C22—H22···O6^{v}	0.93	2.52	3.269 (6)	137
C15—H15···O5^{vi}	0.93	2.55	3.361 (6)	146

Symmetry codes: (i) $x, y+1, z-1$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, -y+2, -z$; (iv) $-x+2, -y+1, -z$; (v) $-x+2, -y+1, -z+1$; (vi) $x, y, z-1$.

Data collection: *APEX2* (Bruker, 2005); 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: AT2344).

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supplementary materials

Acta Cryst. (2007). E**63**, m2198-m2199 [**doi:10.1107/S1600536807035076**]

(Dihydroxyglyoxime-κ^2N,N')bis(1,10-phenanthroline-κ^2N,N')manganese(II) dinitrate dihydrate

T. Liu, Z.-W. Wang, Y.-X. Wang and Z.-P. Xie

Comment

The crystal structure of bis(1,10-phenanthroline-*N*,*N*')(dihydroxy glyoxime) copper(II) dinitrate dihydrate, (II), and bis(1,10-phenanthroline-N,*N*') (dihydroxy glyoxime) cobalt(II) dinitrate dihydrate, (III), has previously been reported (Liu *et al.*, 2007). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II) and (III). We report herein the crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The six N atoms of one dihydroxy glyoxime and two 1,10-phenanthroline (phen) ligands are coordinated to the Mn atom, in a distorted octahedral arrangement (Table 1). The dihydroxy glyoxime and two phen ligands are each planar and the phen ligands are nearly perpendicular to each other, with a dihedral angle of 86.94 (7)°, as in (II) and (III).

In the crystal structure, the molecules are linked into a three-dimensional framework (Fig. 2) by O—H···O, C—H···O, C—H···N and O—H···N hydrogen bonds (Table 2). There are π-π stacking interactions between adjacent phen ligands with centroid-centroid distance of 3.580 (2) Å (symmetry code: 1 − *x*, 2 − *y*, −*z*). These π-π stacking interactions and hydrogen bonds lead to a supramolecular network structure (Fig. 2), as in (II) and (III). The three compounds, (I), (II) and (III), are isostructural.

Experimental

Manganese dinitrate hexahydrate (144 mg, 0.5 mmol), phen (198 mg, 1 mmol) and dihydroxy glyoxime (120 mg, 1 mmol) were dissolved in ethanol (15 ml). The mixture was heated for 5 h under reflux with stirring. It was then filtered to give a clear solution, into which diethyl ether vapour was allowed to condense in a closed vessel. After being allowed to stand for a few days at room temperature, some colourless single crystals suitable for X-ray diffraction analysis precipitated.

Refinement

H atoms of the water molecules were located in a difference synthesis and refined freely. The remaining H atoms were positioned geometrically, with O—H = 0.82 Å (for OH) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C, O)$, where x = 1.2 for aromatic H atoms and x = 1.5 for hydroxyl H atoms.

Figures

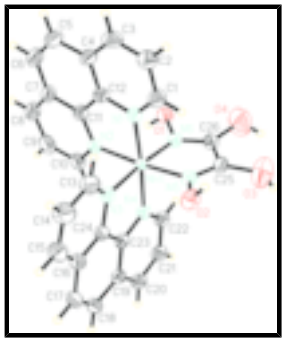

Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Solvent molecules have been omitted for clarity.

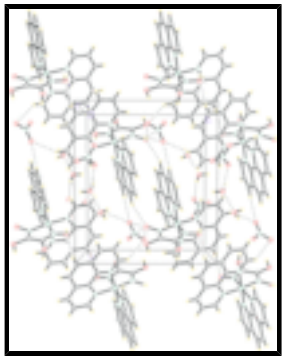

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

(Dihydroxyglyoxime-κ^2*N*,*N*')bis(1,10-phenanthroline-κ^2*N*,*N*')manganese(II) dinitrate dihydrate

Crystal data

$[Mn(C_{12}H_8N_2)_2(C_2H_4N_2O_4)](NO_3)_2·2H_2O$	F_{000} = 1428
M_r = 695.47	D_x = 1.535 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5592 reflections
a = 13.913 (2) Å	θ = 2.1–25.0°
b = 11.998 (5) Å	μ = 0.52 mm^{-1}
c = 18.131 (3) Å	T = 273 (2) K
β = 96.228 (4)°	Prism, colourless
V = 3008.6 (14) Å^3	0.30 × 0.23 × 0.18 mm
Z = 4	

Data collection

Bruker APEX II area-detector diffractometer	6179 independent reflections
Radiation source: fine-focus sealed tube	3132 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 273(2) K	θ_{max} = 26.7°
φ and ω scans	θ_{min} = 2.0°

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.861, T_{max} = 0.912
20095 measured reflections

h = −17→17
k = −15→15
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.166
S = 0.99
6179 reflections
444 parameters
12 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0806P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Extinction correction: none

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	0.77582 (4)	0.75577 (4)	0.03825 (3)	0.03420 (19)
O1	0.7959 (2)	0.9968 (2)	0.04742 (16)	0.0605 (8)
H1A	0.8019	0.9977	0.0029	0.091*
O2	0.8357 (2)	0.6023 (3)	0.14815 (18)	0.0683 (9)
H2A	0.8150	0.5969	0.1887	0.102*
O3	0.9306 (4)	0.7550 (5)	0.2469 (3)	0.1472 (19)
H3A	0.9890	0.7641	0.2467	0.221*
O4	0.9029 (4)	0.9960 (4)	0.1826 (4)	0.155 (2)
H4A	0.9502	0.9809	0.2120	0.233*
O5	0.7738 (3)	0.1306 (3)	0.9096 (2)	0.0962 (13)
O6	0.8934 (2)	0.0146 (3)	0.9287 (2)	0.0783 (10)
O7	0.8897 (4)	0.1357 (4)	0.8427 (3)	0.1356 (19)

O8	0.7404 (6)	0.8835 (8)	0.2850 (4)	0.219 (4)
O9	0.6159 (6)	0.8842 (6)	0.3345 (4)	0.209 (3)
O10	0.6416 (8)	1.0073 (6)	0.2609 (6)	0.388 (11)
O11	0.5552 (13)	0.4230 (13)	0.1434 (9)	0.574 (14)
O12	0.695 (2)	0.3357 (18)	0.2000 (11)	0.64 (2)
N1	0.6533 (2)	0.7803 (3)	0.0767 (2)	0.0492 (9)
N2	0.7067 (2)	0.8181 (3)	−0.05277 (19)	0.0453 (9)
N3	0.7384 (2)	0.6057 (3)	0.00436 (19)	0.0495 (9)
N4	0.8938 (2)	0.7246 (3)	−0.00697 (18)	0.0459 (9)
N5	0.8376 (2)	0.7049 (3)	0.1295 (2)	0.0490 (9)
N6	0.8222 (2)	0.8935 (3)	0.0762 (2)	0.0473 (9)
N7	0.8510 (3)	0.0927 (4)	0.8919 (3)	0.0713 (12)
N8	0.6670 (6)	0.9299 (9)	0.2896 (5)	0.155 (4)
C1	0.6298 (3)	0.7618 (4)	0.1438 (3)	0.0601 (12)
H1	0.6769	0.7353	0.1798	0.072*
C2	0.5368 (4)	0.7804 (4)	0.1633 (3)	0.0707 (14)
H2	0.5236	0.7678	0.2118	0.085*
C3	0.4665 (3)	0.8164 (4)	0.1125 (3)	0.0666 (14)
H3	0.4042	0.8270	0.1253	0.080*
C4	0.4872 (3)	0.8374 (3)	0.0413 (3)	0.0570 (12)
C5	0.4199 (3)	0.8792 (4)	−0.0160 (3)	0.0690 (14)
H5	0.3561	0.8914	−0.0074	0.083*
C6	0.4483 (4)	0.9013 (4)	−0.0837 (3)	0.0729 (15)
H6	0.4035	0.9295	−0.1208	0.088*
C7	0.5460 (3)	0.8824 (4)	−0.0996 (3)	0.0575 (12)
C8	0.5799 (4)	0.9054 (4)	−0.1654 (3)	0.0720 (15)
H8	0.5382	0.9344	−0.2043	0.086*
C9	0.6765 (4)	0.8862 (4)	−0.1753 (3)	0.0742 (15)
H9	0.6999	0.9041	−0.2200	0.089*
C10	0.7378 (3)	0.8397 (3)	−0.1172 (3)	0.0562 (12)
H10	0.8016	0.8238	−0.1242	0.067*
C11	0.6126 (3)	0.8395 (3)	−0.0444 (2)	0.0468 (10)
C12	0.5836 (3)	0.8180 (3)	0.0252 (2)	0.0459 (10)
C13	0.6605 (3)	0.5457 (4)	0.0147 (3)	0.0667 (13)
H13	0.6140	0.5755	0.0422	0.080*
C14	0.6478 (4)	0.4399 (4)	−0.0147 (3)	0.0818 (17)
H14	0.5931	0.3993	−0.0065	0.098*
C15	0.7135 (4)	0.3950 (4)	−0.0549 (3)	0.0762 (15)
H15	0.7036	0.3244	−0.0755	0.091*
C16	0.7964 (3)	0.4549 (3)	−0.0657 (2)	0.0542 (12)
C17	0.8730 (4)	0.4158 (4)	−0.1057 (3)	0.0659 (14)
H17	0.8670	0.3463	−0.1285	0.079*
C18	0.9528 (4)	0.4755 (4)	−0.1116 (2)	0.0607 (13)
H18	1.0010	0.4465	−0.1377	0.073*
C19	0.9653 (3)	0.5827 (4)	−0.0786 (2)	0.0488 (10)
C20	1.0468 (3)	0.6503 (4)	−0.0802 (2)	0.0591 (12)
H20	1.0987	0.6262	−0.1043	0.071*
C21	1.0498 (3)	0.7506 (4)	−0.0466 (2)	0.0591 (12)
H21	1.1040	0.7957	−0.0478	0.071*

C22	0.9729 (3)	0.7873 (3)	−0.0101 (2)	0.0516 (11)
H22	0.9765	0.8569	0.0127	0.062*
C23	0.8909 (3)	0.6235 (3)	−0.0409 (2)	0.0461 (10)
C24	0.8064 (3)	0.5585 (3)	−0.0346 (2)	0.0463 (10)
C25	0.8807 (3)	0.7818 (4)	0.1722 (2)	0.0509 (11)
C26	0.8680 (3)	0.8923 (4)	0.1413 (3)	0.0533 (11)
H11A	0.511 (3)	0.401 (3)	0.111 (3)	0.570 (13)*
H12A	0.674 (8)	0.286 (4)	0.228 (5)	0.64 (3)*
H11B	0.5599 (19)	0.4908 (14)	0.1538 (16)	0.573 (7)*
H12B	0.731 (2)	0.307 (3)	0.1701 (18)	0.642 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0323 (3)	0.0334 (3)	0.0362 (3)	0.0025 (3)	0.0005 (2)	−0.0023 (3)
O1	0.075 (2)	0.0436 (17)	0.061 (2)	0.0081 (14)	−0.0009 (18)	0.0001 (15)
O2	0.075 (2)	0.063 (2)	0.066 (2)	0.0010 (16)	0.0004 (18)	0.0183 (17)
O3	0.143 (4)	0.182 (5)	0.106 (4)	0.004 (4)	−0.031 (3)	0.020 (3)
O4	0.175 (6)	0.125 (4)	0.155 (5)	−0.013 (3)	−0.026 (4)	−0.042 (4)
O5	0.067 (2)	0.104 (3)	0.120 (3)	0.020 (2)	0.021 (2)	0.006 (2)
O6	0.078 (2)	0.059 (2)	0.096 (3)	0.0090 (18)	0.003 (2)	0.018 (2)
O7	0.134 (4)	0.147 (4)	0.136 (4)	0.028 (3)	0.058 (3)	0.064 (3)
O8	0.168 (6)	0.293 (10)	0.204 (8)	−0.064 (7)	0.058 (6)	−0.083 (6)
O9	0.229 (9)	0.218 (8)	0.175 (7)	0.002 (6)	0.000 (6)	−0.022 (6)
O10	0.55 (2)	0.142 (6)	0.380 (14)	−0.070 (8)	−0.355 (14)	0.128 (7)
O11	0.55 (3)	0.76 (3)	0.48 (3)	0.09 (3)	0.39 (2)	0.16 (2)
O12	0.56 (3)	0.94 (5)	0.40 (3)	0.04 (3)	−0.09 (2)	−0.40 (3)
N1	0.048 (2)	0.044 (2)	0.055 (2)	0.0009 (15)	0.0006 (18)	−0.0012 (17)
N2	0.052 (2)	0.039 (2)	0.044 (2)	0.0024 (15)	0.0001 (17)	−0.0074 (16)
N3	0.046 (2)	0.048 (2)	0.054 (2)	−0.0017 (17)	0.0016 (17)	−0.0013 (18)
N4	0.046 (2)	0.040 (2)	0.050 (2)	0.0034 (15)	−0.0021 (16)	−0.0018 (16)
N5	0.046 (2)	0.047 (2)	0.054 (2)	0.0020 (16)	0.0027 (17)	0.0055 (19)
N6	0.045 (2)	0.046 (2)	0.050 (2)	0.0041 (16)	0.0028 (17)	0.0006 (17)
N7	0.063 (3)	0.069 (3)	0.082 (4)	−0.006 (2)	0.010 (2)	0.010 (3)
N8	0.108 (6)	0.245 (12)	0.116 (7)	−0.070 (7)	0.031 (5)	−0.083 (7)
C1	0.055 (3)	0.074 (3)	0.052 (3)	0.007 (2)	0.007 (2)	0.009 (3)
C2	0.061 (3)	0.082 (4)	0.070 (4)	0.006 (3)	0.013 (3)	−0.003 (3)
C3	0.049 (3)	0.068 (3)	0.086 (4)	−0.004 (2)	0.022 (3)	−0.012 (3)
C4	0.044 (3)	0.046 (3)	0.079 (4)	0.002 (2)	−0.002 (2)	−0.010 (2)
C5	0.048 (3)	0.067 (3)	0.090 (4)	0.007 (2)	−0.003 (3)	−0.006 (3)
C6	0.061 (3)	0.061 (3)	0.090 (4)	0.012 (2)	−0.022 (3)	−0.004 (3)
C7	0.061 (3)	0.052 (3)	0.057 (3)	0.005 (2)	−0.009 (2)	−0.003 (2)
C8	0.077 (4)	0.064 (3)	0.069 (4)	0.012 (3)	−0.019 (3)	−0.002 (3)
C9	0.108 (5)	0.058 (3)	0.053 (3)	0.002 (3)	−0.005 (3)	−0.006 (3)
C10	0.070 (3)	0.053 (3)	0.045 (3)	0.002 (2)	0.002 (2)	−0.003 (2)
C11	0.047 (3)	0.038 (2)	0.052 (3)	0.0021 (19)	−0.005 (2)	−0.001 (2)
C12	0.042 (2)	0.038 (2)	0.056 (3)	0.0024 (18)	0.000 (2)	−0.003 (2)
C13	0.055 (3)	0.052 (3)	0.094 (4)	−0.009 (2)	0.010 (3)	−0.004 (3)

C14	0.066 (3)	0.054 (3)	0.125 (5)	−0.015 (3)	0.012 (3)	−0.009 (3)
C15	0.078 (4)	0.047 (3)	0.101 (5)	−0.006 (3)	−0.002 (3)	−0.015 (3)
C16	0.064 (3)	0.039 (2)	0.057 (3)	0.005 (2)	−0.005 (2)	−0.003 (2)
C17	0.093 (4)	0.053 (3)	0.049 (3)	0.018 (3)	−0.005 (3)	−0.007 (2)
C18	0.077 (3)	0.058 (3)	0.046 (3)	0.021 (3)	0.002 (2)	−0.006 (2)
C19	0.050 (3)	0.054 (3)	0.041 (3)	0.013 (2)	0.000 (2)	0.004 (2)
C20	0.054 (3)	0.073 (3)	0.052 (3)	0.015 (2)	0.012 (2)	0.003 (3)
C21	0.048 (3)	0.068 (3)	0.062 (3)	−0.001 (2)	0.006 (2)	0.003 (3)
C22	0.044 (3)	0.051 (2)	0.059 (3)	0.000 (2)	0.002 (2)	−0.003 (2)
C23	0.047 (2)	0.046 (2)	0.043 (3)	0.007 (2)	−0.0049 (19)	0.003 (2)
C24	0.053 (3)	0.042 (2)	0.042 (3)	0.009 (2)	−0.002 (2)	0.000 (2)
C25	0.045 (2)	0.060 (3)	0.046 (3)	0.004 (2)	−0.001 (2)	0.002 (2)
C26	0.052 (3)	0.057 (3)	0.051 (3)	−0.002 (2)	0.001 (2)	−0.011 (2)

Geometric parameters (Å, °)

Mn1—N1	1.933 (3)	C3—C4	1.376 (6)
Mn1—N2	1.966 (3)	C3—H3	0.9300
Mn1—N3	1.955 (3)	C4—C5	1.414 (6)
Mn1—N4	1.949 (3)	C4—C12	1.421 (5)
Mn1—N5	1.881 (4)	C5—C6	1.355 (7)
Mn1—N6	1.877 (3)	C5—H5	0.9300
O1—N6	1.378 (4)	C6—C7	1.437 (7)
O1—H1A	0.8200	C6—H6	0.9300
O2—N5	1.278 (4)	C7—C8	1.359 (6)
O2—H2A	0.8200	C7—C11	1.387 (6)
O3—C25	1.488 (6)	C8—C9	1.395 (7)
O3—H3A	0.8200	C8—H8	0.9300
O4—C26	1.505 (6)	C9—C10	1.398 (6)
O4—H4A	0.8200	C9—H9	0.9300
O5—N7	1.240 (5)	C10—H10	0.9300
O6—N7	1.259 (5)	C11—C12	1.390 (6)
O7—N7	1.207 (5)	C13—C14	1.380 (6)
O8—N8	1.174 (9)	C13—H13	0.9300
O9—N8	1.262 (8)	C14—C15	1.342 (6)
O10—N8	1.104 (11)	C14—H14	0.9300
O11—H11A	0.85 (5)	C15—C16	1.390 (6)
O11—H11B	0.836 (10)	C15—H15	0.9300
O12—H12A	0.86 (8)	C16—C24	1.366 (5)
O12—H12B	0.85 (4)	C16—C17	1.432 (6)
N1—C1	1.313 (5)	C17—C18	1.335 (6)
N1—C12	1.349 (5)	C17—H17	0.9300
N2—C10	1.315 (5)	C18—C19	1.420 (6)
N2—C11	1.358 (5)	C18—H18	0.9300
N3—C13	1.331 (5)	C19—C23	1.390 (5)
N3—C24	1.363 (5)	C19—C20	1.397 (6)
N4—C22	1.340 (5)	C20—C21	1.348 (6)
N4—C23	1.358 (5)	C20—H20	0.9300
N5—C25	1.308 (5)	C21—C22	1.389 (5)

N6—C26	1.280 (5)	C21—H21	0.9300
C1—C2	1.395 (6)	C22—H22	0.9300
C1—H1	0.9300	C23—C24	1.427 (5)
C2—C3	1.339 (7)	C25—C26	1.443 (6)
C2—H2	0.9300		
N1—Mn1—N2	82.79 (15)	C7—C6—H6	119.2
N1—Mn1—N3	92.23 (14)	C8—C7—C11	116.2 (5)
N1—Mn1—N4	175.49 (14)	C8—C7—C6	124.7 (5)
N1—Mn1—N5	93.95 (15)	C11—C7—C6	119.1 (5)
N1—Mn1—N6	90.86 (14)	C7—C8—C9	120.7 (5)
N2—Mn1—N3	89.86 (13)	C7—C8—H8	119.6
N2—Mn1—N4	94.46 (14)	C9—C8—H8	119.6
N2—Mn1—N5	175.53 (14)	C8—C9—C10	119.1 (5)
N2—Mn1—N6	95.16 (14)	C8—C9—H9	120.4
N3—Mn1—N4	84.17 (14)	C10—C9—H9	120.4
N3—Mn1—N5	93.32 (15)	N2—C10—C9	121.0 (5)
N3—Mn1—N6	174.40 (14)	N2—C10—H10	119.5
N4—Mn1—N5	88.99 (14)	C9—C10—H10	119.5
N4—Mn1—N6	92.95 (13)	N2—C11—C7	124.4 (4)
N5—Mn1—N6	81.81 (15)	N2—C11—C12	116.4 (4)
N6—O1—H1A	109.5	C7—C11—C12	119.1 (4)
N5—O2—H2A	109.5	N1—C12—C11	115.6 (4)
C25—O3—H3A	109.5	N1—C12—C4	122.5 (4)
C26—O4—H4A	109.5	C11—C12—C4	121.9 (4)
H11A—O11—H11B	120 (3)	N3—C13—C14	121.0 (5)
H12A—O12—H12B	111 (7)	N3—C13—H13	119.5
C1—N1—C12	117.7 (4)	C14—C13—H13	119.5
C1—N1—Mn1	128.8 (3)	C15—C14—C13	120.9 (5)
C12—N1—Mn1	113.4 (3)	C15—C14—H14	119.6
C10—N2—C11	118.5 (4)	C13—C14—H14	119.6
C10—N2—Mn1	130.0 (3)	C14—C15—C16	119.5 (5)
C11—N2—Mn1	111.6 (3)	C14—C15—H15	120.2
C13—N3—C24	118.0 (4)	C16—C15—H15	120.2
C13—N3—Mn1	130.3 (3)	C24—C16—C15	117.5 (4)
C24—N3—Mn1	111.7 (3)	C24—C16—C17	117.3 (4)
C22—N4—C23	117.8 (4)	C15—C16—C17	125.2 (4)
C22—N4—Mn1	130.0 (3)	C18—C17—C16	122.3 (4)
C23—N4—Mn1	112.1 (3)	C18—C17—H17	118.8
O2—N5—C25	122.9 (4)	C16—C17—H17	118.8
O2—N5—Mn1	121.7 (3)	C17—C18—C19	121.2 (4)
C25—N5—Mn1	115.4 (3)	C17—C18—H18	119.4
C26—N6—O1	116.4 (3)	C19—C18—H18	119.4
C26—N6—Mn1	116.5 (3)	C23—C19—C20	117.0 (4)
O1—N6—Mn1	125.9 (3)	C23—C19—C18	117.5 (4)
O7—N7—O5	120.2 (5)	C20—C19—C18	125.5 (4)
O7—N7—O6	119.3 (5)	C21—C20—C19	119.7 (4)
O5—N7—O6	120.3 (5)	C21—C20—H20	120.1
O10—N8—O8	127.0 (11)	C19—C20—H20	120.1
O10—N8—O9	119.7 (11)	C20—C21—C22	120.7 (4)

O8—N8—O9	113.3 (11)	C20—C21—H21	119.7
N1—C1—C2	122.6 (4)	C22—C21—H21	119.7
N1—C1—H1	118.7	N4—C22—C21	121.4 (4)
C2—C1—H1	118.7	N4—C22—H22	119.3
C3—C2—C1	120.4 (5)	C21—C22—H22	119.3
C3—C2—H2	119.8	N4—C23—C19	123.4 (4)
C1—C2—H2	119.8	N4—C23—C24	115.9 (4)
C2—C3—C4	119.5 (5)	C19—C23—C24	120.7 (4)
C2—C3—H3	120.3	N3—C24—C16	123.1 (4)
C4—C3—H3	120.3	N3—C24—C23	116.0 (4)
C3—C4—C5	124.4 (5)	C16—C24—C23	120.9 (4)
C3—C4—C12	117.4 (4)	N5—C25—C26	112.9 (4)
C5—C4—C12	118.2 (5)	N5—C25—O3	121.7 (4)
C6—C5—C4	120.0 (5)	C26—C25—O3	125.2 (4)
C6—C5—H5	120.0	N6—C26—C25	113.3 (4)
C4—C5—H5	120.0	N6—C26—O4	123.5 (4)
C5—C6—C7	121.7 (5)	C25—C26—O4	123.2 (4)
C5—C6—H6	119.2		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N2	0.82	2.67	2.991 (4)	105
O2—H2A···O3	0.82	2.63	2.791 (7)	93
C1—H1···N5	0.93	2.53	3.009 (5)	112
C13—H13···N1	0.93	2.58	3.037 (6)	111
C22—H22···N6	0.93	2.58	3.030 (5)	110
O1—H1A···O5^{i}	0.82	2.33	2.958 (5)	134
O1—H1A···O6^{i}	0.82	1.96	2.674 (5)	145
C3—H3···O5^{ii}	0.93	2.54	3.385 (6)	151
C5—H5···O1^{iii}	0.93	2.54	3.344 (6)	145
C18—H18···O2^{iv}	0.93	2.37	3.225 (6)	152
C22—H22···O6^{v}	0.93	2.52	3.269 (6)	137
C15—H15···O5^{vi}	0.93	2.55	3.361 (6)	146

Symmetry codes: (i) *x*, *y*+1, *z*−1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*+2, −*z*; (iv) −*x*+2, −*y*+1, −*z*; (v) −*x*+2, −*y*+1, −*z*+1; (vi) *x*, *y*, *z*−1.

Fig. 1

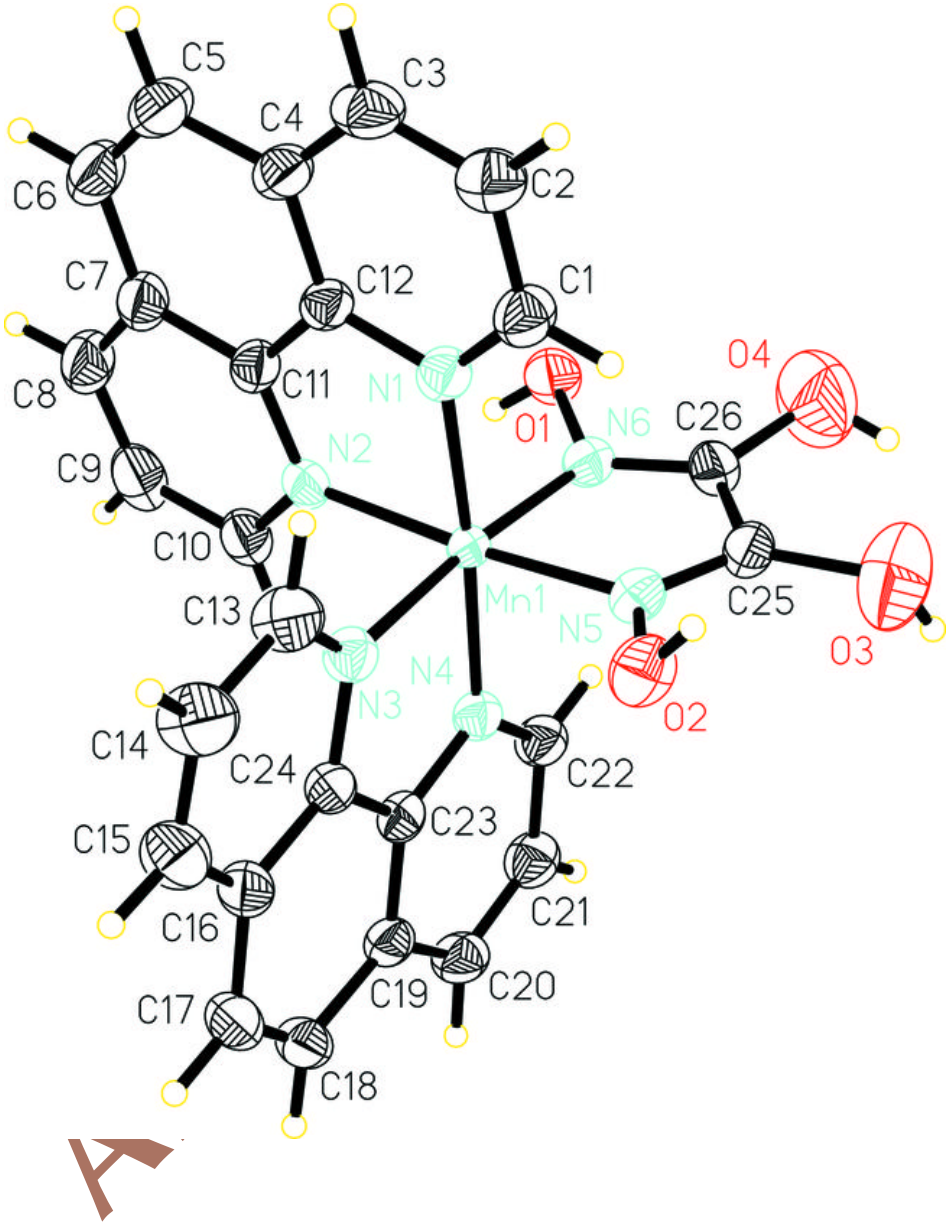
C5
C3
C4
C6
C2
C7
C12
C1
C8
C11
N1
O1
N6
C26
O4
C9
N2
C10
C13
Mn1
N5
C25
O3
N4
N3
O2
C14
C24
C22
C15
C23
C16
C21
C17
C19
C20
C18

Fig. 2