

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

T. Liu,^{a*} Y.-X. Wang,^b Z.-W. Wang,^a Z.-P. Xie^{a,c} and J. Y. Zhu^d

^aCollege of Engineering, Jingtangshan University, Jian 343009, People's Republic of China, ^bCollege of Mathematics and Physics, Jingtangshan University, Jian 343009, People's Republic of China, ^cDepartment of Chemistry, Jiangxi University of Science and Technology, Ganzhou 341000, People's Republic of China, and ^dDepartment of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China
Correspondence e-mail: taoliu07@126.com

Received 20 November 2009; accepted 15 December 2009

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
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)</i>	Liu & Xie (2007a)	10.1107/S1600536807026852	EDUMAS
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')copper(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007b)	10.1107/S1600536807028255	EDUVAB
<i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i>	Liu & Xie (2007b)	10.1107/S1600536807028735	RIGQAA
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i>	Liu, Wang, Wang & Xie (2007c)	10.1107/S1600536807030917	UDUMIQ
<i>Polymeric KNOF₂</i>	Liu Wang, Wang & Xie (2007a)	10.1107/S1600536807027195	ICSD 240891
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')cobalt(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007d)	10.1107/S1600536807031224	WIHJED
<i>Tetrakis(μ-2-pyridyloxyacetato)bis[(1,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i>	Liu, Wang, Wang & Xie (2007e)	10.1107/S1600536807032679	WIHQEK
<i>Tetrakis[μ-(2-pyridyloxy)acetato-κ²O:O']bis[(1,10-phenanthroline-κ²N,N')-(2-pyridyloxy)acetato-κO]neodymium(III)]</i>	Liu, Wang, Wang & Xie (2007f)	10.1107/S1600536807035349	TIGDAP
<i>(Dihydroxyglyoxime-κ²N,N')bis(1,10-phenanthroline-κ²N,N')manganese(II) dinitrate dihydrate</i>	Liu, Wang, Wang & Xie (2007g)	10.1107/S1600536807035076	TIGDET
<i>2-Amino-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Liu & Zhu (2007j)	10.1107/S1600536807040068	KIKQAX
<i>2-Hydroxy-3,5-dinitrobenzamide monohydrate</i>	Liu & Zhu (2007k)	10.1107/S1600536807039712	KIKQEB
<i>2-(1-Hydroxy-2-pyridyl)acetamide monohydrate</i>	Liu & Zhu (2007l)	10.1107/S1600536807040652	CIKQOD
<i>Bis(2,2'-bipyridine-κN,N')bis(thiocyanato-κN)iron(II)</i>	Liu & Zhu (2007a)	10.1107/S1600536807043486	XIFXOA
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(1,10-phenanthroline)disamarium(III)]</i>	Liu & Zhu (2007b)	10.1107/S1600536807045485	XILNAI
<i>3-Hydroxy-2,4,6-trinitropyridine monohydrate</i>	Liu & Zhu (2007m)	10.1107/S1600536807045230	PILNOO
<i>catena-Poly[hexakis(μ₂-anilinoacetamide)bis(1,10-phenanthroline)-dipraseodymium(III)]</i>	Liu & Zhu (2007c)	10.1107/S1600536807047733	SILZET
<i>catena-Poly[[tetra-μ-anilinoacetamidato-bis(1,10-phenanthroline)dicerium(III)]-di-μ-anilinoacetamidato]</i>	Liu & Zhu (2007d)	10.1107/S1600536807050969	GIMZOS
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)chromium(II)</i>	Liu & Zhu (2007e)	10.1107/S1600536807051756	WINFAB
<i>2-Ammonio-3-carboxy-5-nitrobenzoate monohydrate</i>	Liu & Zhu (2007n)	10.1107/S1600536807048477	GINFEP
<i>2-(Benzoylhydrazinocarbonyl)benzoic acid</i>	Liu & Zhu (2007o)	10.1107/S160053680705204X	TINZIA
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)vanadium(II)</i>	Liu & Zhu (2007f)	10.1107/S1600536807054529	HIPZIQ
<i>catena-Poly[[nitrato-κO](1,10-phenanthroline-κ²N,N')nickel(II)]-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007g)	10.1107/S1600536807056504	XIRGIP
<i>catena-Poly[[nitrato-κO](1,10-phenanthroline-κ²N,N')copper(II)]-μ-acetamido-κ²O:N]</i>	Liu & Zhu (2007h)	10.1107/S1600536807059077	HIQROP
<i>catena-Poly[[nitrato-κO](1,10-phenanthroline-κ²N,N')cobalt(II)]-μ-acetamidato-κ²O:N]</i>	Liu & Zhu (2007i)	10.1107/S1600536807060631	YIQMER
<i>N'-Benzoyl-4-nitronicotinohydrazide</i>	Liu & Zhu (2007p)	10.1107/S1600536807053068	CIPVON
<i>N'-(3-Nitro-4-pyridylcarbonyl)pyridine-4-carbohydrazide</i>	Liu & Zhu (2007q)	10.1107/S1600536807054876	RIRWEV

Table 1 (continued)

Title	Reference	DOI	Refcode
<i>Ethylenediammonium sulfate</i>	Liu & Zhu (2007r)	10.1107/S1600536807056280	ETDAMS03
<i>Ethylenediammonium perchlorate</i>	Liu & Zhu (2007s)	10.1107/S1600536807059909	HIRYEN
<i>catena-Poly[[[nitrate-κO](1,10-phenanthroline-κ²N,N')manganese(II)]-μ-nitrate-κ²O:O']</i>	Liu & Zhu (2008)	10.1107/S160053680706254X	MIRROV

References

Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007a). *Acta Cryst.* **E63**, i170.
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007b). *Acta Cryst.* **E63**, m1887–m1888.
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007c). *Acta Cryst.* **E63**, m2020–m2021.
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007d). *Acta Cryst.* **E63**, m2027–m2028.
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007e). *Acta Cryst.* **E63**, m2080–m2081.
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007f). *Acta Cryst.* **E63**, m2196–m2197.
 Liu, T., Wang, Z.-W., Wang, Y.-X. & Xie, Z.-P. (2007g). *Acta Cryst.* **E63**, m2198–m2199.
 Liu, T. & Xie, Z.-P. (2007a). *Acta Cryst.* **E63**, m1820.
 Liu, T. & Xie, Z.-P. (2007b). *Acta Cryst.* **E63**, m1908.
 Liu, T. & Zhu, J. Y. (2007a). *Acta Cryst.* **E63**, m2506–m2507.

Liu, T. & Zhu, J.-Y. (2007b). *Acta Cryst.* **E63**, m2592–m2593.
 Liu, T. & Zhu, J. Y. (2007c). *Acta Cryst.* **E63**, m2659–m2660.
 Liu, T. & Zhu, J. Y. (2007d). *Acta Cryst.* **E63**, m2775–m2776.
 Liu, T. & Zhu, J. Y. (2007e). *Acta Cryst.* **E63**, m2809.
 Liu, T. & Zhu, J. Y. (2007f). *Acta Cryst.* **E63**, m2912.
 Liu, T. & Zhu, J.-Y. (2007g). *Acta Cryst.* **E63**, m2977–m2978.
 Liu, T. & Zhu, J. Y. (2007h). *Acta Cryst.* **E63**, m3108.
 Liu, T. & Zhu, J. Y. (2007i). *Acta Cryst.* **E63**, m3144.
 Liu, T. & Zhu, J.-Y. (2007j). *Acta Cryst.* **E63**, o3829.
 Liu, T. & Zhu, J. Y. (2007k). *Acta Cryst.* **E63**, o3830.
 Liu, T. & Zhu, J.-Y. (2007l). *Acta Cryst.* **E63**, o3860.
 Liu, T. & Zhu, J. Y. (2007m). *Acta Cryst.* **E63**, o4112.
 Liu, T. & Zhu, J. Y. (2007n). *Acta Cryst.* **E63**, o4267.
 Liu, T. & Zhu, J. Y. (2007o). *Acta Cryst.* **E63**, o4441.
 Liu, T. & Zhu, J. Y. (2007p). *Acta Cryst.* **E63**, o4527.
 Liu, T. & Zhu, J. Y. (2007q). *Acta Cryst.* **E63**, o4574.
 Liu, T. & Zhu, J.-Y. (2007r). *Acta Cryst.* **E63**, o4660.
 Liu, T. & Zhu, J. Y. (2007s). *Acta Cryst.* **E63**, o4874.
 Liu, T. & Zhu, J. Y. (2008). *Acta Cryst.* **E64**, m28.

catena-Poly[[*(nitrate-κO)*(1,10-phenanthroline-*κ²N,N')*manganese(II)]-*μ-nitrate-κ²O:O'*]

 T. Liu^{a*} and J. Y. Zhu^b

^aCollege of Engineering, Jinggangshan University, Jian 343009, People's Republic of China, and ^bDepartment of Information Engineering, Jiangxi University of Science and Technology, Nanchang 330013, People's Republic of China
Correspondence e-mail: taoliu07@126.com

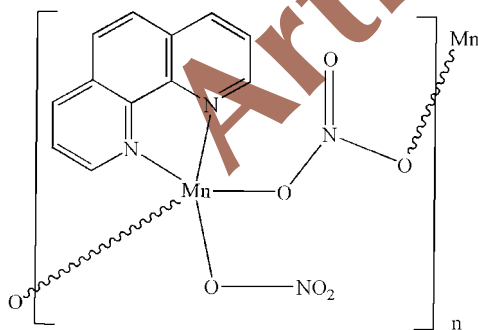
Received 20 November 2007; accepted 23 November 2007

Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.033; wR factor = 0.093; data-to-parameter ratio = 12.2.

In the crystal structure of the title compound, $[\text{Mn}(\text{NO}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)]_n$, the Mn^{II} atoms are linked by nitrate ligands to form a chain. Each Mn^{II} atom is five-coordinated by two N atoms of a 1,10-phenanthroline ligand and three O atoms of two nitrates within a trigonal-bipyramidal coordination geometry. In the crystal structure, the chains are linked by hydrogen bonds into a polymeric ribbon structure.

Related literature

For general background, see: Desiraju (1995, 1997); Braga *et al.* (1998); Wu *et al.* (2003); Pan & Xu (2004); Liu *et al.* (2004); Li *et al.* (2005). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[\text{Mn}(\text{NO}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)]$
 $M_r = 359.16$

Monoclinic, $P2_1/n$
 $a = 8.7116$ (13) Å
 $b = 9.1824$ (11) Å
 $c = 17.1183$ (17) Å
 $\beta = 102.159$ (4)°

$V = 1338.6$ (3) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 1.03$ mm⁻¹
 $T = 273$ (2) K
 $0.42 \times 0.23 \times 0.20$ mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.672$, $T_{\text{max}} = 0.819$

8124 measured reflections
2545 independent reflections
2194 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.093$
 $S = 1.01$
2545 reflections

209 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.36$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Mn1—O1	2.0145 (18)	Mn1—N1	2.018 (2)
Mn1—O2	1.9470 (17)	Mn1—N2	1.988 (2)
Mn1—O5 ⁱ	2.3361 (19)		
O1—Mn1—O5 ⁱ	86.83 (7)	O2—Mn1—N2	174.52 (8)
O2—Mn1—O5 ⁱ	82.09 (7)	O5—Mn1—N1 ⁱ	138.26 (3)
O1—Mn1—N1	165.99 (8)	O5—Mn1—N2 ⁱ	125.23 (4)
O1—Mn1—N2	93.16 (8)	N1—Mn1—N2	82.65 (8)
O2—Mn1—N1	94.35 (9)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots O4 ⁱⁱ	0.93	2.51	3.331 (4)	148
C10—H10 \cdots O2 ⁱⁱⁱ	0.93	2.37	3.276 (3)	165

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

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.

The authors thank the Youth Programme of Jinggangshan University for financial support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2505).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Braga, D., Grepioni, F. & Desiraju, G. R. (1998). *Chem. Rev.* **98**, 1375–1386.
Bruker (2005). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 2311–2315.
Desiraju, G. R. (1997). *J. Chem. Soc. Chem. Commun.* pp. 1475–1476.
Li, H., Yin, K.-L. & Xu, D.-J. (2005). *Acta Cryst.* **C61**, m19–m21.
Liu, B.-X., Su, J.-R. & Xu, D.-J. (2004). *Acta Cryst.* **C60**, m183–m185.
Pan, T.-T. & Xu, D.-J. (2004). *Acta Cryst.* **E60**, m56–m58.
Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
Siemens (1996). SAINT and SHELXTL. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Wu, Z.-Y., Xue, Y.-H. & Xu, D.-J. (2003). *Acta Cryst.* **E59**, m809–m811.

supplementary materials

Article retracted

Acta Cryst. (2008). E64, m28 [doi:10.1107/S160053680706254X]

catena-Poly[[nitrate- κ O](1,10-phenanthroline- κ^2 N,N')manganese(II)]- μ -nitrate- κ^2 O:O']

T. Liu and J. Y. Zhu

Comment

In the synthesis of crystal structures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Aromatic polycyclic compounds, such as phenanthroline, quinoline and benzimidazole, are one of the most important classes of biological ligands, the coordinations of metal-aromatic polycyclic compounds are of critical importance in biological systems, organic materials and coordination chemistry (Wu *et al.*, 2003; Pan & Xu, 2004; Liu *et al.*, 2004; Li *et al.*, 2005). We report herein 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 title compound, $[\text{Mn}(\text{NO}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)]_n$, are linked by nitrate ligands to form a chain. Each Mn^{II} atom is five-coordinated by two N atoms of 1,10-phenanthroline (phen) ligand and three O atoms of two nitrates within a bipyramidal coordination geometry (Table 1). The Mn—O and Mn—N bond are in the range 1.9470 (17)–2.3361 (19) Å and 1.988 (2)–2.018 (2) Å, respectively (Table 1).

In the crystal structure, no classic C—H \cdots O hydrogen bonds (Fig. 2 and Table 2) seem to be effective in the stabilization of the structure, resulting in the formation of a polymeric ribbon structure.

Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Europium (III) nitrate pentahydrate (213.9 mg, 0.5 mmol), manganese (II) nitrate hexahydrate (287.1 mg, 1 mmol), phen (180.2 mg, 1 mmol) and distilled water (7 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colourless solution was decanted from small colourless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

Refinement

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

Figures

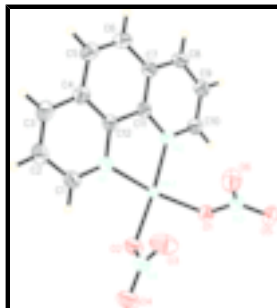


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $-x + 3/2, y + 1/2, -z + 1/2$].

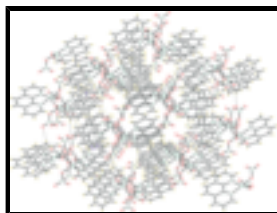


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

catena-Poly[[[(nitrate- κ O)(1,10-phenanthroline- κ^2 N, \backslash N¹)manganese(II)]- μ -nitrate- κ^2 O:O¹]

Crystal data

[Mn(NO₃)₂(C₁₂H₈N₂)]

$M_r = 359.16$

Monoclinic, $P2_1/n$

Hall symbol: $-p\ 2yn$

$a = 8.7116$ (13) Å

$b = 9.1824$ (11) Å

$c = 17.1183$ (17) Å

$\beta = 102.159$ (4)°

$V = 1338.6$ (3) Å³

$Z = 4$

$F_{000} = 724$

$D_x = 1.782$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5711 reflections

$\theta = 2.1$ – 27.1 °

$\mu = 1.03$ mm⁻¹

$T = 273$ (2) K

Prism, colourless

$0.42 \times 0.23 \times 0.20$ mm

Data collection

Bruker APEXII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ (2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.672, T_{\max} = 0.819$

8124 measured reflections

2545 independent reflections

2194 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.017$

$\theta_{\text{max}} = 26.1$ °

$\theta_{\text{min}} = 2.4$ °

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.5483P]$
$wR(F^2) = 0.093$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{\max} = 0.001$
2545 reflections	$\Delta\rho_{\max} = 0.36 \text{ e } \text{\AA}^{-3}$
209 parameters	$\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL, $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0179 (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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.66502 (3)	0.92794 (3)	0.803177 (16)	0.03141 (15)
O1	0.6879 (2)	0.73412 (19)	0.75168 (10)	0.0520 (4)
O2	0.5484 (2)	1.0052 (2)	0.70206 (11)	0.0587 (5)
O3	0.3466 (3)	0.9003 (3)	0.72914 (16)	0.0906 (8)
O4	0.3287 (3)	1.0285 (3)	0.62191 (14)	0.0772 (6)
O5	0.6208 (2)	0.5057 (2)	0.74824 (12)	0.0593 (5)
O6	0.5458 (3)	0.6518 (2)	0.83135 (14)	0.0755 (6)
N1	0.6080 (2)	1.0941 (2)	0.86880 (13)	0.0464 (5)
N2	0.7953 (2)	0.8670 (2)	0.90779 (12)	0.0452 (4)
N3	0.6159 (2)	0.6285 (2)	0.77856 (13)	0.0470 (5)
N4	0.4025 (3)	0.9772 (3)	0.68402 (13)	0.0516 (5)
C1	0.5211 (3)	1.2101 (3)	0.84667 (17)	0.0538 (6)
H1	0.4829	1.2263	0.7924	0.065*
C2	0.4835 (3)	1.3108 (3)	0.90171 (19)	0.0600 (7)
H2	0.4227	1.3922	0.8838	0.072*
C3	0.5365 (3)	1.2882 (3)	0.98057 (19)	0.0601 (7)

supplementary materials

H3	0.5100	1.3523	1.0176	0.072*
C4	0.6324 (3)	1.1667 (3)	1.00645 (15)	0.0488 (6)
C5	0.6988 (3)	1.1334 (3)	1.08805 (16)	0.0568 (6)
H5	0.6749	1.1919	1.1282	0.068*
C6	0.7949 (3)	1.0191 (3)	1.10763 (16)	0.0553 (6)
H6	0.8361	1.0000	1.1613	0.066*
C7	0.8364 (3)	0.9249 (3)	1.04801 (15)	0.0466 (5)
C8	0.9424 (3)	0.8080 (3)	1.06332 (15)	0.0537 (6)
H8	0.9924	0.7863	1.1156	0.064*
C9	0.9722 (3)	0.7263 (3)	1.00167 (17)	0.0564 (6)
H9	1.0438	0.6499	1.0116	0.068*
C10	0.8953 (3)	0.7578 (3)	0.92411 (16)	0.0522 (6)
H10	0.9146	0.7004	0.8825	0.063*
C11	0.7670 (3)	0.9514 (3)	0.96834 (14)	0.0420 (5)
C12	0.6658 (3)	1.0727 (2)	0.94761 (15)	0.0428 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0374 (2)	0.0301 (2)	0.02529 (19)	0.00252 (12)	0.00320 (13)	0.00100 (11)
O1	0.0628 (10)	0.0482 (10)	0.0459 (9)	-0.0052 (8)	0.0131 (8)	-0.0007 (7)
O2	0.0537 (10)	0.0658 (13)	0.0514 (10)	-0.0071 (9)	-0.0008 (8)	0.0128 (9)
O3	0.0735 (14)	0.130 (2)	0.0678 (14)	-0.0247 (14)	0.0136 (12)	0.0269 (15)
O4	0.0677 (12)	0.0828 (14)	0.0691 (14)	-0.0060 (11)	-0.0129 (11)	0.0214 (12)
O5	0.0581 (10)	0.0475 (11)	0.0722 (12)	-0.0049 (8)	0.0134 (9)	-0.0144 (9)
O6	0.0910 (15)	0.0644 (13)	0.0845 (15)	-0.0048 (11)	0.0492 (13)	-0.0075 (11)
N1	0.0483 (11)	0.0441 (11)	0.0460 (11)	0.0003 (9)	0.0084 (9)	0.0041 (9)
N2	0.0508 (11)	0.0414 (10)	0.0424 (10)	0.0015 (9)	0.0074 (8)	-0.0026 (8)
N3	0.0473 (10)	0.0451 (11)	0.0493 (11)	0.0015 (9)	0.0116 (9)	-0.0043 (9)
N4	0.0535 (12)	0.0524 (12)	0.0466 (11)	-0.0017 (10)	0.0053 (10)	0.0018 (10)
C1	0.0558 (14)	0.0469 (14)	0.0563 (14)	0.0055 (12)	0.0066 (12)	0.0070 (12)
C2	0.0587 (15)	0.0467 (14)	0.0740 (18)	0.0118 (12)	0.0123 (13)	0.0039 (13)
C3	0.0628 (16)	0.0506 (15)	0.0707 (17)	0.0072 (12)	0.0227 (14)	-0.0085 (13)
C4	0.0494 (13)	0.0478 (13)	0.0526 (13)	-0.0020 (11)	0.0185 (11)	-0.0032 (11)
C5	0.0626 (15)	0.0618 (16)	0.0490 (14)	-0.0020 (13)	0.0187 (12)	-0.0102 (12)
C6	0.0608 (15)	0.0638 (16)	0.0419 (13)	0.0004 (13)	0.0121 (11)	-0.0010 (12)
C7	0.0505 (13)	0.0471 (13)	0.0419 (12)	-0.0048 (10)	0.0087 (10)	0.0029 (10)
C8	0.0596 (14)	0.0527 (14)	0.0449 (13)	-0.0003 (12)	0.0025 (11)	0.0060 (11)
C9	0.0594 (15)	0.0464 (14)	0.0592 (15)	0.0089 (12)	0.0026 (12)	0.0028 (12)
C10	0.0589 (14)	0.0439 (13)	0.0519 (14)	0.0078 (11)	0.0072 (12)	-0.0025 (11)
C11	0.0445 (12)	0.0393 (11)	0.0431 (12)	-0.0042 (9)	0.0114 (10)	-0.0007 (9)
C12	0.0428 (11)	0.0400 (12)	0.0468 (12)	-0.0047 (9)	0.0119 (10)	0.0017 (9)

Geometric parameters (\AA , $^\circ$)

Mn1—O1	2.0145 (18)	C2—C3	1.348 (4)
Mn1—O2	1.9470 (17)	C2—H2	0.9300
Mn1—O5 ⁱ	2.3361 (19)	C3—C4	1.408 (4)

Mn1—N1	2.018 (2)	C3—H3	0.9300
Mn1—N2	1.988 (2)	C4—C12	1.403 (3)
O1—N3	1.291 (3)	C4—C5	1.428 (4)
O2—N4	1.269 (3)	C5—C6	1.341 (4)
O3—N4	1.221 (3)	C5—H5	0.9300
O4—N4	1.216 (3)	C6—C7	1.441 (4)
O5—N3	1.246 (3)	C6—H6	0.9300
O5—Mn1 ⁱⁱⁱ	2.3362 (19)	C7—C11	1.392 (4)
O6—N3	1.212 (3)	C7—C8	1.404 (4)
N1—C1	1.316 (3)	C8—C9	1.364 (4)
N1—C12	1.351 (3)	C8—H8	0.9300
N2—C10	1.319 (3)	C9—C10	1.386 (4)
N2—C11	1.358 (3)	C9—H9	0.9300
C1—C2	1.407 (4)	C10—H10	0.9300
C1—H1	0.9300	C11—C12	1.419 (3)
O1—Mn1—O5 ⁱ	86.83 (7)	C2—C3—C4	119.5 (3)
O2—Mn1—O5 ⁱ	82.09 (7)	C2—C3—H3	120.2
O1—Mn1—N1	165.99 (8)	C4—C3—H3	120.2
O1—Mn1—N2	93.16 (8)	C12—C4—C3	117.4 (2)
O2—Mn1—N1	94.35 (9)	C12—C4—C5	117.9 (2)
O2—Mn1—N2	174.52 (8)	C3—C4—C5	124.7 (2)
O5—Mn1—N1 ⁱ	138.26 (3)	C6—C5—C4	121.0 (2)
O5—Mn1—N2 ⁱ	125.23 (4)	C6—C5—H5	119.5
N1—Mn1—N2	82.65 (8)	C4—C5—H5	119.5
N3—O1—Mn1	114.06 (14)	C5—C6—C7	122.0 (2)
N4—O2—Mn1	116.78 (15)	C5—C6—H6	119.0
N3—O5—Mn1 ⁱⁱ	122.25 (15)	C7—C6—H6	119.0
C1—N1—C12	118.4 (2)	C11—C7—C8	116.7 (2)
C1—N1—Mn1	130.26 (19)	C11—C7—C6	117.8 (2)
C12—N1—Mn1	111.27 (16)	C8—C7—C6	125.4 (2)
C10—N2—C11	119.4 (2)	C9—C8—C7	120.1 (2)
C10—N2—Mn1	129.13 (17)	C9—C8—H8	120.0
C11—N2—Mn1	111.47 (16)	C7—C8—H8	120.0
O6—N3—O5	122.5 (2)	C8—C9—C10	119.6 (2)
O6—N3—O1	119.4 (2)	C8—C9—H9	120.2
O5—N3—O1	118.0 (2)	C10—C9—H9	120.2
O4—N4—O3	124.7 (2)	N2—C10—C9	121.7 (2)
O4—N4—O2	116.9 (2)	N2—C10—H10	119.1
O3—N4—O2	118.4 (2)	C9—C10—H10	119.1
N1—C1—C2	122.7 (3)	N2—C11—C7	122.5 (2)
N1—C1—H1	118.7	N2—C11—C12	117.4 (2)
C2—C1—H1	118.7	C7—C11—C12	120.1 (2)
C3—C2—C1	119.4 (3)	N1—C12—C4	122.5 (2)
C3—C2—H2	120.3	N1—C12—C11	116.4 (2)
C1—C2—H2	120.3	C4—C12—C11	121.0 (2)

Symmetry codes: (i) $-x+3/2, y+1/2, -z+3/2$; (ii) $-x+3/2, y-1/2, -z+3/2$.

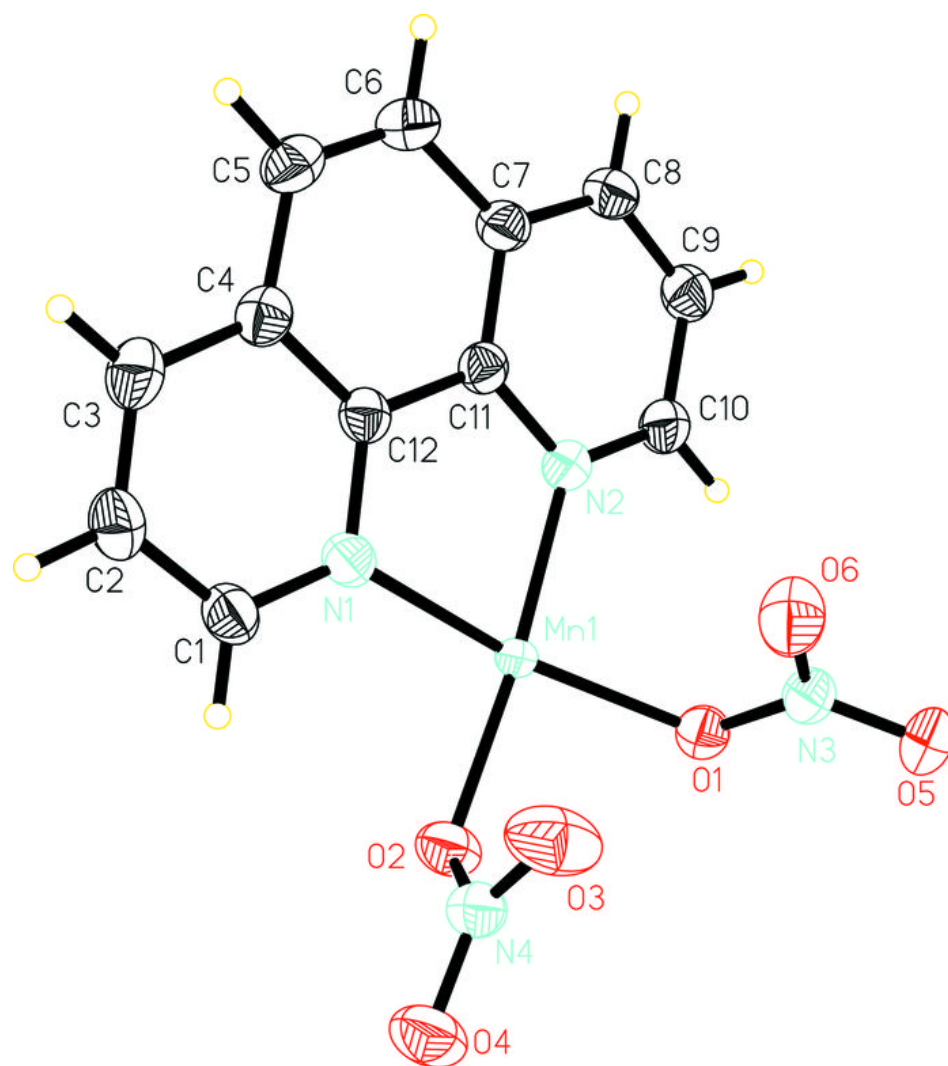
Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C2—H2···O4 ⁱⁱⁱ	0.93	2.51	3.331 (4)	148
C10—H10···O2 ⁱⁱ	0.93	2.37	3.276 (3)	165

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

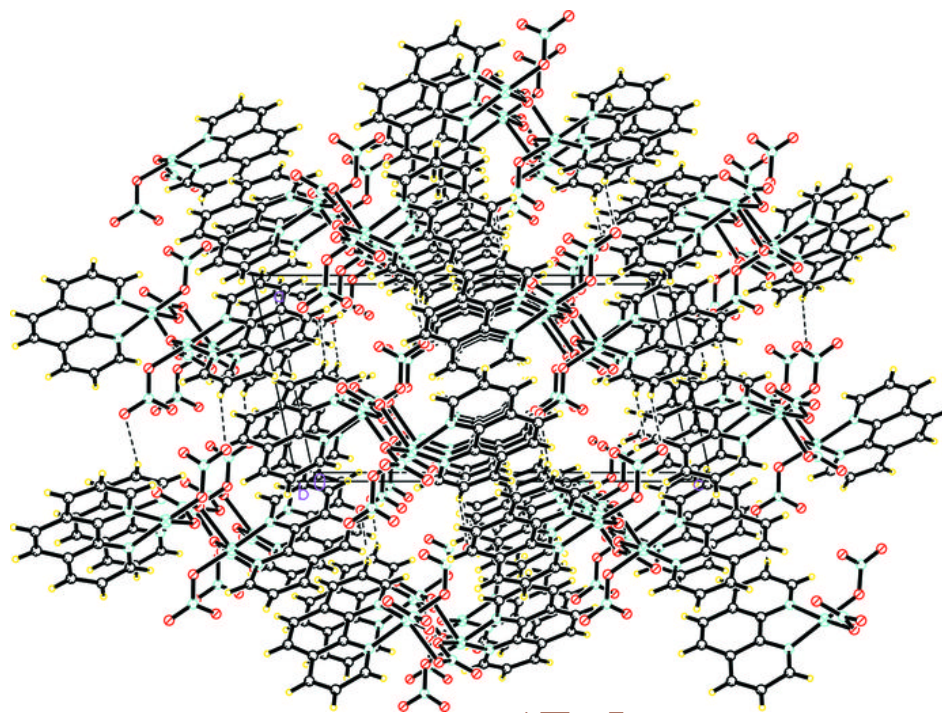
Article retracted

Fig. 1



Arc

Fig. 2



Article ref.