

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 |
|--|---|--|-----------------------|
| <i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)manganese(II)</i> <i>(Dihydroxyglyoxime-κ²N,N')bis(I,10-phenanthroline-κ²N,N')copper(II) dinitrate dihydrate</i> | Liu & Xie (2007a) Liu, Wang, Wang & Xie (2007b) | 10.1107/S1600536807026852 10.1107/S1600536807028255 | EDUMAS EDUVAB |
| <i>Tetrakis(pyrazine-κN)bis(thiocyanato-κN)zinc(II)</i> | Liu & Xie (2007b) | 10.1107/S1600536807028735 | RIGQAA |
| <i>Tetrakis(μ-2-pyridyloxyacetato)bis[(I,10-phenanthroline)(2-pyridyloxyacetato)-lanthanum(III)]</i> | Liu, Wang, Wang & Xie (2007c) | 10.1107/S1600536807030917 | UDUMIQ |
| <i>Polymeric KNO₂</i> <i>(Dihydroxyglyoxime-κ²N,N')bis(I,10-phenanthroline-κ²N,N')cobalt(II) dinitrate dihydrate</i> | Liu Wang, Wang & Xie (2007a) Liu, Wang, Wang & Xie (2007d) | 10.1107/S1600536807027195 10.1107/S1600536807031224 | ICSD 240891 WIHIED |
| <i>Tetrakis(μ-2-pyridyloxyacetato)bis[(I,10-phenanthroline)(2-pyridyloxyacetato)-praseodymium(III)]</i> | Liu, Wang, Wang & Xie (2007e) | 10.1107/S1600536807032679 | WIHQEK |
| <i>Tetrakis[μ-(2-pyridyloxyacetato-κ²O:O')bis(I,10-phenanthroline-κ²N,N')-(2-pyridyloxyacetato-κO)neodymium(III)]</i> | Liu, Wang, Wang & Xie (2007f) | 10.1107/S1600536807035349 | TIGDAP |
| <i>(Dihydroxyglyoxime-κ²N,N')bis(I,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-ammonium (I/I)</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(I,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(I,10-phenanthroline)-dipraseodymium(III)]</i> | Liu & Zhu (2007c) | 10.1107/S1600536807047733 | SILZET |
| <i>catena-Poly[[tetra-μ-anilinoacetamido-bis(I,10-phenanthroline)dicerium(III)-di-μ-anilinoacetamido]</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](I,10-phenanthroline-κ²N,N')nickel(II)-μ-acetamido-κ²O:N]</i> | Liu & Zhu (2007g) | 10.1107/S1600536807056504 | XIRGIP |
| <i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ²N,N')copper(II)-μ-acetamido-κ²O:N]</i> | Liu & Zhu (2007h) | 10.1107/S1600536807059077 | HIQROP |
| <i>catena-Poly[[nitrato-κO](I,10-phenanthroline-κ²N,N')cobalt(II)-μ-acetamido-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 |

addenda and errata

Table 1 (continued)

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

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catena-Poly[[$(\text{nitrato}-\kappa^2\text{O})(1,10\text{-phenanthroline}-\kappa^2\text{N},\text{N}')$ manganese(II)]- μ -nitrato- $\kappa^2\text{O}: \text{O}'$]

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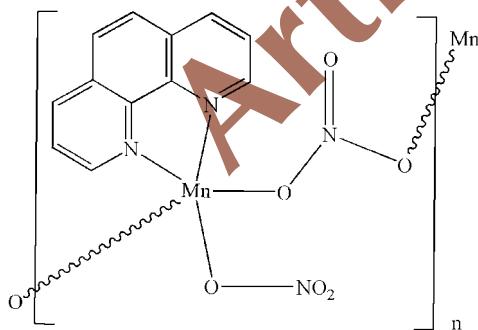
Received 20 November 2007; accepted 23 November 2007

Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C-C}) = 0.004$ 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)

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

8124 measured reflections

2545 independent reflections

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

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

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, °).

| $D\cdots H\cdots A$ | $D\cdots H$ | $H\cdots A$ | $D\cdots A$ | $D\cdots H\cdots A$ |
|-----------------------------|-------------|-------------|-------------|---------------------|
| C2—H2···O4 ⁱⁱ | 0.93 | 2.51 | 3.331 (4) | 148 |
| C10—H10···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.

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

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supplementary materials

Article retracted

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

catena-Poly[[(nitrato- κO)(1,10-phenanthroline- $\kappa^2 N,N'$)manganese(II)]- μ -nitrato- $\kappa^2 O:O'$]

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, $[Mn(NO_3)_2(C_{12}H_8N_2)]_n$, 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 $U_{iso}(H) = 1.2U_{eq}(C)$.

supplementary materials

Figures

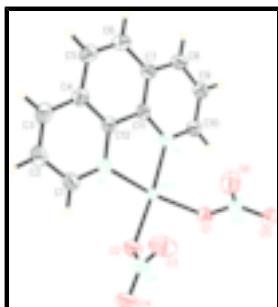


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A): $-x + 3/2, y + 1/2, -z + 1/2$].

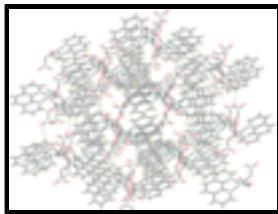


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.



Crystal data

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

$M_r = 359.16$

Monoclinic, $P2_1/n$

Hall symbol: -p 2yn

$a = 8.7116 (13)$ Å

$b = 9.1824 (11)$ Å

$c = 17.1183 (17)$ Å

$\beta = 102.159 (4)^\circ$

$V = 1338.6 (3)$ Å 3

$Z = 4$

$F_{000} = 724$

$D_x = 1.782$ Mg m $^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5711 reflections

$\theta = 2.1\text{--}27.1^\circ$

$\mu = 1.03$ mm $^{-1}$

$T = 273 (2)$ K

Prism, colourless

$0.42 \times 0.23 \times 0.20$ mm

Data collection

Bruker APEXII area-detector diffractometer

2545 independent reflections

Radiation source: fine-focus sealed tube

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

Monochromator: graphite

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

$T = 273(2)$ K

$\theta_{\text{max}} = 26.1^\circ$

φ and ω scans

$\theta_{\text{min}} = 2.4^\circ$

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

$h = -10 \rightarrow 10$

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

$k = -11 \rightarrow 11$

8124 measured reflections

$l = -21 \rightarrow 21$

*Refinement*Refinement on F^2

Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

H-atom parameters constrained

$$R[F^2 > 2\sigma(F^2)] = 0.033$$

$$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.5483P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$$wR(F^2) = 0.093$$

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

$$S = 1.01$$

$$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$$

2545 reflections

$$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$$

209 parameters

Extinction correction: SHELXL,
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{1/4}$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.0179 (16)

Secondary atom site location: difference Fourier map

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)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|---------------|----------------------------------|
| 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 ⁱⁱ | 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) $-x+3/2, y-1/2, -z+3/2$.

supplementary materials

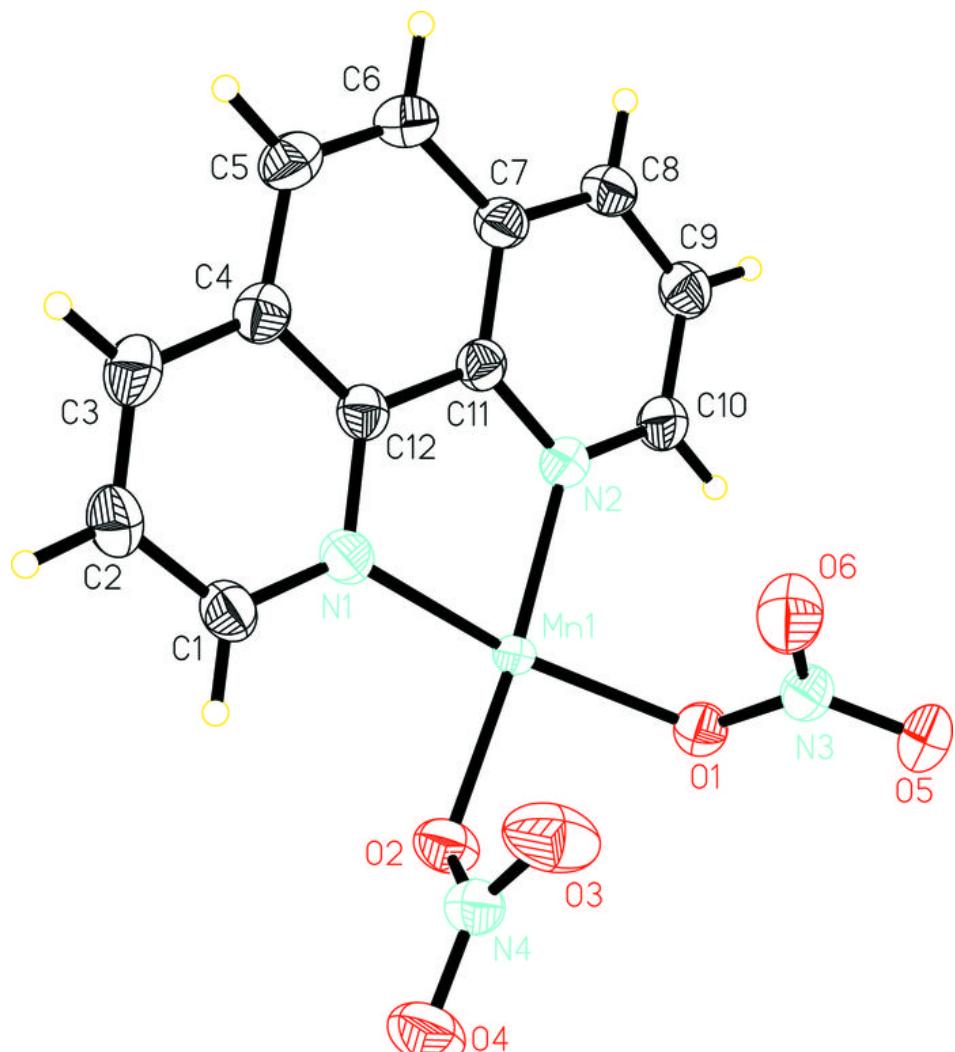
Hydrogen-bond geometry (Å, °)

| <i>D—H···A</i> | <i>D—H</i> | <i>H···A</i> | <i>D···A</i> | <i>D—H···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

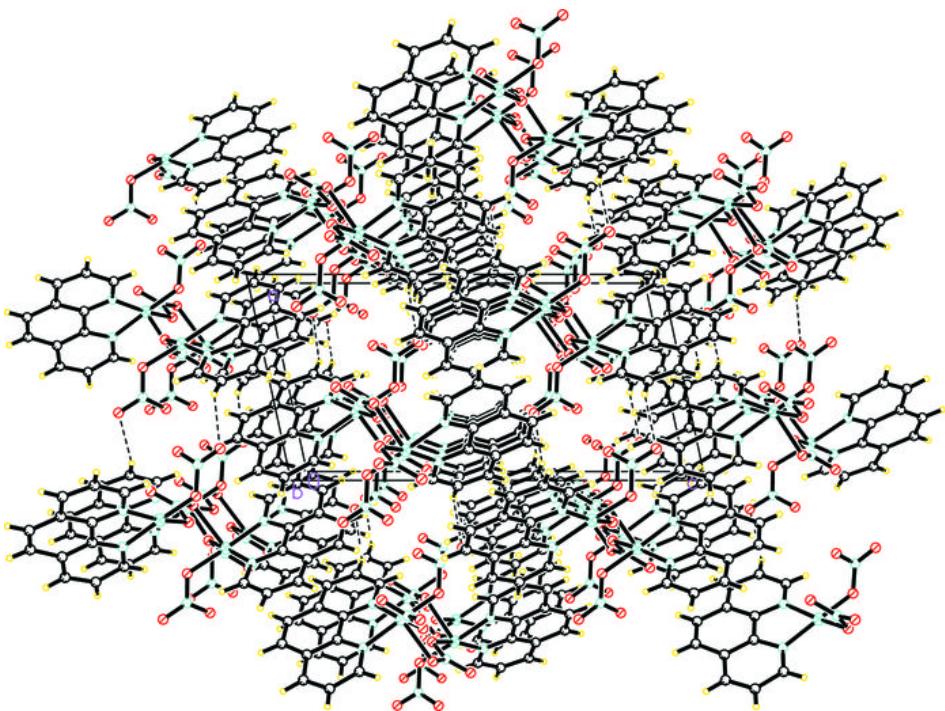
Fig. 1



Arc

supplementary materials

Fig. 2



Article rev.