

Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted 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	Retracted by	DOI	Refcode
<i>trans</i> -Bis[1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato]copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
<i>Bis</i> (4-bromo-2-formylphenolato- $\kappa^2 O, O'$)copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
<i>Bis</i> (salicylaldehyde)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
<i>Bis</i> (4-bromo-2-formylphenolato- $\kappa^2 O, O'$)zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
<i>Bis</i> (2-formylphenolato- $\kappa^2 O, O'$)nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
<i>Bis</i> (2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
<i>Bis</i> (2-formylphenolato- $\kappa^2 O, O'$)manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)copper(II) naphthalene-1,5-disulfonate dihydrate	Liu <i>et al.</i> (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui <i>et al.</i> (2006)	Journal	10.1107/S160053680604565X	HESPEP
<i>Bis</i> (2-formylphenolato- $\kappa^2 O, O'$)iron(II)	Yang <i>et al.</i> (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer <i>et al.</i> (2007a)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer <i>et al.</i> (2007b)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2007)	Author	10.1107/S1600536807031121	WIHKEE
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen <i>et al.</i> (2007)	Author	10.1107/S1600536807032540	WIHRIP
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li <i>et al.</i> (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1 $\kappa^4 O^1, O^2, O^3, O^4$:2 $\kappa^4 O^1, N, N', N''$ }(methanol-1 κO)- μ -nitrate-1:2 $\kappa^2 O:O'$ -dinitrate-1 $\kappa^4 O, O'$ -cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol- μ -nitrate-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol- μ -nitrate-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol- μ -nitrate-dinitratolutetium(III)zinc(II)	Sui, Sui <i>et al.</i> (2007)	Author	10.1107/S1600536807037737	AFEF0H
catena-Poly[[chloridonickel(II)]-di- μ -chlorido-[chloridonickel(II)]- μ -4,4'-methylenebis(3,5-dimethylpyrazole)- $\kappa^2 N^2, N^2$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
[2,2'-[<i>o</i> -Phenylenebis(nitrilomethylidyne)]diphenolato]zinc(II)	Liu <i>et al.</i> (2007a)	Author	10.1107/S1600536807040640	DIKYUS
<i>trans</i> -Bis(ethylenediamine- $\kappa^2 N, N'$)bis(nitrate- κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[<i>N, N'</i> -(<i>o</i> -Phenylene)bis(picolinamido)- $\kappa^4 N, N', N'', N'''$]cobalt(II)	Liu & Zeng (2007a)	Author	10.1107/S1600536807044571	XILFII
[<i>N, N'</i> -(<i>o</i> -Phenylene)dipicolinamide- $\kappa^4 N$]nickel(II)	Liu & Zeng (2007b)	Author	10.1107/S1600536807048386	WINWEW
[2,2'-[<i>o</i> -Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu <i>et al.</i> (2007b)	Author	10.1107/S1600536807052993	VIQPIV
<i>N</i> -(2-Amino-3-pyridyl)urea monohydrate	Li <i>et al.</i> (2007)	Author	10.1107/S1600536807047526	SIMFEA
<i>N</i> -(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime- $\kappa^2 N, N'$)(3,5-dinitro-2-oxidobenzooato- $\kappa^2 O^1, O^2$)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ -Acetato-tri- μ -ferrocenecarboxylatobis[(<i>N, N</i> -dimethylformamide)-copper(II)]	Liu, Lin <i>et al.</i> (2007)	Journal	10.1107/S1600536807059041	HIQQEE

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li <i>et al.</i> (2008)	Author	10.1107/S1600536807056309	RISTET
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoerbium(III)zinc(II)	Chen <i>et al.</i> (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato- $\kappa^2 O^1, O^6$)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoholmium(III)zinc(II)	Xiao, Sui <i>et al.</i> (2008)	Author	10.1107/S1600536808013743	BIZTUA
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu <i>et al.</i> (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid-4,4'-bipyridine (2I)	Wang <i>et al.</i> (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato- $1\kappa^4 O^1, O^1, O^6, O^6:2\kappa^4 O^1, N, N', O^1$ }(ethanol- $1\kappa O$)- μ -nitrate- $1:2\kappa^2 O:O'$ -dinitrate- $1\kappa^2 O, O'$ -samarium(III)zinc(II)	Huang <i>et al.</i> (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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{2,2'-[*o*-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)

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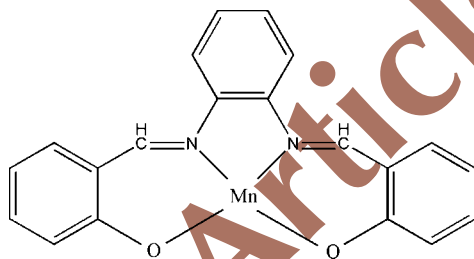
Received 19 October 2007; accepted 25 October 2007

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; R factor = 0.059; wR factor = 0.161; data-to-parameter ratio = 12.9.

The title complex, $[\text{Mn}(\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_2)]$, is a mononuclear manganese(II) compound. The manganese(II) ion is four-coordinated in a square-planar geometry by two imine N and two phenolate O atoms from one 2,2'-[*o*-phenylenebis(nitrilomethylidyne)]diphenolate Schiff base ligand. No strong hydrogen bonds were found in the crystal structure.

Related literature

For related literature, see: Liu *et al.* (2007).



Experimental

Crystal data

$[\text{Mn}(\text{C}_{20}\text{H}_{14}\text{N}_2\text{O}_2)]$
 $M_r = 369.27$
 Orthorhombic, $P2_12_12_1$
 $a = 5.4676$ (6) Å
 $b = 16.6244$ (19) Å
 $c = 17.324$ (2) Å

$V = 1574.7$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.85$ mm⁻¹
 $T = 293$ (2) K
 $0.25 \times 0.08 \times 0.07$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: none
 9864 measured reflections

2930 independent reflections
 2298 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$
 $wR(F^2) = 0.161$
 $S = 1.06$
 2930 reflections
 227 parameters
 H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.81$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.37$ e Å⁻³
 Absolute structure: Flack (1983),
 1204 Friedel pairs
 Flack parameter: -0.13 (5)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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 are grateful to the Key Laboratory of Coordination Chemistry, JingGangShan University, People's Republic of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2322).

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supplementary materials

Article retracted

Acta Cryst. (2007). E63, m2854 [doi:10.1107/S1600536807052993]

{2,2'-[*o*-Phenylenebis(nitrilomethylidene)]diphenolato}manganese(II)

Y.-Q. Liu, X.-R. Zeng, Q.-Y. Luo and Y.-P. Xu

Comment

The X-ray structure determination shows the title complex to be a discrete molecular compound (Fig. 1). Each manganese(II) ion is four-coordinated in a square-planar geometry by two imine N and two phenolate O atoms from one 2,2'-[*o*-phenylenebis(nitrilomethylidene)]-diphenolate Schiff base ligand, coordination bond lengths are listed as: Mn1—N1 1.853 (5) Å; Mn1—N2 1.852 (5) Å; Mn1—O1 1.834 (4) Å; Mn1—O2 1.841 (4) Å. Atom O1, O2, N1 and N2 are approximately coplanar with the central Mn cation, the maximum deviation from the least-squares plane through all five atoms being 0.0141 Å for atom O1. The structure of a related complex, $\text{ZnC}_{20}\text{H}_{14}\text{N}_2\text{O}_2$ has been reported (Liu *et al.*, 2007). No strong hydrogen bonds are found with the three-dimensional framework of the crystal mainly constructed by weak intermolecular interactions.

Experimental

A mixture of 2,2'-[*o*-phenylenebis(nitrilomethylidene)]-diphenolate Schiff base (0.341 g, 0.001 mol) and $\text{MnSO}_4 \cdot \text{H}_2\text{O}$ (0.169 g, 0.001 mol) in the molar ratio of 1:1 was added to methanol. The mixture was heated at 365 K or so for 5 h under reflux with stirring. The resulting solution was then filtered off. Single crystals suitable for X-ray diffraction analysis formed after a week by slow evaporation of the solvent.

Refinement

All H atoms were located at calculated positions and refined as riding on their parent C atoms with the C—H bond length fixed to 0.93 Å with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$.

Figures

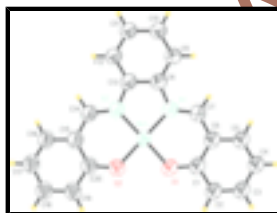


Fig. 1. The asymmetric unit of (I), showing atom labelling and 50% probability displacement ellipsoids for the non-hydrogen atoms.

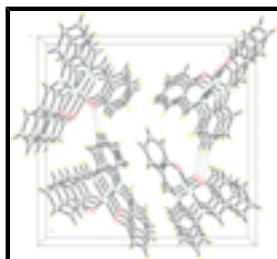


Fig. 2. The packing diagram of (I), viewed along the *a* axis.

{2,2'-[o-Phenylenebis(nitrilomethylidene)]diphenolato}manganese(II)

Crystal data

[Mn(C₂₀H₁₄N₂O₂)]

M_r = 369.27

Orthorhombic, *P*2₁2₁2₁

Hall symbol: P 2ac 2ab

a = 5.4676 (6) Å

b = 16.6244 (19) Å

c = 17.324 (2) Å

V = 1574.7 (3) Å³

Z = 4

*F*₀₀₀ = 756.0

D_x = 1.558 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 3944 reflections

θ = 1.0–28.3°

μ = 0.85 mm⁻¹

T = 293 (2) K

Block, brown

0.25 × 0.08 × 0.07 mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 293(2) K

φ and ω scans

Absorption correction: none

9864 measured reflections

2930 independent reflections

2298 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.046

θ_{max} = 25.5°

θ_{min} = 1.7°

h = -6→6

k = -20→20

l = -20→20

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.059

wR (*F*²) = 0.161

S = 1.06

2930 reflections

227 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

$$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 2.0762P]$$

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.81 e Å⁻³

Δρ_{min} = -0.37 e Å⁻³

Extinction correction: SHELXL97 (Sheldrick, 1997),

$$F_c^* = kF_c [1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$$

Extinction coefficient: 0.020 (3)

Absolute structure: Flack (1983)

Flack parameter: -0.13 (5)

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 $F^2 > 2\sigma(F^2)$ 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	0.15024 (15)	0.77722 (5)	0.31030 (4)	0.0471 (3)
O1	0.1505 (9)	0.8737 (2)	0.3616 (2)	0.0654 (11)
O2	0.4255 (9)	0.8173 (2)	0.2628 (2)	0.0626 (12)
N1	-0.1267 (10)	0.7379 (3)	0.3591 (3)	0.0609 (13)
N2	0.1512 (11)	0.6815 (3)	0.2556 (3)	0.0602 (13)
C1	-0.0151 (14)	0.9022 (4)	0.4090 (4)	0.0649 (17)
C2	0.0095 (13)	0.9814 (4)	0.4377 (4)	0.0660 (17)
H2	0.1447	1.0119	0.4235	0.079*
C3	-0.1621 (14)	1.0137 (4)	0.4859 (4)	0.0668 (16)
H3	-0.1421	1.0664	0.5028	0.080*
C4	-0.3658 (14)	0.9706 (4)	0.5105 (4)	0.0674 (17)
H4	-0.4777	0.9933	0.5446	0.081*
C5	-0.3974 (13)	0.8939 (4)	0.4834 (4)	0.0664 (18)
H5	-0.5348	0.8648	0.4982	0.080*
C6	-0.2241 (13)	0.8582 (4)	0.4332 (4)	0.0648 (17)
C7	-0.2680 (13)	0.7784 (4)	0.4071 (3)	0.0625 (15)
H7	-0.4076	0.7527	0.4253	0.075*
C8	-0.1898 (13)	0.6582 (4)	0.3369 (4)	0.0616 (16)
C9	-0.3811 (13)	0.6121 (4)	0.3653 (4)	0.0635 (16)
H9	-0.4812	0.6321	0.4042	0.076*
C10	-0.4224 (13)	0.5357 (4)	0.3353 (4)	0.0648 (17)
H10	-0.5559	0.5057	0.3520	0.078*
C11	-0.2629 (14)	0.5040 (4)	0.2800 (4)	0.0649 (17)
H11	-0.2875	0.4521	0.2617	0.078*
C12	-0.0690 (14)	0.5489 (4)	0.2523 (4)	0.0636 (17)
H12	0.0362	0.5275	0.2155	0.076*
C13	-0.0334 (13)	0.6267 (4)	0.2803 (4)	0.0615 (16)
C14	0.2948 (12)	0.6644 (4)	0.1966 (4)	0.0618 (16)
H14	0.2688	0.6156	0.1717	0.074*
C15	0.4841 (13)	0.7136 (4)	0.1683 (4)	0.0639 (16)
C16	0.6217 (13)	0.6860 (4)	0.1047 (4)	0.0657 (17)
H16	0.5813	0.6371	0.0820	0.079*
C17	0.8115 (12)	0.7291 (4)	0.0758 (4)	0.0670 (16)

supplementary materials

H17	0.8961	0.7108	0.0327	0.080*
C18	0.8798 (14)	0.8022 (4)	0.1118 (4)	0.0663 (17)
H18	1.0134	0.8312	0.0936	0.080*
C19	0.7471 (13)	0.8303 (4)	0.1739 (4)	0.0650 (17)
H19	0.7913	0.8789	0.1965	0.078*
C20	0.5471 (13)	0.7875 (4)	0.2040 (4)	0.0632 (16)

Atomic displacement parameters (\AA^2)

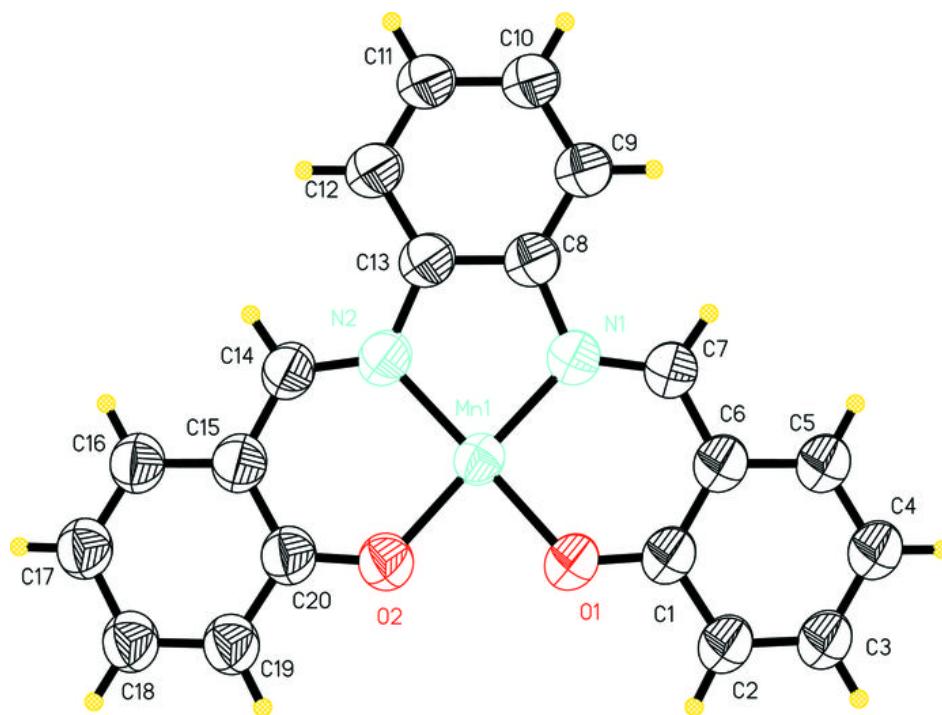
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0554 (5)	0.0423 (4)	0.0437 (4)	0.0039 (4)	-0.0010 (4)	0.0021 (3)
O1	0.075 (3)	0.056 (2)	0.065 (3)	-0.003 (2)	0.009 (3)	-0.0109 (19)
O2	0.067 (3)	0.057 (2)	0.064 (3)	0.000 (2)	0.010 (2)	0.001 (2)
N1	0.068 (3)	0.055 (3)	0.059 (3)	-0.003 (3)	0.009 (3)	-0.004 (2)
N2	0.070 (3)	0.052 (3)	0.058 (3)	0.001 (3)	0.006 (3)	-0.005 (2)
C1	0.075 (5)	0.056 (4)	0.064 (4)	-0.001 (3)	0.008 (4)	-0.010 (3)
C2	0.076 (4)	0.057 (3)	0.065 (4)	0.000 (3)	0.007 (4)	-0.010 (3)
C3	0.077 (4)	0.058 (3)	0.065 (4)	0.001 (4)	0.007 (4)	-0.010 (3)
C4	0.076 (5)	0.060 (4)	0.066 (4)	0.001 (4)	0.008 (4)	-0.009 (3)
C5	0.074 (5)	0.060 (4)	0.065 (4)	0.001 (3)	0.008 (3)	-0.008 (3)
C6	0.073 (4)	0.058 (4)	0.063 (4)	0.000 (3)	0.008 (3)	-0.007 (3)
C7	0.069 (4)	0.058 (3)	0.061 (3)	-0.001 (4)	0.009 (3)	-0.005 (3)
C8	0.070 (4)	0.054 (3)	0.060 (3)	-0.004 (3)	0.006 (3)	-0.003 (3)
C9	0.072 (4)	0.056 (3)	0.063 (4)	-0.005 (3)	0.005 (3)	-0.002 (3)
C10	0.074 (5)	0.056 (4)	0.064 (4)	-0.006 (3)	0.005 (3)	-0.003 (3)
C11	0.075 (4)	0.055 (4)	0.065 (4)	-0.005 (3)	0.004 (3)	-0.004 (3)
C12	0.074 (5)	0.054 (3)	0.063 (4)	-0.004 (3)	0.004 (3)	-0.004 (3)
C13	0.072 (4)	0.053 (3)	0.060 (3)	-0.003 (3)	0.004 (3)	-0.004 (3)
C14	0.071 (4)	0.055 (3)	0.059 (3)	0.003 (3)	0.007 (3)	-0.005 (3)
C15	0.071 (4)	0.059 (4)	0.062 (4)	0.004 (3)	0.008 (3)	0.000 (3)
C16	0.072 (5)	0.062 (4)	0.063 (4)	0.004 (4)	0.009 (4)	0.000 (3)
C17	0.072 (4)	0.064 (4)	0.065 (4)	0.005 (4)	0.010 (3)	0.002 (3)
C18	0.070 (4)	0.063 (4)	0.065 (4)	0.004 (3)	0.011 (4)	0.004 (3)
C19	0.069 (4)	0.061 (4)	0.065 (4)	0.003 (3)	0.011 (3)	0.003 (3)
C20	0.068 (4)	0.058 (4)	0.063 (4)	0.002 (3)	0.010 (3)	0.002 (3)

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

Mn1—O1	1.834 (4)	C8—C9	1.387 (9)
Mn1—O2	1.841 (4)	C8—C13	1.402 (9)
Mn1—N2	1.852 (5)	C9—C10	1.390 (9)
Mn1—N1	1.853 (5)	C9—H9	0.9300
O1—C1	1.310 (7)	C10—C11	1.399 (9)
O2—C20	1.314 (7)	C10—H10	0.9300
N1—C7	1.320 (7)	C11—C12	1.383 (9)
N1—C8	1.422 (8)	C11—H11	0.9300
N2—C14	1.320 (8)	C12—C13	1.396 (8)
N2—C13	1.425 (8)	C12—H12	0.9300
C1—C2	1.414 (9)	C14—C15	1.408 (9)

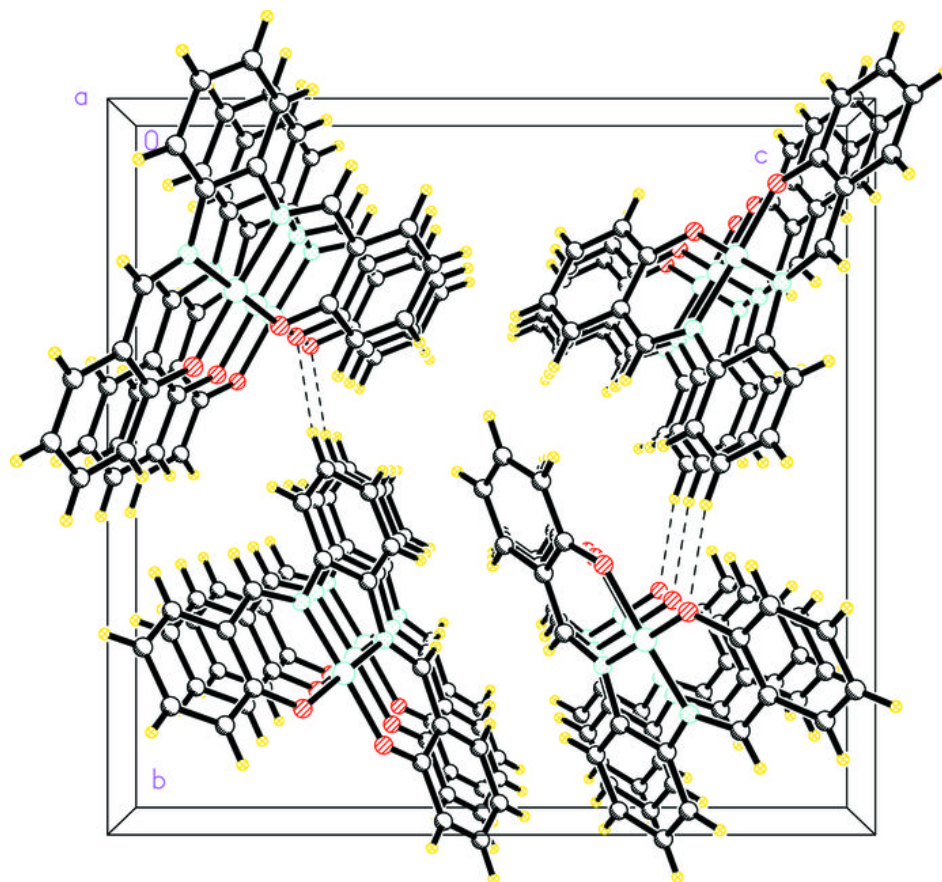
C1—C6	1.419 (10)	C14—H14	0.9300
C2—C3	1.366 (9)	C15—C16	1.410 (9)
C2—H2	0.9300	C15—C20	1.418 (9)
C3—C4	1.392 (9)	C16—C17	1.357 (9)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.369 (8)	C17—C18	1.416 (9)
C4—H4	0.9300	C17—H17	0.9300
C5—C6	1.417 (9)	C18—C19	1.379 (9)
C5—H5	0.9300	C18—H18	0.9300
C6—C7	1.422 (9)	C19—C20	1.405 (9)
C7—H7	0.9300	C19—H19	0.9300
O1—Mn1—O2	84.2 (2)	C13—C8—N1	112.8 (6)
O1—Mn1—N2	178.2 (2)	C8—C9—C10	119.7 (6)
O2—Mn1—N2	94.6 (2)	C8—C9—H9	120.2
O1—Mn1—N1	95.1 (2)	C10—C9—H9	120.2
O2—Mn1—N1	179.3 (2)	C9—C10—C11	119.9 (6)
N2—Mn1—N1	86.1 (2)	C9—C10—H10	120.0
C1—O1—Mn1	128.2 (4)	C11—C10—H10	120.0
C20—O2—Mn1	128.6 (4)	C12—C11—C10	120.8 (6)
C7—N1—C8	120.2 (6)	C12—C11—H11	119.6
C7—N1—Mn1	125.8 (4)	C10—C11—H11	119.6
C8—N1—Mn1	113.8 (4)	C11—C12—C13	119.1 (6)
C14—N2—C13	121.1 (5)	C11—C12—H12	120.4
C14—N2—Mn1	125.6 (4)	C13—C12—H12	120.4
C13—N2—Mn1	113.2 (4)	C12—C13—C8	120.2 (6)
O1—C1—C2	119.4 (6)	C12—C13—N2	125.9 (6)
O1—C1—C6	123.7 (6)	C8—C13—N2	113.8 (5)
C2—C1—C6	116.9 (6)	N2—C14—C15	125.6 (6)
C3—C2—C1	121.0 (7)	N2—C14—H14	117.2
C3—C2—H2	119.5	C15—C14—H14	117.2
C1—C2—H2	119.5	C14—C15—C16	118.4 (6)
C2—C3—C4	122.3 (6)	C14—C15—C20	122.0 (6)
C2—C3—H3	118.8	C16—C15—C20	119.5 (6)
C4—C3—H3	118.8	C17—C16—C15	121.6 (6)
C5—C4—C3	118.4 (7)	C17—C16—H16	119.2
C5—C4—H4	120.8	C15—C16—H16	119.2
C3—C4—H4	120.8	C16—C17—C18	119.6 (6)
C4—C5—C6	121.1 (7)	C16—C17—H17	120.2
C4—C5—H5	119.5	C18—C17—H17	120.2
C6—C5—H5	119.5	C19—C18—C17	119.6 (7)
C5—C6—C1	120.3 (6)	C19—C18—H18	120.2
C5—C6—C7	118.2 (6)	C17—C18—H18	120.2
C1—C6—C7	121.5 (6)	C18—C19—C20	121.9 (7)
N1—C7—C6	125.3 (6)	C18—C19—H19	119.1
N1—C7—H7	117.4	C20—C19—H19	119.1
C6—C7—H7	117.4	O2—C20—C19	119.3 (6)
C9—C8—C13	120.1 (6)	O2—C20—C15	122.9 (6)
C9—C8—N1	127.0 (6)	C19—C20—C15	117.8 (6)

Fig. 1



Article re

Fig. 2



Article