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Bis(benzoato-κ^2O,O')(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')manganese(II)

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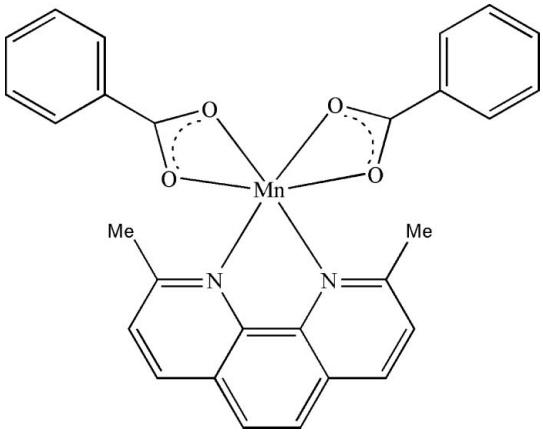
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.033; wR factor = 0.094; data-to-parameter ratio = 12.7.

In the title compound, $[Mn(C_7H_5O_2)_2(C_{14}H_{12}N_2)]$, the Mn^{II} ion is located on a twofold rotation axis and is coordinated by a bidentate 2,9-dimethyl-1,10-phenanthroline ligand and two bidentate benzoate anions in a distorted octahedral environment. The phenyl ring is disordered over two positions, with site occupancy factors of *ca* 0.57 and 0.43. The crystal packing is stabilized by π–π interactions between the 2,9-dimethyl-1,10-phenanthroline rings of neighboring molecules, with a distance between their ring planes of 3.443 Å.

Related literature

For related literature, see: Ruttingter & Dismukes (1997); Wang *et al.* (1996); Wall *et al.* (1999); Naing *et al.* (1995); Xuan *et al.* (2007).



Experimental

Crystal data

$[Mn(C_7H_5O_2)_2(C_{14}H_{12}N_2)]$
M_r = 505.42
Monoclinic, $C2/c$
a = 17.7020 (19) Å
b = 14.3903 (16) Å
c = 9.5678 (11) Å
β = 91.431 (1)°
V = 2436.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.58 mm^{-1}
T = 291 (2) K
0.43 × 0.24 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.789, T_{max} = 0.886
9141 measured reflections
2274 independent reflections
1940 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.094
S = 1.06
2274 reflections
179 parameters
93 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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* (Bruker, 1997); 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: HG2237).

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supplementary materials

Acta Cryst. (2007). E**63**, m2127 [**doi:10.1107/S1600536807033302**]

Bis(benzoato-κ^2O,O')(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')manganese(II)

P.-Z. Zhao, X.-P. Xuan and J.-G. Wang

Comment

It is general believed that manganese plays an important role in biological systems (Ruttingter & Dismukes, 1997). In addition, metal-phenanthroline complexes and their derivatives have attracted much attention because of their peculiar features (Wang *et al.*, 1996; Wall *et al.*, 1999; Naing *et al.*, 1995). The title complex, (I), was recently obtained from the reaction of 2,9-dimethyl-1,10-phenanthroline, sodium benzoate and $Mn(NO_3)_2$ in an ethanol/water mixture. Here we report its structure.

Each Mn^{II} ion is located on a twofold symmetry axis and is six-coordinated by two N atoms from a 2,9-dimethyl-1,10-phenanthroline ligand, and four O atoms from two benzoate anions. The MnO_4N_2 unit forms a distorted octahedron geometry, with two O atoms occupying the axial positions with the axial O—Mn—O angle 168.60 (7)° (Fig.1). The Mn—N bond length is 2.2360 (13)Å and the Mn—O bond lengths are 2.1611 (13) and 2.2971 (14)Å respectively

In the crystal structure, molecules are linked into a one dimensional network by π-π interactions between the 2,9-dimethyl-1,10-phenanthroline ring systems (Fig. 2). These intermolecular interactions occur between the parallel rings within offset face-to-face packing. The distance of neighboring molecules parallel ring planes is 3.4432 Å.

Experimental

To a solution of 2,9-dimethyl-1,10-phenanthroline hemihydrate ($C_{14}H_{12}N_20.5H_2O$, 0.109 g, 0.5 mmol) in ethanol(10 ml) and sodium benzoate (0.073 g, 0.5 mmol) in 1:1 (*v*/*v*) ethanol/water (20 ml) was added a 0.205 g 50% solution of $Mn(NO_3)_2$ (0.089 g, 0.5 mmol) in distilled water(5 ml). The mixture solution was stirred and refluxed for 4 h at 333 K. The hot solution was then filtered into a bottle. Yellow single crystals of (I) were appeared over a period of one week by slow evaporation at room temperature.

Refinement

The H atoms were positioned geometrically and treated as riding, with C—H distances in the range 0.95–0.99Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. The disordered benzene ring has been put into two parts and site occupation refined. 93 least-squares restraints were used to the benzene ring to get reasonable shape and U_{eq}.

Figures

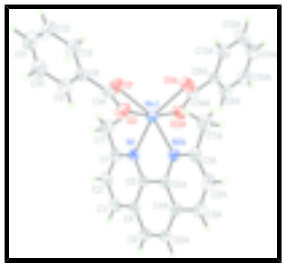


Fig. 1. The molecular stucture of the title complex(I),with atome labels and 30% probability displacement ellipsoids for non-H atoms. Symmetry code for the symbol 'A': $-x + 2$, y, $-z + 1/2$

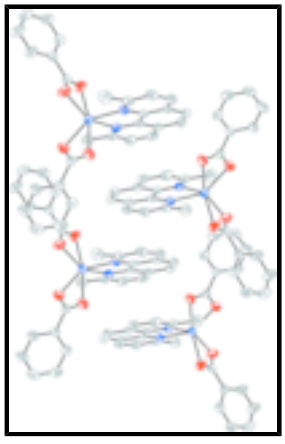


Fig. 2. The π-π interaction between 2,9-dimethyl-1,10-phenanthroline ligands in the crystal structure of (I). H atoms have been omitted for clarity.

Bis(benzoato-κ^2*O*,*O*')(2,9-dimethyl-1,10-phenanthroline-\ κ^2*N*,*N*')manganese(II)

Crystal data

$[Mn(C_7H_5O_2)_2(C_{14}H_{12}N_2)]$	F_{000} = 1044
M_r = 505.42	D_x = 1.378 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3415 reflections
a = 17.7020 (19) Å	θ = 2.3–26.5º
b = 14.3903 (16) Å	μ = 0.58 mm^{-1}
c = 9.5678 (11) Å	*T* = 291 (2) K
β = 91.431 (1)º	Block, yellow
V = 2436.5 (5) Å^3	0.43 × 0.24 × 0.21 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2274 independent reflections
Radiation source: fine-focus sealed tube	1940 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 291(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.3º

Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -20 \rightarrow 21$
$T_{min} = 0.789$, $T_{max} = 0.886$	$k = -17 \rightarrow 17$
9141 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.094$	$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 1.3028P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.002$
2274 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
179 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}
93 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}	Occ. (<1)

C8	0.87920 (18)	0.1290 (2)	0.5538 (3)	0.0514 (5)	0.567 (2)
C9	0.8162 (2)	0.1670 (3)	0.6115 (3)	0.0608 (6)	0.567 (2)
H9	0.7996	0.2253	0.5820	0.073*	0.567 (2)
C10	0.7767 (2)	0.1203 (3)	0.7128 (4)	0.0759 (6)	0.567 (2)
H10	0.7341	0.1469	0.7512	0.091*	0.567 (2)
C11	0.8011 (2)	0.0343 (3)	0.7557 (4)	0.0850 (11)	0.567 (2)
H11	0.7748	0.0023	0.8235	0.102*	0.567 (2)
C12	0.8638 (2)	−0.0046 (3)	0.7000 (4)	0.0937 (11)	0.567 (2)
H12	0.8802	−0.0628	0.7302	0.112*	0.567 (2)
C13	0.9028 (2)	0.0422 (3)	0.5988 (4)	0.0749 (9)	0.567 (2)
H13	0.9453	0.0152	0.5606	0.090*	0.567 (2)
C8'	0.8885 (3)	0.1355 (2)	0.5663 (4)	0.0514 (5)	0.433 (2)
C9'	0.8128 (3)	0.1519 (3)	0.5892 (6)	0.0608 (6)	0.433 (2)
H9'	0.7848	0.1894	0.5280	0.073*	0.433 (2)
C10'	0.7790 (3)	0.1121 (4)	0.7040 (6)	0.0759 (6)	0.433 (2)
H10'	0.7281	0.1230	0.7196	0.091*	0.433 (2)
C11'	0.8198 (3)	0.0572 (4)	0.7940 (6)	0.0850 (11)	0.433 (2)
H11'	0.7968	0.0309	0.8709	0.102*	0.433 (2)
C12'	0.8948 (3)	0.0407 (4)	0.7712 (5)	0.0937 (11)	0.433 (2)
H12'	0.9224	0.0028	0.8325	0.112*	0.433 (2)
C13'	0.9296 (3)	0.0801 (3)	0.6571 (5)	0.0749 (9)	0.433 (2)
H13'	0.9806	0.0690	0.6422	0.090*	0.433 (2)
Mn1	1.0000	0.25641 (2)	0.2500	0.05121 (11)	
O1	0.99102 (8)	0.15840 (10)	0.41993 (15)	0.0780 (4)	
O2	0.89099 (8)	0.24055 (9)	0.37312 (15)	0.0713 (4)	
N1	0.94460 (7)	0.37936 (9)	0.14787 (12)	0.0455 (3)	
C1	0.88955 (9)	0.37836 (13)	0.04959 (17)	0.0539 (4)	
C2	0.86000 (10)	0.46112 (15)	−0.00559 (18)	0.0633 (5)	
H2	0.8220	0.4588	−0.0744	0.076*	
C3	0.88607 (11)	0.54461 (14)	0.04000 (18)	0.0614 (5)	
H3	0.8664	0.5992	0.0020	0.074*	
C4	0.94303 (10)	0.54831 (12)	0.14496 (16)	0.0518 (4)	
C5	0.97064 (9)	0.46279 (11)	0.19584 (14)	0.0434 (4)	
C6	0.97268 (11)	0.63307 (12)	0.19948 (18)	0.0636 (5)	
H6	0.9542	0.6893	0.1651	0.076*	
C7	0.86054 (12)	0.28554 (16)	0.0018 (2)	0.0756 (6)	
H7A	0.9015	0.2496	−0.0339	0.113*	
H7B	0.8226	0.2941	−0.0705	0.113*	
H7C	0.8390	0.2535	0.0792	0.113*	
C14	0.92396 (11)	0.17951 (11)	0.44429 (17)	0.0541 (4)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C8	0.0568 (11)	0.0505 (10)	0.0472 (9)	0.0018 (8)	0.0059 (8)	0.0010 (8)
C9	0.0614 (11)	0.0606 (14)	0.0605 (14)	0.0018 (10)	0.0022 (10)	−0.0056 (11)
C10	0.0597 (11)	0.0969 (16)	0.0718 (13)	−0.0051 (11)	0.0176 (10)	−0.0054 (12)
C11	0.077 (2)	0.111 (2)	0.068 (2)	−0.0111 (18)	0.0173 (16)	0.0230 (18)

C12	0.091 (2)	0.102 (2)	0.089 (2)	0.0151 (19)	0.0176 (18)	0.0505 (18)
C13	0.0684 (18)	0.079 (2)	0.078 (2)	0.0173 (15)	0.0184 (15)	0.0289 (16)
C8'	0.0568 (11)	0.0505 (10)	0.0472 (9)	0.0018 (8)	0.0059 (8)	0.0010 (8)
C9'	0.0614 (11)	0.0606 (14)	0.0605 (14)	0.0018 (10)	0.0022 (10)	−0.0056 (11)
C10'	0.0597 (11)	0.0969 (16)	0.0718 (13)	−0.0051 (11)	0.0176 (10)	−0.0054 (12)
C11'	0.077 (2)	0.111 (2)	0.068 (2)	−0.0111 (18)	0.0173 (16)	0.0230 (18)
C12'	0.091 (2)	0.102 (2)	0.089 (2)	0.0151 (19)	0.0176 (18)	0.0505 (18)
C13'	0.0684 (18)	0.079 (2)	0.078 (2)	0.0173 (15)	0.0184 (15)	0.0289 (16)
Mn1	0.0594 (2)	0.0447 (2)	0.0499 (2)	0.000	0.00940 (16)	0.000
O1	0.0753 (8)	0.0800 (9)	0.0799 (9)	0.0175 (7)	0.0294 (7)	0.0247 (7)
O2	0.0771 (9)	0.0648 (8)	0.0726 (8)	0.0061 (6)	0.0113 (7)	0.0217 (6)
N1	0.0461 (7)	0.0515 (7)	0.0391 (6)	−0.0034 (6)	0.0057 (5)	0.0023 (5)
C1	0.0464 (9)	0.0705 (11)	0.0450 (8)	−0.0074 (8)	0.0047 (7)	0.0030 (8)
C2	0.0506 (9)	0.0911 (14)	0.0483 (9)	0.0032 (9)	0.0004 (8)	0.0127 (9)
C3	0.0633 (11)	0.0702 (11)	0.0511 (9)	0.0139 (9)	0.0091 (8)	0.0160 (8)
C4	0.0599 (10)	0.0554 (9)	0.0410 (8)	0.0071 (8)	0.0144 (7)	0.0071 (7)
C5	0.0476 (8)	0.0493 (8)	0.0337 (7)	0.0003 (7)	0.0114 (6)	0.0017 (6)
C6	0.0907 (14)	0.0461 (9)	0.0547 (10)	0.0077 (9)	0.0166 (9)	0.0051 (7)
C7	0.0678 (12)	0.0875 (14)	0.0709 (12)	−0.0233 (11)	−0.0113 (10)	−0.0018 (11)
C14	0.0697 (11)	0.0424 (8)	0.0506 (9)	−0.0007 (8)	0.0063 (8)	−0.0035 (7)

Geometric parameters (Å, °)

C8—C9	1.371 (5)	Mn1—O1	2.1611 (13)
C8—C13	1.383 (5)	Mn1—N1	2.2360 (13)
C8—C14	1.515 (4)	Mn1—N1^{i}	2.2360 (13)
C9—C10	1.383 (5)	Mn1—O2^{i}	2.2971 (14)
C9—H9	0.9300	Mn1—O2	2.2972 (14)
C10—C11	1.370 (6)	Mn1—C14^{i}	2.5723 (17)
C10—H10	0.9300	Mn1—C14	2.5724 (17)
C11—C12	1.363 (6)	O1—C14	1.253 (2)
C11—H11	0.9300	O2—C14	1.247 (2)
C12—C13	1.379 (5)	N1—C1	1.337 (2)
C12—H12	0.9300	N1—C5	1.3616 (19)
C13—H13	0.9300	C1—C2	1.399 (3)
C8'—C13'	1.375 (6)	C1—C7	1.498 (3)
C8'—C9'	1.383 (7)	C2—C3	1.355 (3)
C8'—C14	1.481 (5)	C2—H2	0.9300
C9'—C10'	1.388 (7)	C3—C4	1.406 (2)
C9'—H9'	0.9300	C3—H3	0.9300
C10'—C11'	1.363 (8)	C4—C5	1.407 (2)
C10'—H10'	0.9300	C4—C6	1.422 (2)
C11'—C12'	1.372 (7)	C5—C5^{i}	1.449 (3)
C11'—H11'	0.9300	C6—C6^{i}	1.350 (4)
C12'—C13'	1.388 (6)	C6—H6	0.9300
C12'—H12'	0.9300	C7—H7A	0.9600
C13'—H13'	0.9300	C7—H7B	0.9600
Mn1—O1^{i}	2.1611 (13)	C7—H7C	0.9600

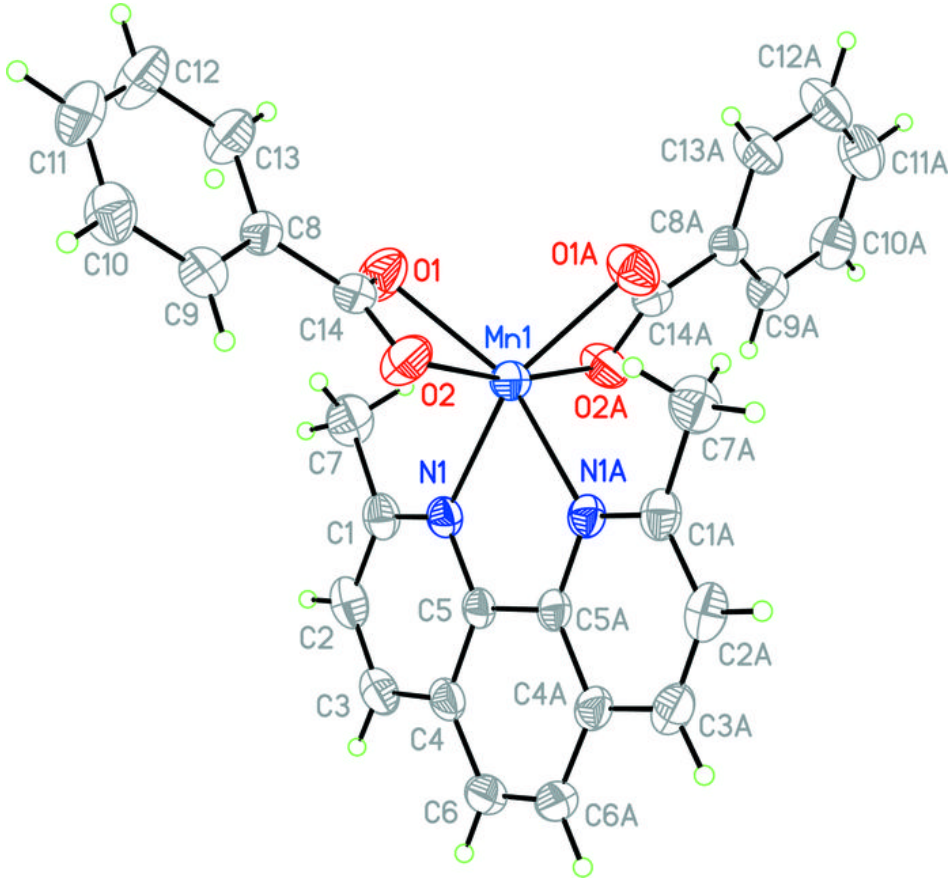
C9—C8—C13	118.5 (3)	O1—Mn1—C14^{i}	108.21 (5)
C9—C8—C14	122.1 (3)	N1—Mn1—C14^{i}	104.85 (5)
C13—C8—C14	119.3 (3)	N1^{i}—Mn1—C14^{i}	115.12 (5)
C8—C9—C10	121.2 (4)	O2^{i}—Mn1—C14^{i}	28.98 (5)
C8—C9—H9	119.4	O2—Mn1—C14^{i}	142.12 (6)
C10—C9—H9	119.4	O1^{i}—Mn1—C14	108.21 (5)
C11—C10—C9	119.2 (4)	O1—Mn1—C14	29.07 (5)
C11—C10—H10	120.4	N1—Mn1—C14	115.12 (5)
C9—C10—H10	120.4	N1^{i}—Mn1—C14	104.85 (5)
C12—C11—C10	120.5 (4)	O2^{i}—Mn1—C14	142.12 (6)
C12—C11—H11	119.8	O2—Mn1—C14	28.98 (5)
C10—C11—H11	119.8	C14^{i}—Mn1—C14	129.04 (7)
C11—C12—C13	120.1 (4)	C14—O1—Mn1	93.99 (11)
C11—C12—H12	120.0	C14—O2—Mn1	87.84 (11)
C13—C12—H12	120.0	C1—N1—C5	118.76 (14)
C12—C13—C8	120.5 (3)	C1—N1—Mn1	127.07 (11)
C12—C13—H13	119.8	C5—N1—Mn1	114.16 (10)
C8—C13—H13	119.8	N1—C1—C2	121.02 (16)
C13'—C8'—C9'	119.9 (4)	N1—C1—C7	117.53 (16)
C13'—C8'—C14	121.2 (4)	C2—C1—C7	121.45 (16)
C9'—C8'—C14	118.9 (4)	C3—C2—C1	120.80 (17)
C8'—C9'—C10'	119.6 (5)	C3—C2—H2	119.6
C8'—C9'—H9'	120.2	C1—C2—H2	119.6
C10'—C9'—H9'	120.2	C2—C3—C4	119.73 (17)
C11'—C10'—C9'	120.5 (5)	C2—C3—H3	120.1
C11'—C10'—H10'	119.7	C4—C3—H3	120.1
C9'—C10'—H10'	119.7	C3—C4—C5	116.79 (16)
C10'—C11'—C12'	120.0 (5)	C3—C4—C6	123.10 (16)
C10'—C11'—H11'	120.0	C5—C4—C6	120.11 (15)
C12'—C11'—H11'	120.0	N1—C5—C4	122.88 (14)
C11'—C12'—C13'	120.3 (5)	N1—C5—C5^{i}	118.15 (8)
C11'—C12'—H12'	119.8	C4—C5—C5^{i}	118.96 (9)
C13'—C12'—H12'	119.8	C6^{i}—C6—C4	120.93 (10)
C8'—C13'—C12'	119.7 (4)	C6^{i}—C6—H6	119.5
C8'—C13'—H13'	120.1	C4—C6—H6	119.5
C12'—C13'—H13'	120.1	C1—C7—H7A	109.5
O1^{i}—Mn1—O1	98.53 (8)	C1—C7—H7B	109.5
O1^{i}—Mn1—N1	103.14 (5)	H7A—C7—H7B	109.5
O1—Mn1—N1	143.66 (5)	C1—C7—H7C	109.5
O1^{i}—Mn1—N1^{i}	143.66 (5)	H7A—C7—H7C	109.5
O1—Mn1—N1^{i}	103.14 (5)	H7B—C7—H7C	109.5
N1—Mn1—N1^{i}	75.38 (7)	O2—C14—O1	120.11 (16)
O1^{i}—Mn1—O2^{i}	58.05 (5)	O2—C14—C8'	122.0 (2)
O1—Mn1—O2^{i}	113.54 (5)	O1—C14—C8'	117.7 (2)
N1—Mn1—O2^{i}	102.68 (5)	O2—C14—C8	118.01 (19)

N1^{i}—Mn1—O2^{i}	86.43 (4)	O1—C14—C8	121.78 (19)
O1^{i}—Mn1—O2	113.54 (5)	C8'—C14—C8	8.4 (2)
O1—Mn1—O2	58.05 (5)	O2—C14—Mn1	63.17 (10)
N1—Mn1—O2	86.43 (4)	O1—C14—Mn1	56.94 (9)
N1^{i}—Mn1—O2	102.68 (5)	C8'—C14—Mn1	173.3 (2)
O2^{i}—Mn1—O2	168.59 (7)	C8—C14—Mn1	176.64 (15)
O1^{i}—Mn1—C14^{i}	29.07 (5)		
C13—C8—C9—C10	0.1 (2)	N1—C1—C2—C3	−0.5 (3)
C14—C8—C9—C10	−179.1 (3)	C7—C1—C2—C3	179.08 (17)
C8—C9—C10—C11	−0.1 (2)	C1—C2—C3—C4	−0.6 (3)
C9—C10—C11—C12	0.3 (4)	C2—C3—C4—C5	0.8 (2)
C10—C11—C12—C13	−0.4 (6)	C2—C3—C4—C6	−179.22 (17)
C11—C12—C13—C8	0.4 (5)	C1—N1—C5—C4	−1.0 (2)
C9—C8—C13—C12	−0.3 (4)	Mn1—N1—C5—C4	−179.99 (11)
C14—C8—C13—C12	179.0 (3)	C1—N1—C5—C5^{i}	178.91 (16)
C13'—C8'—C9'—C10'	0.0 (2)	Mn1—N1—C5—C5^{i}	0.0 (2)
C14—C8'—C9'—C10'	−179.2 (3)	C3—C4—C5—N1	0.0 (2)
C8'—C9'—C10'—C11'	0.0 (3)	C6—C4—C5—N1	−179.98 (14)
C9'—C10'—C11'—C12'	−0.2 (5)	C3—C4—C5—C5^{i}	−179.96 (16)
C10'—C11'—C12'—C13'	0.4 (7)	C6—C4—C5—C5^{i}	0.1 (3)
C9'—C8'—C13'—C12'	0.2 (5)	C3—C4—C6—C6^{i}	179.9 (2)
C14—C8'—C13'—C12'	179.4 (4)	C5—C4—C6—C6^{i}	−0.2 (3)
C11'—C12'—C13'—C8'	−0.4 (6)	Mn1—O2—C14—O1	0.18 (17)
O1^{i}—Mn1—O1—C14	−112.38 (12)	Mn1—O2—C14—C8'	175.0 (2)
N1—Mn1—O1—C14	13.89 (16)	Mn1—O2—C14—C8	−176.45 (17)
N1^{i}—Mn1—O1—C14	97.00 (11)	Mn1—O1—C14—O2	−0.20 (18)
O2^{i}—Mn1—O1—C14	−171.16 (10)	Mn1—O1—C14—C8'	−175.22 (19)
O2—Mn1—O1—C14	0.11 (10)	Mn1—O1—C14—C8	176.31 (17)
C14^{i}—Mn1—O1—C14	−140.61 (10)	C13'—C8'—C14—O2	−169.1 (3)
O1^{i}—Mn1—O2—C14	85.24 (11)	C9'—C8'—C14—O2	10.1 (4)
O1—Mn1—O2—C14	−0.11 (10)	C13'—C8'—C14—O1	5.8 (4)
N1—Mn1—O2—C14	−171.97 (11)	C9'—C8'—C14—O1	−175.0 (2)
N1^{i}—Mn1—O2—C14	−97.83 (10)	C13'—C8'—C14—C8	126.9 (18)
O2^{i}—Mn1—O2—C14	44.60 (10)	C9'—C8'—C14—C8	−54.0 (17)
C14^{i}—Mn1—O2—C14	78.26 (16)	C9—C8—C14—O2	−23.5 (3)
O1^{i}—Mn1—N1—C1	38.62 (13)	C13—C8—C14—O2	157.3 (2)
O1—Mn1—N1—C1	−86.43 (15)	C9—C8—C14—O1	159.9 (2)
N1^{i}—Mn1—N1—C1	−178.83 (15)	C13—C8—C14—O1	−19.3 (3)
O2^{i}—Mn1—N1—C1	98.32 (13)	C9—C8—C14—C8'	96.7 (17)
O2—Mn1—N1—C1	−74.74 (13)	C13—C8—C14—C8'	−82.5 (17)
C14^{i}—Mn1—N1—C1	68.55 (13)	O1^{i}—Mn1—C14—O2	−105.89 (11)
C14—Mn1—N1—C1	−79.02 (13)	O1—Mn1—C14—O2	179.81 (17)
O1^{i}—Mn1—N1—C5	−142.54 (10)	N1—Mn1—C14—O2	8.85 (12)
O1—Mn1—N1—C5	92.42 (13)	N1^{i}—Mn1—C14—O2	89.41 (11)

N1^{i}—Mn1—N1—C5	0.01 (7)	O2^{i}—Mn1—C14—O2	−166.93 (8)
O2^{i}—Mn1—N1—C5	−82.83 (10)	C14^{i}—Mn1—C14—O2	−129.28 (11)
O2—Mn1—N1—C5	104.11 (10)	O1^{i}—Mn1—C14—O1	74.30 (14)
C14^{i}—Mn1—N1—C5	−112.61 (10)	N1—Mn1—C14—O1	−170.96 (11)
C14—Mn1—N1—C5	99.82 (10)	N1^{i}—Mn1—C14—O1	−90.40 (11)
C5—N1—C1—C2	1.3 (2)	O2^{i}—Mn1—C14—O1	13.26 (15)
Mn1—N1—C1—C2	−179.91 (11)	O2—Mn1—C14—O1	−179.81 (17)
C5—N1—C1—C7	−178.30 (14)	C14^{i}—Mn1—C14—O1	50.91 (10)
Mn1—N1—C1—C7	0.5 (2)		

Symmetry codes: (i) −*x*+2, *y*, −*z*+1/2.

Fig. 1


C12
C11
C13
C10
C8
C9
C14
O1
O2
Mn1
O1A
O2A
C14A
C8A
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C13A
C11A
C10A
C9A
C7
N1
N1A
C7A
C1
C1A
C5
C5A
C2
C2A
C3
C4A
C3A
C4
C6
C6A

Fig. 2