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# (Acetylacetonato-$\kappa^2O,O'$)aqua[2-(2-nitrophenoxy)-*N*′-(2-oxidobenzylidene-$\kappa O$)acetohydrazidato-$\kappa^2O,N'$]-manganese(III)

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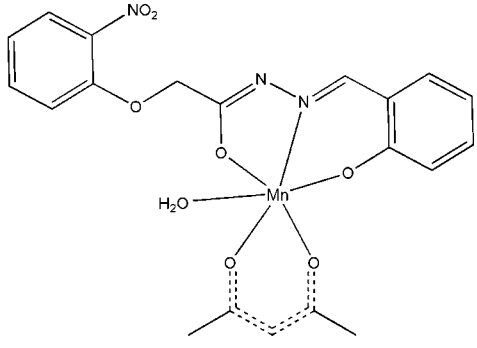
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.038; $wR$ factor = 0.086; data-to-parameter ratio = 16.2.

In the title complex, $[Mn(C_{15}H_{11}N_3O_5)(C_5H_7O_2)(H_2O)]$, the $Mn^{III}$ ion has a distorted octahedral coordination geometry. It is coordinated by a phenoxy O atom, a hydrazine N atom and a carbonyl O atom of the 2-(2-nitrophenoxy)-*N*′-(2-oxidobenzylidene-$\kappa O$)acetohydrazidate dianion, by two O atoms of the acetylacetonate anion and by the O atom of a coordinated water molecule. In the crystal structure, complex molecules are linked into centrosymmetric dimeric units through four intermolecular O—H···O hydrogen bonds involving both H atoms of the coordinated water molecule.

## Related literature

For the biological activity and chemical versatility of hydrazone complexes, see: Liu & Gao (1998); Iskander *et al.* (2001); Cariati *et al.* (2002); Sreekanth *et al.* (2004); Bai *et al.* (2006); Mondal *et al.* (2008). For phenoxyacetylhydrazone complexes, see: Chen & Liu (2004); Sun *et al.* (2005); Chen & Liu (2006).




## Experimental

### Crystal data

$[Mn(C_{15}H_{11}N_3O_5)(C_5H_7O_2)(H_2O)]$
$M_r$ = 485.33
Monoclinic, $P2_1/c$
$a$ = 8.5217 (6) Å
$b$ = 13.9263 (10) Å
$c$ = 17.6311 (10) Å
$\beta$ = 92.725 (3)°
$V$ = 2090.0 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.69 mm$^{-1}$
$T$ = 293 K
0.58 × 0.32 × 0.27 mm

### Data collection

Rigaku R-AXIS RAPID Imaging Plate diffractometer
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
$T_{min}$ = 0.766, $T_{max}$ = 0.832
4921 measured reflections
4735 independent reflections
3155 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.046

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.086
$S$ = 0.88
4735 reflections
293 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H01···O4$^{i}$ | 0.88 | 2.16 | 2.955 (2) | 150 |
| O1$W$—H02···O2$^{i}$ | 0.88 | 1.96 | 2.829 (2) | 169 |

Symmetry code: (i) $-x+1, -y, -z+1$.

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS98* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL98* (Sheldrick, 2008); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2221).

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# supporting information

*Acta Cryst.* (2009). E**65**, m986 [doi:10.1107/S1600536809028177]

# (Acetylacetonato-$\kappa^2O,O'$)aqua[2-(2-nitrophenoxy)-*N*′-(2-oxidobenzylidene-$\kappa O$)acetohydrazidato-$\kappa^2O,N'$]manganese(III)

**Zi-Jing Xiao**

## S1. Comment

The design and construction of hydrazone complexes are of great interest due to their various structures and their biological activities and chemical versatility (Liu & Gao, 1998; Iskander *et al.*, 2001; Cariati *et al.*, 2002; Sreekanth *et al.*, 2004; Bai *et al.*, 2006; Mondal *et al.*, 2008). Relatively speaking, only a few crystal structures of phenoxyacetyl-hydrazone complexes have been studied (Chen & Liu, 2004; Sun *et al.*, 2005; Chen & Liu, 2006).

As shown in Fig. 1, the $Mn^{III}$ ion in (I) is octahedrally coordinated by phenol atom O1, hydrazine atom N1 and carbonyl atom O2 from the phenoxyacetylhydrazone ligand $L^{2-}$, two oxygen atoms (O6 and O7) from an $acac^-$ ligand, and O1W atom from coordinated water molecule. Atoms O1, N1, O2 and O7 form the equatorial plane, while the atoms O6 and O1W occupy the two axial positions. The bond distance of Mn1—O6($acac^-$) (2.130 (2) Å) is much longer than the one of Mn1—O7($acac^-$) (1.921 (1) Å) due to the Jahn-Teller effect of Mn(III) ion.

In most of phenoxyacetylhydrazone complexes, the phenoxy oxygen atom is not coordinated to metal atom. This structural phenomenon is found in the title complex (I) and was also found in several known complexes (Chen & Liu, 2004; Sun *et al.*, 2005; Chen & Liu, 2006).

The complex $Co(C_2H_3O_2)(C_4H_9NO)_2(C_{15}H_{11}N_3O_5)$ (II) (Sun *et al.*, 2005) and the title complex $Mn(C_{15}H_{11}N_3O_5)(C_5H_7O_2)(H_2O)$ (I) have the same *N*-salicylaldehyde-N′– (*o*-nitrophenoxyacyl) hydrazone ligand. The dihedral angles between the two benzene rings of the phenoxyacyl hydrazone ligand in complex (I) is 89.48 (8)°, while the corresponding one in (II) is 44.1 (1)°. This big difference of the two dihedral angles may come from the different sizes of the second ligands in the two complexes.

As shown in Fig. 2, two neighboring complex molecules are linked by four hydrogen bonds O—H(coordinated water molecule)···*O*(carbonyl O or oxygen in *o*-nitrate group) to form a centrosymmetrical dimer.

## S2. Experimental

The *N*-salicylaldehyde-*N*′- (*o*-nitrophenoxyacyl) hydrazone ligand, ($H_2L$) was prepared according the reference (Sun *et al.*, 2005). $H_2L$ (0.05 mmol) and $Mn(acac)_3$ (0.05 mmol) were dissolved in a mixed solution of 10 ml 95% EtOH and 1 ml DMF. The mixture was stirred for 3 h. After one week, Dark-brown crystals of (I) were obtained.

## S3. Refinement

The water H atoms (H01 and H02) were located from the difference Fourier map and refined isotropically, with O—H distance restraints of 0.88 Å. The other H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

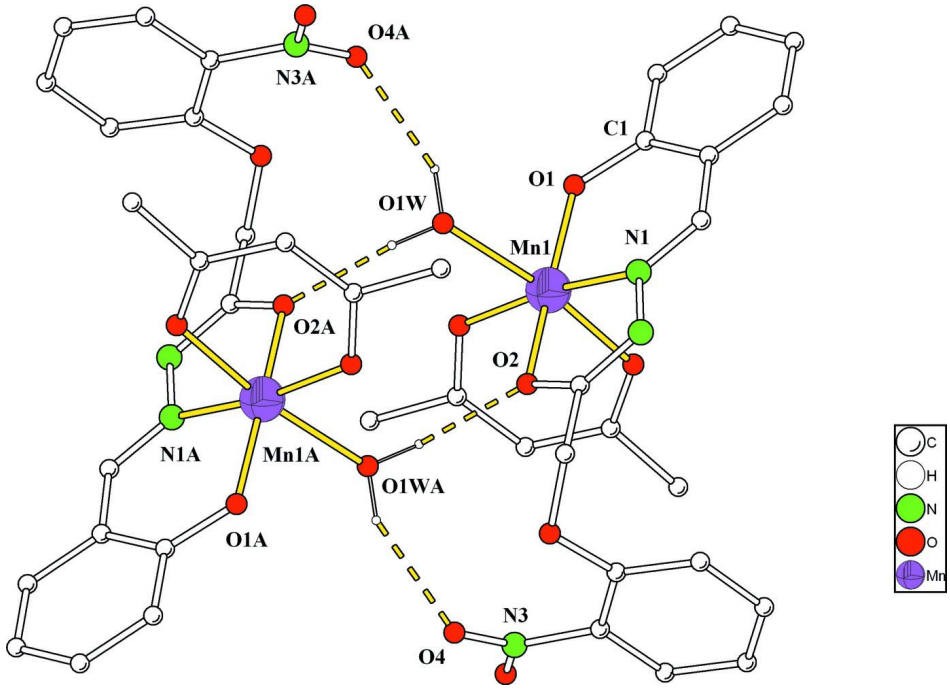


**Figure 1**

The molecular structure of (I), showing 20% probability displacement ellipsoids and the atom numbering scheme.

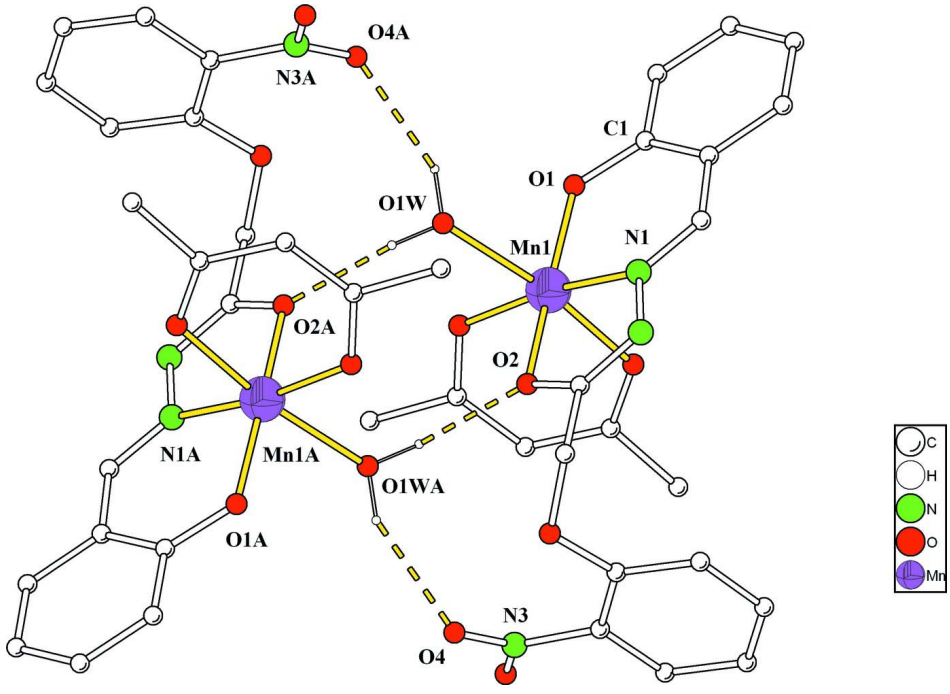


**Figure 2**

Extended centrosymmetrical dimer structure of (I).

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*Crystal data*

$[Mn(C_{15}H_{11}N_3O_5)(C_5H_7O_2)(H_2O)]$
$M_r = 485.33$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.5217\ (6)$ Å
$b = 13.9263\ (10)$ Å
$c = 17.6311\ (10)$ Å
$\beta = 92.725\ (3)°$
$V = 2090.0\ (2)$ Å$^3$
$Z = 4$
$F(000) = 1000$
$D_x = 1.542$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4921 reflections
$\theta = 2.3–27.5°$
$\mu = 0.69$ mm$^{-1}$
$T = 293$ K
Prism, red-black
0.58 × 0.32 × 0.27 mm

*Data collection*

Rigaku R-AXIS RAPID Imaging Plate diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
$T_{min} = 0.766$, $T_{max} = 0.832$
4735 measured reflections
4735 independent reflections
3155 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = 0\rightarrow11$
$k = 0\rightarrow18$
$l = -22\rightarrow22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.086$
$S = 0.88$
4735 reflections
293 parameters
2 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.042P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å$^{-3}$
$\Delta\rho_{min} = -0.26$ e Å$^{-3}$

*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 | 0.42210 (3) | 0.18422 (2) | 0.481380 (18) | 0.03308 (10) |
| N1 | 0.57698 (19) | 0.27034 (12) | 0.53316 (9) | 0.0331 (4) |

| | | | | |
|---|---|---|---|---|
| N2 | 0.73611 (19) | 0.24037 (13) | 0.53073 (10) | 0.0375 (4) |
| N3 | 0.8041 (2) | 0.02849 (16) | 0.26015 (12) | 0.0533 (5) |
| O1 | 0.25674 (16) | 0.25554 (11) | 0.52037 (9) | 0.0418 (4) |
| O2 | 0.61556 (15) | 0.11671 (10) | 0.46352 (8) | 0.0378 (3) |
| O3 | 0.90604 (16) | 0.07570 (10) | 0.41027 (8) | 0.0388 (3) |
| O4 | 0.8243 (2) | −0.04084 (13) | 0.30114 (10) | 0.0592 (5) |
| O5 | 0.7271 (3) | 0.02349 (18) | 0.20070 (14) | 0.1154 (10) |
| O6 | 0.44030 (18) | 0.26593 (11) | 0.38003 (9) | 0.0456 (4) |
| O7 | 0.29877 (16) | 0.09269 (10) | 0.42284 (8) | 0.0378 (3) |
| O1W | 0.39896 (18) | 0.07903 (11) | 0.57926 (8) | 0.0445 (4) |
| H01 | 0.3227 | 0.0898 | 0.6102 | 0.084 (10)* |
| H02 | 0.3985 | 0.0165 | 0.5720 | 0.059 (8)* |
| C1 | 0.2598 (2) | 0.34515 (15) | 0.54655 (12) | 0.0363 (5) |
| C2 | 0.3993 (2) | 0.39648 (15) | 0.56558 (11) | 0.0356 (5) |
| C3 | 0.3901 (3) | 0.49157 (16) | 0.59191 (12) | 0.0447 (6) |
| H3A | 0.4822 | 0.5254 | 0.6036 | 0.054* |
| C4 | 0.2482 (3) | 0.53520 (17) | 0.60058 (14) | 0.0545 (6) |
| H4A | 0.2434 | 0.5984 | 0.6173 | 0.065* |
| C5 | 0.1116 (3) | 0.48358 (19) | 0.58401 (14) | 0.0547 (7) |
| H5A | 0.0149 | 0.5125 | 0.5907 | 0.066* |
| C6 | 0.1161 (3) | 0.39072 (17) | 0.55798 (13) | 0.0474 (6) |
| H6A | 0.0226 | 0.3576 | 0.5478 | 0.057* |
| C7 | 0.5521 (2) | 0.35502 (15) | 0.55894 (11) | 0.0364 (5) |
| H7A | 0.6389 | 0.3919 | 0.5743 | 0.044* |
| C8 | 0.7392 (2) | 0.16010 (15) | 0.49417 (12) | 0.0342 (5) |
| C9 | 0.8935 (2) | 0.10965 (16) | 0.48634 (12) | 0.0398 (5) |
| H9A | 0.9791 | 0.1536 | 0.4990 | 0.048* |
| H9B | 0.9013 | 0.0559 | 0.5213 | 0.048* |
| C10 | 0.9278 (2) | 0.14196 (15) | 0.35479 (12) | 0.0361 (5) |
| C11 | 0.8798 (2) | 0.11932 (16) | 0.27964 (13) | 0.0406 (5) |
| C12 | 0.9049 (3) | 0.18249 (19) | 0.22091 (14) | 0.0531 (6) |
| H12A | 0.8707 | 0.1669 | 0.1716 | 0.064* |
| C13 | 0.9798 (3) | 0.26774 (18) | 0.23514 (16) | 0.0570 (7) |
| H13A | 0.9990 | 0.3095 | 0.1955 | 0.068* |
| C14 | 1.0266 (3) | 0.29151 (18) | 0.30817 (16) | 0.0552 (7) |
| H14A | 1.0773 | 0.3497 | 0.3177 | 0.066* |
| C15 | 0.9996 (3) | 0.23052 (17) | 0.36756 (13) | 0.0457 (6) |
| H15A | 1.0297 | 0.2488 | 0.4169 | 0.055* |
| C16 | 0.4860 (4) | 0.28832 (19) | 0.25042 (16) | 0.0682 (8) |
| H16A | 0.4550 | 0.3539 | 0.2572 | 0.102* |
| H16B | 0.4391 | 0.2643 | 0.2036 | 0.102* |
| H16C | 0.5983 | 0.2848 | 0.2489 | 0.102* |
| C17 | 0.4325 (3) | 0.22903 (17) | 0.31512 (13) | 0.0446 (5) |
| C18 | 0.3747 (3) | 0.13544 (18) | 0.29967 (13) | 0.0479 (6) |
| H18A | 0.3812 | 0.1129 | 0.2503 | 0.057* |
| C19 | 0.3099 (2) | 0.07523 (16) | 0.35096 (12) | 0.0378 (5) |
| C20 | 0.2423 (3) | −0.01982 (16) | 0.32597 (13) | 0.0471 (6) |
| H20A | 0.1363 | −0.0249 | 0.3417 | 0.071* |

| | | | | |
|---|---|---|---|---|
| H20B | 0.3044 | −0.0707 | 0.3486 | 0.071* |
| H20C | 0.2430 | −0.0246 | 0.2717 | 0.071* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mn1 | 0.03206 (16) | 0.03084 (17) | 0.03640 (18) | 0.00197 (14) | 0.00244 (12) | −0.00560 (15) |
| N1 | 0.0330 (9) | 0.0332 (10) | 0.0331 (9) | 0.0030 (7) | 0.0021 (8) | −0.0026 (8) |
| N2 | 0.0315 (9) | 0.0399 (11) | 0.0413 (10) | 0.0049 (8) | 0.0021 (8) | −0.0051 (8) |
| N3 | 0.0568 (12) | 0.0530 (14) | 0.0498 (13) | −0.0075 (11) | −0.0001 (11) | −0.0056 (11) |
| O1 | 0.0340 (8) | 0.0387 (8) | 0.0533 (9) | 0.0027 (6) | 0.0078 (7) | −0.0123 (7) |
| O2 | 0.0343 (7) | 0.0318 (8) | 0.0475 (9) | 0.0009 (6) | 0.0037 (7) | −0.0063 (7) |
| O3 | 0.0420 (8) | 0.0379 (8) | 0.0371 (8) | 0.0071 (7) | 0.0087 (7) | −0.0008 (7) |
| O4 | 0.0740 (12) | 0.0437 (10) | 0.0604 (11) | −0.0057 (9) | 0.0091 (9) | −0.0050 (9) |
| O5 | 0.158 (2) | 0.0944 (18) | 0.0865 (16) | −0.0486 (17) | −0.0697 (17) | 0.0141 (13) |
| O6 | 0.0578 (10) | 0.0365 (9) | 0.0425 (9) | −0.0007 (7) | 0.0016 (8) | 0.0018 (7) |
| O7 | 0.0405 (8) | 0.0375 (8) | 0.0353 (8) | −0.0033 (6) | 0.0028 (7) | −0.0057 (6) |
| O1W | 0.0534 (9) | 0.0368 (9) | 0.0437 (9) | 0.0019 (7) | 0.0092 (8) | −0.0013 (7) |
| C1 | 0.0419 (11) | 0.0358 (12) | 0.0314 (11) | 0.0069 (9) | 0.0029 (9) | −0.0015 (9) |
| C2 | 0.0431 (12) | 0.0333 (11) | 0.0308 (11) | 0.0058 (9) | 0.0046 (9) | −0.0037 (9) |
| C3 | 0.0544 (14) | 0.0377 (13) | 0.0417 (13) | 0.0053 (11) | 0.0009 (11) | −0.0045 (10) |
| C4 | 0.0717 (17) | 0.0369 (13) | 0.0547 (15) | 0.0181 (13) | 0.0010 (13) | −0.0090 (11) |
| C5 | 0.0528 (15) | 0.0583 (16) | 0.0531 (15) | 0.0241 (13) | 0.0040 (12) | −0.0089 (13) |
| C6 | 0.0435 (12) | 0.0493 (14) | 0.0496 (14) | 0.0105 (11) | 0.0046 (11) | −0.0072 (12) |
| C7 | 0.0390 (11) | 0.0357 (12) | 0.0345 (12) | −0.0007 (9) | 0.0009 (9) | −0.0056 (10) |
| C8 | 0.0368 (11) | 0.0346 (12) | 0.0317 (11) | 0.0044 (9) | 0.0055 (9) | 0.0018 (9) |
| C9 | 0.0390 (11) | 0.0450 (13) | 0.0356 (11) | 0.0108 (10) | 0.0033 (10) | 0.0003 (10) |
| C10 | 0.0312 (10) | 0.0357 (12) | 0.0418 (12) | 0.0075 (9) | 0.0060 (9) | 0.0010 (10) |
| C11 | 0.0383 (11) | 0.0377 (12) | 0.0458 (13) | 0.0023 (10) | 0.0029 (10) | 0.0002 (11) |
| C12 | 0.0585 (15) | 0.0573 (16) | 0.0432 (13) | 0.0045 (13) | 0.0004 (12) | 0.0036 (12) |
| C13 | 0.0642 (16) | 0.0482 (16) | 0.0591 (17) | 0.0034 (13) | 0.0090 (14) | 0.0146 (13) |
| C14 | 0.0601 (15) | 0.0359 (13) | 0.0701 (18) | −0.0029 (11) | 0.0095 (14) | −0.0009 (12) |
| C15 | 0.0488 (13) | 0.0409 (14) | 0.0476 (14) | 0.0043 (11) | 0.0052 (11) | −0.0057 (11) |
| C16 | 0.096 (2) | 0.0565 (17) | 0.0538 (16) | 0.0007 (16) | 0.0162 (15) | 0.0136 (14) |
| C17 | 0.0465 (13) | 0.0467 (14) | 0.0407 (13) | 0.0076 (11) | 0.0050 (11) | 0.0033 (11) |
| C18 | 0.0598 (15) | 0.0477 (14) | 0.0368 (12) | 0.0032 (12) | 0.0082 (11) | −0.0041 (11) |
| C19 | 0.0361 (11) | 0.0377 (12) | 0.0394 (12) | 0.0066 (9) | −0.0007 (10) | −0.0084 (10) |
| C20 | 0.0523 (14) | 0.0431 (14) | 0.0456 (13) | 0.0005 (11) | 0.0000 (11) | −0.0126 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Mn1—O1 | 1.8806 (14) | C5—C6 | 1.373 (3) |
| Mn1—O7 | 1.9214 (14) | C5—H5A | 0.9300 |
| Mn1—O2 | 1.9366 (13) | C6—H6A | 0.9300 |
| Mn1—N1 | 1.9746 (16) | C7—H7A | 0.9300 |
| Mn1—O6 | 2.1303 (15) | C8—C9 | 1.503 (3) |
| Mn1—O1W | 2.2793 (15) | C9—H9A | 0.9700 |
| N1—C7 | 1.285 (3) | C9—H9B | 0.9700 |

| | | | |
|---|---|---|---|
| N1—N2 | 1.421 (2) | C10—C15 | 1.390 (3) |
| N2—C8 | 1.291 (3) | C10—C11 | 1.404 (3) |
| N3—O5 | 1.212 (3) | C11—C12 | 1.383 (3) |
| N3—O4 | 1.213 (2) | C12—C13 | 1.366 (4) |
| N3—C11 | 1.454 (3) | C12—H12A | 0.9300 |
| O1—C1 | 1.330 (2) | C13—C14 | 1.370 (4) |
| O2—C8 | 1.309 (2) | C13—H13A | 0.9300 |
| O3—C10 | 1.364 (2) | C14—C15 | 1.376 (3) |
| O3—C9 | 1.431 (2) | C14—H14A | 0.9300 |
| O6—C17 | 1.253 (3) | C15—H15A | 0.9300 |
| O7—C19 | 1.298 (2) | C16—C17 | 1.497 (3) |
| O1W—H01 | 0.8802 | C16—H16A | 0.9600 |
| O1W—H02 | 0.8799 | C16—H16B | 0.9600 |
| C1—C6 | 1.402 (3) | C16—H16C | 0.9600 |
| C1—C2 | 1.414 (3) | C17—C18 | 1.415 (3) |
| C2—C3 | 1.407 (3) | C18—C19 | 1.368 (3) |
| C2—C7 | 1.435 (3) | C18—H18A | 0.9300 |
| C3—C4 | 1.368 (3) | C19—C20 | 1.501 (3) |
| C3—H3A | 0.9300 | C20—H20A | 0.9600 |
| C4—C5 | 1.387 (4) | C20—H20B | 0.9600 |
| C4—H4A | 0.9300 | C20—H20C | 0.9600 |

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| O1—Mn1—O7 | 98.43 (6) | C2—C7—H7A | 117.8 |
| O1—Mn1—O2 | 166.98 (7) | N2—C8—O2 | 124.81 (18) |
| O7—Mn1—O2 | 92.22 (6) | N2—C8—C9 | 119.28 (19) |
| O1—Mn1—N1 | 90.36 (7) | O2—C8—C9 | 115.90 (18) |
| O7—Mn1—N1 | 171.05 (6) | O3—C9—C8 | 110.20 (16) |
| O2—Mn1—N1 | 79.31 (6) | O3—C9—H9A | 109.6 |
| O1—Mn1—O6 | 96.33 (7) | C8—C9—H9A | 109.6 |
| O7—Mn1—O6 | 87.91 (6) | O3—C9—H9B | 109.6 |
| O2—Mn1—O6 | 91.51 (6) | C8—C9—H9B | 109.6 |
| N1—Mn1—O6 | 89.40 (6) | H9A—C9—H9B | 108.1 |
| O1—Mn1—O1W | 88.25 (6) | O3—C10—C15 | 123.9 (2) |
| O7—Mn1—O1W | 85.15 (6) | O3—C10—C11 | 118.78 (19) |
| O2—Mn1—O1W | 85.19 (6) | C15—C10—C11 | 117.3 (2) |
| N1—Mn1—O1W | 96.91 (6) | C12—C11—C10 | 121.0 (2) |
| O6—Mn1—O1W | 172.19 (6) | C12—C11—N3 | 117.3 (2) |
| C7—N1—N2 | 116.98 (17) | C10—C11—N3 | 121.6 (2) |
| C7—N1—Mn1 | 127.08 (14) | C13—C12—C11 | 120.2 (2) |
| N2—N1—Mn1 | 115.18 (12) | C13—C12—H12A | 119.9 |
| C8—N2—N1 | 108.13 (16) | C11—C12—H12A | 119.9 |
| O5—N3—O4 | 121.7 (2) | C12—C13—C14 | 119.7 (2) |
| O5—N3—C11 | 118.1 (2) | C12—C13—H13A | 120.2 |
| O4—N3—C11 | 120.2 (2) | C14—C13—H13A | 120.2 |
| C1—O1—Mn1 | 128.29 (13) | C13—C14—C15 | 120.9 (2) |
| C8—O2—Mn1 | 112.55 (12) | C13—C14—H14A | 119.5 |
| C10—O3—C9 | 117.88 (17) | C15—C14—H14A | 119.5 |
| C17—O6—Mn1 | 122.95 (15) | C14—C15—C10 | 120.8 (2) |

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| C19—O7—Mn1 | 125.80 (13) | C14—C15—H15A | 119.6 |
| Mn1—O1W—H01 | 116.9 | C10—C15—H15A | 119.6 |
| Mn1—O1W—H02 | 121.7 | C17—C16—H16A | 109.5 |
| H01—O1W—H02 | 105.0 | C17—C16—H16B | 109.5 |
| O1—C1—C6 | 118.1 (2) | H16A—C16—H16B | 109.5 |
| O1—C1—C2 | 123.98 (18) | C17—C16—H16C | 109.5 |
| C6—C1—C2 | 117.85 (19) | H16A—C16—H16C | 109.5 |
| C3—C2—C1 | 119.68 (19) | H16B—C16—H16C | 109.5 |
| C3—C2—C7 | 118.1 (2) | O6—C17—C18 | 123.8 (2) |
| C1—C2—C7 | 122.25 (18) | O6—C17—C16 | 117.7 (2) |
| C4—C3—C2 | 121.2 (2) | C18—C17—C16 | 118.5 (2) |
| C4—C3—H3A | 119.4 | C19—C18—C17 | 125.8 (2) |
| C2—C3—H3A | 119.4 | C19—C18—H18A | 117.1 |
| C3—C4—C5 | 118.9 (2) | C17—C18—H18A | 117.1 |
| C3—C4—H4A | 120.5 | O7—C19—C18 | 125.5 (2) |
| C5—C4—H4A | 120.5 | O7—C19—C20 | 113.99 (19) |
| C6—C5—C4 | 121.5 (2) | C18—C19—C20 | 120.5 (2) |
| C6—C5—H5A | 119.3 | C19—C20—H20A | 109.5 |
| C4—C5—H5A | 119.3 | C19—C20—H20B | 109.5 |
| C5—C6—C1 | 120.8 (2) | H20A—C20—H20B | 109.5 |
| C5—C6—H6A | 119.6 | C19—C20—H20C | 109.5 |
| C1—C6—H6A | 119.6 | H20A—C20—H20C | 109.5 |
| N1—C7—C2 | 124.32 (19) | H20B—C20—H20C | 109.5 |
| N1—C7—H7A | 117.8 | | |

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| O1—Mn1—N1—C7 | −18.44 (18) | O1—C1—C6—C5 | −179.2 (2) |
| O2—Mn1—N1—C7 | 169.54 (18) | C2—C1—C6—C5 | 2.5 (3) |
| O6—Mn1—N1—C7 | 77.89 (17) | N2—N1—C7—C2 | −179.77 (19) |
| O1W—Mn1—N1—C7 | −106.72 (17) | Mn1—N1—C7—C2 | 10.7 (3) |
| O1—Mn1—N1—N2 | 171.88 (14) | C3—C2—C7—N1 | −177.42 (19) |
| O2—Mn1—N1—N2 | −0.15 (13) | C1—C2—C7—N1 | 2.5 (3) |
| O6—Mn1—N1—N2 | −91.80 (14) | N1—N2—C8—O2 | 1.6 (3) |
| O1W—Mn1—N1—N2 | 83.60 (13) | N1—N2—C8—C9 | −177.13 (17) |
| C7—N1—N2—C8 | −171.41 (17) | Mn1—O2—C8—N2 | −1.8 (3) |
| Mn1—N1—N2—C8 | −0.6 (2) | Mn1—O2—C8—C9 | 176.98 (14) |
| O7—Mn1—O1—C1 | −157.85 (17) | C10—O3—C9—C8 | 71.6 (2) |
| O2—Mn1—O1—C1 | 57.6 (4) | N2—C8—C9—O3 | −136.04 (19) |
| N1—Mn1—O1—C1 | 20.41 (17) | O2—C8—C9—O3 | 45.1 (2) |
| O6—Mn1—O1—C1 | −69.03 (17) | C9—O3—C10—C15 | 27.0 (3) |
| O1W—Mn1—O1—C1 | 117.32 (17) | C9—O3—C10—C11 | −155.01 (18) |
| O1—Mn1—O2—C8 | −37.1 (3) | O3—C10—C11—C12 | −177.42 (19) |
| O7—Mn1—O2—C8 | 177.99 (13) | C15—C10—C11—C12 | 0.7 (3) |
| N1—Mn1—O2—C8 | 0.91 (13) | O3—C10—C11—N3 | 1.6 (3) |
| O6—Mn1—O2—C8 | 90.02 (14) | C15—C10—C11—N3 | 179.81 (19) |
| O1W—Mn1—O2—C8 | −97.07 (13) | O5—N3—C11—C12 | −21.3 (4) |
| O1—Mn1—O6—C17 | −125.31 (18) | O4—N3—C11—C12 | 155.4 (2) |
| O7—Mn1—O6—C17 | −27.06 (18) | O5—N3—C11—C10 | 159.6 (2) |
| O2—Mn1—O6—C17 | 65.11 (18) | O4—N3—C11—C10 | −23.7 (3) |

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| N1—Mn1—O6—C17 | 144.40 (18) | C10—C11—C12—C13 | 1.1 (4) |
| O1—Mn1—O7—C19 | 125.06 (16) | N3—C11—C12—C13 | −178.0 (2) |
| O2—Mn1—O7—C19 | −62.46 (16) | C11—C12—C13—C14 | −1.6 (4) |
| O6—Mn1—O7—C19 | 28.97 (16) | C12—C13—C14—C15 | 0.2 (4) |
| O1W—Mn1—O7—C19 | −147.44 (16) | C13—C14—C15—C10 | 1.7 (4) |
| Mn1—O1—C1—C6 | 166.84 (16) | O3—C10—C15—C14 | 175.9 (2) |
| Mn1—O1—C1—C2 | −15.0 (3) | C11—C10—C15—C14 | −2.2 (3) |
| O1—C1—C2—C3 | 179.15 (19) | Mn1—O6—C17—C18 | 15.6 (3) |
| C6—C1—C2—C3 | −2.6 (3) | Mn1—O6—C17—C16 | −165.12 (17) |
| O1—C1—C2—C7 | −0.8 (3) | O6—C17—C18—C19 | 4.8 (4) |
| C6—C1—C2—C7 | 177.4 (2) | C16—C17—C18—C19 | −174.5 (2) |
| C1—C2—C3—C4 | 1.0 (3) | Mn1—O7—C19—C18 | −20.4 (3) |
| C7—C2—C3—C4 | −179.1 (2) | Mn1—O7—C19—C20 | 160.21 (14) |
| C2—C3—C4—C5 | 1.0 (4) | C17—C18—C19—O7 | −3.8 (4) |
| C3—C4—C5—C6 | −1.1 (4) | C17—C18—C19—C20 | 175.6 (2) |
| C4—C5—C6—C1 | −0.6 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H01···O4$^{i}$ | 0.88 | 2.16 | 2.955 (2) | 150 |
| O1*W*—H02···O2$^{i}$ | 0.88 | 1.96 | 2.829 (2) | 169 |

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.