Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cis-Tetraaquabis{5-[4-(1*H*-imidazol-1-yl-κN^3)phenyl]tetrazolido}manganese(II) dihydrate

Shao-Wei Tong,[a] Wen-Dong Song,[b]* Dong-Liang Miao,[a] Shi-Jie Li[c] and Jing-Bo An[a]

[a]College of Food Science and Technology, Guangdong Ocean University, Zhanjiang 524088, People's Republic of China, [b]College of Science, Guangdong Ocean University, Zhanjiang 524088, People's Republic of China, and [c]School of Enviroment Science and Engineering, Donghua University, Shanghai 200051, People's Republic of China
Correspondence e-mail: songwd60@163.com

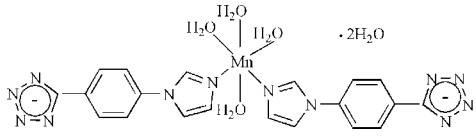
Received 9 February 2012; accepted 9 March 2012

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.056; wR factor = 0.142; data-to-parameter ratio = 11.4.

In the title compound, $[Mn(C_{10}H_7N_6)_2(H_2O)_4]\cdot 2H_2O$, the Mn^{2+} lies on a twofold rotation axis and is six-coordinated by two N atoms from the *cis*-related monodentate 5-[4-(imidazol-1-yl)phenyl]tetrazolide ligands and four O atoms from the coordinated water molecules. The complex molecules are connected *via* water O—H···O and O—H···N hydrogen bonds and weak π–π stacking interactions between the benzene rings [minimum ring centroid separation = 3.750 (6) Å] into a three-dimensional polymeric structure. The imidazolyl group of the ligand is partially disordered over two sets of sites with refined occupancies of 0.531 (7):0.469 (7).

Related literature

For our previous work based on imidazole derivatives as ligands, see: Li, Song *et al.* (2011); Li, Ma *et al.* (2011); Fan *et al.* (2010); Li *et al.* (2010). For related structures, see: Huang *et al.* (2009); Cheng (2011). An independent determination of the title structure is reported by Wang *et al.* (2012).



Experimental

Crystal data

$[Mn(C_{10}H_7N_6)_2(H_2O)_4]\cdot 2H_2O$
M_r = 585.47
Monoclinic, $C2/c$
a = 19.1342 (18) Å
b = 13.2100 (4) Å
c = 13.3280 (13) Å
β = 131.056 (2)°
V = 2540.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.58 mm^{-1}
T = 294 K
0.80 × 0.11 × 0.10 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.653, T_{max} = 0.944
8421 measured reflections
2239 independent reflections
1957 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.142
S = 1.31
2239 reflections
196 parameters
512 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3E···N5^{i}	0.85	2.65	3.397 (4)	147
O3—H3E···N6^{i}	0.85	1.89	2.726 (4)	169
O3—H3D···N4^{ii}	0.85	2.63	3.261 (5)	132
O3—H3D···N3^{ii}	0.85	1.95	2.774 (5)	162
O2—H2D···O3^{iii}	0.85	1.84	2.684 (4)	170
O2—H2C···O3	0.85	1.90	2.745 (4)	170
O1—H1D···N5^{iv}	0.85	1.96	2.811 (4)	179
O1—H1C···N5^{v}	0.85	2.62	3.396 (4)	152
O1—H1C···N4^{v}	0.85	1.99	2.835 (4)	179

Symmetry codes: (i) $x, y, z-1$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+1, -y, -z+1$; (iv) $-x+1, y, -z+\frac{5}{2}$; (v) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku/MSC, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We acknowledge the public science and technology research funds projects of ocean (grant No. 2000905021), the Guangdong Oceanic Fisheries Technology Promotion Project [grant No. A2009003?018(c)], the Guangdong Chinese Academy of Science comprehensive strategic cooperation project (grant No. 2009B091300121) and the Guangdong Province key project in the field of social development [grant No. A2009011-007(c)].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2182).

References

Cheng, X.-C. (2011). *Acta Cryst.* E**67**, m1757.
Fan, R.-Z., Li, S.-J., Song, W.-D., Miao, D.-L. & Hu, S.-W. (2010). *Acta Cryst.* E**66**, m897–m898.
Huang, R. Y., Zhu, K., Chen, H., Liu, G. X. & Ren, X. M. (2009). *Wuji Huaxue Xuebao*, **25**, 162–165.
Li, S.-J., Ma, X.-T., Song, W.-D., Li, X.-F. & Liu, J.-H. (2011). *Acta Cryst.* E**67**, m295–m296.
Li, S.-J., Miao, D.-L., Song, W.-D., Li, S.-H. & Yan, J.-B. (2010). *Acta Cryst.* E**66**, m1096–m1097.

Li, S. J., Song, W. D., Miao, D. L., Hu, S. W., Ji, L. L. & Ma, D. Y. (2011). *Z. Anorg. Allg. Chem.* **637**, 1246–1252.
Rigaku/MSC (1998). *RAPID-AUTO*. Rigaku/MSC, The Woodlands, Texas, USA.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, X., Yan, S.-W., Chang, S.-C., Liang, Y.-C. & Zhang, F.-T. (2012). *Acta Cryst.* E**68**, m413–m414.

supplementary materials

Acta Cryst. (2012). E**68**, m433–m434 [doi:10.1107/S1600536812010446]

cis-Tetraaquabis{5-[4-(1*H*-imidazol-1-yl-κN^3)phenyl]tetrazolido}manganese(II) dihydrate

Shao-Wei Tong, Wen-Dong Song, Dong-Liang Miao, Shi-Jie Li and Jing-Bo An

Comment

In recent years, our research group has shown great interest in the design and synthesis of interesting metal–organic comlexes with imidazole derivatives such as 2-propyl-imidazole-4,5-dicarboxylic acid (Fan *et al.*, 2010; Li *et al.*, 2010) and 2-ethyl-1*H*-imidazole-4,5-dicarboxylic acid (Li, Song *et al.*, 2011; Li, Ma *et al.*, 2011). In this paper, we report the synthesis and structure of a new Mn^{II} complex, $[Mn(C_{10}H_7N_6)_2(H_2O)_4]$. $2(H_2O)$ and the structure is reported here.

As shown in the Fig. 1, the title complex molecule comprises the Mn^{2+} ion which lies on a crystallographic twofold rotation axis and is six-coordinated by two N atoms from the *cis*-related monodentate 5-[4-(imidazol-1-yl)phenyl]-tetrazolide ligands and four O atoms from the coordinated water molecules. The complex has a slightly distorted octahedral geometry [Mn—N = 2.256 (4) Å; Mn—O = 2.177 (3) and 2.204 (3) Å]. In the crystal structure, the complex molecules are connected *via* water O—H···O and O—H···N hydrogen bonds (Table 1) into a three-dimensional supramolecular structure which is further stabilized by weak π–π stacking interactions between benzene rings [minimum ring centroid distance, 3.750 (6) Å]. The atoms C2 and C3 of the imidazolyl ring of the ligand are disordered over two sites (C2′ and C3′) with refined occupancies of 0.531 (7):0.469 (7), respectively. The structure of the anhydrous *trans* isomer of this complex has previosly been reported (Cheng, 2011).

Experimental

A mixture of manganese(II) chloride (0.1 mmol, 0.020 g) and 5-[4-(imidazol-1-yl)phenyl]tetrazole (1-tetrazole-4-imidazole-benzene) (0.2 mmol, 0.043 g) in 15 ml of water was sealed in an autoclave equipped with a Teflon liner (25 ml) and then heated at 413 K for 3 days. Crystals of the title compound were obtained by slow evaporation of the solvent at room temperature.

Refinement

H atoms of the water molecule were located in a difference-Fourier map and refined as riding with an O—H distance restraint of 0.85 Å, with U_{iso}(H) = 1.5 U_{eq}. The imidazolyl and phenyl H atoms were located in a difference-Fourier but were refined as riding with C—H = 0.93 Å and U_{iso}(H) = 1.5U_{eq}(C). The imidazolyl groups of the ligand are partially disordered over two sets of sites (C2, C2′ and C3, C3′) with refined occupancies of 0.531 (7) : 0.469 (7).

Computing details

Data collection: *RAPID-AUTO* (Rigaku/MSC, 1998); cell refinement: *RAPID-AUTO* (Rigaku/MSC, 1998); data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

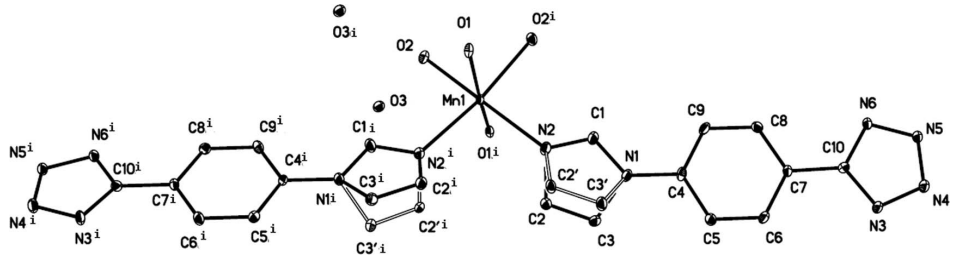


Figure 1

The molecular configuration and atom numbering scheme of the title compound, with non-H atoms shown as 30% probability displacement ellipsoids. For symmetry code (i): -*x* + 1, *y*, -*z* + 3/2.

cis-Tetraaquabis{5-[4-(1*H*-imidazol-1-yl- κN^3)phenyl]tetrazolido}manganese(II) dihydrate

Crystal data

$[Mn(C_{10}H_7N_6)_2(H_2O)_4]\cdot 2H_2O$
M_r = 585.47
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 19.1342 (18) Å
b = 13.2100 (4) Å
c = 13.3280 (13) Å
β = 131.056 (2)°
V = 2540.3 (4) Å^3
Z = 4
F(000) = 1212
D_x = 1.531 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 3180 reflections
θ = 3.1–30.0°
μ = 0.58 mm^{-1}
T = 294 K
Block, colourless
0.80 × 0.11 × 0.10 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.653, T_{max} = 0.944
8421 measured reflections
2239 independent reflections
1957 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 25.0°, θ_{min} = 3.1°
h = −22→22
k = −15→15
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.142
S = 1.31
2239 reflections
196 parameters
512 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
$w = 1/[\sigma^2(F_o^2) + (0.0076P)^2 + 23.3787P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mn1	0.5000	0.14050 (7)	0.7500	0.0114 (2)	
N1	0.4195 (3)	0.3148 (3)	0.9401 (4)	0.0197 (8)	
N2	0.4707 (3)	0.2569 (3)	0.8420 (4)	0.0189 (8)	
N3	0.2780 (3)	0.3910 (3)	1.2697 (4)	0.0190 (8)	
N4	0.2668 (3)	0.3553 (3)	1.3534 (4)	0.0201 (8)	
N5	0.2945 (2)	0.2610 (3)	1.3831 (3)	0.0158 (8)	
N6	0.3247 (2)	0.2320 (3)	1.3206 (3)	0.0149 (7)	
O1	0.65066 (19)	0.1248 (2)	0.9144 (3)	0.0164 (7)	
H1C	0.6860	0.1315	0.8971	0.020*	
H1D	0.6680	0.1664	0.9757	0.020*	
O2	0.5016 (2)	0.0210 (2)	0.6390 (3)	0.0172 (7)	
H2C	0.4550	0.0260	0.5564	0.021*	
H2D	0.5483	0.0045	0.6477	0.021*	
O3	0.3656 (2)	0.0306 (2)	0.3671 (3)	0.0178 (7)	
H3D	0.3190	−0.0069	0.3354	0.021*	
H3E	0.3466	0.0912	0.3426	0.021*	
C1	0.4461 (3)	0.2365 (3)	0.9100 (5)	0.0227 (10)	
H1	0.4471	0.1708	0.9362	0.027*	
C2	0.4225 (6)	0.3504 (6)	0.7794 (8)	0.0186 (17)	0.531 (7)
H2	0.4149	0.3814	0.7102	0.022*	0.531 (7)
C3	0.3898 (6)	0.3863 (6)	0.8365 (8)	0.0184 (17)	0.531 (7)
H3	0.3553	0.4450	0.8139	0.022*	0.531 (7)
C2′	0.5005 (7)	0.3579 (7)	0.8818 (9)	0.0181 (19)	0.469 (7)
H2′	0.5348	0.3938	0.8669	0.022*	0.469 (7)
C3′	0.4721 (7)	0.3956 (7)	0.9450 (9)	0.0192 (19)	0.469 (7)
H3′	0.4840	0.4593	0.9828	0.023*	0.469 (7)
C4	0.3907 (3)	0.3145 (3)	1.0161 (4)	0.0148 (8)	
C5	0.3558 (3)	0.4030 (3)	1.0259 (4)	0.0172 (9)	
H5	0.3501	0.4616	0.9822	0.021*	
C6	0.3299 (3)	0.4027 (3)	1.1017 (4)	0.0178 (9)	
H6	0.3060	0.4613	1.1080	0.021*	
C7	0.3392 (3)	0.3158 (3)	1.1684 (4)	0.0133 (8)	
C8	0.3722 (3)	0.2276 (3)	1.1547 (4)	0.0153 (9)	
H8	0.3767	0.1684	1.1963	0.018*	
C9	0.3986 (3)	0.2275 (3)	1.0794 (4)	0.0180 (9)	
H9	0.4216	0.1687	1.0718	0.022*	
C10	0.3140 (3)	0.3136 (3)	1.2521 (4)	0.0139 (9)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0141 (5)	0.0116 (4)	0.0135 (5)	0.000	0.0113 (4)	0.000
N1	0.031 (2)	0.0127 (17)	0.031 (2)	0.0007 (15)	0.0271 (18)	−0.0012 (15)
N2	0.026 (2)	0.0149 (18)	0.0275 (19)	−0.0026 (16)	0.0226 (17)	−0.0031 (15)
N3	0.027 (2)	0.0169 (19)	0.026 (2)	0.0046 (16)	0.0230 (18)	0.0029 (15)
N4	0.029 (2)	0.0180 (18)	0.0255 (19)	0.0026 (17)	0.0233 (18)	0.0018 (16)
N5	0.0204 (19)	0.0150 (18)	0.0179 (18)	0.0006 (15)	0.0152 (16)	0.0009 (14)
N6	0.0191 (18)	0.0152 (18)	0.0150 (17)	0.0001 (15)	0.0132 (15)	0.0001 (14)
O1	0.0183 (15)	0.0209 (16)	0.0174 (15)	−0.0029 (13)	0.0148 (14)	−0.0036 (13)
O2	0.0157 (16)	0.0216 (16)	0.0178 (15)	0.0008 (13)	0.0124 (14)	−0.0021 (13)
O3	0.0195 (16)	0.0145 (15)	0.0229 (16)	0.0009 (13)	0.0155 (14)	−0.0001 (13)
C1	0.038 (3)	0.015 (2)	0.031 (2)	0.0024 (19)	0.030 (2)	−0.0001 (18)
C2	0.026 (4)	0.015 (4)	0.024 (4)	0.001 (3)	0.020 (3)	0.001 (3)
C3	0.025 (4)	0.012 (3)	0.026 (4)	0.002 (3)	0.020 (3)	0.001 (3)
C2′	0.028 (4)	0.013 (4)	0.024 (4)	−0.006 (3)	0.022 (3)	−0.003 (3)
C3′	0.026 (4)	0.018 (4)	0.024 (4)	−0.003 (3)	0.021 (3)	−0.001 (3)
C4	0.015 (2)	0.017 (2)	0.019 (2)	−0.0056 (16)	0.0138 (17)	−0.0053 (16)
C5	0.024 (2)	0.013 (2)	0.021 (2)	−0.0015 (17)	0.0177 (18)	0.0002 (17)
C6	0.022 (2)	0.016 (2)	0.024 (2)	0.0031 (17)	0.0188 (19)	−0.0001 (17)
C7	0.014 (2)	0.016 (2)	0.0128 (19)	0.0001 (16)	0.0102 (17)	−0.0004 (16)
C8	0.018 (2)	0.013 (2)	0.0155 (19)	−0.0002 (17)	0.0114 (17)	0.0010 (16)
C9	0.021 (2)	0.017 (2)	0.023 (2)	0.0031 (17)	0.0173 (18)	−0.0016 (17)
C10	0.014 (2)	0.0125 (19)	0.016 (2)	0.0001 (16)	0.0098 (17)	−0.0007 (16)

Geometric parameters (Å, º)

Mn1—O2^{i}	2.177 (3)	O2—H2D	0.8500
Mn1—O2	2.177 (3)	O3—H3D	0.8500
Mn1—O1	2.204 (3)	O3—H3E	0.8499
Mn1—O1^{i}	2.204 (3)	C1—H1	0.9300
Mn1—N2	2.256 (4)	C2—C3	1.349 (11)
Mn1—N2^{i}	2.256 (4)	C2—H2	0.9300
N1—C1	1.327 (6)	C3—H3	0.9300
N1—C4	1.436 (5)	C2′—C3′	1.361 (12)
N1—C3′	1.438 (10)	C2′—H2′	0.9300
N1—C3	1.446 (9)	C3′—H3′	0.9300
N2—C1	1.293 (5)	C4—C9	1.374 (6)
N2—C2′	1.410 (10)	C4—C5	1.393 (6)
N2—C2	1.436 (9)	C5—C6	1.389 (6)
N3—C10	1.336 (5)	C5—H5	0.9300
N3—N4	1.352 (5)	C6—C7	1.390 (6)
N4—N5	1.309 (5)	C6—H6	0.9300
N5—N6	1.346 (5)	C7—C8	1.393 (6)
N6—C10	1.338 (5)	C7—C10	1.478 (5)
O1—H1C	0.8500	C8—C9	1.388 (6)
O1—H1D	0.8501	C8—H8	0.9300
O2—H2C	0.8500	C9—H9	0.9300

O2^{i}—Mn1—O2	87.07 (16)	H3D—O3—H3E	108.3
O2^{i}—Mn1—O1	81.34 (11)	N2—C1—N1	115.9 (4)
O2—Mn1—O1	90.81 (11)	N2—C1—H1	122.0
O2^{i}—Mn1—O1^{i}	90.81 (11)	N1—C1—H1	122.0
O2—Mn1—O1^{i}	81.34 (11)	C3—C2—N2	109.5 (7)
O1—Mn1—O1^{i}	169.20 (16)	C3—C2—H2	125.3
O2^{i}—Mn1—N2	90.29 (12)	N2—C2—H2	125.3
O2—Mn1—N2	169.50 (12)	C2—C3—N1	105.8 (7)
O1—Mn1—N2	98.84 (12)	C2—C3—H3	127.1
O1^{i}—Mn1—N2	88.54 (12)	N1—C3—H3	127.1
O2^{i}—Mn1—N2^{i}	169.50 (12)	C3′—C2′—N2	110.6 (7)
O2—Mn1—N2^{i}	90.29 (12)	C3′—C2′—H2′	124.7
O1—Mn1—N2^{i}	88.54 (12)	N2—C2′—H2′	124.7
O1^{i}—Mn1—N2^{i}	98.84 (12)	C2′—C3′—N1	104.6 (7)
N2—Mn1—N2^{i}	94.05 (18)	C2′—C3′—H3′	127.7
C1—N1—C4	127.8 (4)	N1—C3′—H3′	127.7
C1—N1—C3′	101.3 (5)	C9—C4—C5	120.7 (4)
C4—N1—C3′	123.5 (5)	C9—C4—N1	119.8 (4)
C1—N1—C3	102.0 (4)	C5—C4—N1	119.5 (4)
C4—N1—C3	125.7 (4)	C6—C5—C4	119.2 (4)
C3′—N1—C3	51.9 (5)	C6—C5—H5	120.4
C1—N2—C2′	100.2 (5)	C4—C5—H5	120.4
C1—N2—C2	101.3 (4)	C5—C6—C7	120.8 (4)
C2′—N2—C2	49.6 (5)	C5—C6—H6	119.6
C1—N2—Mn1	125.0 (3)	C7—C6—H6	119.6
C2′—N2—Mn1	131.7 (4)	C6—C7—C8	119.0 (4)
C2—N2—Mn1	124.4 (4)	C6—C7—C10	122.0 (4)
C10—N3—N4	104.9 (3)	C8—C7—C10	119.0 (4)
N5—N4—N3	109.2 (3)	C9—C8—C7	120.5 (4)
N4—N5—N6	109.8 (3)	C9—C8—H8	119.7
C10—N6—N5	104.8 (3)	C7—C8—H8	119.7
Mn1—O1—H1C	118.3	C4—C9—C8	119.8 (4)
Mn1—O1—H1D	108.9	C4—C9—H9	120.1
H1C—O1—H1D	108.4	C8—C9—H9	120.1
Mn1—O2—H2C	110.6	N3—C10—N6	111.3 (4)
Mn1—O2—H2D	125.2	N3—C10—C7	125.3 (4)
H2C—O2—H2D	108.1	N6—C10—C7	123.4 (4)

O2^{i}—Mn1—N2—C1	−11.2 (4)	C1—N2—C2′—C3′	−13.7 (9)
O2—Mn1—N2—C1	64.1 (9)	C2—N2—C2′—C3′	82.6 (9)
O1—Mn1—N2—C1	−92.5 (4)	Mn1—N2—C2′—C3′	−173.9 (5)
O1^{i}—Mn1—N2—C1	79.6 (4)	N2—C2′—C3′—N1	−1.9 (10)
N2^{i}—Mn1—N2—C1	178.3 (5)	C1—N1—C3′—C2′	16.4 (8)
O2^{i}—Mn1—N2—C2′	144.8 (6)	C4—N1—C3′—C2′	168.1 (6)
O2—Mn1—N2—C2′	−139.8 (8)	C3—N1—C3′—C2′	−80.2 (8)
O1—Mn1—N2—C2′	63.5 (6)	C1—N1—C4—C9	7.3 (7)
O1^{i}—Mn1—N2—C2′	−124.4 (6)	C3′—N1—C4—C9	−136.7 (6)
N2^{i}—Mn1—N2—C2′	−25.6 (6)	C3—N1—C4—C9	159.1 (5)
O2^{i}—Mn1—N2—C2	−151.5 (5)	C1—N1—C4—C5	−173.4 (5)

O2—Mn1—N2—C2	−76.1 (9)	C3′—N1—C4—C5	42.6 (7)
O1—Mn1—N2—C2	127.2 (5)	C3—N1—C4—C5	−21.6 (7)
O1^{i}—Mn1—N2—C2	−60.7 (5)	C9—C4—C5—C6	0.6 (7)
N2^{i}—Mn1—N2—C2	38.1 (4)	N1—C4—C5—C6	−178.7 (4)
C10—N3—N4—N5	−0.3 (5)	C4—C5—C6—C7	0.6 (7)
N3—N4—N5—N6	0.1 (5)	C5—C6—C7—C8	−2.0 (7)
N4—N5—N6—C10	0.2 (4)	C5—C6—C7—C10	178.7 (4)
C2′—N2—C1—N1	27.0 (6)	C6—C7—C8—C9	2.3 (6)
C2—N2—C1—N1	−23.5 (6)	C10—C7—C8—C9	−178.5 (4)
Mn1—N2—C1—N1	−170.9 (3)	C5—C4—C9—C8	−0.4 (7)
C4—N1—C1—N2	−178.7 (4)	N1—C4—C9—C8	178.9 (4)
C3′—N1—C1—N2	−28.7 (6)	C7—C8—C9—C4	−1.0 (7)
C3—N1—C1—N2	24.4 (6)	N4—N3—C10—N6	0.5 (5)
C1—N2—C2—C3	12.3 (8)	N4—N3—C10—C7	−179.7 (4)
C2′—N2—C2—C3	−81.5 (8)	N5—N6—C10—N3	−0.4 (5)
Mn1—N2—C2—C3	160.0 (5)	N5—N6—C10—C7	179.7 (4)
N2—C2—C3—N1	1.1 (9)	C6—C7—C10—N3	2.2 (7)
C1—N1—C3—C2	−13.8 (7)	C8—C7—C10—N3	−177.1 (4)
C4—N1—C3—C2	−171.3 (5)	C6—C7—C10—N6	−178.0 (4)
C3′—N1—C3—C2	81.2 (8)	C8—C7—C10—N6	2.8 (6)

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*E*···N5^{ii}	0.85	2.65	3.397 (4)	147
O3—H3*E*···N6^{ii}	0.85	1.89	2.726 (4)	169
O3—H3*D*···N4^{iii}	0.85	2.63	3.261 (5)	132
O3—H3*D*···N3^{iii}	0.85	1.95	2.774 (5)	162
O2—H2*D*···O3^{iv}	0.85	1.84	2.684 (4)	170
O2—H2*C*···O3	0.85	1.90	2.745 (4)	170
O1—H1*D*···N5^{v}	0.85	1.96	2.811 (4)	179
O1—H1*C*···N5^{vi}	0.85	2.62	3.396 (4)	152
O1—H1*C*···N4^{vi}	0.85	1.99	2.835 (4)	179

Symmetry codes: (ii) *x*, *y*, *z*−1; (iii) −*x*+1/2, *y*−1/2, −*z*+3/2; (iv) −*x*+1, −*y*, −*z*+1; (v) −*x*+1, *y*, −*z*+5/2; (vi) *x*+1/2, −*y*+1/2, *z*−1/2.