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

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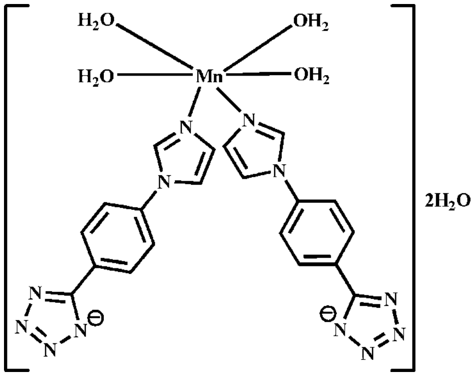
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.037; wR factor = 0.099; data-to-parameter ratio = 13.5.

In the title compound, $[Mn(C_{10}H_7N_6)_2(H_2O)_4]\cdot 2H_2O$, the complex unit comprises an Mn^{2+} ion, coordinated by two imidazole N atoms from *cis*-related monodentate 5-[4-(imidazol-1-yl)phenyl]tetrazolide ligands and four water molecules, together with two water molecules of solvation. The Mn^{2+} ion lies on a twofold rotation axis and has a slightly distorted octahedral geometry. The molecules are connected by O—H···N and O—H···O hydrogen bonds involving both coordinated and solvent water molecules, generating a three-dimensional structure. Two C atoms of the imidazole ring of the ligand are each disordered over two sites with occupancy factors of 0.75 and 0.25.

Related literature

For general background to the use of nitrogen-containing ligands in the construction of supramolecular coordination compounds, see: Qi *et al.* (2008). For the structure of the anhydrous *trans*-isomer of the title complex, see: Cheng (2011).



Experimental

Crystal data

$[Mn(C_{10}H_7N_6)_2(H_2O)_4]\cdot 2H_2O$
M_r = 585.47
Monoclinic, $C2/c$
a = 19.239 (3) Å
b = 13.141 (2) Å
c = 13.417 (2) Å
β = 129.912 (2)°
V = 2601.8 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 296 K
0.50 × 0.45 × 0.35 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.764, T_{max} = 0.826
7759 measured reflections
2962 independent reflections
2246 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.04
2962 reflections
219 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H11W···O3W	0.79 (4)	1.91 (4)	2.690 (4)	169 (2)
O1W—H12W···O3W^{i}	0.82 (3)	1.95 (3)	2.762 (3)	168 (4)
O2W—H21W···N4^{ii}	0.79 (4)	2.07 (4)	2.847 (4)	169 (3)
O2W—H22W···N5^{iii}	0.85 (3)	1.97 (3)	2.812 (3)	170 (4)
O3W—H31W···N3^{iv}	0.83 (4)	1.97 (3)	2.786 (3)	167 (3)
O3W—H31W···N4^{iv}	0.83 (4)	2.62 (3)	3.308 (3)	142 (3)
O3W—H32W···N6^{v}	0.82 (3)	1.95 (3)	2.757 (3)	172 (2)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2184).

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supplementary materials

Acta Cryst. (2012). E**68**, m413–m414 [doi:10.1107/S1600536812010380]

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

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Comment

In recent years, much study has been focused on using nitrogen-containing ligands and 1,4-benzenedicarboxylic acid to construct supramolecular coordination compounds. The reason is that these supramolecular coordination assemblies exhibit not only a variety of architectures but also have potential applications as functional materials (Qi *et al.*, 2008). In this paper, we report the synthesis and structure of the title complex $[Mn(timb)_2(H_2O)_4] . 2H_2O$, {Htimb = 5-[4-imidazol-1-yl)phenyl]tetrazole}, synthesized by the hydrothermal reaction of manganese(II) acetate with Htimb in the presence of 1,4-benzenedicarboxylic acid.

In the title compound the coordination polyhedron comprises a Mn^{2+} ion, two monodentate *cis*-related timb$^-$ ligands and four coordinated water molecules, together with two water molecules of solvation (Fig. 1). The Mn^{2+} lies on a twofold rotation axis and the complex has a slightly distorted octahedral geometry. Both the coordinated and solvent water molecules form intermolecular O—H···O and O—H···N hydrogen-bonding interactions (Table 1) to form a three-dimensional supramolecular network. Two atoms of the imidazole ring (C2, C3) are disordered over two sites (C2*A* and C3*A*, respectively), with occupancy factors of 0.75 and 0.25. The structure of the anhydrous *trans*-isomer of the title complex has previously been reported (Cheng, 2011).

Experimental

A mixture of $Mn(OAc)_2$ (0.098 g, 0.4 mmol), 5-[4-imidazol-1-yl)phenyl]tetrazole (Htimb) (0.064 g, 0.3 mmol), 1,4-benzendicarboxylic acid (0.066 g, 0.4 mmol) and water (9 ml) was stirred for 30 min in air. The mixture was then transferred to a 18 ml Teflon-lined hydrothermal bomb. The bomb was kept at 433 K for 75 h under autogenous pressure. The product was washed with distilled water and dried, giving the yellow title compound.

Refinement

Hydrogen atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in a difference-Fourier analysis and both positional and isotropic displacement parameters were allowed to refine. Atom pairs C2, C2*A* and C3, C3*A* represent disordered atoms of the imidazole ring of the ligand, having site occupancies of 0.75 and 0.25.

Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); 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: *SHELXL97* (Sheldrick, 2008).

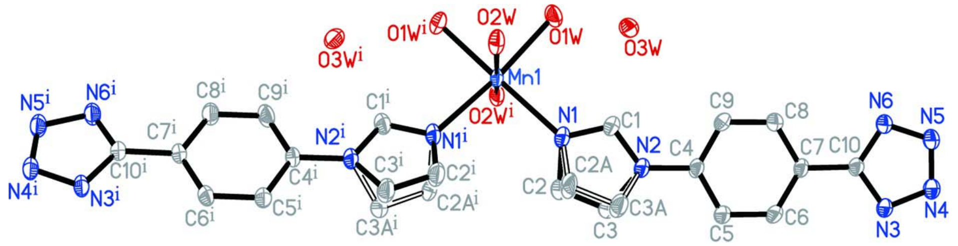

Figure 1

Molecular configuration and atom numbering scheme for the title complex, showing the partial disorder in the imidaziole ring of the ligand. Displacement ellipsoids are drawn at the 30% probability level. For symmetry code (i): -*x* - 1, *y*, -*z* + 5/2.

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Crystal data

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$M_r = 585.47$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 19.239$ (3) Å
$b = 13.141$ (2) Å
$c = 13.417$ (2) Å
$\beta = 129.912$ (2)°
$V = 2601.8$ (7) Å^3
$Z = 4$

$F(000) = 1212$
$D_x = 1.495$ Mg m^{-3}
Mo *Kα* radiation, $\lambda = 0.71073$ Å
Cell parameters from 7759 reflections
$\theta = 2.1–27.5°$
$\mu = 0.57$ mm^{-1}
$T = 296$ K
Block, yellow
0.50 × 0.45 × 0.35 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.764$, $T_{max} = 0.826$

7759 measured reflections
2962 independent reflections
2246 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.1°$
$h = -24 \rightarrow 24$
$k = -17 \rightarrow 16$
$l = -12 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.099$
$S = 1.04$
2962 reflections
219 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 1.08P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
Mn1	0.50000	0.64609 (3)	1.25000	0.0381 (2)	
O1W	0.50199 (14)	0.52591 (12)	1.13954 (19)	0.0494 (6)	
O2W	0.35299 (11)	0.62992 (13)	1.09094 (17)	0.0487 (6)	
N1	0.53170 (13)	0.76342 (13)	1.16074 (18)	0.0471 (6)	
N2	0.58359 (12)	0.81830 (13)	1.06351 (18)	0.0439 (6)	
N3	0.72694 (13)	0.88544 (13)	0.73642 (18)	0.0457 (6)	
N4	0.73655 (13)	0.84944 (13)	0.65176 (19)	0.0476 (6)	
N5	0.70484 (12)	0.75736 (14)	0.61811 (17)	0.0476 (7)	
N6	0.67343 (12)	0.72992 (13)	0.67890 (17)	0.0452 (6)	
C1	0.54836 (16)	0.74146 (16)	1.0828 (2)	0.0499 (8)	
C2	0.5739 (3)	0.8554 (3)	1.2134 (4)	0.0586 (16)	0.750
C3	0.6063 (3)	0.8903 (3)	1.1558 (4)	0.0600 (15)	0.750
C4	0.61025 (13)	0.81709 (14)	0.98504 (19)	0.0371 (6)	
C5	0.64673 (17)	0.90308 (16)	0.9751 (2)	0.0500 (8)	
C6	0.67239 (17)	0.90067 (16)	0.8996 (2)	0.0503 (8)	
C7	0.66198 (13)	0.81344 (14)	0.83318 (19)	0.0358 (6)	
C8	0.62672 (15)	0.72795 (16)	0.8463 (2)	0.0469 (7)	
C9	0.60114 (15)	0.72957 (16)	0.9219 (2)	0.0495 (8)	
C10	0.68777 (13)	0.80981 (14)	0.75070 (19)	0.0358 (6)	
C2A	0.5081 (10)	0.8671 (8)	1.1261 (14)	0.067 (5)	0.250
C3A	0.5379 (10)	0.9036 (8)	1.0642 (14)	0.070 (5)	0.250
O3W	0.63171 (12)	0.47411 (14)	1.12748 (17)	0.0481 (6)	
H1	0.53660	0.67790	1.04430	0.0600*	
H5	0.65400	0.96230	1.01900	0.0600*	
H2	0.57970	0.88850	1.27980	0.0710*	0.750
H3	0.63730	0.95100	1.17400	0.0710*	0.750
H9	0.57770	0.67120	0.93000	0.0590*	
H11W	0.5443 (19)	0.510 (2)	1.146 (2)	0.065 (9)*	
H12W	0.457 (2)	0.524 (2)	1.062 (3)	0.069 (9)*	
H21W	0.3226 (18)	0.6277 (18)	1.111 (3)	0.063 (8)*	
H22W	0.329 (2)	0.666 (2)	1.023 (3)	0.078 (10)*	
H6	0.69710	0.95870	0.89330	0.0600*	
H8	0.62010	0.66830	0.80350	0.0560*	
H21A	0.47760	0.90570	1.14540	0.0810*	0.250
H31A	0.52910	0.96810	1.02920	0.0830*	0.250
H31W	0.6792 (19)	0.508 (2)	1.171 (3)	0.070 (9)*	
H32W	0.6465 (17)	0.415 (2)	1.150 (2)	0.060 (8)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0532 (3)	0.0388 (2)	0.0477 (3)	0.0000	0.0440 (2)	0.0000
O1W	0.0568 (11)	0.0558 (10)	0.0539 (11)	0.0025 (8)	0.0439 (10)	−0.0081 (8)
O2W	0.0539 (10)	0.0631 (10)	0.0514 (10)	0.0093 (8)	0.0440 (9)	0.0084 (8)
N1	0.0636 (12)	0.0482 (10)	0.0584 (11)	−0.0029 (9)	0.0524 (10)	0.0005 (8)
N2	0.0619 (11)	0.0410 (9)	0.0575 (11)	−0.0042 (8)	0.0515 (10)	−0.0015 (8)
N3	0.0657 (12)	0.0424 (9)	0.0591 (12)	−0.0070 (8)	0.0539 (11)	−0.0051 (8)
N4	0.0638 (12)	0.0487 (10)	0.0596 (11)	−0.0038 (9)	0.0530 (11)	−0.0039 (9)
N5	0.0626 (12)	0.0505 (11)	0.0531 (11)	−0.0060 (9)	0.0479 (10)	−0.0068 (8)
N6	0.0611 (11)	0.0448 (10)	0.0509 (10)	−0.0094 (8)	0.0456 (10)	−0.0075 (8)
C1	0.0740 (16)	0.0430 (11)	0.0625 (14)	−0.0077 (11)	0.0574 (14)	−0.0020 (10)
C2	0.089 (3)	0.052 (2)	0.080 (3)	−0.017 (2)	0.075 (2)	−0.0164 (19)
C3	0.092 (3)	0.0465 (18)	0.084 (3)	−0.0215 (19)	0.076 (3)	−0.0183 (18)
C4	0.0430 (11)	0.0414 (10)	0.0436 (11)	0.0005 (8)	0.0354 (10)	0.0034 (8)
C5	0.0795 (16)	0.0366 (11)	0.0686 (15)	−0.0057 (10)	0.0634 (14)	−0.0049 (10)
C6	0.0797 (16)	0.0372 (11)	0.0717 (15)	−0.0079 (10)	0.0658 (15)	−0.0016 (10)
C7	0.0413 (11)	0.0400 (10)	0.0390 (11)	−0.0004 (8)	0.0317 (10)	0.0022 (8)
C8	0.0650 (14)	0.0426 (11)	0.0553 (13)	−0.0131 (10)	0.0488 (13)	−0.0109 (10)
C9	0.0695 (15)	0.0439 (12)	0.0624 (14)	−0.0187 (11)	0.0548 (13)	−0.0082 (10)
C10	0.0420 (11)	0.0375 (10)	0.0399 (11)	0.0011 (8)	0.0318 (10)	0.0019 (8)
C2A	0.108 (10)	0.058 (6)	0.100 (9)	0.028 (7)	0.096 (9)	0.021 (6)
C3A	0.120 (11)	0.045 (5)	0.106 (10)	0.021 (6)	0.101 (9)	0.020 (6)
O3W	0.0543 (11)	0.0420 (9)	0.0597 (10)	0.0019 (8)	0.0420 (9)	−0.0048 (8)

Geometric parameters (Å, º)

Mn1—O1W	2.183 (2)	N4—N5	1.299 (3)
Mn1—O2W	2.203 (2)	N5—N6	1.339 (4)
Mn1—N1	2.263 (2)	N6—C10	1.329 (3)
Mn1—O1W^{i}	2.183 (2)	C2—C3	1.347 (9)
Mn1—O2W^{i}	2.203 (2)	C2A—C3A	1.36 (3)
Mn1—N1^{i}	2.263 (2)	C4—C5	1.381 (4)
O1W—H12W	0.82 (3)	C4—C9	1.371 (3)
O1W—H11W	0.79 (4)	C5—C6	1.383 (5)
O2W—H21W	0.79 (4)	C6—C7	1.385 (3)
O2W—H22W	0.85 (3)	C7—C10	1.476 (4)
O3W—H32W	0.82 (3)	C7—C8	1.381 (3)
O3W—H31W	0.83 (4)	C8—C9	1.383 (4)
N1—C2	1.372 (5)	C1—H1	0.9300
N1—C1	1.308 (4)	C2—H2	0.9300
N1—C2A	1.417 (11)	C2A—H21A	0.9300
N2—C4	1.437 (4)	C3—H3	0.9300
N2—C3	1.388 (5)	C3A—H31A	0.9300
N2—C3A	1.428 (16)	C5—H5	0.9300
N2—C1	1.331 (4)	C6—H6	0.9300
N3—C10	1.333 (3)	C8—H8	0.9300
N3—N4	1.348 (3)	C9—H9	0.9300

O1W—Mn1—O2W	80.99 (9)	N1—C1—N2	113.9 (2)
O1W—Mn1—N1	90.32 (8)	N1—C2—C3	110.1 (4)
O1W—Mn1—O1W^{i}	87.31 (8)	N1—C2A—C3A	111.5 (15)
O1W—Mn1—O2W^{i}	90.98 (8)	N2—C3—C2	106.5 (4)
O1W—Mn1—N1^{i}	168.63 (10)	N2—C3A—C2A	103.2 (9)
O2W—Mn1—N1	99.64 (8)	N2—C4—C9	119.9 (2)
O1W^{i}—Mn1—O2W	90.98 (8)	C5—C4—C9	119.9 (3)
O2W—Mn1—O2W^{i}	168.93 (7)	N2—C4—C5	120.27 (19)
O2W—Mn1—N1^{i}	87.94 (8)	C4—C5—C6	119.6 (2)
O1W^{i}—Mn1—N1	168.63 (10)	C5—C6—C7	121.2 (2)
O2W^{i}—Mn1—N1	87.94 (8)	C6—C7—C10	122.0 (2)
N1—Mn1—N1^{i}	94.10 (8)	C8—C7—C10	119.89 (19)
O1W^{i}—Mn1—O2W^{i}	80.99 (9)	C6—C7—C8	118.1 (3)
O1W^{i}—Mn1—N1^{i}	90.32 (8)	C7—C8—C9	121.1 (2)
O2W^{i}—Mn1—N1^{i}	99.64 (8)	C4—C9—C8	120.1 (2)
H11W—O1W—H12W	108 (3)	N3—C10—C7	125.22 (18)
Mn1—O1W—H11W	125.7 (18)	N6—C10—C7	123.8 (2)
Mn1—O1W—H12W	115 (2)	N3—C10—N6	111.0 (2)
H21W—O2W—H22W	112 (4)	N2—C1—H1	123.00
Mn1—O2W—H21W	117 (2)	N1—C1—H1	123.00
Mn1—O2W—H22W	117 (3)	N1—C2—H2	125.00
H31W—O3W—H32W	107 (3)	C3—C2—H2	125.00
Mn1—N1—C1	124.09 (14)	C3A—C2A—H21A	124.00
Mn1—N1—C2A	133.7 (9)	N1—C2A—H21A	124.00
C1—N1—C2	103.8 (3)	C2—C3—H3	127.00
C1—N1—C2A	98.1 (8)	N2—C3—H3	127.00
Mn1—N1—C2	126.8 (2)	N2—C3A—H31A	129.00
C3A—N2—C4	121.6 (7)	C2A—C3A—H31A	128.00
C1—N2—C3A	101.7 (8)	C4—C5—H5	120.00
C3—N2—C4	127.3 (3)	C6—C5—H5	120.00
C1—N2—C4	126.86 (19)	C5—C6—H6	119.00
C1—N2—C3	104.6 (3)	C7—C6—H6	119.00
N4—N3—C10	104.79 (18)	C9—C8—H8	120.00
N3—N4—N5	109.4 (2)	C7—C8—H8	119.00
N4—N5—N6	109.5 (2)	C8—C9—H9	120.00
N5—N6—C10	105.31 (19)	C4—C9—H9	120.00

O1W—Mn1—N1—C1	−4.3 (2)	N4—N3—C10—N6	0.1 (3)
O1W—Mn1—N1—C2	−154.2 (4)	N4—N3—C10—C7	−179.0 (2)
O2W—Mn1—N1—C1	−85.2 (2)	N3—N4—N5—N6	0.1 (3)
O2W—Mn1—N1—C2	124.9 (4)	N4—N5—N6—C10	0.0 (3)
O2W^{i}—Mn1—N1—C1	86.7 (2)	N5—N6—C10—N3	−0.1 (3)
O2W^{i}—Mn1—N1—C2	−63.3 (4)	N5—N6—C10—C7	179.1 (2)
N1^{i}—Mn1—N1—C1	−173.8 (2)	N1—C2—C3—N2	0.2 (5)
N1^{i}—Mn1—N1—C2	36.3 (4)	N2—C4—C5—C6	179.8 (2)
Mn1—N1—C1—N2	−166.66 (17)	C9—C4—C5—C6	1.1 (4)
C2—N1—C1—N2	−11.0 (3)	N2—C4—C9—C8	−180.0 (2)
Mn1—N1—C2—C3	161.0 (3)	C5—C4—C9—C8	−1.3 (4)
C1—N1—C2—C3	6.3 (5)	C4—C5—C6—C7	0.2 (4)

C3—N2—C1—N1	11.3 (4)	C5—C6—C7—C8	−1.2 (4)
C4—N2—C1—N1	179.0 (2)	C5—C6—C7—C10	179.1 (2)
C1—N2—C3—C2	−6.5 (5)	C6—C7—C8—C9	1.0 (4)
C4—N2—C3—C2	−174.1 (3)	C10—C7—C8—C9	−179.3 (2)
C1—N2—C4—C5	−179.5 (2)	C6—C7—C10—N3	3.6 (4)
C1—N2—C4—C9	−0.8 (4)	C6—C7—C10—N6	−175.4 (2)
C3—N2—C4—C5	−14.5 (4)	C8—C7—C10—N3	−176.1 (2)
C3—N2—C4—C9	164.2 (3)	C8—C7—C10—N6	4.9 (4)
C10—N3—N4—N5	−0.1 (3)	C7—C8—C9—C4	0.2 (4)

Symmetry code: (i) −*x*+1, *y*, −*z*+5/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H11*W*···O3*W*	0.79 (4)	1.91 (4)	2.690 (4)	169 (2)
O1*W*—H12*W*···O3*W*^{ii}	0.82 (3)	1.95 (3)	2.762 (3)	168 (4)
O2*W*—H21*W*···N4^{iii}	0.79 (4)	2.07 (4)	2.847 (4)	169 (3)
O2*W*—H22*W*···N5^{iv}	0.85 (3)	1.97 (3)	2.812 (3)	170 (4)
O3*W*—H31*W*···N3^{v}	0.83 (4)	1.97 (3)	2.786 (3)	167 (3)
O3*W*—H31*W*···N4^{v}	0.83 (4)	2.62 (3)	3.308 (3)	142 (3)
O3*W*—H32*W*···N6^{vi}	0.82 (3)	1.95 (3)	2.757 (3)	172 (2)

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