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4,4′,6,6′-Tetramethyl-2,2′-bipyrimidine hexahydrate

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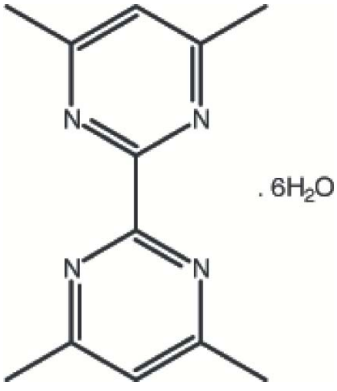
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.148; data-to-parameter ratio = 15.7.

In the title compound, $C_{12}H_{14}N_4\cdot 6H_2O$, the two pyrimidine rings make a dihedral angle of 5.285 (6)°. Intermolecular O—H···O hydrogen bonds link the six water molecules, generating edge-fused four-, five- or six-membered ring motifs and forming two-dimensional sheets. The sheets are stabilized by the formation of O—H···N hydrogen bonds between the water molecules and the bipyrimidine molecules, resulting in a three-dimensional network.

Related literature

For 2,2′-bipyrimidine and its derivatives, see: Ji *et al.* (2000); Baumann *et al.* (1998). For hydrogen-bonded water clusters, see: Buck & Huisken (2000); Lakshminarayanan *et al.* (2006). For water–water interactions in bulk water or ice, see: Zhang *et al.* (2005). For bond lengths and angles, see: Berg *et al.* (2002). For the preparation of the compound by the Ullmann coupling method, see: Vlad & Horvath (2002).



Experimental

Crystal data

$C_{12}H_{14}N_4\cdot 6H_2O$
M_r = 322.37
Triclinic, $P\overline{1}$
a = 6.8622 (19) Å
b = 11.098 (3) Å
c = 11.750 (3) Å
α = 98.233 (3)°
β = 91.774 (4)°
γ = 102.599 (4)°
V = 862.4 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.41 × 0.31 × 0.21 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.980
6492 measured reflections
3196 independent reflections
2026 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.148
S = 1.04
3196 reflections
204 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1W···O3^{i}	0.84	2.08	2.914 (2)	172
O1—H2W···O6	0.84	2.00	2.837 (2)	175
O2—H3W···N2	0.83	2.20	2.995 (2)	158
O2—H3W···N1	0.83	2.49	3.083 (2)	129
O2—H4W···O5^{ii}	0.84	2.04	2.872 (2)	167
O3—H5W···O5^{iii}	0.83	2.04	2.847 (2)	163
O3—H6W···O2	0.83	2.01	2.832 (2)	177
O4—H7W···O2	0.84	2.01	2.841 (2)	180
O4—H8W···O1^{iv}	0.84	1.92	2.755 (2)	171
O5—H9W···N4^{v}	0.83	2.31	3.007 (2)	142
O5—H9W···N3^{v}	0.83	2.46	3.196 (2)	149
O5—H10W···O3	0.83	2.04	2.849 (2)	166
O6—H11W···O4^{i}	0.83	2.05	2.851 (2)	162
O6—H12W···O4	0.84	2.06	2.886 (2)	173

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXS97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2743).

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4,4′,6,6′-Tetramethyl-2,2′-bipyrimidine hexahydrate

Yanni Ma, Le Zhou, Dongsheng Deng and Baoming Ji

S1. Comment

2,2′-Bipyrimidine and its derivatives have been used as the ligands in inorganic and organometallic chemistry (Ji *et al.* 2000; Baumann *et al.* 1998). On the other hand, the investigations of hydrogen-bonded water clusters in compound have recently attracted a great deal of interest (Buck *et al.* 2000; Lakshminarayanan *et al.* 2006). These studies can provided clues to understand the nature of water-water interactions in bulk water or ice (Zhang *et al.* 2005). In view of the importance of these compound, we herein report the synthesis and crystal structure of the title compound.

The molecule of the title compound (Fig. 1.), is built up form one pyrimidine ring connected to the other pyrimidine ring through the 2 and 2′ carbon atoms, in which the bond lengths and angles are within ranges as reported by Berg *et al.* (2002). In the crystal structure, the four substituent methyl groups lie in the corresponding pyrimidine ring plane, respectively. And, the dihedral angle between the two pyrimidine rings is 5.285 (6)°. It must be pointed out that the striking feature of the title compound is the interesting arrangement of the six water molecules, which connected each other by the formation of intermolecular O—H···O hydrogen bonds, generating the edge-fused four-, five-, or six-membered ring motifs, to form a two-dimensional sheet (Fig.2.). Interestingly, every water O atom in the sheet is tri-coordination, which unlike the water at the surface of ice or in liquid water shows four coordination. Furthermore, the sheets are anchored in four nitrogen atoms of the titlelte molecule by the formation of O—H···N hydrogen bonds, resulting in a three-dimensional network, in which these hydrogen bonding interactions, with O—H···O hydrogen bonds may be effective in the stabilization of the crystal packing. Detail hydrogen bonds are given in Table 1.

S2. Experimental

The title compound was prepared according to the reported Ullmann coupling method (Vlad & Horvath, 2002). Under nitrogen-protected, 4,6-dimethyl-2-iodopyrimidine (351 mg, 1.5 mmol), absolute DMF (2.0 ml) and activated copper powder (508 mg, 8.0 mmol) were placed in a 25 ml flask. The reaction mixture was heated to 358 K with vigorous stirring. After 4 h, 127 mg (2 mmol) of activated copper powder was added to the mixture. After another 3.5 h, the temperature was increased to 398 K and the stirring was continued for 2 h. The suspension was then cooled to 273 K, carefully drowned into a solution of 1.4 g potassium cyanide in 6 ml of 25% aqueous solution of ammonia, and filtered. The solid residue on the filter was extracted with the same amount of cyanide solution and filtered again. The combined filtrates were treated with 58 mg of potassium cyanide and extracted with chloroform (5 times 20 ml). Washed with water and dried. Recrystallization of the crude product from ethyl acetate-petroleum ether gave 81 mg. The crystalline compound was luckily obtained by the reaction of the title compound with $NdCl_3$ under the hydrothermal condition.

S3. Refinement

All H atoms were positioned geometrically and treated as riding, with C—H bond lengths constrained to 0.93 Å (aromatic CH), 0.96 Å (methyl CH_3), and 0.83 or 0.84 Å (OH), and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methylene C or

OH).

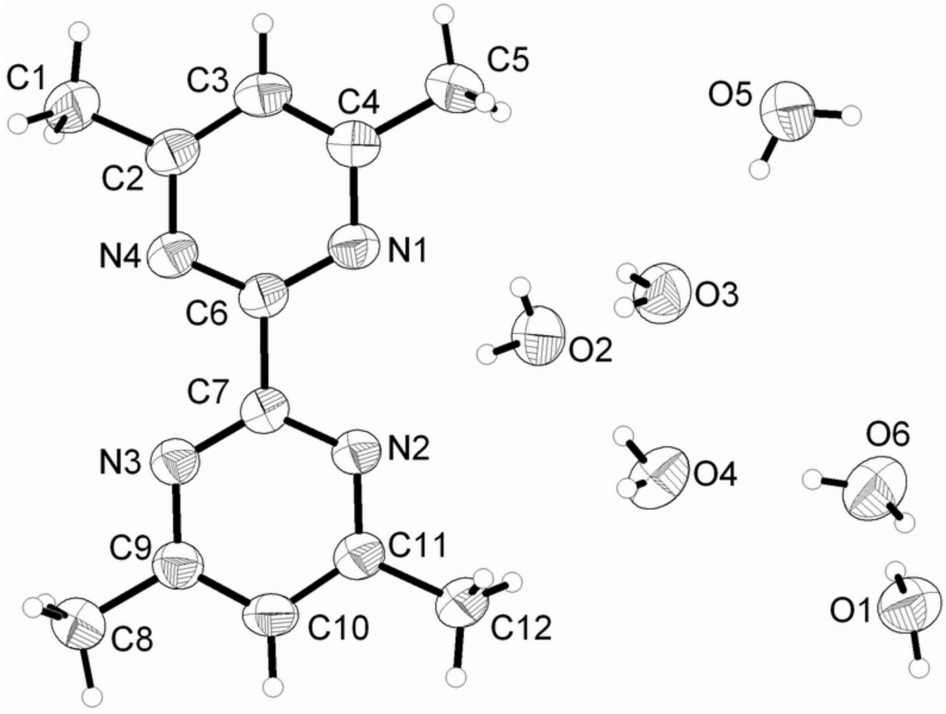

Figure 1

View of the title molecular structure with atom numbering scheme and 30% probability displacement ellipsoids for non-hydrogen atoms.

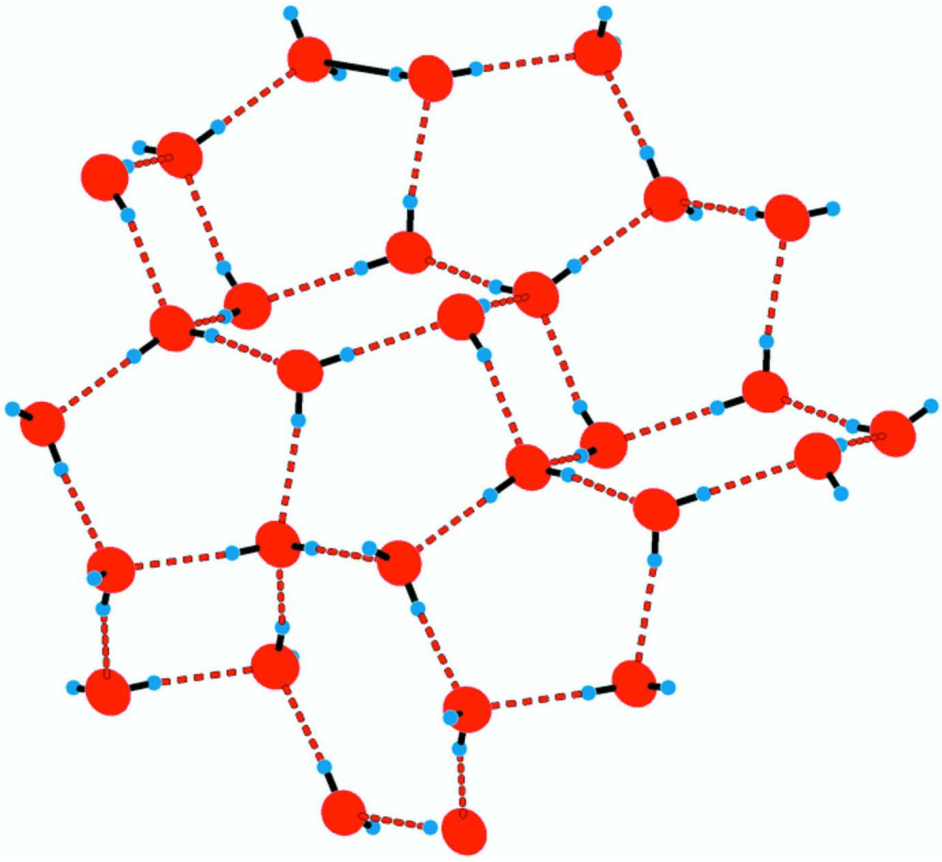

Figure 2

View of the two-dimensional sheet constructed by the lattice water molecules (O—H···O hydrogen bonds are represented as dashed lines).

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Crystal data

$C_{12}H_{14}N_4 \cdot 6H_2O$
$M_r = 322.37$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.8622\ (19)$ Å
$b = 11.098\ (3)$ Å
$c = 11.750\ (3)$ Å
$\alpha = 98.233\ (3)°$
$\beta = 91.774\ (4)°$
$\gamma = 102.599\ (4)°$
$V = 862.4\ (4)$ Å^3
$Z = 2$
$F(000) = 348$
$D_x = 1.241$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1270 reflections
$\theta = 1.0–1.0°$
$\mu = 0.10$ mm^{-1}
$T = 296$ K
Block, colourless
0.41 × 0.31 × 0.21 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.961$, $T_{max} = 0.980$
6492 measured reflections
3196 independent reflections
2026 reflections with $I > 2\sigma(I)$

R_{int} = 0.023
θ_{max} = 25.5°, θ_{min} = 2.4°
h = −8→8
k = −13→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.148
S = 1.04
3196 reflections
204 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.074P)^2 + 0.0388P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXS97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.045 (6)

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}
O1	1.0078 (2)	0.66049 (15)	0.38126 (13)	0.0642 (5)
H1W	0.9576	0.6341	0.3142	0.096*
H2W	0.9194	0.6501	0.4285	0.096*
O2	0.4638 (2)	0.32153 (14)	0.82784 (13)	0.0576 (5)
H3W	0.3978	0.2491	0.8284	0.086*
H4W	0.5591	0.3379	0.8787	0.086*
O3	0.1279 (3)	0.42962 (14)	0.85957 (13)	0.0620 (5)
H5W	0.0432	0.3909	0.8985	0.093*
H6W	0.2226	0.3952	0.8493	0.093*
O4	0.6255 (3)	0.40256 (16)	0.62491 (14)	0.0672 (5)
H7W	0.5777	0.3790	0.6846	0.101*
H8W	0.7336	0.3788	0.6155	0.101*
O5	0.2031 (2)	0.66114 (14)	1.01180 (14)	0.0624 (5)
H9W	0.2119	0.7281	0.9869	0.094*
H10W	0.1897	0.6013	0.9586	0.094*
O6	0.7043 (3)	0.63916 (16)	0.54052 (14)	0.0705 (5)

H11W	0.6024	0.6411	0.5015	0.106*
H12W	0.6844	0.5744	0.5710	0.106*
N1	0.2840 (3)	0.14305 (16)	0.99505 (14)	0.0417 (4)
N2	0.2855 (3)	0.04691 (15)	0.77127 (13)	0.0417 (4)
N3	0.2336 (2)	−0.15832 (15)	0.82104 (14)	0.0403 (4)
N4	0.2327 (2)	−0.06158 (15)	1.04606 (14)	0.0407 (4)
C1	0.1870 (4)	−0.1038 (2)	1.24073 (18)	0.0559 (6)
H1A	0.0530	−0.1535	1.2264	0.084*
H1B	0.2033	−0.0587	1.3178	0.084*
H1C	0.2801	−0.1572	1.2319	0.084*
C2	0.2256 (3)	−0.0134 (2)	1.15686 (17)	0.0414 (5)
C3	0.2480 (3)	0.1139 (2)	1.18979 (17)	0.0452 (5)
H3	0.2434	0.1471	1.2667	0.054*
C4	0.2775 (3)	0.19090 (19)	1.10592 (17)	0.0432 (5)
C5	0.3011 (4)	0.3293 (2)	1.1331 (2)	0.0632 (7)
H5A	0.4190	0.3704	1.1002	0.095*
H5B	0.3133	0.3543	1.2152	0.095*
H5C	0.1861	0.3522	1.1015	0.095*
C6	0.2612 (3)	0.01975 (18)	0.97125 (16)	0.0365 (5)
C7	0.2621 (3)	−0.03399 (18)	0.84670 (16)	0.0363 (5)
C8	0.1946 (4)	−0.3443 (2)	0.6791 (2)	0.0617 (7)
H8A	0.3139	−0.3691	0.7017	0.093*
H8B	0.1661	−0.3685	0.5975	0.093*
H8C	0.0846	−0.3845	0.7189	0.093*
C9	0.2245 (3)	−0.20604 (19)	0.70895 (17)	0.0432 (5)
C10	0.2398 (3)	−0.1290 (2)	0.62551 (18)	0.0496 (6)
H10	0.2286	−0.1625	0.5477	0.060*
C11	0.2719 (3)	−0.00161 (19)	0.65939 (17)	0.0449 (5)
C12	0.2935 (4)	0.0891 (2)	0.57525 (19)	0.0644 (7)
H12A	0.1977	0.1402	0.5887	0.097*
H12B	0.2705	0.0442	0.4982	0.097*
H12C	0.4262	0.1413	0.5849	0.097*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0689 (12)	0.0708 (11)	0.0513 (10)	0.0119 (9)	0.0050 (8)	0.0098 (8)
O2	0.0637 (11)	0.0499 (9)	0.0589 (10)	0.0082 (8)	0.0062 (8)	0.0138 (8)
O3	0.0686 (11)	0.0632 (11)	0.0583 (10)	0.0187 (8)	0.0111 (8)	0.0151 (8)
O4	0.0691 (12)	0.0825 (12)	0.0556 (10)	0.0191 (9)	0.0074 (8)	0.0251 (9)
O5	0.0743 (12)	0.0495 (9)	0.0617 (10)	0.0089 (8)	0.0045 (9)	0.0101 (8)
O6	0.0698 (12)	0.0794 (12)	0.0626 (11)	0.0096 (9)	0.0030 (9)	0.0231 (9)
N1	0.0440 (10)	0.0440 (10)	0.0355 (9)	0.0073 (8)	0.0036 (8)	0.0043 (8)
N2	0.0505 (11)	0.0413 (10)	0.0332 (9)	0.0100 (8)	0.0055 (8)	0.0052 (8)
N3	0.0430 (10)	0.0412 (10)	0.0365 (9)	0.0090 (8)	0.0047 (8)	0.0057 (8)
N4	0.0407 (10)	0.0472 (10)	0.0349 (9)	0.0105 (8)	0.0049 (7)	0.0076 (8)
C1	0.0706 (16)	0.0596 (15)	0.0415 (13)	0.0177 (12)	0.0136 (11)	0.0141 (11)
C2	0.0357 (11)	0.0537 (13)	0.0351 (11)	0.0096 (10)	0.0038 (9)	0.0082 (9)

C3	0.0448 (13)	0.0571 (14)	0.0328 (11)	0.0124 (10)	0.0058 (9)	0.0023 (10)
C4	0.0422 (12)	0.0469 (12)	0.0387 (12)	0.0091 (10)	0.0017 (9)	0.0021 (9)
C5	0.0879 (19)	0.0528 (15)	0.0461 (14)	0.0161 (13)	0.0047 (13)	−0.0024 (11)
C6	0.0326 (11)	0.0438 (12)	0.0330 (11)	0.0083 (9)	0.0031 (8)	0.0060 (9)
C7	0.0317 (10)	0.0417 (11)	0.0356 (11)	0.0079 (9)	0.0035 (8)	0.0067 (9)
C8	0.0899 (19)	0.0485 (14)	0.0475 (14)	0.0197 (13)	0.0058 (13)	0.0033 (11)
C9	0.0462 (13)	0.0427 (12)	0.0397 (12)	0.0088 (9)	0.0047 (9)	0.0044 (9)
C10	0.0640 (15)	0.0482 (13)	0.0322 (11)	0.0072 (11)	0.0025 (10)	0.0002 (10)
C11	0.0523 (13)	0.0462 (13)	0.0361 (11)	0.0098 (10)	0.0050 (10)	0.0078 (9)
C12	0.103 (2)	0.0525 (15)	0.0378 (13)	0.0139 (14)	0.0069 (13)	0.0121 (11)

Geometric parameters (Å, º)

O1—H1W	0.8358	C1—H1B	0.9600
O1—H2W	0.8355	C1—H1C	0.9600
O2—H3W	0.8334	C2—C3	1.383 (3)
O2—H4W	0.8431	C3—C4	1.386 (3)
O3—H5W	0.8342	C3—H3	0.9300
O3—H6W	0.8269	C4—C5	1.496 (3)
O4—H7W	0.8351	C5—H5A	0.9600
O4—H8W	0.8443	C5—H5B	0.9600
O5—H9W	0.8278	C5—H5C	0.9600
O5—H10W	0.8314	C6—C7	1.500 (3)
O6—H11W	0.8302	C8—C9	1.492 (3)
O6—H12W	0.8353	C8—H8A	0.9600
N1—C6	1.330 (2)	C8—H8B	0.9600
N1—C4	1.340 (3)	C8—H8C	0.9600
N2—C7	1.338 (2)	C9—C10	1.383 (3)
N2—C11	1.340 (3)	C10—C11	1.379 (3)
N3—C7	1.339 (2)	C10—H10	0.9300
N3—C9	1.341 (3)	C11—C12	1.498 (3)
N4—C6	1.337 (2)	C12—H12A	0.9600
N4—C2	1.341 (3)	C12—H12B	0.9600
C1—C2	1.493 (3)	C12—H12C	0.9600
C1—H1A	0.9600		

H1W—O1—H2W	110.2	H5A—C5—H5C	109.5
H3W—O2—H4W	109.0	H5B—C5—H5C	109.5
H5W—O3—H6W	111.2	N1—C6—N4	126.97 (18)
H7W—O4—H8W	108.4	N1—C6—C7	116.44 (17)
H9W—O5—H10W	111.6	N4—C6—C7	116.57 (18)
H11W—O6—H12W	109.9	N3—C7—N2	126.13 (18)
C6—N1—C4	116.54 (17)	N3—C7—C6	117.13 (17)
C7—N2—C11	116.80 (17)	N2—C7—C6	116.70 (17)
C7—N3—C9	116.70 (17)	C9—C8—H8A	109.5
C6—N4—C2	116.31 (18)	C9—C8—H8B	109.5
C2—C1—H1A	109.5	H8A—C8—H8B	109.5
C2—C1—H1B	109.5	C9—C8—H8C	109.5

H1A—C1—H1B	109.5	H8A—C8—H8C	109.5
C2—C1—H1C	109.5	H8B—C8—H8C	109.5
H1A—C1—H1C	109.5	N3—C9—C10	120.62 (19)
H1B—C1—H1C	109.5	N3—C9—C8	117.30 (18)
N4—C2—C3	120.80 (18)	C10—C9—C8	122.07 (19)
N4—C2—C1	116.81 (19)	C11—C10—C9	118.96 (19)
C3—C2—C1	122.37 (19)	C11—C10—H10	120.5
C2—C3—C4	118.69 (19)	C9—C10—H10	120.5
C2—C3—H3	120.7	N2—C11—C10	120.71 (18)
C4—C3—H3	120.7	N2—C11—C12	116.59 (19)
N1—C4—C3	120.68 (19)	C10—C11—C12	122.71 (19)
N1—C4—C5	116.81 (19)	C11—C12—H12A	109.5
C3—C4—C5	122.50 (19)	C11—C12—H12B	109.5
C4—C5—H5A	109.5	H12A—C12—H12B	109.5
C4—C5—H5B	109.5	C11—C12—H12C	109.5
H5A—C5—H5B	109.5	H12A—C12—H12C	109.5
C4—C5—H5C	109.5	H12B—C12—H12C	109.5
C6—N4—C2—C3	−0.3 (3)	C11—N2—C7—N3	2.5 (3)
C6—N4—C2—C1	178.04 (18)	C11—N2—C7—C6	−175.32 (18)
N4—C2—C3—C4	0.2 (3)	N1—C6—C7—N3	−178.13 (16)
C1—C2—C3—C4	−178.1 (2)	N4—C6—C7—N3	0.3 (3)
C6—N1—C4—C3	−0.1 (3)	N1—C6—C7—N2	−0.1 (3)
C6—N1—C4—C5	−179.45 (19)	N4—C6—C7—N2	178.33 (16)
C2—C3—C4—N1	0.1 (3)	C7—N3—C9—C10	−1.4 (3)
C2—C3—C4—C5	179.3 (2)	C7—N3—C9—C8	179.46 (19)
C4—N1—C6—N4	0.0 (3)	N3—C9—C10—C11	2.3 (3)
C4—N1—C6—C7	178.16 (17)	C8—C9—C10—C11	−178.5 (2)
C2—N4—C6—N1	0.3 (3)	C7—N2—C11—C10	−1.4 (3)
C2—N4—C6—C7	−177.94 (17)	C7—N2—C11—C12	178.63 (19)
C9—N3—C7—N2	−1.1 (3)	C9—C10—C11—N2	−0.9 (3)
C9—N3—C7—C6	176.71 (17)	C9—C10—C11—C12	179.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*W*···O3^{i}	0.84	2.08	2.914 (2)	172
O1—H2*W*···O6	0.84	2.00	2.837 (2)	175
O2—H3*W*···N2	0.83	2.20	2.995 (2)	158
O2—H3*W*···N1	0.83	2.49	3.083 (2)	129
O2—H4*W*···O5^{ii}	0.84	2.04	2.872 (2)	167
O3—H5*W*···O5^{iii}	0.83	2.04	2.847 (2)	163
O3—H6*W*···O2	0.83	2.01	2.832 (2)	177
O4—H7*W*···O2	0.84	2.01	2.841 (2)	180
O4—H8*W*···O1^{iv}	0.84	1.92	2.755 (2)	171
O5—H9*W*···N4^{v}	0.83	2.31	3.007 (2)	142
O5—H9*W*···N3^{v}	0.83	2.46	3.196 (2)	149
O5—H10*W*···O3	0.83	2.04	2.849 (2)	166

O6—H11*W*···O4^{i}	0.83	2.05	2.851 (2)	162
O6—H12*W*···O4	0.84	2.06	2.886 (2)	173

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