

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

4-[4,5-Bis(pyridin-2-yl)-1H-imidazol-2-yl]phenol monohydrate

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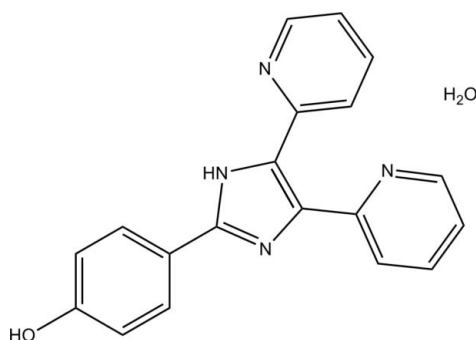
Received 11 December 2010; accepted 12 December 2010

 Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.038; wR factor = 0.109; data-to-parameter ratio = 11.5.

In the title hydrate, $\text{C}_{19}\text{H}_{14}\text{N}_4\text{O}\cdot\text{H}_2\text{O}$, the dihedral angle between the two pyridine rings is 38.0 (2)°. The dihedral angle between the imidazole and benzene rings is 25.3 (2)°. The crystal structure is stabilized by intermolecular $\text{O}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For early studies of lophine (2,4,5-triphenylimidazole), see: Radziszewsky (1877). For further synthetic details, see: Nakashima *et al.* (1995); Kuroda *et al.* (1993).



Experimental

Crystal data

 $\text{C}_{19}\text{H}_{14}\text{N}_4\text{O}\cdot\text{H}_2\text{O}$
 $M_r = 332.36$

 Triclinic, $P\bar{1}$
 $a = 8.5875$ (17) Å
 $b = 9.0151$ (18) Å
 $c = 11.353$ (2) Å
 $\alpha = 77.89$ (3)°
 $\beta = 69.96$ (3)°
 $\gamma = 73.66$ (3)°

 $V = 786.0$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 113$ K
 $0.22 \times 0.20 \times 0.16$ mm

Data collection

 Bruker SMART CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 1998)
 $T_{\min} = 0.980$, $T_{\max} = 0.985$

 5731 measured reflections
 2746 independent reflections
 2155 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.109$
 $S = 1.09$
 2746 reflections
 239 parameters
 4 restraints

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{O2}^{\text{i}}$	0.82	1.89	2.7003 (17)	171
$\text{O2}-\text{H2A}\cdots\text{N3}^{\text{ii}}$	0.88 (1)	1.91 (1)	2.7655 (16)	167 (2)
$\text{N2}-\text{H2C}\cdots\text{O2}^{\text{ii}}$	0.91 (1)	2.09 (1)	2.9715 (19)	164 (2)
$\text{O2}-\text{H2B}\cdots\text{N4}^{\text{iii}}$	0.87 (1)	1.99 (1)	2.8254 (17)	162 (2)

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

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); 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: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5769).

References

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 Nakashima, K., Yamasaki, H., Kuroda, N. & Akiyama, S. (1995). *Anal. Chim. Acta*, **303**, 103–107.
 Radziszewsky, B. (1877). *Chem. Ber.* **10**, 70–75.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2011). E67, o161 [https://doi.org/10.1107/S1600536810052062]

4-[4,5-Bis(pyridin-2-yl)-1*H*-imidazol-2-yl]phenol monohydrate**Guo-Yong Xiao, Hai-Jun Chi, Peng Lei, Jiang-Long Yu and Zhi-Zhi Hu****S1. Comment**

Lophine, 2,4,5-triphenylimidazole, is a well known potential chemiluminescent (CL) compound (Radziszewsky, 1877). 2-(4-Hydroxyphenyl)-4,5-di(2-pyridyl)imidazole was synthesized by the methods similar to those previously reported (Nakashima *et al.*, 1995; Kuroda *et al.*, 1993). Recently, we have synthesized an analogic structure of imidazole derivative, namely, the title compound, 2-(4-hydroxyphenyl)-4,5-di(2-pyridyl)imidazole. We present its crystal structure here.

The compound consists of a 2-(4-hydroxyphenyl)-4,5-di(2-pyridyl)imidazole molecule and a water molecule of crystallization (Fig. 1). The central imidazole ring forms dihedral angles of 25.3 (2), 22.5 (2), and 29.2 (2)°, respectively, with the C1—C6 benzene ring, C9—C13/N3 pyridine ring, and C15—C19/N4 pyridine ring. The dihedral angle between the two pyridine rings is 38.0 (2)°. The dihedral angle between the central imidazole ring and the benzene ring is 25.3 (2)°. The crystal structure is stabilized by intermolecular O—H···O, O—H···N, and N—H···O hydrogen bonds (Fig. 2, and Table 1).

S2. Experimental

The title compound was prepared by the reaction of 2, 2'-pyridyl (1.0 mmol), 4-hydroxybenzaldehyde (1.0 mmol) and ammonium acetate (10 mmol) in 8 ml acetic acid refluxed for 6 h. After cooling to room temperature, the mixture was poured into water, the precipitate was filtered off and dried to give the target compound in 20% yield. Colourless prisms of the title compound were grown by slow evaporation of a solution in methanol.

S3. Refinement

H2A, H2B, and H2C atoms were located in a difference Fourier map, with N—H, O—H and H···H distances restrained to 0.90 (1), 0.85 (1), and 1.45 (2) Å, respectively. The remaining H atoms were placed in calculated positions (C—H = 0.93 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

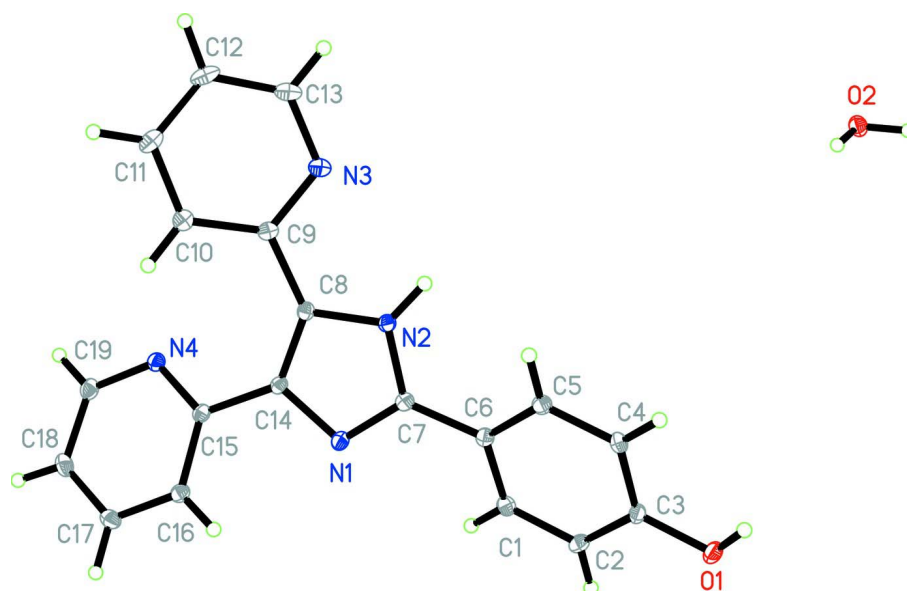


Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids for the non-hydrogen atoms.

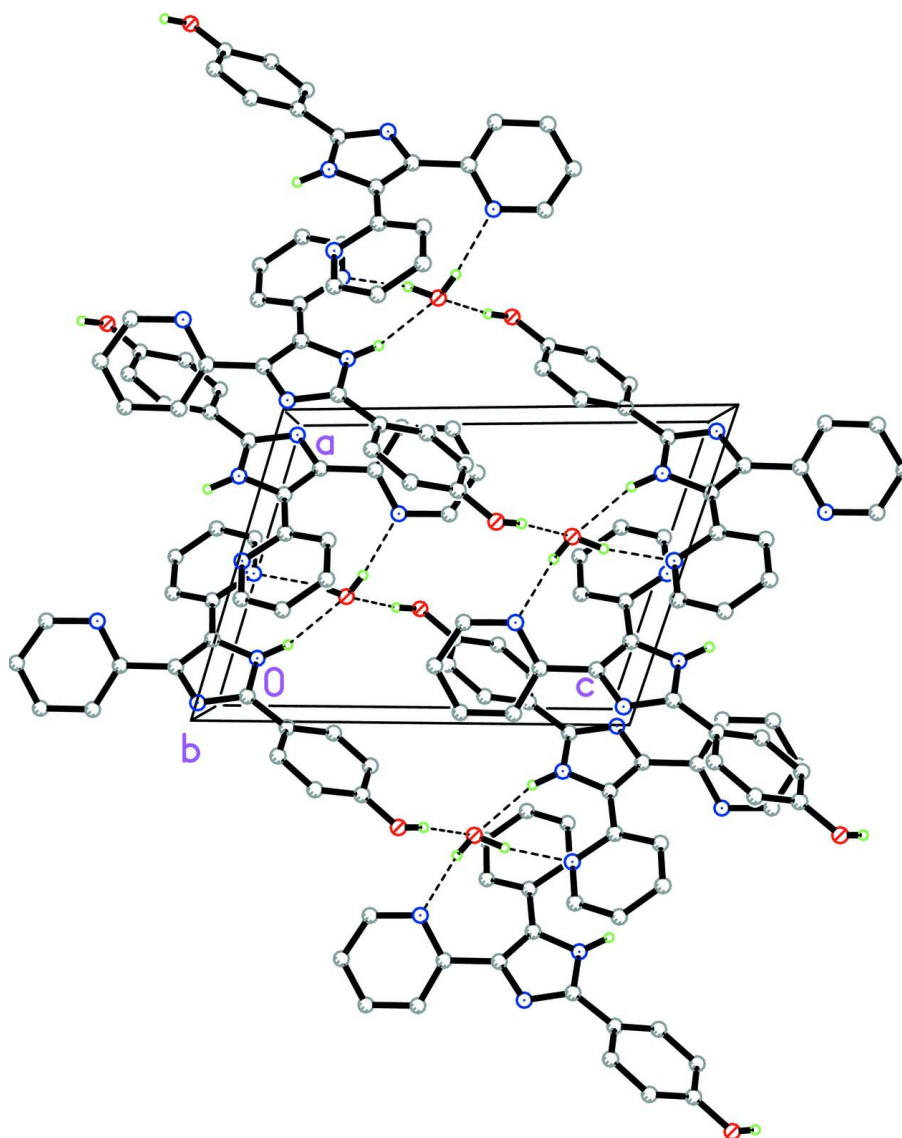


Figure 2

The packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

4-[4,5-Bis(pyridin-2-yl)-1H-imidazol-2-yl]phenol monohydrate

Crystal data

$C_{19}H_{14}N_4O \cdot H_2O$

$M_r = 332.36$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.5875$ (17) Å

$b = 9.0151$ (18) Å

$c = 11.353$ (2) Å

$\alpha = 77.89$ (3)°

$\beta = 69.96$ (3)°

$\gamma = 73.66$ (3)°

$V = 786.0$ (3) Å³

$Z = 2$

$F(000) = 348$

$D_x = 1.404$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2376 reflections

$\theta = 2.6$ – 27.9 °

$\mu = 0.10$ mm⁻¹

$T = 113$ K

Prism, colourless

$0.22 \times 0.20 \times 0.16$ mm

Data collection

Bruker SMART CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 1998)
 $T_{\min} = 0.980$, $T_{\max} = 0.985$

5731 measured reflections
2746 independent reflections
2155 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.6^\circ$
 $h = -10 \rightarrow 10$
 $k = -10 \rightarrow 10$
 $l = -13 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.109$
 $S = 1.09$
2746 reflections
239 parameters
4 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
 $w = 1/[\sigma^2(F_o^2) + (0.0736P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	1.35444 (13)	0.11009 (12)	0.44275 (9)	0.0221 (3)
H1	1.3597	0.1807	0.3838	0.033*
N1	0.95455 (15)	0.27226 (13)	1.01220 (10)	0.0162 (3)
N2	0.80962 (15)	0.46738 (13)	0.90993 (10)	0.0152 (3)
N3	0.52123 (15)	0.70299 (13)	0.99216 (10)	0.0187 (3)
N4	0.68226 (15)	0.36680 (13)	1.32116 (10)	0.0175 (3)
C1	1.12180 (18)	0.11950 (15)	0.77615 (12)	0.0175 (3)
H1A	1.1067	0.0502	0.8503	0.021*
C2	1.22861 (18)	0.06627 (16)	0.66424 (12)	0.0179 (3)
H2	1.2854	-0.0381	0.6633	0.022*
C3	1.25179 (18)	0.16872 (16)	0.55213 (12)	0.0160 (3)
C4	1.16603 (18)	0.32453 (16)	0.55465 (12)	0.0173 (3)
H4	1.1808	0.3935	0.4804	0.021*
C5	1.05921 (18)	0.37679 (16)	0.66722 (12)	0.0174 (3)
H5	1.0018	0.4810	0.6679	0.021*

C6	1.03582 (17)	0.27565 (15)	0.78036 (12)	0.0155 (3)
C7	0.93382 (17)	0.33457 (15)	0.90045 (12)	0.0154 (3)
C8	0.74579 (17)	0.49413 (15)	1.03485 (12)	0.0144 (3)
C9	0.61392 (17)	0.63503 (15)	1.07191 (12)	0.0153 (3)
C10	0.58923 (18)	0.69920 (15)	1.18034 (13)	0.0187 (3)
H10	0.6575	0.6535	1.2325	0.022*
C11	0.46215 (19)	0.83145 (16)	1.20923 (14)	0.0232 (3)
H11	0.4441	0.8763	1.2809	0.028*
C12	0.3623 (2)	0.89615 (17)	1.13019 (15)	0.0272 (4)
H12	0.2730	0.9828	1.1493	0.033*
C13	0.39737 (19)	0.83010 (16)	1.02306 (14)	0.0244 (4)
H13	0.3318	0.8759	0.9689	0.029*
C14	0.83707 (18)	0.37066 (15)	1.09693 (12)	0.0145 (3)
C15	0.83185 (18)	0.32729 (15)	1.23068 (12)	0.0151 (3)
C16	0.97916 (18)	0.24099 (15)	1.25986 (12)	0.0174 (3)
H16	1.0801	0.2143	1.1956	0.021*
C17	0.97453 (19)	0.19538 (16)	1.38436 (13)	0.0203 (3)
H17	1.0713	0.1362	1.4053	0.024*
C18	0.8229 (2)	0.23941 (16)	1.47772 (13)	0.0220 (3)
H18	0.8166	0.2130	1.5627	0.026*
C19	0.68134 (19)	0.32344 (16)	1.44204 (12)	0.0202 (3)
H19	0.5796	0.3516	1.5053	0.024*
O2	0.39964 (13)	0.34896 (12)	0.25546 (9)	0.0233 (3)
H2A	0.439 (2)	0.337 (3)	0.1750 (10)	0.068 (7)*
H2B	0.473 (2)	0.374 (2)	0.2803 (15)	0.066 (7)*
H2C	0.764 (2)	0.5192 (18)	0.8472 (12)	0.042 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0213 (6)	0.0233 (6)	0.0160 (5)	-0.0012 (4)	-0.0004 (4)	-0.0043 (4)
N1	0.0174 (7)	0.0154 (6)	0.0144 (6)	-0.0033 (5)	-0.0028 (5)	-0.0028 (5)
N2	0.0153 (7)	0.0152 (6)	0.0131 (6)	-0.0023 (5)	-0.0035 (5)	-0.0010 (5)
N3	0.0157 (7)	0.0175 (6)	0.0214 (6)	-0.0030 (5)	-0.0060 (5)	0.0004 (5)
N4	0.0180 (7)	0.0177 (6)	0.0151 (6)	-0.0027 (5)	-0.0039 (5)	-0.0027 (5)
C1	0.0196 (8)	0.0167 (7)	0.0160 (7)	-0.0056 (6)	-0.0056 (6)	0.0006 (6)
C2	0.0164 (8)	0.0150 (7)	0.0215 (7)	-0.0023 (6)	-0.0038 (6)	-0.0054 (6)
C3	0.0141 (7)	0.0204 (7)	0.0141 (7)	-0.0045 (6)	-0.0026 (6)	-0.0057 (6)
C4	0.0207 (8)	0.0189 (7)	0.0128 (7)	-0.0061 (6)	-0.0059 (6)	0.0006 (5)
C5	0.0199 (8)	0.0139 (7)	0.0184 (7)	-0.0025 (6)	-0.0065 (6)	-0.0028 (5)
C6	0.0141 (7)	0.0177 (7)	0.0159 (7)	-0.0057 (6)	-0.0041 (6)	-0.0027 (6)
C7	0.0154 (8)	0.0142 (7)	0.0166 (7)	-0.0041 (6)	-0.0038 (6)	-0.0024 (6)
C8	0.0140 (7)	0.0158 (7)	0.0131 (7)	-0.0050 (6)	-0.0021 (6)	-0.0022 (5)
C9	0.0130 (7)	0.0142 (7)	0.0168 (7)	-0.0053 (6)	-0.0016 (6)	0.0003 (5)
C10	0.0184 (8)	0.0184 (7)	0.0185 (7)	-0.0061 (6)	-0.0036 (6)	-0.0011 (6)
C11	0.0230 (8)	0.0176 (7)	0.0245 (8)	-0.0049 (6)	0.0009 (6)	-0.0063 (6)
C12	0.0187 (8)	0.0173 (7)	0.0375 (9)	0.0024 (6)	-0.0018 (7)	-0.0064 (7)
C13	0.0180 (8)	0.0203 (8)	0.0317 (8)	-0.0009 (6)	-0.0092 (7)	0.0015 (6)

C14	0.0129 (7)	0.0150 (7)	0.0150 (7)	-0.0034 (5)	-0.0025 (6)	-0.0034 (5)
C15	0.0171 (8)	0.0119 (7)	0.0166 (7)	-0.0039 (5)	-0.0045 (6)	-0.0030 (5)
C16	0.0179 (8)	0.0145 (7)	0.0193 (7)	-0.0030 (6)	-0.0048 (6)	-0.0036 (6)
C17	0.0230 (8)	0.0166 (7)	0.0245 (8)	-0.0040 (6)	-0.0129 (7)	-0.0004 (6)
C18	0.0304 (9)	0.0217 (8)	0.0168 (7)	-0.0085 (7)	-0.0104 (7)	0.0005 (6)
C19	0.0230 (9)	0.0208 (8)	0.0145 (7)	-0.0053 (6)	-0.0024 (6)	-0.0022 (6)
O2	0.0195 (6)	0.0314 (6)	0.0179 (6)	-0.0060 (5)	-0.0058 (4)	-0.0005 (5)

Geometric parameters (Å, °)

O1—C3	1.3644 (17)	C8—C14	1.382 (2)
O1—H1	0.8200	C8—C9	1.4702 (19)
N1—C7	1.3252 (17)	C9—C10	1.3950 (19)
N1—C14	1.3854 (18)	C10—C11	1.381 (2)
N2—C7	1.3563 (18)	C10—H10	0.9300
N2—C8	1.3807 (16)	C11—C12	1.381 (2)
N2—H2C	0.908 (9)	C11—H11	0.9300
N3—C13	1.3397 (19)	C12—C13	1.370 (2)
N3—C9	1.3473 (18)	C12—H12	0.9300
N4—C19	1.3436 (17)	C13—H13	0.9300
N4—C15	1.3505 (18)	C14—C15	1.4747 (18)
C1—C2	1.3767 (19)	C15—C16	1.393 (2)
C1—C6	1.3958 (19)	C16—C17	1.3767 (18)
C1—H1A	0.9300	C16—H16	0.9300
C2—C3	1.3961 (19)	C17—C18	1.384 (2)
C2—H2	0.9300	C17—H17	0.9300
C3—C4	1.392 (2)	C18—C19	1.381 (2)
C4—C5	1.3794 (19)	C18—H18	0.9300
C4—H4	0.9300	C19—H19	0.9300
C5—C6	1.3986 (19)	O2—H2A	0.876 (9)
C5—H5	0.9300	O2—H2B	0.870 (9)
C6—C7	1.4601 (18)		
C3—O1—H1	109.5	C10—C9—C8	122.56 (12)
C7—N1—C14	105.45 (12)	C11—C10—C9	119.19 (14)
C7—N2—C8	108.44 (11)	C11—C10—H10	120.4
C7—N2—H2C	124.9 (11)	C9—C10—H10	120.4
C8—N2—H2C	125.9 (11)	C10—C11—C12	119.02 (14)
C13—N3—C9	118.20 (12)	C10—C11—H11	120.5
C19—N4—C15	117.30 (12)	C12—C11—H11	120.5
C2—C1—C6	121.15 (13)	C13—C12—C11	118.64 (14)
C2—C1—H1A	119.4	C13—C12—H12	120.7
C6—C1—H1A	119.4	C11—C12—H12	120.7
C1—C2—C3	120.07 (13)	N3—C13—C12	123.43 (14)
C1—C2—H2	120.0	N3—C13—H13	118.3
C3—C2—H2	120.0	C12—C13—H13	118.3
O1—C3—C4	122.37 (12)	C8—C14—N1	110.41 (12)
O1—C3—C2	118.14 (12)	C8—C14—C15	132.74 (13)

C4—C3—C2	119.45 (13)	N1—C14—C15	116.85 (12)
C5—C4—C3	120.07 (12)	N4—C15—C16	122.02 (12)
C5—C4—H4	120.0	N4—C15—C14	118.81 (13)
C3—C4—H4	120.0	C16—C15—C14	119.11 (13)
C4—C5—C6	121.06 (13)	C17—C16—C15	119.66 (14)
C4—C5—H5	119.5	C17—C16—H16	120.2
C6—C5—H5	119.5	C15—C16—H16	120.2
C1—C6—C5	118.19 (12)	C16—C17—C18	118.66 (14)
C1—C6—C7	121.05 (12)	C16—C17—H17	120.7
C5—C6—C7	120.62 (12)	C18—C17—H17	120.7
N1—C7—N2	111.15 (12)	C19—C18—C17	118.60 (13)
N1—C7—C6	125.50 (13)	C19—C18—H18	120.7
N2—C7—C6	123.27 (12)	C17—C18—H18	120.7
N2—C8—C14	104.55 (12)	N4—C19—C18	123.71 (13)
N2—C8—C9	120.20 (11)	N4—C19—H19	118.1
C14—C8—C9	135.20 (12)	C18—C19—H19	118.1
N3—C9—C10	121.40 (13)	H2A—O2—H2B	111.3 (13)
N3—C9—C8	116.00 (11)		
C6—C1—C2—C3	-0.4 (2)	C14—C8—C9—C10	21.5 (2)
C1—C2—C3—O1	-177.92 (12)	N3—C9—C10—C11	2.8 (2)
C1—C2—C3—C4	-0.1 (2)	C8—C9—C10—C11	-179.71 (12)
O1—C3—C4—C5	177.80 (12)	C9—C10—C11—C12	0.3 (2)
C2—C3—C4—C5	0.0 (2)	C10—C11—C12—C13	-2.5 (2)
C3—C4—C5—C6	0.4 (2)	C9—N3—C13—C12	1.3 (2)
C2—C1—C6—C5	0.8 (2)	C11—C12—C13—N3	1.8 (2)
C2—C1—C6—C7	-174.87 (12)	N2—C8—C14—N1	0.65 (14)
C4—C5—C6—C1	-0.9 (2)	C9—C8—C14—N1	-176.67 (13)
C4—C5—C6—C7	174.85 (12)	N2—C8—C14—C15	-179.37 (13)
C14—N1—C7—N2	0.11 (14)	C9—C8—C14—C15	3.3 (3)
C14—N1—C7—C6	176.81 (12)	C7—N1—C14—C8	-0.48 (14)
C8—N2—C7—N1	0.29 (15)	C7—N1—C14—C15	179.53 (11)
C8—N2—C7—C6	-176.50 (11)	C19—N4—C15—C16	1.93 (18)
C1—C6—C7—N1	24.1 (2)	C19—N4—C15—C14	179.00 (11)
C5—C6—C7—N1	-151.45 (13)	C8—C14—C15—N4	30.9 (2)
C1—C6—C7—N2	-159.53 (12)	N1—C14—C15—N4	-149.14 (12)
C5—C6—C7—N2	24.87 (19)	C8—C14—C15—C16	-151.97 (15)
C7—N2—C8—C14	-0.56 (14)	N1—C14—C15—C16	28.01 (17)
C7—N2—C8—C9	177.25 (11)	N4—C15—C16—C17	-0.8 (2)
C13—N3—C9—C10	-3.58 (19)	C14—C15—C16—C17	-177.87 (11)
C13—N3—C9—C8	178.78 (11)	C15—C16—C17—C18	-1.13 (19)
N2—C8—C9—N3	22.10 (17)	C16—C17—C18—C19	1.86 (19)
C14—C8—C9—N3	-160.90 (14)	C15—N4—C19—C18	-1.17 (19)
N2—C8—C9—C10	-155.51 (12)	C17—C18—C19—N4	-0.7 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1···O2 ⁱ	0.82	1.89	2.7003 (17)	171
O2—H2A···N3 ⁱⁱ	0.88 (1)	1.91 (1)	2.7655 (16)	167 (2)
N2—H2C···O2 ⁱⁱ	0.91 (1)	2.09 (1)	2.9715 (19)	164 (2)
O2—H2B···N4 ⁱⁱⁱ	0.87 (1)	1.99 (1)	2.8254 (17)	162 (2)

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