Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4-Benzyl-6-bromo-2-(4-methoxyphenyl)-4*H*-imidazo[4,5-*b*]pyridine monohydrate

**Y. Ouzidan,[a] Y. Kandri Rodi,[b] S. Obbade,[b] El Mokhtar Essassi[c] and Seik Weng Ng[d]***

[a]Laboratoire de Chimie Organique Appliquée, Faculté des Sciences et Techniques, Université Sidi Mohamed Ben Abdallah, Fés, Morocco, [b]Laboratoire d'Electrochimie et de Physicochimie des Matériaux et des Interfaces, A313 Domaine Universitaire, 38402 St Martin d'Hères, Grenoble, France, [c]Laboratoire de Chimie Organique Hétérocyclique, Pôle de Compétences Pharmacochimie, Université Mohammed V-Agdal, BP 1014 Avenue Ibn Batout, Rabat, Morocco, and [d]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

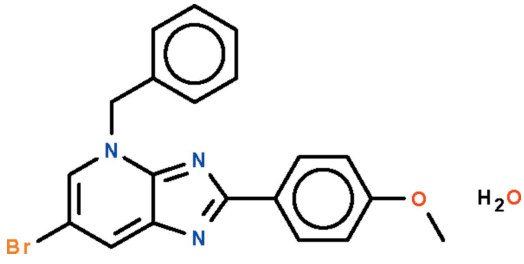
Received 11 March 2010; accepted 19 March 2010

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.035; $wR$ factor = 0.098; data-to-parameter ratio = 21.2.

The imidazopyridine fused ring in the title compound, $C_{20}H_{16}BrN_3O\cdot H_2O$, is coplanar with the aromatic ring at the 2-position [dihedral angle = 5.2 (1)°]. In the five-membered imidazo portion, the C—N bond whose C atom is also connected to the pyridine N atom has predominantly double-bond character [1.334 (2) Å] whereas the C—N bond whose atom is connected to the pyridine C atom has predominantly single-bond character [1.371 (2) Å]. The water molecule engages in hydrogen bonding with the latter N atom; it is also connected to a symmetry-related water molecule, generating a linear chain structure.

## Related literature

For the crystal structure of 4-benzyl-6-bromo-2-phenyl-4*H*-imidazo[4,5-*b*]pyridine, see: Ouzidan *et al.* (2010).




## Experimental

### Crystal data

$C_{20}H_{16}BrN_3O\cdot H_2O$
$M_r$ = 412.28
Monoclinic, $P2_1/c$
$a$ = 10.5924 (2) Å
$b$ = 5.4544 (1) Å
$c$ = 31.7444 (7) Å
$\beta$ = 100.292 (1)°
$V$ = 1804.53 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.30 mm$^{-1}$
$T$ = 293 K
0.29 × 0.13 × 0.09 mm

### Data collection

Bruker X8 APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.556, $T_{max}$ = 0.820
25327 measured reflections
5183 independent reflections
3751 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.098
$S$ = 1.02
5183 reflections
244 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1w—H11···N2 | 0.85 (1) | 2.30 (2) | 3.092 (3) | 155 (5) |
| O1w—H12···O1$W^{i}$ | 0.85 (1) | 2.30 (2) | 3.119 (2) | 162 (5) |

Symmetry code: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Université Sidi Mohammed Ben Abdallah, Université Mohammed V-Agdal and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2233).

## References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ouzidan, Y., Obbade, S., Capet, F., Essassi, E. M. & Ng, S. W. (2010). *Acta Cryst.* E**66**, o947.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *publCIF*. In preparation.

# supporting information

*Acta Cryst.* (2010). E**66**, o947 [doi:10.1107/S1600536810010391]

# 4-Benzyl-6-bromo-2-(4-methoxyphenyl)-4*H*-imidazo[4,5-*b*]pyridine monohydrate

**Y. Ouzidan, Y. Kandri Rodi, S. Obbade, El Mokhtar Essassi and Seik Weng Ng**

## S1. Comment

Imidazo[4,5-*b*]pyridines are a class of sedative drugs. In the previous study, we reacted 6-bromo-2-phenyl-1*H*-imidazo[4,5-*b*]pyridine with benzyl chloride in the presence of a catalytic quantity of tetra-*n*-butylammonium bromide under mild conditions to form 4-benzyl-6-bromo-2-phenyl-4*H*-imidazo[4,5-*b*]pyridine (Ouzidan *et al.*, 2010). The study is extended to the synthesis of the 2(4-methoxyphenyl) analog to furnish the title hydrate (Scheme I, Fig. 1). The imidazopyridine fused-ring in the $C_{20}H_{16}BrN_3O$ molecule is co-planar with the aromatic ring at the 2-position [dihedral angle 5.2 (1) °]. In the five-membered imidazo portion, the carbon–nitrogen bond whose carbon atom is also connected to the pyridine nitrogen atom is a double bond [1.334 (2) Å] whereas the carbon–nitrogen bond whose atom is connected to the pyridine carbon atom is a single bond [1.371 (2) Å]. The water molecule engages in hydrogen bonding with the latter nitrogen atom; it is also connected to a symmetry-related water molecule to generate a linear chain structure.

## S2. Experimental

To a solution of the 6-bromo-2-(4-methoxyphenyl)-1*H*-imidazo[4,5-*b*]pyridine (0.33 g, 1.21 mmol), potassium carbonate (0.20 g, 1.42 mmol) and tetra-*n*-butylammonium bromide (0.04 g (0,1 mmol) in DMF (15 ml) was added benzyl chloride (0.15 ml, 1.31 mmol). Stirring was continued at room temperature for 12 hours. The salt was removed by filtration and the filtrate concentrated under reduced pressure. The residue was chromatographed on a column of silica gel with ethyl acetate/hexane (1/1) as eluent. Yellow crystals were isolated when the solvent was allowed to evaporate.

## S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C). The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H 0.84 (1) Å.

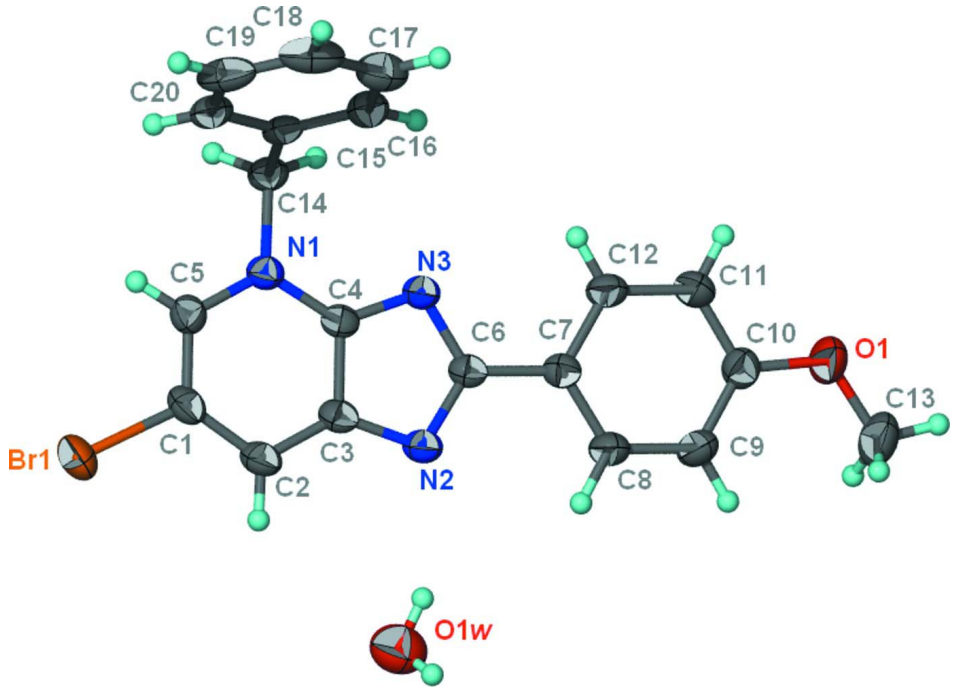



**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of $C_{20}H_{16}BrN_3O\cdot H_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

**4-Benzyl-6-bromo-2-(4-methoxyphenyl)-4*H*-imidazo[4,5-*b*]pyridine monohydrate**

*Crystal data*

$C_{20}H_{16}BrN_3O\cdot H_2O$
$M_r = 412.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.5924\ (2)$ Å
$b = 5.4544\ (1)$ Å
$c = 31.7444\ (7)$ Å
$\beta = 100.292\ (1)°$
$V = 1804.53\ (6)$ Å$^3$
$Z = 4$
$F(000) = 840$
$D_x = 1.518$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6654 reflections
$\theta = 3.0–28.2°$
$\mu = 2.30$ mm$^{-1}$
$T = 293$ K
Prism, yellow
0.29 × 0.13 × 0.09 mm

*Data collection*

Bruker X8 APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.556$, $T_{max} = 0.820$
25327 measured reflections
5183 independent reflections
3751 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 29.8°$, $\theta_{min} = 3.0°$
$h = -14\rightarrow14$
$k = -7\rightarrow7$
$l = -40\rightarrow44$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.098$
$S = 1.02$
5183 reflections
244 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.4879P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{min} = -0.38$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.33516 (2) | 0.25313 (4) | 0.229786 (7) | 0.06505 (10) |
| O1W | 0.0347 (2) | 1.0524 (4) | 0.27301 (7) | 0.0809 (5) |
| H11 | 0.091 (3) | 1.063 (10) | 0.2955 (9) | 0.18 (2)* |
| H12 | 0.032 (5) | 1.199 (4) | 0.2641 (17) | 0.16 (2)* |
| N1 | 0.49030 (13) | 0.4485 (3) | 0.35254 (4) | 0.0370 (3) |
| N2 | 0.25772 (13) | 0.9195 (3) | 0.34637 (4) | 0.0397 (3) |
| N3 | 0.43173 (14) | 0.7798 (2) | 0.39573 (5) | 0.0368 (3) |
| O1 | 0.24437 (17) | 1.6309 (3) | 0.50907 (5) | 0.0663 (4) |
| C1 | 0.36408 (17) | 0.4170 (3) | 0.28302 (5) | 0.0437 (4) |
| C2 | 0.28596 (17) | 0.6138 (4) | 0.28937 (5) | 0.0438 (4) |
| H2 | 0.2193 | 0.6666 | 0.2682 | 0.053* |
| C3 | 0.31304 (16) | 0.7260 (3) | 0.32892 (6) | 0.0380 (4) |
| C4 | 0.41915 (15) | 0.6437 (3) | 0.36032 (5) | 0.0351 (3) |
| C5 | 0.46265 (17) | 0.3344 (3) | 0.31392 (6) | 0.0417 (4) |
| H5 | 0.5108 | 0.1995 | 0.3084 | 0.050* |
| C6 | 0.33092 (15) | 0.9407 (3) | 0.38565 (5) | 0.0355 (3) |
| C7 | 0.30567 (16) | 1.1232 (3) | 0.41692 (5) | 0.0374 (3) |
| C8 | 0.20011 (19) | 1.2782 (3) | 0.40877 (6) | 0.0466 (4) |
| H8 | 0.1446 | 1.2678 | 0.3826 | 0.056* |
| C9 | 0.17580 (19) | 1.4476 (4) | 0.43868 (6) | 0.0501 (5) |
| H9 | 0.1041 | 1.5485 | 0.4327 | 0.060* |
| C10 | 0.25837 (19) | 1.4669 (3) | 0.47759 (6) | 0.0462 (4) |
| C11 | 0.3644 (2) | 1.3137 (4) | 0.48642 (6) | 0.0501 (5) |
| H11A | 0.4197 | 1.3246 | 0.5126 | 0.060* |
| C12 | 0.38781 (18) | 1.1462 (4) | 0.45650 (5) | 0.0448 (4) |
| H12A | 0.4597 | 1.0458 | 0.4626 | 0.054* |
| C13 | 0.1389 (3) | 1.7962 (4) | 0.50100 (10) | 0.0722 (7) |
| H13A | 0.1424 | 1.9056 | 0.5249 | 0.108* |
| H13B | 0.0601 | 1.7054 | 0.4971 | 0.108* |
| H13C | 0.1431 | 1.8891 | 0.4756 | 0.108* |
| C14 | 0.60115 (17) | 0.3669 (3) | 0.38527 (6) | 0.0409 (4) |
| H14A | 0.6095 | 0.1901 | 0.3839 | 0.049* |
| H14B | 0.5856 | 0.4091 | 0.4136 | 0.049* |

| | | | | |
|---|---|---|---|---|
| C15 | 0.72405 (16) | 0.4858 (3) | 0.37807 (5) | 0.0376 (4) |
| C16 | 0.76570 (19) | 0.7021 (3) | 0.39913 (6) | 0.0460 (4) |
| H16 | 0.7194 | 0.7703 | 0.4185 | 0.055* |
| C17 | 0.8757 (2) | 0.8163 (4) | 0.39140 (8) | 0.0592 (5) |
| H17 | 0.9033 | 0.9607 | 0.4057 | 0.071* |
| C18 | 0.9443 (2) | 0.7187 (5) | 0.36287 (8) | 0.0675 (7) |
| H18 | 1.0174 | 0.7983 | 0.3574 | 0.081* |
| C19 | 0.9054 (2) | 0.5027 (5) | 0.34216 (7) | 0.0644 (7) |
| H19 | 0.9529 | 0.4356 | 0.3230 | 0.077* |
| C20 | 0.79559 (18) | 0.3847 (4) | 0.34969 (6) | 0.0495 (5) |
| H20 | 0.7698 | 0.2382 | 0.3358 | 0.059* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.06531 (16) | 0.07264 (17) | 0.05167 (13) | 0.00232 (11) | −0.00455 (10) | −0.02553 (10) |
| O1W | 0.0702 (12) | 0.0877 (14) | 0.0805 (13) | −0.0048 (10) | 0.0017 (10) | 0.0014 (11) |
| N1 | 0.0327 (7) | 0.0387 (7) | 0.0383 (7) | −0.0010 (6) | 0.0027 (5) | 0.0004 (6) |
| N2 | 0.0325 (7) | 0.0490 (8) | 0.0361 (7) | 0.0033 (6) | 0.0020 (5) | 0.0001 (6) |
| N3 | 0.0330 (7) | 0.0413 (8) | 0.0349 (7) | 0.0013 (6) | 0.0024 (5) | 0.0003 (5) |
| O1 | 0.0887 (11) | 0.0604 (9) | 0.0474 (8) | 0.0241 (9) | 0.0063 (7) | −0.0108 (7) |
| C1 | 0.0387 (9) | 0.0493 (10) | 0.0411 (8) | −0.0084 (8) | 0.0018 (7) | −0.0091 (7) |
| C2 | 0.0340 (9) | 0.0543 (11) | 0.0402 (8) | −0.0023 (8) | −0.0016 (7) | −0.0028 (8) |
| C3 | 0.0296 (8) | 0.0457 (10) | 0.0375 (8) | −0.0033 (7) | 0.0025 (6) | 0.0006 (7) |
| C4 | 0.0292 (8) | 0.0397 (8) | 0.0357 (8) | −0.0028 (7) | 0.0041 (6) | 0.0022 (6) |
| C5 | 0.0388 (9) | 0.0396 (9) | 0.0460 (9) | −0.0031 (7) | 0.0061 (7) | −0.0059 (7) |
| C6 | 0.0307 (8) | 0.0414 (9) | 0.0340 (7) | −0.0010 (7) | 0.0044 (6) | 0.0027 (6) |
| C7 | 0.0354 (8) | 0.0419 (9) | 0.0343 (8) | 0.0007 (7) | 0.0049 (6) | 0.0026 (7) |
| C8 | 0.0423 (10) | 0.0532 (11) | 0.0407 (9) | 0.0102 (8) | −0.0019 (7) | −0.0005 (7) |
| C9 | 0.0486 (11) | 0.0530 (11) | 0.0469 (10) | 0.0175 (9) | 0.0036 (8) | 0.0006 (8) |
| C10 | 0.0568 (11) | 0.0437 (10) | 0.0382 (8) | 0.0056 (8) | 0.0090 (8) | 0.0002 (7) |
| C11 | 0.0555 (11) | 0.0559 (11) | 0.0347 (9) | 0.0090 (9) | −0.0035 (8) | −0.0017 (8) |
| C12 | 0.0424 (10) | 0.0513 (10) | 0.0380 (8) | 0.0099 (8) | 0.0000 (7) | 0.0035 (8) |
| C13 | 0.0841 (18) | 0.0593 (14) | 0.0763 (17) | 0.0176 (12) | 0.0229 (14) | −0.0141 (12) |
| C14 | 0.0414 (9) | 0.0387 (9) | 0.0406 (8) | 0.0037 (7) | 0.0015 (7) | 0.0072 (7) |
| C15 | 0.0337 (8) | 0.0409 (9) | 0.0359 (8) | 0.0094 (7) | −0.0001 (6) | 0.0084 (6) |
| C16 | 0.0436 (10) | 0.0443 (10) | 0.0477 (10) | 0.0036 (8) | 0.0020 (8) | 0.0036 (7) |
| C17 | 0.0487 (12) | 0.0578 (12) | 0.0652 (13) | −0.0073 (10) | −0.0060 (10) | 0.0126 (10) |
| C18 | 0.0383 (11) | 0.097 (2) | 0.0640 (14) | −0.0018 (11) | −0.0006 (10) | 0.0325 (13) |
| C19 | 0.0426 (11) | 0.107 (2) | 0.0454 (10) | 0.0293 (12) | 0.0118 (9) | 0.0190 (12) |
| C20 | 0.0471 (11) | 0.0600 (12) | 0.0386 (9) | 0.0204 (9) | 0.0006 (8) | 0.0025 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C1 | 1.8877 (17) | C9—C10 | 1.384 (3) |
| O1w—H11 | 0.85 (1) | C9—H9 | 0.9300 |
| O1w—H12 | 0.85 (1) | C10—C11 | 1.388 (3) |
| N1—C4 | 1.352 (2) | C11—C12 | 1.372 (3) |

| | | | |
|---|---|---|---|
| N1—C5 | 1.359 (2) | C11—H11A | 0.9300 |
| N1—C14 | 1.490 (2) | C12—H12A | 0.9300 |
| N2—C6 | 1.351 (2) | C13—H13A | 0.9600 |
| N2—C3 | 1.371 (2) | C13—H13B | 0.9600 |
| N3—C4 | 1.334 (2) | C13—H13C | 0.9600 |
| N3—C6 | 1.375 (2) | C14—C15 | 1.508 (2) |
| O1—C10 | 1.369 (2) | C14—H14A | 0.9700 |
| O1—C13 | 1.423 (3) | C14—H14B | 0.9700 |
| C1—C5 | 1.374 (3) | C15—C16 | 1.389 (3) |
| C1—C2 | 1.392 (3) | C15—C20 | 1.390 (3) |
| C2—C3 | 1.380 (2) | C16—C17 | 1.381 (3) |
| C2—H2 | 0.9300 | C16—H16 | 0.9300 |
| C3—C4 | 1.435 (2) | C17—C18 | 1.366 (4) |
| C5—H5 | 0.9300 | C17—H17 | 0.9300 |
| C6—C7 | 1.464 (2) | C18—C19 | 1.376 (4) |
| C7—C8 | 1.389 (2) | C18—H18 | 0.9300 |
| C7—C12 | 1.400 (2) | C19—C20 | 1.387 (3) |
| C8—C9 | 1.382 (3) | C19—H19 | 0.9300 |
| C8—H8 | 0.9300 | C20—H20 | 0.9300 |

| | | | |
|---|---|---|---|
| H11—O1W—H12 | 101 (5) | C12—C11—C10 | 120.05 (17) |
| C4—N1—C5 | 119.19 (14) | C12—C11—H11A | 120.0 |
| C4—N1—C14 | 120.23 (14) | C10—C11—H11A | 120.0 |
| C5—N1—C14 | 120.53 (15) | C11—C12—C7 | 121.39 (17) |
| C6—N2—C3 | 102.87 (13) | C11—C12—H12A | 119.3 |
| C4—N3—C6 | 101.69 (13) | C7—C12—H12A | 119.3 |
| C10—O1—C13 | 117.82 (18) | O1—C13—H13A | 109.5 |
| C5—C1—C2 | 123.00 (16) | O1—C13—H13B | 109.5 |
| C5—C1—Br1 | 117.70 (14) | H13A—C13—H13B | 109.5 |
| C2—C1—Br1 | 119.29 (13) | O1—C13—H13C | 109.5 |
| C3—C2—C1 | 116.21 (16) | H13A—C13—H13C | 109.5 |
| C3—C2—H2 | 121.9 | H13B—C13—H13C | 109.5 |
| C1—C2—H2 | 121.9 | N1—C14—C15 | 111.09 (13) |
| N2—C3—C2 | 132.43 (16) | N1—C14—H14A | 109.4 |
| N2—C3—C4 | 107.37 (14) | C15—C14—H14A | 109.4 |
| C2—C3—C4 | 120.19 (16) | N1—C14—H14B | 109.4 |
| N3—C4—N1 | 128.09 (14) | C15—C14—H14B | 109.4 |
| N3—C4—C3 | 111.05 (15) | H14A—C14—H14B | 108.0 |
| N1—C4—C3 | 120.84 (15) | C16—C15—C20 | 119.06 (18) |
| N1—C5—C1 | 120.50 (17) | C16—C15—C14 | 120.06 (16) |
| N1—C5—H5 | 119.8 | C20—C15—C14 | 120.86 (17) |
| C1—C5—H5 | 119.8 | C17—C16—C15 | 120.2 (2) |
| N2—C6—N3 | 116.99 (15) | C17—C16—H16 | 119.9 |
| N2—C6—C7 | 122.69 (15) | C15—C16—H16 | 119.9 |
| N3—C6—C7 | 120.31 (14) | C18—C17—C16 | 120.5 (2) |
| C8—C7—C12 | 117.59 (16) | C18—C17—H17 | 119.8 |
| C8—C7—C6 | 121.75 (15) | C16—C17—H17 | 119.8 |
| C12—C7—C6 | 120.66 (15) | C17—C18—C19 | 120.1 (2) |

| | | | |
|---|---|---|---|
| C9—C8—C7 | 121.45 (17) | C17—C18—H18 | 120.0 |
| C9—C8—H8 | 119.3 | C19—C18—H18 | 120.0 |
| C7—C8—H8 | 119.3 | C18—C19—C20 | 120.3 (2) |
| C8—C9—C10 | 119.90 (17) | C18—C19—H19 | 119.9 |
| C8—C9—H9 | 120.0 | C20—C19—H19 | 119.9 |
| C10—C9—H9 | 120.0 | C19—C20—C15 | 119.9 (2) |
| O1—C10—C9 | 124.58 (17) | C19—C20—H20 | 120.0 |
| O1—C10—C11 | 115.81 (17) | C15—C20—H20 | 120.0 |
| C9—C10—C11 | 119.61 (17) | | |

| | | | |
|---|---|---|---|
| C5—C1—C2—C3 | 0.4 (3) | N2—C6—C7—C12 | −176.91 (17) |
| Br1—C1—C2—C3 | −179.58 (13) | N3—C6—C7—C12 | 3.7 (2) |
| C6—N2—C3—C2 | −178.68 (19) | C12—C7—C8—C9 | −0.7 (3) |
| C6—N2—C3—C4 | −0.05 (18) | C6—C7—C8—C9 | 179.03 (18) |
| C1—C2—C3—N2 | −179.63 (18) | C7—C8—C9—C10 | 0.7 (3) |
| C1—C2—C3—C4 | 1.9 (3) | C13—O1—C10—C9 | −1.2 (3) |
| C6—N3—C4—N1 | −177.47 (17) | C13—O1—C10—C11 | 178.4 (2) |
| C6—N3—C4—C3 | 1.19 (18) | C8—C9—C10—O1 | 178.8 (2) |
| C5—N1—C4—N3 | −179.48 (17) | C8—C9—C10—C11 | −0.7 (3) |
| C14—N1—C4—N3 | −2.2 (3) | O1—C10—C11—C12 | −178.8 (2) |
| C5—N1—C4—C3 | 2.0 (2) | C9—C10—C11—C12 | 0.7 (3) |
| C14—N1—C4—C3 | 179.30 (15) | C10—C11—C12—C7 | −0.8 (3) |
| N2—C3—C4—N3 | −0.77 (19) | C8—C7—C12—C11 | 0.7 (3) |
| C2—C3—C4—N3 | 178.06 (16) | C6—C7—C12—C11 | −178.99 (18) |
| N2—C3—C4—N1 | 178.00 (15) | C4—N1—C14—C15 | −92.30 (18) |
| C2—C3—C4—N1 | −3.2 (3) | C5—N1—C14—C15 | 84.99 (19) |
| C4—N1—C5—C1 | 0.3 (3) | N1—C14—C15—C16 | 93.17 (18) |
| C14—N1—C5—C1 | −176.98 (16) | N1—C14—C15—C20 | −85.35 (19) |
| C2—C1—C5—N1 | −1.6 (3) | C20—C15—C16—C17 | 0.9 (3) |
| Br1—C1—C5—N1 | 178.39 (13) | C14—C15—C16—C17 | −177.60 (17) |
| C3—N2—C6—N3 | 0.88 (19) | C15—C16—C17—C18 | 0.3 (3) |
| C3—N2—C6—C7 | −178.50 (15) | C16—C17—C18—C19 | −1.2 (3) |
| C4—N3—C6—N2 | −1.33 (19) | C17—C18—C19—C20 | 0.8 (3) |
| C4—N3—C6—C7 | 178.06 (15) | C18—C19—C20—C15 | 0.4 (3) |
| N2—C6—C7—C8 | 3.4 (3) | C16—C15—C20—C19 | −1.3 (2) |
| N3—C6—C7—C8 | −175.95 (17) | C14—C15—C20—C19 | 177.23 (15) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1w—H11···N2 | 0.85 (1) | 2.30 (2) | 3.092 (3) | 155 (5) |
| O1w—H12···O1*W*$^{i}$ | 0.85 (1) | 2.30 (2) | 3.119 (2) | 162 (5) |

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