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

# 4-(1*H*-Pyrrolo[2,3-*b*]pyridin-2-yl)-pyridine

**Ping-Hsin Huang,[a]* Yuh-Sheng Wen[b] and Jiun-Yi Shen[c]**

[a]Cardinal Tien College of Healthcare & Management, Taipei, Taiwan 231, Republic of China, [b]Institute of Chemistry, Academia Sinica, Nankang, Taipei, Taiwan, Republic of China, and [c]Department of Chemistry, National Taiwan University, Taipei, Taiwan, Republic of China
Correspondence e-mail: pshuang@ctcn.edu.tw

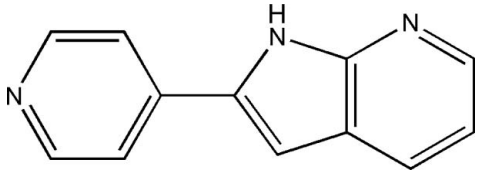
Received 12 March 2013; accepted 29 March 2013

Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.058; $wR$ factor = 0.124; data-to-parameter ratio = 12.3.

The asymmetric unit of the title compound, $C_{12}H_9N_3$, contains two independent molecules in which the dihedral angle between the pyridine and azaindole rings are 8.23 (6) and 9.89 (2)°. In the crystal, both types of molecule are connected by pairs of N—H—N hydrogen bonds into inversion dimers.

## Related literature

For the production of luminescent organic compounds, see: Liu *et al.* (2000); Parcerisa *et al.* (2008). For related structures, see: Huang *et al.* (2012).



## Experimental

### Crystal data

$C_{12}H_9N_3$
$M_r$ = 195.22
Triclinic, $P\overline{1}$
$a$ = 6.5529 (5) Å
$b$ = 10.0457 (8) Å
$c$ = 14.5282 (11) Å
$\alpha$ = 83.372 (2)°
$\beta$ = 86.697 (2)°
$\gamma$ = 87.427 (2)°
$V$ = 947.69 (13) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 295 K
0.30 × 0.20 × 0.05 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.975, $T_{max}$ = 0.996
10193 measured reflections
3329 independent reflections
2573 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.124
$S$ = 1.14
3329 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···N2$^{i}$ | 0.86 | 2.22 | 3.061 (3) | 167 |
| N4—H4$A$···N5$^{ii}$ | 0.86 | 2.22 | 3.066 (3) | 169 |

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

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: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

This work is partially supported by the instrumentation center, National Taiwan University, and Cardinal Tien College of Healthcare & Management.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2308).

## References

Bruker (2001). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Huang, P.-H., Wen, Y.-S. & Shen, J.-Y. (2012). *Acta Cryst.* E**68**, o1943.
Liu, S. F., Wu, Q., Schmider, H. L., Aziz, H., Hu, N. X., Popovic, Z. & Wang, S. (2000). *J. Am. Chem. Soc.* **122**, 3671–3678.
Parcerisa, J., Romero, M. & Pujol, M. D. (2008). *Tetrahedron*, **64**, 500–507.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2013). E**69**, o674 [https://doi.org/10.1107/S1600536813008672]

## 4-(1*H*-Pyrrolo[2,3-*b*]pyridin-2-yl)pyridine

**Ping-Hsin Huang, Yuh-Sheng Wen and Jiun-Yi Shen**

### S1. Comment

The title compound has been shown to be an precursor for the production of luminescent organic compound (Liu *et al.*, 2000). In the crystal structure of the title compound two crystallographically independent molecules are found which shows no large structural differences. Both molecules are nearly coplanar, the dihedral angles between the pyridine and the azaindole rings is 8.23 (6)° and 9.89 (2)° (Huang *et al.*, 2012). Each of these molecules is connected into centrosymmetrically dimers by intermolecular N—H—N hydrogen bonding.

### S2. Experimental

The compound was synthesized by the following procedure (Parcerisa *et al.*, 2008). A solution of [3-(2-hydroxy-2-pyridin-4-yl-ethyl)-pyridin-2-yl]-carbamic acid *tert*-butyl ester (1 mmol and acetonitrile (12 ml) was cooled to ice temperature. Afterwards triethylamine (1.2 mmol) and trifluoromethanesulfonic anhydride (1.1 mmol) was added over a period of 5 min. The mixture was stirred at room temperature for 2 h, trifluoroacetic acid was added (1.5 mmol) and afterwards the mixture was heated under reflux for 1 h. The mixture was cooled to room temperature and neutralized using 2 N NaOH. The aqueous layer was extracted with ethyl ether and the organic extract was washed with brine and aqueous $Na_2SO_4$, dried and concentrated. The residue was purified by column chromatography using hexane/ethyl acetate (2:8) as eluent, followed by recrystallization in $CH_2Cl_2$ and hexane to give a white solid in 64% yield. Crystals suitable for X-ray diffraction were grown from a $CH_2Cl_2$ solution layered with hexane at room temperature. $^1$H NMR ($CDCl_3$, 300 MHz): 8.62 (dd, 2 H, J= 1.0, 3.1 Hz), 8.29 (dd, 1 H, J= 1.0, 3.4 Hz), 8.00 (dd, 1 H, J = 1.0, 5.3 Hz), 7.72 (dd, 2 H, J = 1.0, 3.1 Hz), 7.13 (dd, 1 H, J= 3.4, 5.3 Hz), 6.99 (s, 1 H), Anal. Calcd for $C_{12}H_9N_3$: C, 73.83; H, 4.65; N, 21.52. Found: C, 74.21; H, 4.40; N, 21.34.

### S3. Refinement

H atoms were located in difference map but were positioned with idealized geometry and refined isotropic with $U_{iso}$(H) = 1.2$U_{eq}$(C,N).

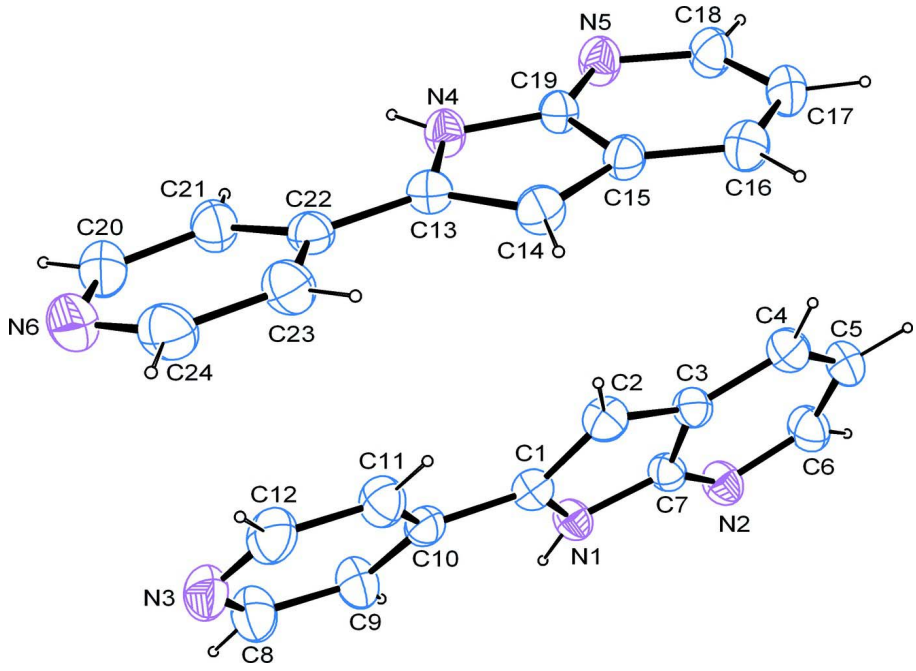



**Figure 1**

Molecular structure of the title compound with labeling and displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

**4-(1*H*-Pyrrolo[2,3-*b*]pyridin-2-yl)pyridine**

*Crystal data*

$C_{12}H_9N_3$
$M_r = 195.22$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.5529\ (5)$ Å
$b = 10.0457\ (8)$ Å
$c = 14.5282\ (11)$ Å
$\alpha = 83.372\ (2)°$
$\beta = 86.697\ (2)°$
$\gamma = 87.427\ (2)°$
$V = 947.69\ (13)$ Å$^3$
$Z = 4$
$F(000) = 408$
$D_x = 1.368$ Mg m$^{-3}$
$D_m = 1.368$ Mg m$^{-3}$
$D_m$ measured by not measured
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1585 reflections
$\theta = 2.6–23.3°$
$\mu = 0.09$ mm$^{-1}$
$T = 295$ K
Plate, colorless
0.30 × 0.20 × 0.05 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.975$, $T_{max} = 0.996$
10193 measured reflections
3329 independent reflections
2573 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.4°$
$h = -7\rightarrow7$
$k = -11\rightarrow11$
$l = -17\rightarrow17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.124$
$S = 1.14$
3329 reflections
271 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
$w = 1/[\sigma^2(F_o^2) + (0.0442P)^2 + 0.126P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å$^{-3}$
$\Delta\rho_{min} = -0.17$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.2449 (3) | 0.99700 (17) | 0.92427 (12) | 0.0443 (5) |
| H1 | 0.1787 | 1.0568 | 0.9532 | 0.053* |
| N2 | −0.0037 (3) | 0.82637 (19) | 0.94609 (13) | 0.0523 (5) |
| N3 | 0.7664 (4) | 1.3698 (2) | 0.86462 (16) | 0.0704 (6) |
| N4 | 0.7252 (3) | 0.97632 (17) | 0.57580 (12) | 0.0452 (5) |
| H4A | 0.6651 | 1.0437 | 0.5450 | 0.054* |
| N5 | 0.4869 (3) | 0.80868 (19) | 0.55706 (13) | 0.0524 (5) |
| N6 | 1.2240 (4) | 1.3404 (2) | 0.62691 (16) | 0.0710 (6) |
| C1 | 0.4379 (3) | 1.0098 (2) | 0.88094 (14) | 0.0423 (5) |
| C2 | 0.4911 (3) | 0.8951 (2) | 0.84219 (15) | 0.0493 (6) |
| H2 | 0.6131 | 0.8780 | 0.8089 | 0.059* |
| C3 | 0.3285 (3) | 0.8067 (2) | 0.86152 (15) | 0.0435 (5) |
| C4 | 0.2881 (4) | 0.6784 (2) | 0.84216 (16) | 0.0548 (6) |
| H4 | 0.3826 | 0.6290 | 0.8083 | 0.066* |
| C5 | 0.1035 (4) | 0.6273 (2) | 0.87473 (17) | 0.0576 (7) |
| H5 | 0.0713 | 0.5418 | 0.8630 | 0.069* |
| C6 | −0.0344 (4) | 0.7025 (2) | 0.92484 (17) | 0.0589 (7) |
| H6 | −0.1580 | 0.6644 | 0.9454 | 0.071* |
| C7 | 0.1773 (3) | 0.8734 (2) | 0.91330 (14) | 0.0416 (5) |
| C8 | 0.5755 (5) | 1.3615 (3) | 0.90108 (19) | 0.0712 (8) |
| H8 | 0.5140 | 1.4376 | 0.9232 | 0.085* |
| C9 | 0.4636 (4) | 1.2481 (2) | 0.90816 (18) | 0.0603 (7) |
| H9 | 0.3301 | 1.2493 | 0.9337 | 0.072* |
| C10 | 0.5497 (3) | 1.1326 (2) | 0.87731 (14) | 0.0445 (5) |
| C11 | 0.7495 (4) | 1.1396 (2) | 0.84044 (16) | 0.0561 (6) |

| | | | | |
|---|---|---|---|---|
| H11 | 0.8162 | 1.0644 | 0.8193 | 0.067* |
| C12 | 0.8479 (4) | 1.2578 (3) | 0.83527 (18) | 0.0678 (7) |
| H12 | 0.9811 | 1.2597 | 0.8094 | 0.081* |
| C13 | 0.9063 (3) | 0.9796 (2) | 0.61960 (14) | 0.0424 (5) |
| C14 | 0.9524 (3) | 0.8542 (2) | 0.66219 (15) | 0.0485 (6) |
| H14 | 1.0656 | 0.8293 | 0.6969 | 0.058* |
| C15 | 0.7970 (3) | 0.7688 (2) | 0.64396 (14) | 0.0436 (5) |
| C16 | 0.7536 (4) | 0.6348 (2) | 0.66723 (16) | 0.0554 (6) |
| H16 | 0.8395 | 0.5771 | 0.7035 | 0.066* |
| C17 | 0.5792 (4) | 0.5904 (2) | 0.63473 (17) | 0.0573 (6) |
| H17 | 0.5454 | 0.5012 | 0.6486 | 0.069* |
| C18 | 0.4535 (4) | 0.6788 (2) | 0.58133 (17) | 0.0557 (6) |
| H18 | 0.3366 | 0.6450 | 0.5607 | 0.067* |
| C19 | 0.6574 (3) | 0.8490 (2) | 0.58945 (14) | 0.0415 (5) |
| C20 | 1.0412 (5) | 1.3402 (3) | 0.59264 (18) | 0.0692 (8) |
| H20 | 0.9818 | 1.4225 | 0.5701 | 0.083* |
| C21 | 0.9327 (4) | 1.2275 (2) | 0.58795 (16) | 0.0566 (6) |
| H21 | 0.8044 | 1.2350 | 0.5631 | 0.068* |
| C22 | 1.0152 (3) | 1.1027 (2) | 0.62031 (14) | 0.0444 (5) |
| C23 | 1.2075 (4) | 1.1013 (2) | 0.65608 (17) | 0.0559 (6) |
| H23 | 1.2712 | 1.0205 | 0.6787 | 0.067* |
| C24 | 1.3034 (4) | 1.2199 (3) | 0.65792 (18) | 0.0672 (7) |
| H24 | 1.4319 | 1.2159 | 0.6824 | 0.081* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0419 (10) | 0.0413 (11) | 0.0508 (11) | −0.0013 (8) | 0.0011 (9) | −0.0113 (8) |
| N2 | 0.0454 (11) | 0.0507 (12) | 0.0623 (13) | −0.0102 (9) | 0.0003 (9) | −0.0112 (9) |
| N3 | 0.0765 (16) | 0.0626 (16) | 0.0714 (15) | −0.0247 (13) | −0.0063 (12) | 0.0053 (12) |
| N4 | 0.0435 (11) | 0.0392 (11) | 0.0524 (11) | −0.0022 (8) | −0.0088 (9) | −0.0003 (8) |
| N5 | 0.0511 (12) | 0.0480 (12) | 0.0583 (12) | −0.0112 (9) | −0.0108 (9) | 0.0003 (9) |
| N6 | 0.0781 (17) | 0.0669 (16) | 0.0707 (15) | −0.0277 (13) | 0.0007 (13) | −0.0125 (12) |
| C1 | 0.0354 (12) | 0.0475 (14) | 0.0435 (13) | −0.0009 (10) | −0.0020 (10) | −0.0034 (10) |
| C2 | 0.0432 (13) | 0.0539 (15) | 0.0498 (14) | 0.0005 (11) | 0.0038 (11) | −0.0054 (11) |
| C3 | 0.0457 (13) | 0.0409 (13) | 0.0441 (13) | 0.0020 (10) | −0.0037 (10) | −0.0057 (10) |
| C4 | 0.0627 (16) | 0.0474 (15) | 0.0542 (15) | 0.0029 (12) | 0.0004 (12) | −0.0089 (11) |
| C5 | 0.0703 (17) | 0.0414 (14) | 0.0629 (16) | −0.0094 (12) | −0.0066 (13) | −0.0096 (11) |
| C6 | 0.0570 (15) | 0.0540 (16) | 0.0674 (17) | −0.0163 (12) | −0.0014 (13) | −0.0095 (13) |
| C7 | 0.0408 (12) | 0.0412 (13) | 0.0439 (13) | −0.0038 (10) | −0.0064 (10) | −0.0062 (10) |
| C8 | 0.080 (2) | 0.0510 (17) | 0.083 (2) | −0.0045 (14) | −0.0019 (16) | −0.0076 (14) |
| C9 | 0.0568 (15) | 0.0499 (16) | 0.0747 (18) | −0.0087 (12) | 0.0038 (13) | −0.0109 (13) |
| C10 | 0.0477 (13) | 0.0461 (14) | 0.0394 (12) | −0.0052 (10) | −0.0064 (10) | 0.0002 (10) |
| C11 | 0.0500 (14) | 0.0573 (16) | 0.0607 (16) | −0.0104 (12) | 0.0045 (12) | −0.0049 (12) |
| C12 | 0.0593 (17) | 0.076 (2) | 0.0665 (18) | −0.0216 (15) | 0.0066 (13) | 0.0018 (15) |
| C13 | 0.0394 (12) | 0.0457 (14) | 0.0423 (12) | −0.0011 (10) | −0.0029 (10) | −0.0059 (10) |
| C14 | 0.0448 (13) | 0.0499 (15) | 0.0509 (14) | 0.0019 (11) | −0.0111 (11) | −0.0034 (11) |
| C15 | 0.0465 (13) | 0.0395 (13) | 0.0439 (13) | 0.0006 (10) | −0.0027 (10) | −0.0016 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16 | 0.0632 (16) | 0.0461 (15) | 0.0559 (15) | 0.0016 (12) | −0.0070 (12) | −0.0009 (11) |
| C17 | 0.0707 (17) | 0.0407 (14) | 0.0604 (16) | −0.0123 (12) | −0.0045 (13) | −0.0010 (11) |
| C18 | 0.0556 (15) | 0.0524 (16) | 0.0595 (15) | −0.0157 (12) | −0.0078 (12) | −0.0004 (12) |
| C19 | 0.0431 (12) | 0.0385 (13) | 0.0429 (12) | −0.0062 (10) | −0.0006 (10) | −0.0040 (9) |
| C20 | 0.087 (2) | 0.0538 (17) | 0.0668 (18) | −0.0156 (15) | −0.0081 (16) | 0.0007 (13) |
| C21 | 0.0595 (15) | 0.0505 (15) | 0.0601 (16) | −0.0079 (12) | −0.0115 (12) | −0.0013 (12) |
| C22 | 0.0440 (13) | 0.0497 (14) | 0.0403 (13) | −0.0053 (10) | 0.0007 (10) | −0.0083 (10) |
| C23 | 0.0494 (14) | 0.0582 (16) | 0.0618 (16) | −0.0072 (12) | −0.0079 (12) | −0.0093 (12) |
| C24 | 0.0570 (16) | 0.082 (2) | 0.0658 (18) | −0.0206 (15) | −0.0063 (13) | −0.0156 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C7 | 1.366 (2) | C8—H8 | 0.9300 |
| N1—C1 | 1.384 (2) | C9—C10 | 1.378 (3) |
| N1—H1 | 0.8600 | C9—H9 | 0.9300 |
| N2—C7 | 1.338 (3) | C10—C11 | 1.387 (3) |
| N2—C6 | 1.343 (3) | C11—C12 | 1.368 (3) |
| N3—C12 | 1.329 (3) | C11—H11 | 0.9300 |
| N3—C8 | 1.332 (3) | C12—H12 | 0.9300 |
| N4—C19 | 1.362 (3) | C13—C14 | 1.367 (3) |
| N4—C13 | 1.382 (2) | C13—C22 | 1.457 (3) |
| N4—H4A | 0.8600 | C14—C15 | 1.416 (3) |
| N5—C19 | 1.334 (3) | C14—H14 | 0.9300 |
| N5—C18 | 1.336 (3) | C15—C16 | 1.388 (3) |
| N6—C20 | 1.324 (3) | C15—C19 | 1.408 (3) |
| N6—C24 | 1.336 (3) | C16—C17 | 1.373 (3) |
| C1—C2 | 1.362 (3) | C16—H16 | 0.9300 |
| C1—C10 | 1.457 (3) | C17—C18 | 1.384 (3) |
| C2—C3 | 1.413 (3) | C17—H17 | 0.9300 |
| C2—H2 | 0.9300 | C18—H18 | 0.9300 |
| C3—C4 | 1.390 (3) | C20—C21 | 1.374 (3) |
| C3—C7 | 1.403 (3) | C20—H20 | 0.9300 |
| C4—C5 | 1.373 (3) | C21—C22 | 1.384 (3) |
| C4—H4 | 0.9300 | C21—H21 | 0.9300 |
| C5—C6 | 1.381 (3) | C22—C23 | 1.390 (3) |
| C5—H5 | 0.9300 | C23—C24 | 1.375 (3) |
| C6—H6 | 0.9300 | C23—H23 | 0.9300 |
| C8—C9 | 1.373 (3) | C24—H24 | 0.9300 |
| | | | |
| C7—N1—C1 | 108.49 (17) | C12—C11—H11 | 120.1 |
| C7—N1—H1 | 125.8 | C10—C11—H11 | 120.1 |
| C1—N1—H1 | 125.8 | N3—C12—C11 | 124.5 (3) |
| C7—N2—C6 | 113.4 (2) | N3—C12—H12 | 117.7 |
| C12—N3—C8 | 115.3 (2) | C11—C12—H12 | 117.7 |
| C19—N4—C13 | 108.82 (17) | C14—C13—N4 | 108.76 (19) |
| C19—N4—H4A | 125.6 | C14—C13—C22 | 128.8 (2) |
| C13—N4—H4A | 125.6 | N4—C13—C22 | 122.39 (19) |
| C19—N5—C18 | 113.62 (19) | C13—C14—C15 | 107.79 (19) |

| | | | |
|---|---|---|---|
| C20—N6—C24 | 115.3 (2) | C13—C14—H14 | 126.1 |
| C2—C1—N1 | 108.75 (19) | C15—C14—H14 | 126.1 |
| C2—C1—C10 | 129.1 (2) | C16—C15—C19 | 117.3 (2) |
| N1—C1—C10 | 122.06 (19) | C16—C15—C14 | 136.3 (2) |
| C1—C2—C3 | 108.01 (19) | C19—C15—C14 | 106.40 (18) |
| C1—C2—H2 | 126.0 | C17—C16—C15 | 117.6 (2) |
| C3—C2—H2 | 126.0 | C17—C16—H16 | 121.2 |
| C4—C3—C7 | 117.2 (2) | C15—C16—H16 | 121.2 |
| C4—C3—C2 | 136.3 (2) | C16—C17—C18 | 119.9 (2) |
| C7—C3—C2 | 106.46 (19) | C16—C17—H17 | 120.0 |
| C5—C4—C3 | 117.6 (2) | C18—C17—H17 | 120.0 |
| C5—C4—H4 | 121.2 | N5—C18—C17 | 125.2 (2) |
| C3—C4—H4 | 121.2 | N5—C18—H18 | 117.4 |
| C4—C5—C6 | 120.1 (2) | C17—C18—H18 | 117.4 |
| C4—C5—H5 | 119.9 | N5—C19—N4 | 125.41 (19) |
| C6—C5—H5 | 119.9 | N5—C19—C15 | 126.4 (2) |
| N2—C6—C5 | 125.0 (2) | N4—C19—C15 | 108.23 (18) |
| N2—C6—H6 | 117.5 | N6—C20—C21 | 124.8 (3) |
| C5—C6—H6 | 117.5 | N6—C20—H20 | 117.6 |
| N2—C7—N1 | 125.10 (19) | C21—C20—H20 | 117.6 |
| N2—C7—C3 | 126.6 (2) | C20—C21—C22 | 119.7 (2) |
| N1—C7—C3 | 108.29 (18) | C20—C21—H21 | 120.2 |
| N3—C8—C9 | 124.4 (3) | C22—C21—H21 | 120.2 |
| N3—C8—H8 | 117.8 | C21—C22—C23 | 116.1 (2) |
| C9—C8—H8 | 117.8 | C21—C22—C13 | 122.5 (2) |
| C8—C9—C10 | 119.7 (2) | C23—C22—C13 | 121.3 (2) |
| C8—C9—H9 | 120.1 | C24—C23—C22 | 119.7 (2) |
| C10—C9—H9 | 120.1 | C24—C23—H23 | 120.1 |
| C9—C10—C11 | 116.3 (2) | C22—C23—H23 | 120.1 |
| C9—C10—C1 | 122.5 (2) | N6—C24—C23 | 124.3 (2) |
| C11—C10—C1 | 121.1 (2) | N6—C24—H24 | 117.8 |
| C12—C11—C10 | 119.7 (2) | C23—C24—H24 | 117.8 |

| | | | |
|---|---|---|---|
| C7—N1—C1—C2 | 0.5 (2) | C19—N4—C13—C14 | −0.7 (2) |
| C7—N1—C1—C10 | 177.80 (18) | C19—N4—C13—C22 | −178.17 (19) |
| N1—C1—C2—C3 | −0.2 (2) | N4—C13—C14—C15 | 0.6 (2) |
| C10—C1—C2—C3 | −177.3 (2) | C22—C13—C14—C15 | 177.8 (2) |
| C1—C2—C3—C4 | 179.9 (2) | C13—C14—C15—C16 | −179.2 (3) |
| C1—C2—C3—C7 | −0.1 (2) | C13—C14—C15—C19 | −0.3 (2) |
| C7—C3—C4—C5 | 0.3 (3) | C19—C15—C16—C17 | 0.5 (3) |
| C2—C3—C4—C5 | −179.7 (2) | C14—C15—C16—C17 | 179.3 (2) |
| C3—C4—C5—C6 | 0.0 (4) | C15—C16—C17—C18 | −0.4 (4) |
| C7—N2—C6—C5 | 0.4 (3) | C19—N5—C18—C17 | 0.0 (3) |
| C4—C5—C6—N2 | −0.3 (4) | C16—C17—C18—N5 | 0.1 (4) |
| C6—N2—C7—N1 | 179.2 (2) | C18—N5—C19—N4 | −179.1 (2) |
| C6—N2—C7—C3 | −0.1 (3) | C18—N5—C19—C15 | 0.2 (3) |
| C1—N1—C7—N2 | −179.9 (2) | C13—N4—C19—N5 | 180.0 (2) |
| C1—N1—C7—C3 | −0.5 (2) | C13—N4—C19—C15 | 0.6 (2) |

| | | | |
|---|---|---|---|
| C4—C3—C7—N2 | −0.2 (3) | C16—C15—C19—N5 | −0.5 (3) |
| C2—C3—C7—N2 | 179.8 (2) | C14—C15—C19—N5 | −179.6 (2) |
| C4—C3—C7—N1 | −179.60 (18) | C16—C15—C19—N4 | 178.96 (19) |
| C2—C3—C7—N1 | 0.4 (2) | C14—C15—C19—N4 | −0.2 (2) |
| C12—N3—C8—C9 | −0.9 (4) | C24—N6—C20—C21 | 0.4 (4) |
| N3—C8—C9—C10 | 0.8 (4) | N6—C20—C21—C22 | −0.3 (4) |
| C8—C9—C10—C11 | 0.2 (4) | C20—C21—C22—C23 | −0.1 (3) |
| C8—C9—C10—C1 | −178.6 (2) | C20—C21—C22—C13 | 178.4 (2) |
| C2—C1—C10—C9 | 170.0 (2) | C14—C13—C22—C21 | −168.3 (2) |
| N1—C1—C10—C9 | −6.7 (3) | N4—C13—C22—C21 | 8.6 (3) |
| C2—C1—C10—C11 | −8.7 (4) | C14—C13—C22—C23 | 10.1 (3) |
| N1—C1—C10—C11 | 174.5 (2) | N4—C13—C22—C23 | −173.0 (2) |
| C9—C10—C11—C12 | −0.9 (3) | C21—C22—C23—C24 | 0.2 (3) |
| C1—C10—C11—C12 | 177.9 (2) | C13—C22—C23—C24 | −178.2 (2) |
| C8—N3—C12—C11 | 0.0 (4) | C20—N6—C24—C23 | −0.2 (4) |
| C10—C11—C12—N3 | 0.9 (4) | C22—C23—C24—N6 | −0.1 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···N2$^{i}$ | 0.86 | 2.22 | 3.061 (3) | 167 |
| N4—H4*A*···N5$^{ii}$ | 0.86 | 2.22 | 3.066 (3) | 169 |

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