# organic compounds

# 3-Ethyl-5-(4-methoxyphenoxy)-2-(pyridin-4-yl)-3*H*-imidazo[4,5-*b*]pyridine

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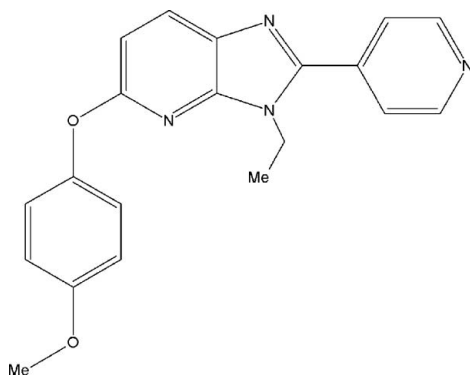Correspondence e-mail: a_sp59@yahoo.in

In the title compound, $C_{20}H_{18}N_4O_2$, the imidazopyridine fused ring system is almost perpendicular to the benzene ring [dihedral angle = 87.6 (5)°]. The pyridine ring makes a dihedral angle of 35.5 (5)° with the mean plane of the imidazopyridine fragment. The crystal structure is stabilized by an aromatic $\pi$–$\pi$ stacking interaction between the phenyl rings of neighbouring molecules [centroid–centroid distance = 3.772 (2) Å, interplanar distance = 3.546 (2) Å and slippage = 1.286 (2) Å].

## Related literature

For the biological activity of pyridine derivatives, see: Passannanti *et al.* (1998); Jiyeon *et al.* (2010); Abdel-Alim *et al.* (2005); Girgis *et al.* (2006); Slominska *et al.* (2008); Spanka *et al.* (2010). For a related structure, see: Ouzidan *et al.* (2010). For $sp^3$ hybridization, see: Beddoes *et al.* (1986).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{20}H_{18}N_4O_2$ | $V = 1723.74$ (8) Å$^3$ |
| $M_r = 346.38$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 13.6591$ (4) Å | $\mu = 0.09$ mm$^{-1}$ |
| $b = 13.7104$ (4) Å | $T = 293$ K |
| $c = 9.3177$ (2) Å | $0.25 \times 0.22 \times 0.19$ mm |
| $\beta = 98.940$ (1)° | |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 24827 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 5887 independent reflections |
| | 3938 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.981$, $T_{max} = 0.985$ | $R_{int} = 0.027$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | 237 parameters |
| $wR(F^2) = 0.140$ | H-atom parameters constrained |
| $S = 1.00$ | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| 5887 reflections | $\Delta\rho_{min} = -0.20$ e Å$^{-3}$ |

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: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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# supporting information

# 3-Ethyl-5-(4-methoxyphenoxy)-2-(pyridin-4-yl)-3*H*-imidazo[4,5-*b*]pyridine

## S. Ranjith, A. SubbiahPandi, A. D. Suresh and K. Pitchumani

### S1. Comment

Pyridine derivatives has numerous applications in medicinal chemistry (Passannanti *et al.*, 1998). Furthermore, the imidazo[4,5-*b*]pyridine moiety is also an important heterocyclic nucleus which has been used extensively in medicinal chemistry. In fact, the heterocycles derived from these intermediates have been tested for their potential as anti-neuroinflammatory (Jiyeon *et al.*, 2010). Pyridine-3-carboxamides have gained attention because of their diverse pharmacological properties such as anti-inflammatory (Abdel-Alim *et al.*, 2005), anticancer (Girgis *et al.*, 2006), cytoprotective (Slominska *et al.*, 2008), and anxiolytic (Spanka *et al.*, 2010) activities. Against this background, and in order to obtain detailed information on molecular conformations in the solid state, an X-ray study of the title compound was carried out.

The bond lengths and angles in (Fig. 1) agree with those observed in other imidazopyridine derivatives (Ouzidan *et al.*, 2010). The imidazopyridine ring system is essentially planar, with maximum deviation of 0.013 (1)° for atom C1. The sum of bond angles around N2[359.2 (9)°] of the imidazole ring is in accordance with $sp^3$ hybridization (Beddoes *et al.*, 1986). The imidazopyridine ring system makes dihedral angles of 35.5 (5) and 87.6 (5)°, respectively, with the pyridine and phenyl rings and also the dihedral angle between the pyridine and phenyl ring is 87.0 (6)°. It shows that the phenyl ring is perpendicular to both the imidazopyridine and pyridine rings. The atoms O1 and O2 are deviated by 0.039 (1) and - 0.021 (1)Å from the leastsquares plane of the phenyl ring.

The molecules lack hydrogen bonding functionality and pack in layers parallel to the (100) planes. The crystal structure is stabilized by an aromatic *π*–*π* stacking interaction between the phenyl rings of adjacent molecules, with a Cg···Cg distance of 3.772 (2) Å and an interplanar distance of 3.546 (3) Å resulting in a slippage of 1.286 (3) Å (Cg is the centroid of the C14–C19 phenyl ring).

### S2. Experimental

*N*-ethyl-6-(4-methoxyphenoxy)pyridin-2-amine (0.23 g, 1 mmol) and amide (0.12 g, 1 mmol) successively added to Al$^{3+}$– Y in xylene at 145°C. After stirring for 16 h, the mixture was diluted with dichloromethane. After removing the catalyst by filtration, followed by solvent evaporation, the resulting crude product was finally purified by column chromatography (silica gel). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution of the title compound in ethylacetate at room temperature.

### S3. Refinement

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with C—H distances fixed in the range 0.93–0.97 Å with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H 1.2$U_{eq}(C)$ for other H atoms.
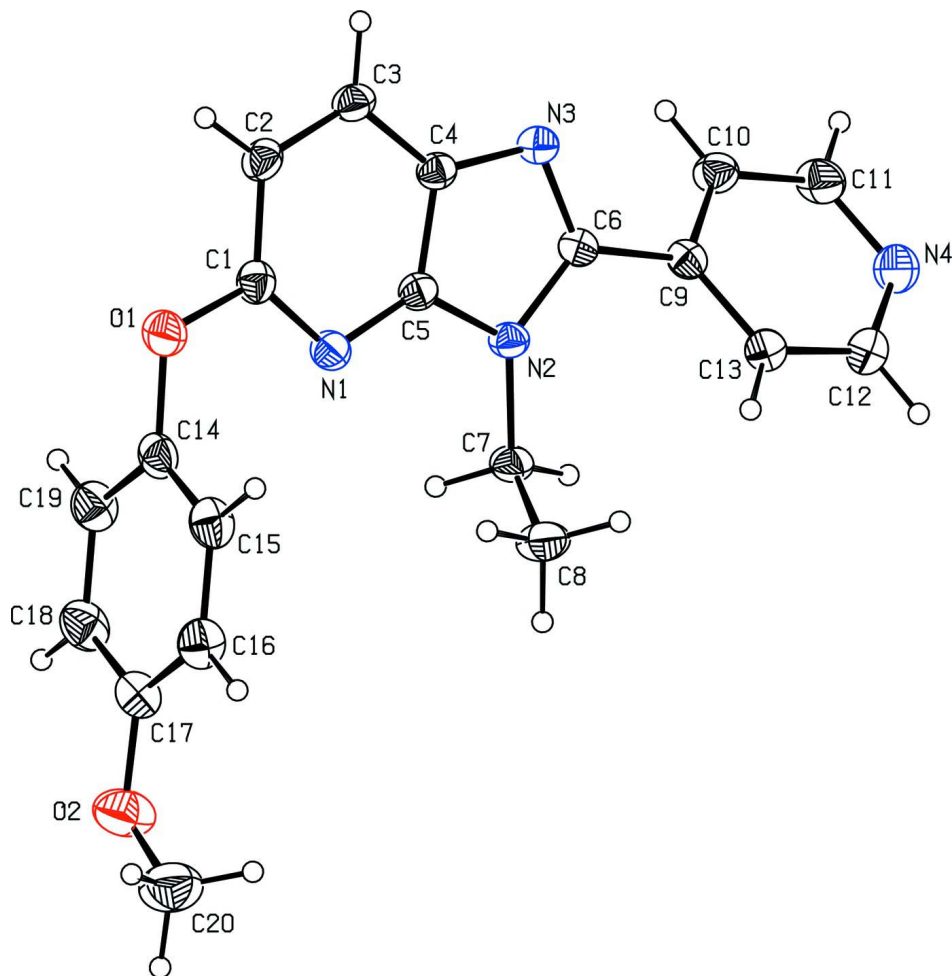
**Figure 1**

The structure of showing the atom-numbering scheme. The displacement ellipsoids are drawn at the 30% probability level.

**3-Ethyl-5-(4-methoxyphenoxy)-2-(pyridin-4-yl)-3*H*- imidazo[4,5-*b*]pyridine**

*Crystal data*

| | |
|---|---|
| $C_{20}H_{18}N_4O_2$ | $F(000) = 728$ |
| $M_r = 346.38$ | $D_x = 1.335$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 5887 reflections |
| $a = 13.6591$ (4) Å | $\theta = 1.5–32.0°$ |
| $b = 13.7104$ (4) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 9.3177$ (2) Å | $T = 293$ K |
| $\beta = 98.940$ (1)° | Block, white crystalline |
| $V = 1723.74$ (8) Å$^3$ | $0.25 \times 0.22 \times 0.19$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | Graphite monochromator |
| Radiation source: fine-focus sealed tube | Detector resolution: 10.0 pixels mm$^{-1}$ |
| | $\omega$ and $\varphi$ scans |

Absorption correction: multi-scan
  (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.981$, $T_{max} = 0.985$
24827 measured reflections
5887 independent reflections
3938 reflections with $I > 2\sigma(I)$

$R_{int} = 0.027$
$\theta_{max} = 32.1°$, $\theta_{min} = 1.5°$
$h = -20 \rightarrow 20$
$k = -20 \rightarrow 20$
$l = -13 \rightarrow 12$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.140$
$S = 1.00$
5887 reflections
237 parameters
0 restraints
Primary atom site location: structure-invariant
  direct methods

Secondary atom site location: difference Fourier
  map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.2334P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.20$ 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 (Å$^2$)*

|      | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|------|-----|-----|-----|---------------------|
| C1   | 0.34424 (9)  | 0.10472 (9)   | 0.42615 (13) | 0.0383 (3) |
| C2   | 0.34457 (9)  | 0.18018 (9)   | 0.52777 (14) | 0.0406 (3) |
| H2   | 0.3850       | 0.2344        | 0.5240       | 0.049*     |
| C3   | 0.28465 (9)  | 0.17335 (9)   | 0.63296 (13) | 0.0389 (3) |
| H3   | 0.2834       | 0.2222        | 0.7020       | 0.047*     |
| C4   | 0.22585 (8)  | 0.09028 (8)   | 0.63192 (12) | 0.0335 (2) |
| C5   | 0.23419 (8)  | 0.02078 (8)   | 0.52553 (12) | 0.0330 (2) |
| C6   | 0.12671 (8)  | −0.02604 (8)  | 0.66320 (12) | 0.0332 (2) |
| C7   | 0.16889 (10) | −0.14643 (8)  | 0.46766 (13) | 0.0403 (3) |
| H7A  | 0.1356       | −0.1952       | 0.5182       | 0.048*     |
| H7B  | 0.2363       | −0.1683       | 0.4670       | 0.048*     |
| C8   | 0.11655 (12) | −0.13785 (11) | 0.31346 (15) | 0.0547 (4) |
| H8A  | 0.0490       | −0.1186       | 0.3137       | 0.082*     |
| H8B  | 0.1181       | −0.1997       | 0.2655       | 0.082*     |
| H8C  | 0.1493       | −0.0897       | 0.2629       | 0.082*     |
| C9   | 0.05197 (8)  | −0.08407 (8)  | 0.72257 (12) | 0.0341 (2) |
| C10  | 0.05089 (10) | −0.08248 (9)  | 0.87147 (13) | 0.0427 (3) |
| H10  | 0.0986       | −0.0476       | 0.9329       | 0.051*     |
| C11  | −0.02193 (11)| −0.13343 (10) | 0.92665 (15) | 0.0500 (3) |

| | | | |
|---|---|---|---|
| H11 | −0.0225 | −0.1305 | 1.0262 | 0.060* |
| C12 | −0.08936 (10) | −0.18810 (10) | 0.70402 (15) | 0.0459 (3) |
| H12 | −0.1370 | −0.2251 | 0.6457 | 0.055* |
| C13 | −0.02073 (9) | −0.13820 (9) | 0.63755 (13) | 0.0386 (3) |
| H13 | −0.0233 | −0.1409 | 0.5373 | 0.046* |
| C14 | 0.40351 (9) | 0.04175 (9) | 0.22118 (14) | 0.0425 (3) |
| C15 | 0.33767 (10) | 0.04307 (10) | 0.09494 (15) | 0.0488 (3) |
| H15 | 0.2913 | 0.0930 | 0.0769 | 0.059* |
| C16 | 0.34062 (10) | −0.03057 (11) | −0.00606 (15) | 0.0508 (3) |
| H16 | 0.2964 | −0.0299 | −0.0927 | 0.061* |
| C17 | 0.40900 (10) | −0.10480 (10) | 0.02181 (15) | 0.0479 (3) |
| C18 | 0.47462 (11) | −0.10467 (11) | 0.14910 (16) | 0.0546 (4) |
| H18 | 0.5211 | −0.1544 | 0.1679 | 0.066* |
| C19 | 0.47204 (10) | −0.03162 (11) | 0.24862 (16) | 0.0512 (3) |
| H19 | 0.5167 | −0.0318 | 0.3348 | 0.061* |
| C20 | 0.35584 (16) | −0.18189 (16) | −0.2055 (2) | 0.0799 (5) |
| H20A | 0.2878 | −0.1767 | −0.1920 | 0.120* |
| H20B | 0.3653 | −0.2416 | −0.2555 | 0.120* |
| H20C | 0.3727 | −0.1276 | −0.2621 | 0.120* |
| N1 | 0.29165 (7) | 0.02406 (7) | 0.42238 (11) | 0.0374 (2) |
| N2 | 0.17080 (7) | −0.05379 (7) | 0.54614 (10) | 0.0340 (2) |
| N3 | 0.15774 (7) | 0.05932 (7) | 0.71772 (10) | 0.0357 (2) |
| N4 | −0.09155 (9) | −0.18655 (9) | 0.84645 (13) | 0.0512 (3) |
| O1 | 0.40353 (7) | 0.11775 (7) | 0.32231 (11) | 0.0511 (2) |
| O2 | 0.41700 (9) | −0.18162 (9) | −0.06945 (12) | 0.0716 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0354 (6) | 0.0366 (6) | 0.0433 (6) | −0.0005 (4) | 0.0079 (5) | 0.0034 (5) |
| C2 | 0.0382 (6) | 0.0315 (6) | 0.0517 (7) | −0.0044 (5) | 0.0052 (5) | −0.0009 (5) |
| C3 | 0.0407 (6) | 0.0313 (5) | 0.0433 (6) | −0.0008 (5) | 0.0022 (5) | −0.0056 (5) |
| C4 | 0.0353 (5) | 0.0304 (5) | 0.0338 (5) | 0.0009 (4) | 0.0027 (4) | −0.0008 (4) |
| C5 | 0.0350 (5) | 0.0299 (5) | 0.0338 (5) | 0.0000 (4) | 0.0042 (4) | 0.0004 (4) |
| C6 | 0.0364 (5) | 0.0316 (5) | 0.0318 (5) | 0.0020 (4) | 0.0057 (4) | 0.0008 (4) |
| C7 | 0.0471 (7) | 0.0287 (5) | 0.0468 (7) | −0.0017 (5) | 0.0128 (5) | −0.0070 (5) |
| C8 | 0.0681 (9) | 0.0502 (8) | 0.0454 (7) | −0.0077 (7) | 0.0075 (7) | −0.0135 (6) |
| C9 | 0.0375 (6) | 0.0297 (5) | 0.0360 (5) | 0.0038 (4) | 0.0084 (4) | 0.0031 (4) |
| C10 | 0.0508 (7) | 0.0416 (6) | 0.0365 (6) | −0.0059 (5) | 0.0091 (5) | −0.0021 (5) |
| C11 | 0.0647 (9) | 0.0483 (7) | 0.0403 (7) | −0.0071 (6) | 0.0187 (6) | 0.0014 (6) |
| C12 | 0.0408 (7) | 0.0469 (7) | 0.0496 (7) | −0.0049 (5) | 0.0064 (5) | 0.0004 (6) |
| C13 | 0.0394 (6) | 0.0402 (6) | 0.0357 (6) | 0.0012 (5) | 0.0044 (5) | 0.0025 (5) |
| C14 | 0.0419 (6) | 0.0421 (6) | 0.0470 (7) | −0.0027 (5) | 0.0181 (5) | 0.0038 (5) |
| C15 | 0.0454 (7) | 0.0443 (7) | 0.0571 (8) | 0.0077 (6) | 0.0097 (6) | 0.0095 (6) |
| C16 | 0.0489 (7) | 0.0559 (8) | 0.0462 (7) | 0.0039 (6) | 0.0025 (6) | 0.0070 (6) |
| C17 | 0.0490 (7) | 0.0491 (7) | 0.0473 (7) | 0.0052 (6) | 0.0129 (6) | 0.0019 (6) |
| C18 | 0.0499 (8) | 0.0579 (9) | 0.0554 (8) | 0.0177 (7) | 0.0060 (6) | 0.0030 (7) |
| C19 | 0.0466 (7) | 0.0594 (9) | 0.0468 (7) | 0.0080 (6) | 0.0045 (6) | 0.0042 (6) |

| C20 | 0.0881 (13) | 0.0854 (13) | 0.0627 (11) | 0.0002 (11) | 0.0005 (9) | −0.0198 (10) |
| N1 | 0.0399 (5) | 0.0342 (5) | 0.0396 (5) | −0.0011 (4) | 0.0109 (4) | −0.0010 (4) |
| N2 | 0.0402 (5) | 0.0285 (4) | 0.0342 (5) | −0.0025 (4) | 0.0085 (4) | −0.0030 (4) |
| N3 | 0.0396 (5) | 0.0329 (5) | 0.0346 (5) | 0.0001 (4) | 0.0060 (4) | −0.0017 (4) |
| N4 | 0.0538 (7) | 0.0511 (7) | 0.0517 (7) | −0.0089 (5) | 0.0174 (5) | 0.0016 (5) |
| O1 | 0.0557 (6) | 0.0447 (5) | 0.0585 (6) | −0.0112 (4) | 0.0262 (5) | −0.0036 (4) |
| O2 | 0.0796 (8) | 0.0689 (7) | 0.0634 (7) | 0.0212 (6) | 0.0021 (6) | −0.0142 (6) |

## Geometric parameters (Å, º)

| | | | |
|---|---|---|---|
| C1—N1 | 1.3161 (15) | C10—H10 | 0.9300 |
| C1—O1 | 1.3667 (14) | C11—N4 | 1.3312 (18) |
| C1—C2 | 1.4020 (17) | C11—H11 | 0.9300 |
| C2—C3 | 1.3744 (17) | C12—N4 | 1.3322 (17) |
| C2—H2 | 0.9300 | C12—C13 | 1.3823 (17) |
| C3—C4 | 1.3928 (16) | C12—H12 | 0.9300 |
| C3—H3 | 0.9300 | C13—H13 | 0.9300 |
| C4—N3 | 1.3842 (14) | C14—C15 | 1.365 (2) |
| C4—C5 | 1.3924 (15) | C14—C19 | 1.3708 (19) |
| C5—N1 | 1.3328 (14) | C14—O1 | 1.4048 (16) |
| C5—N2 | 1.3724 (14) | C15—C16 | 1.385 (2) |
| C6—N3 | 1.3192 (14) | C15—H15 | 0.9300 |
| C6—N2 | 1.3788 (13) | C16—C17 | 1.3784 (19) |
| C6—C9 | 1.4686 (15) | C16—H16 | 0.9300 |
| C7—N2 | 1.4638 (14) | C17—O2 | 1.3687 (17) |
| C7—C8 | 1.5066 (19) | C17—C18 | 1.371 (2) |
| C7—H7A | 0.9700 | C18—C19 | 1.369 (2) |
| C7—H7B | 0.9700 | C18—H18 | 0.9300 |
| C8—H8A | 0.9600 | C19—H19 | 0.9300 |
| C8—H8B | 0.9600 | C20—O2 | 1.406 (2) |
| C8—H8C | 0.9600 | C20—H20A | 0.9600 |
| C9—C13 | 1.3857 (17) | C20—H20B | 0.9600 |
| C9—C10 | 1.3899 (16) | C20—H20C | 0.9600 |
| C10—C11 | 1.3786 (18) | | |
| | | | |
| N1—C1—O1 | 118.16 (10) | N4—C12—C13 | 124.07 (13) |
| N1—C1—C2 | 125.63 (11) | N4—C12—H12 | 118.0 |
| O1—C1—C2 | 116.21 (10) | C13—C12—H12 | 118.0 |
| C3—C2—C1 | 119.44 (11) | C12—C13—C9 | 118.98 (11) |
| C3—C2—H2 | 120.3 | C12—C13—H13 | 120.5 |
| C1—C2—H2 | 120.3 | C9—C13—H13 | 120.5 |
| C2—C3—C4 | 117.22 (11) | C15—C14—C19 | 120.64 (13) |
| C2—C3—H3 | 121.4 | C15—C14—O1 | 119.97 (12) |
| C4—C3—H3 | 121.4 | C19—C14—O1 | 119.35 (13) |
| N3—C4—C5 | 109.76 (10) | C14—C15—C16 | 119.40 (13) |
| N3—C4—C3 | 133.26 (10) | C14—C15—H15 | 120.3 |
| C5—C4—C3 | 116.98 (10) | C16—C15—H15 | 120.3 |
| N1—C5—N2 | 125.53 (10) | C17—C16—C15 | 120.04 (13) |

| | | | |
|---|---|---|---|
| N1—C5—C4 | 127.79 (10) | C17—C16—H16 | 120.0 |
| N2—C5—C4 | 106.68 (9) | C15—C16—H16 | 120.0 |
| N3—C6—N2 | 113.32 (9) | O2—C17—C18 | 115.72 (12) |
| N3—C6—C9 | 122.41 (10) | O2—C17—C16 | 124.63 (13) |
| N2—C6—C9 | 124.27 (10) | C18—C17—C16 | 119.66 (13) |
| N2—C7—C8 | 112.19 (10) | C19—C18—C17 | 120.31 (13) |
| N2—C7—H7A | 109.2 | C19—C18—H18 | 119.8 |
| C8—C7—H7A | 109.2 | C17—C18—H18 | 119.8 |
| N2—C7—H7B | 109.2 | C18—C19—C14 | 119.94 (13) |
| C8—C7—H7B | 109.2 | C18—C19—H19 | 120.0 |
| H7A—C7—H7B | 107.9 | C14—C19—H19 | 120.0 |
| C7—C8—H8A | 109.5 | O2—C20—H20A | 109.5 |
| C7—C8—H8B | 109.5 | O2—C20—H20B | 109.5 |
| H8A—C8—H8B | 109.5 | H20A—C20—H20B | 109.5 |
| C7—C8—H8C | 109.5 | O2—C20—H20C | 109.5 |
| H8A—C8—H8C | 109.5 | H20A—C20—H20C | 109.5 |
| H8B—C8—H8C | 109.5 | H20B—C20—H20C | 109.5 |
| C13—C9—C10 | 117.46 (11) | C1—N1—C5 | 112.91 (10) |
| C13—C9—C6 | 123.59 (10) | C5—N2—C6 | 105.53 (9) |
| C10—C9—C6 | 118.91 (11) | C5—N2—C7 | 122.62 (9) |
| C11—C10—C9 | 118.99 (12) | C6—N2—C7 | 131.19 (9) |
| C11—C10—H10 | 120.5 | C6—N3—C4 | 104.72 (9) |
| C9—C10—H10 | 120.5 | C11—N4—C12 | 116.31 (11) |
| N4—C11—C10 | 124.17 (12) | C1—O1—C14 | 116.08 (9) |
| N4—C11—H11 | 117.9 | C17—O2—C20 | 117.96 (13) |
| C10—C11—H11 | 117.9 | | |
| | | | |
| N1—C1—C2—C3 | −1.3 (2) | O1—C14—C19—C18 | −178.17 (12) |
| O1—C1—C2—C3 | 178.21 (11) | O1—C1—N1—C5 | −177.83 (11) |
| C1—C2—C3—C4 | −0.17 (18) | C2—C1—N1—C5 | 1.63 (18) |
| C2—C3—C4—N3 | −179.45 (12) | N2—C5—N1—C1 | 179.15 (11) |
| C2—C3—C4—C5 | 0.96 (16) | C4—C5—N1—C1 | −0.73 (17) |
| N3—C4—C5—N1 | 179.77 (11) | N1—C5—N2—C6 | −179.62 (11) |
| C3—C4—C5—N1 | −0.54 (18) | C4—C5—N2—C6 | 0.28 (12) |
| N3—C4—C5—N2 | −0.12 (13) | N1—C5—N2—C7 | 8.72 (18) |
| C3—C4—C5—N2 | 179.56 (10) | C4—C5—N2—C7 | −171.38 (10) |
| N3—C6—C9—C13 | 142.45 (12) | N3—C6—N2—C5 | −0.36 (13) |
| N2—C6—C9—C13 | −37.09 (17) | C9—C6—N2—C5 | 179.21 (10) |
| N3—C6—C9—C10 | −35.08 (17) | N3—C6—N2—C7 | 170.30 (11) |
| N2—C6—C9—C10 | 145.39 (12) | C9—C6—N2—C7 | −10.13 (19) |
| C13—C9—C10—C11 | −0.54 (19) | C8—C7—N2—C5 | −76.72 (15) |
| C6—C9—C10—C11 | 177.14 (12) | C8—C7—N2—C6 | 113.98 (14) |
| C9—C10—C11—N4 | 1.3 (2) | N2—C6—N3—C4 | 0.28 (13) |
| N4—C12—C13—C9 | 1.1 (2) | C9—C6—N3—C4 | −179.30 (10) |
| C10—C9—C13—C12 | −0.60 (17) | C5—C4—N3—C6 | −0.09 (13) |
| C6—C9—C13—C12 | −178.16 (11) | C3—C4—N3—C6 | −179.70 (13) |
| C19—C14—C15—C16 | −0.1 (2) | C10—C11—N4—C12 | −0.8 (2) |
| O1—C14—C15—C16 | 177.83 (11) | C13—C12—N4—C11 | −0.4 (2) |

| | | | |
|---|---|---|---|
| C14—C15—C16—C17 | 0.6 (2) | N1—C1—O1—C14 | −0.86 (17) |
| C15—C16—C17—O2 | 178.89 (13) | C2—C1—O1—C14 | 179.63 (11) |
| C15—C16—C17—C18 | −0.7 (2) | C15—C14—O1—C1 | 90.64 (14) |
| O2—C17—C18—C19 | −179.25 (14) | C19—C14—O1—C1 | −91.40 (14) |
| C16—C17—C18—C19 | 0.4 (2) | C18—C17—O2—C20 | −175.90 (15) |
| C17—C18—C19—C14 | 0.1 (2) | C16—C17—O2—C20 | 4.5 (2) |
| C15—C14—C19—C18 | −0.2 (2) | | |