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# 1-[(*Z*)-(5-Methyl-2-pyridyl)iminiomethyl]-2-naphtholate

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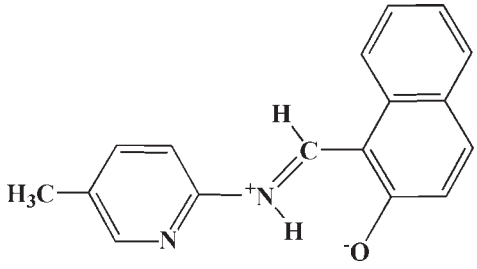
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.038; $wR$ factor = 0.109; data-to-parameter ratio = 9.1.

In the zwitterionic title compound, $C_{17}H_{14}N_2O$, the dihedral angle between the naphthalene and pyridine ring systems is 3.56 (9)° and an intramolecular N—H···O hydrogen bond generates an $S$(6) ring. In the crystal, molecules are linked by C—H···O interactions.

## Related literature

For a related structure, see: Eltayeb *et al.* (2007).



## Experimental

### Crystal data

$C_{17}H_{14}N_2O$
$M_r$ = 262.30
Monoclinic, $P2_1$
$a$ = 4.8703 (2) Å
$b$ = 9.5525 (5) Å
$c$ = 14.0804 (6) Å
$\beta$ = 98.353 (2)°
$V$ = 648.12 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
0.47 × 0.10 × 0.09 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.961, $T_{max}$ = 0.992
6930 measured reflections
1660 independent reflections
1321 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.109
$S$ = 0.98
1660 reflections
182 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 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···$A$ |
|---|---|---|---|---|
| N2—H2···O1 | 0.86 | 1.89 | 2.571 (3) | 135 |
| C3—H3···O1$^{i}$ | 0.93 | 2.46 | 3.346 (3) | 159 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5298).

## References

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Eltayeb, N. E., Teoh, S. G., Teh, J. B.-J., Fun, H.-K. & Ibrahim, K. (2007). *Acta Cryst.* E**63**, o117–o119.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2010). E**66**, o309 [https://doi.org/10.1107/S1600536810000346]

## 1-[(*Z*)-(5-Methyl-2-pyridyl)iminiomethyl]-2-naphtholate

**Xin-Yu Liu, Yu-Hua Fan, Qiang Wang, Cai-Feng Bi and Yu-Fang Wang**

### S1. Comment

One similar compound as 1-{2-[(2-hydroxy-1-naphthyl)methyleneamino] phenyliminiomethyl}-2-naphtholate methanol hemisolvate has been synthesized and characterized by X-ray diffraction (Eltayeb *et al.*, 2007). We now report on the title compound, (I), whose structure was determined by X-ray diffraction (Fig. 1).

This compound, which has a non-planar molecular structure, contains two aromatic rings linked through a imine group. The dihedral angle between the two aromatic rings C2—C3—C4—C5—N1—C6 and C8—C9—C14—C15—C16—C17 is 3.46(0.16)°. Intramolecular N—H···O hydrogen bonds are observed in the molecular structure, similar to those reported structure (Eltayeb *et al.*, 2007). The molecules is formed a one-dimensional zigzag chain through intermolecular C—H···O hydrogen bonds, which make the molecule more stabile.

As seen in Fig. 2, the molecules are linked into a one-dimensional chain by intermolecular C—H···O hydrogen bonds (Table 2).

### S2. Experimental

2-Hydroxy-1-naphthaldehyde (1 mmol, 172.2 mg) were added with stirring to anhydrous ethanol (30 ml) to make a solution. It was slowly dropped into the anhydrous ethanol solution (15 ml) containing (1 mmol, 108.1 mg) 5-methyl-pyridin-2-amine at 339 K and mixture was stirred at 339 K for 4 h, a mass of deep yellow grain was separated out. The product was collected by filtration and washed several times with anhydrous ethanol and dried under vacuum. Yellow needles of (I) were obtained by slow evaporation at room temperature from anhydrous ethanol solution after 4 days.

### S3. Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement. All H-atoms were positioned geometrically (C—H = 0.93–0.96Å, N—H = 0.86Å) and refined as riding with $U_{iso}$(H) =1.2$U_{eq}$(carrier).

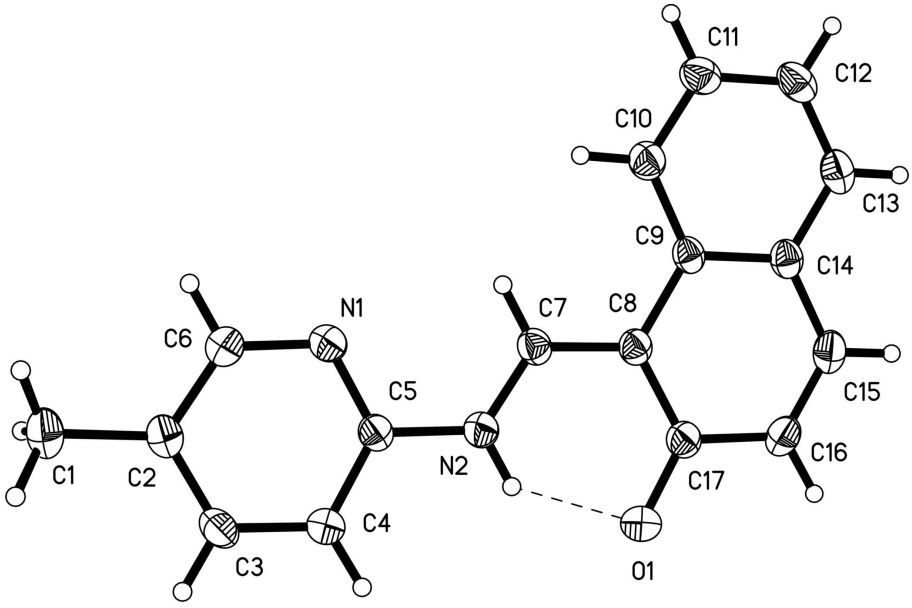


**Figure 1**

The structure of (I) showing 30% probability displacement ellipsoids.

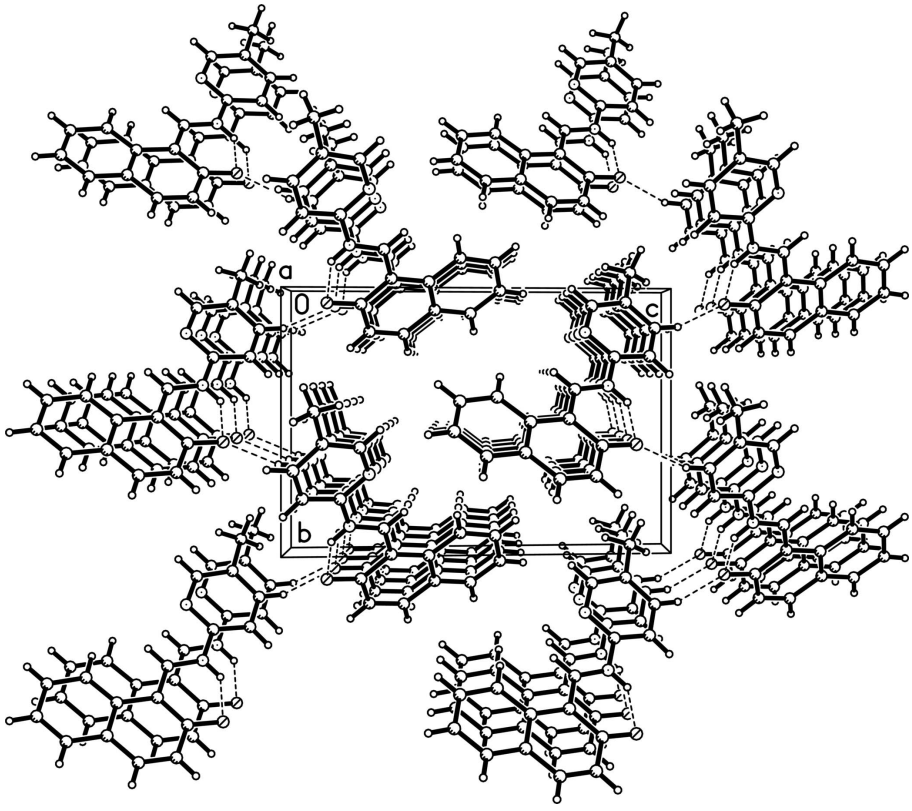


**Figure 2**

The crystal packing of (I), viewed approximately along the *a* axis.

**1-[(*Z*)-(5-Methyl-2-pyridyl)iminiomethyl]-2-naphtholate**

*Crystal data*

$C_{17}H_{14}N_2O$
$M_r = 262.30$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 4.8703$ (2) Å
$b = 9.5525$ (5) Å
$c = 14.0804$ (6) Å
$\beta = 98.353$ (2)°
$V = 648.12$ (5) Å$^3$
$Z = 2$
$F(000) = 276$
$D_x = 1.344$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1877 reflections
$\theta = 2.6$–25.6°
$\mu = 0.09$ mm$^{-1}$
$T = 296$ K
Needle, yellow
0.47 × 0.10 × 0.09 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.961$, $T_{max} = 0.992$
6930 measured reflections
1660 independent reflections
1321 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 28.1°$, $\theta_{min} = 2.6°$
$h = -6 \rightarrow 6$
$k = -12 \rightarrow 11$
$l = -18 \rightarrow 15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.109$
$S = 0.98$
1660 reflections
182 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.0757P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å$^{-3}$
$\Delta\rho_{min} = -0.15$ 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 | −0.5458 (5) | −0.0508 (3) | 0.8827 (2) | 0.0561 (6) |
| H1A | −0.6558 | −0.0735 | 0.8224 | 0.084* |
| H1B | −0.6646 | −0.0178 | 0.9266 | 0.084* |
| H1C | −0.4484 | −0.1328 | 0.9086 | 0.084* |

| | | | | |
|---|---|---|---|---|
| C2 | −0.3401 (5) | 0.0616 (2) | 0.86752 (16) | 0.0431 (5) |
| C3 | −0.2411 (5) | 0.1558 (3) | 0.93834 (17) | 0.0518 (6) |
| H3 | −0.3011 | 0.1508 | 0.9980 | 0.062* |
| C4 | −0.0533 (5) | 0.2576 (3) | 0.92116 (16) | 0.0492 (6) |
| H4 | 0.0127 | 0.3223 | 0.9683 | 0.059* |
| C5 | 0.0341 (4) | 0.2610 (2) | 0.83229 (15) | 0.0382 (5) |
| C6 | −0.2414 (5) | 0.0762 (3) | 0.78108 (16) | 0.0478 (6) |
| H6 | −0.3082 | 0.0143 | 0.7322 | 0.057* |
| C7 | 0.3255 (4) | 0.3752 (2) | 0.73144 (15) | 0.0398 (5) |
| H7 | 0.2584 | 0.3151 | 0.6815 | 0.048* |
| C8 | 0.5254 (4) | 0.4749 (2) | 0.71574 (15) | 0.0383 (5) |
| C9 | 0.6227 (4) | 0.4846 (2) | 0.62325 (15) | 0.0371 (5) |
| C10 | 0.5226 (5) | 0.3996 (3) | 0.54463 (16) | 0.0468 (6) |
| H10 | 0.3905 | 0.3315 | 0.5518 | 0.056* |
| C11 | 0.6141 (5) | 0.4140 (3) | 0.45734 (16) | 0.0501 (6) |
| H11 | 0.5423 | 0.3566 | 0.4064 | 0.060* |
| C12 | 0.8133 (5) | 0.5138 (3) | 0.44477 (17) | 0.0525 (6) |
| H12 | 0.8743 | 0.5238 | 0.3855 | 0.063* |
| C13 | 0.9182 (5) | 0.5968 (3) | 0.51987 (18) | 0.0510 (6) |
| H13 | 1.0539 | 0.6623 | 0.5116 | 0.061* |
| C14 | 0.8257 (4) | 0.5857 (2) | 0.60997 (16) | 0.0413 (5) |
| C15 | 0.9323 (5) | 0.6740 (3) | 0.68904 (18) | 0.0499 (6) |
| H15 | 1.0677 | 0.7395 | 0.6804 | 0.060* |
| C16 | 0.8457 (5) | 0.6663 (3) | 0.77458 (18) | 0.0484 (6) |
| H16 | 0.9224 | 0.7259 | 0.8236 | 0.058* |
| C17 | 0.6352 (5) | 0.5673 (2) | 0.79247 (16) | 0.0430 (5) |
| N1 | −0.0571 (4) | 0.1724 (2) | 0.76194 (13) | 0.0462 (5) |
| N2 | 0.2284 (4) | 0.3625 (2) | 0.81358 (13) | 0.0424 (4) |
| H2 | 0.2877 | 0.4203 | 0.8588 | 0.051* |
| O1 | 0.5562 (4) | 0.5643 (2) | 0.87507 (11) | 0.0567 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0517 (14) | 0.0467 (15) | 0.0725 (16) | −0.0048 (12) | 0.0176 (12) | 0.0080 (13) |
| C2 | 0.0391 (10) | 0.0397 (12) | 0.0520 (12) | 0.0037 (10) | 0.0115 (9) | 0.0067 (11) |
| C3 | 0.0604 (14) | 0.0536 (15) | 0.0459 (12) | −0.0031 (13) | 0.0230 (11) | 0.0044 (12) |
| C4 | 0.0581 (14) | 0.0484 (14) | 0.0438 (12) | −0.0078 (12) | 0.0163 (10) | −0.0060 (11) |
| C5 | 0.0403 (10) | 0.0341 (11) | 0.0416 (11) | 0.0036 (9) | 0.0108 (8) | 0.0026 (9) |
| C6 | 0.0525 (13) | 0.0435 (13) | 0.0478 (12) | −0.0049 (11) | 0.0081 (10) | −0.0027 (11) |
| C7 | 0.0436 (11) | 0.0356 (11) | 0.0418 (11) | 0.0025 (9) | 0.0116 (8) | 0.0036 (9) |
| C8 | 0.0411 (10) | 0.0322 (11) | 0.0429 (11) | 0.0033 (9) | 0.0106 (8) | 0.0024 (9) |
| C9 | 0.0370 (10) | 0.0337 (11) | 0.0421 (10) | 0.0038 (9) | 0.0103 (8) | 0.0058 (9) |
| C10 | 0.0496 (13) | 0.0447 (14) | 0.0481 (12) | −0.0016 (11) | 0.0136 (10) | 0.0000 (11) |
| C11 | 0.0555 (14) | 0.0529 (15) | 0.0437 (12) | 0.0054 (12) | 0.0135 (10) | −0.0005 (11) |
| C12 | 0.0590 (14) | 0.0553 (15) | 0.0475 (13) | 0.0092 (12) | 0.0225 (10) | 0.0091 (11) |
| C13 | 0.0504 (13) | 0.0447 (14) | 0.0615 (15) | 0.0012 (11) | 0.0203 (11) | 0.0108 (12) |
| C14 | 0.0404 (11) | 0.0356 (12) | 0.0493 (12) | 0.0033 (10) | 0.0113 (9) | 0.0055 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 0.0486 (12) | 0.0385 (13) | 0.0645 (14) | −0.0057 (11) | 0.0145 (10) | 0.0025 (12) |
| C16 | 0.0508 (13) | 0.0365 (12) | 0.0582 (14) | −0.0035 (11) | 0.0086 (10) | −0.0055 (11) |
| C17 | 0.0492 (12) | 0.0356 (12) | 0.0460 (12) | 0.0033 (10) | 0.0125 (9) | 0.0016 (10) |
| N1 | 0.0536 (11) | 0.0441 (11) | 0.0430 (10) | −0.0029 (10) | 0.0146 (8) | −0.0014 (9) |
| N2 | 0.0497 (11) | 0.0370 (10) | 0.0425 (9) | −0.0017 (9) | 0.0134 (8) | −0.0010 (8) |
| O1 | 0.0721 (11) | 0.0548 (11) | 0.0463 (9) | −0.0073 (10) | 0.0187 (8) | −0.0083 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.504 (3) | C8—C9 | 1.452 (3) |
| C1—H1A | 0.9600 | C9—C10 | 1.402 (3) |
| C1—H1B | 0.9600 | C9—C14 | 1.413 (3) |
| C1—H1C | 0.9600 | C10—C11 | 1.374 (3) |
| C2—C3 | 1.377 (4) | C10—H10 | 0.9300 |
| C2—C6 | 1.379 (3) | C11—C12 | 1.390 (4) |
| C3—C4 | 1.380 (4) | C11—H11 | 0.9300 |
| C3—H3 | 0.9300 | C12—C13 | 1.360 (4) |
| C4—C5 | 1.379 (3) | C12—H12 | 0.9300 |
| C4—H4 | 0.9300 | C13—C14 | 1.410 (3) |
| C5—N1 | 1.329 (3) | C13—H13 | 0.9300 |
| C5—N2 | 1.407 (3) | C14—C15 | 1.433 (3) |
| C6—N1 | 1.339 (3) | C15—C16 | 1.335 (3) |
| C6—H6 | 0.9300 | C15—H15 | 0.9300 |
| C7—N2 | 1.317 (3) | C16—C17 | 1.444 (3) |
| C7—C8 | 1.402 (3) | C16—H16 | 0.9300 |
| C7—H7 | 0.9300 | C17—O1 | 1.277 (3) |
| C8—C17 | 1.436 (3) | N2—H2 | 0.8600 |
| | | | |
| C2—C1—H1A | 109.5 | C14—C9—C8 | 119.20 (19) |
| C2—C1—H1B | 109.5 | C11—C10—C9 | 121.8 (2) |
| H1A—C1—H1B | 109.5 | C11—C10—H10 | 119.1 |
| C2—C1—H1C | 109.5 | C9—C10—H10 | 119.1 |
| H1A—C1—H1C | 109.5 | C10—C11—C12 | 120.4 (2) |
| H1B—C1—H1C | 109.5 | C10—C11—H11 | 119.8 |
| C3—C2—C6 | 116.3 (2) | C12—C11—H11 | 119.8 |
| C3—C2—C1 | 122.3 (2) | C13—C12—C11 | 119.4 (2) |
| C6—C2—C1 | 121.5 (2) | C13—C12—H12 | 120.3 |
| C2—C3—C4 | 120.3 (2) | C11—C12—H12 | 120.3 |
| C2—C3—H3 | 119.8 | C12—C13—C14 | 121.5 (2) |
| C4—C3—H3 | 119.8 | C12—C13—H13 | 119.3 |
| C5—C4—C3 | 118.4 (2) | C14—C13—H13 | 119.3 |
| C5—C4—H4 | 120.8 | C13—C14—C9 | 119.4 (2) |
| C3—C4—H4 | 120.8 | C13—C14—C15 | 121.8 (2) |
| N1—C5—C4 | 123.2 (2) | C9—C14—C15 | 118.72 (19) |
| N1—C5—N2 | 117.42 (18) | C16—C15—C14 | 122.9 (2) |
| C4—C5—N2 | 119.4 (2) | C16—C15—H15 | 118.6 |
| N1—C6—C2 | 125.2 (2) | C14—C15—H15 | 118.6 |
| N1—C6—H6 | 117.4 | C15—C16—C17 | 121.3 (2) |

| | | | |
|---|---|---|---|
| C2—C6—H6 | 117.4 | C15—C16—H16 | 119.4 |
| N2—C7—C8 | 123.2 (2) | C17—C16—H16 | 119.4 |
| N2—C7—H7 | 118.4 | O1—C17—C8 | 122.9 (2) |
| C8—C7—H7 | 118.4 | O1—C17—C16 | 119.3 (2) |
| C7—C8—C17 | 119.32 (18) | C8—C17—C16 | 117.86 (19) |
| C7—C8—C9 | 120.61 (19) | C5—N1—C6 | 116.61 (19) |
| C17—C8—C9 | 120.07 (19) | C7—N2—C5 | 124.41 (19) |
| C10—C9—C14 | 117.45 (19) | C7—N2—H2 | 117.8 |
| C10—C9—C8 | 123.34 (19) | C5—N2—H2 | 117.8 |

| | | | |
|---|---|---|---|
| C6—C2—C3—C4 | −0.1 (4) | C10—C9—C14—C13 | 0.0 (3) |
| C1—C2—C3—C4 | −179.7 (2) | C8—C9—C14—C13 | −179.1 (2) |
| C2—C3—C4—C5 | −0.8 (4) | C10—C9—C14—C15 | −179.9 (2) |
| C3—C4—C5—N1 | 1.1 (4) | C8—C9—C14—C15 | 1.0 (3) |
| C3—C4—C5—N2 | −179.1 (2) | C13—C14—C15—C16 | 179.2 (2) |
| C3—C2—C6—N1 | 0.9 (4) | C9—C14—C15—C16 | −0.9 (4) |
| C1—C2—C6—N1 | −179.5 (2) | C14—C15—C16—C17 | −0.3 (4) |
| N2—C7—C8—C17 | 1.0 (3) | C7—C8—C17—O1 | −1.0 (3) |
| N2—C7—C8—C9 | −179.45 (19) | C9—C8—C17—O1 | 179.5 (2) |
| C7—C8—C9—C10 | 1.4 (3) | C7—C8—C17—C16 | 178.5 (2) |
| C17—C8—C9—C10 | −179.1 (2) | C9—C8—C17—C16 | −1.1 (3) |
| C7—C8—C9—C14 | −179.55 (19) | C15—C16—C17—O1 | −179.3 (2) |
| C17—C8—C9—C14 | 0.0 (3) | C15—C16—C17—C8 | 1.2 (3) |
| C14—C9—C10—C11 | −0.8 (3) | C4—C5—N1—C6 | −0.3 (3) |
| C8—C9—C10—C11 | 178.3 (2) | N2—C5—N1—C6 | 179.8 (2) |
| C9—C10—C11—C12 | 0.6 (4) | C2—C6—N1—C5 | −0.7 (3) |
| C10—C11—C12—C13 | 0.4 (4) | C8—C7—N2—C5 | −178.1 (2) |
| C11—C12—C13—C14 | −1.2 (4) | N1—C5—N2—C7 | −0.1 (3) |
| C12—C13—C14—C9 | 1.0 (3) | C4—C5—N2—C7 | −180.0 (2) |
| C12—C13—C14—C15 | −179.1 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O1 | 0.86 | 1.89 | 2.571 (3) | 135 |
| C3—H3···O1$^{i}$ | 0.93 | 2.46 | 3.346 (3) | 159 |

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