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

# 2,5-Dimethyl-*N*-[1-(1*H*-pyrrol-2-yl)ethylidene]aniline

**Bi-Yun Su,[a]* Wen-Long Qin[b] and Jia-Xiang Wang[a]**

[a]College of Chemistry and Chemical Engineering, Xi'an ShiYou University, Xi'an, Shaanxi 710065, People's Republic of China, and [b]College of Petroleum Engineering, Xi'an ShiYou University, Xi'an, Shaanxi 710065, People's Republic of China
Correspondence e-mail: subiyun@xsyu.edu.cn

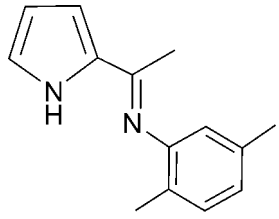
Received 21 September 2012; accepted 27 September 2012

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.045; $wR$ factor = 0.156; data-to-parameter ratio = 16.4.

In the title compound, $C_{14}H_{16}N_2$, the pyrrole and benzene rings form a dihedral angle of 72.37 (8)°. In the crystal, centrosymmetrically related molecules are assembled into dimers by by pairs of N—H···N hydrogen bonds, generating rings of $R_2^2(10)$ graph-set motif. C—H···$\pi$ interactions also occur.

## Related literature

For general background to the iminopyrrole unit, see: Britovsek *et al.* (2003); Dawson *et al.* (2000); Wu *et al.* (2003). For the pyrrole diimine unit, see: Matsuo *et al.* (2001) and for the pyrrole monoimine unit, see: He *et al.* (2009); Su *et al.* (2009*a*,*b*).



## Experimental

### Crystal data

$C_{14}H_{16}N_2$
$M_r$ = 212.29
Monoclinic, $P2_1/n$
$a$ = 12.5894 (17) Å
$b$ = 7.3109 (10) Å
$c$ = 14.8425 (19) Å
$\beta$ = 113.118 (2)°
$V$ = 1256.4 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 296 K
0.37 × 0.28 × 0.15 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.976, $T_{max}$ = 0.990
6463 measured reflections
2441 independent reflections
1885 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.156
$S$ = 0.96
2441 reflections
149 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

*Cg1* is the centroid of the C7–C12 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···N2$^{i}$ | 0.86 | 2.34 | 3.1354 (18) | 155 |
| C1—H1$A$···$Cg1^{i}$ | 0.93 | 2.65 | 3.4298 (16) | 142 |

Symmetry code: (i) $-x, -y+2, -z$.

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

This work was supported by the Natural Science Basic Research Plan of Shaanxi Province (No. 2009JQ2006) and the Scientific Research Plan Project of Shaanxi Education Department (Nos. 12 J K0620 and 2010 J K784).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5010).

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# supporting information

*Acta Cryst.* (2012). E**68**, o3088 [doi:10.1107/S1600536812040858]

## 2,5-Dimethyl-*N*-[1-(1*H*-pyrrol-2-yl)ethylidene]aniline

**Bi-Yun Su, Wen-Long Qin and Jia-Xiang Wang**

### S1. Comment

Bis(imino)pyrrole is usually prepared from Schiff bases condensation of 2,5-diacetylpyrrole and the aromatic amine (Matsuo *et al.*, 2001). Schiff bases containing pyrrole units have been extensively investigated because of their excellent and flexible coordination abilities (Wu *et al.*, 2003). As the five-memberd ring substitute of pyridine six-memberd ring (Matsuo *et al.*, 2001; He *et al.*, 2009), pyrrole has been frequently introduced into the skeleton of the bis(imino)pyridine ligand to design new ligands and corresponding metal complexes as catalysts of olefin polymerizations (Britovsek *et al.*, 2003; Dawson *et al.*, 2000). As a part of our studies on mono(imino)pyrrole ligands (Su *et al.*, 2009*a*,*b*), the crystal structure of the title compound is reported here.

The X-ray analysis of the title compound (Fig. 1) shows that the molecule is non-planar, with a dihedral angle of 72.37 (8)° formed by the pyrrole and benzene rings. The imino N—C bond length (1.288 (2) Å) indicates a C═N double bond character. In the crystal (Fig. 2), a pair of classical N–H···N hydrogen bonds (Table 1) link centrosymmetrically related molecules into a dimer, generating a ring of $R_2^2(10)$ graph-set motif. The dimer is further enforced by C—H···$\pi$ hydrogen interactions.

### S2. Experimental

The reagents 2-acetyl pyrrole (0.1528 g, 1.40 mmol) and 2,5-dimethylaniline (0.3393 g, 2.80 mmol) were placed in a 50-ml flask. A few drops of acetic acid was then added in, and the mixture was subjected to radiation in a 800 W microwave oven for 3 min and 2 min on a medium–heat setting. The reaction was monitored by TLC, and the crude product was purified by silica gel column chromatography (eluant: petroleum ether/ethyl acetate, 5:1 *v*/*v*). Plate-like colourless single crystals used in X-ray diffraction studies were grown from an ethanolic solution by slow evaporation of the solvent at room temperature; yield 72.79%, 0.2982 g. *M*.p. 396.8–398.4 K. The purity and the composition of the compound were checked and characterized by IR, $^1$H NMR, mass spectrum, as well as elemental analysis. IR (KBr): $\nu_{C=N}$ 1659 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ 7.12 (d, 1H, benzene ring aromatic H), $\delta$ 7.09 (d, 1H, benzene ring aromatic H), 6.88 (m, 1H, benzene ring aromatic H), 6.56 (d, 1H, pyrrole ring aromatic H), 6.37 (s, 1H, pyrrole ring aromatic H), 6.18 (d, 1H, pyrrole ring aromatic H), 2.18 (s, 6H, phenyl-$CH_3$), 2.05 (s, 3H, –N=C($CH_3$)-). MS (EI): m/*z* 212 (*M*). Anal. Calcd. for $C_{14}H_{16}N_2$: C, 79.21; H, 7.60; N, 13.20. Found: C, 79.72; H, 7.13; N, 12.84.

### S3. Refinement

All H atoms were placed at calculated positions and refined as riding, with C—H = 0.93–0.96 Å, N—H = 0.86 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C, N) or 1.5 $U_{eq}$(C) for methyl H atoms.

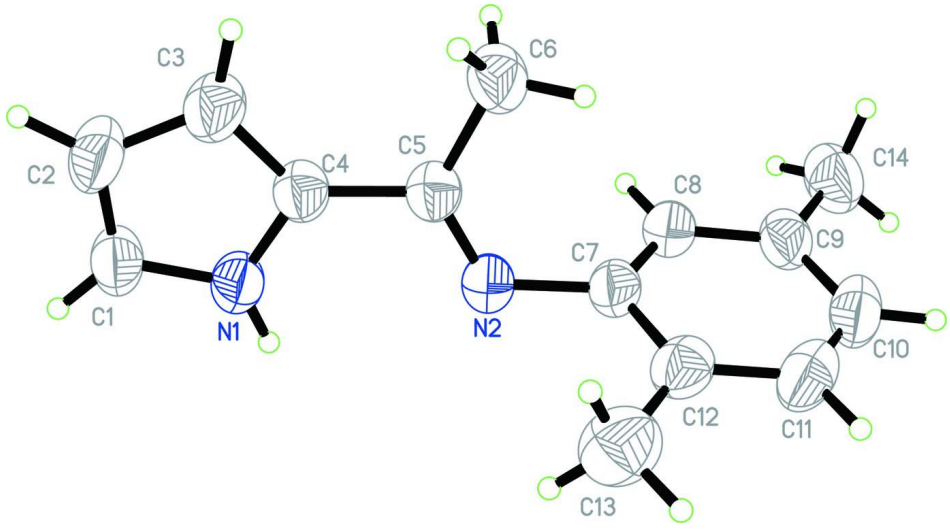


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

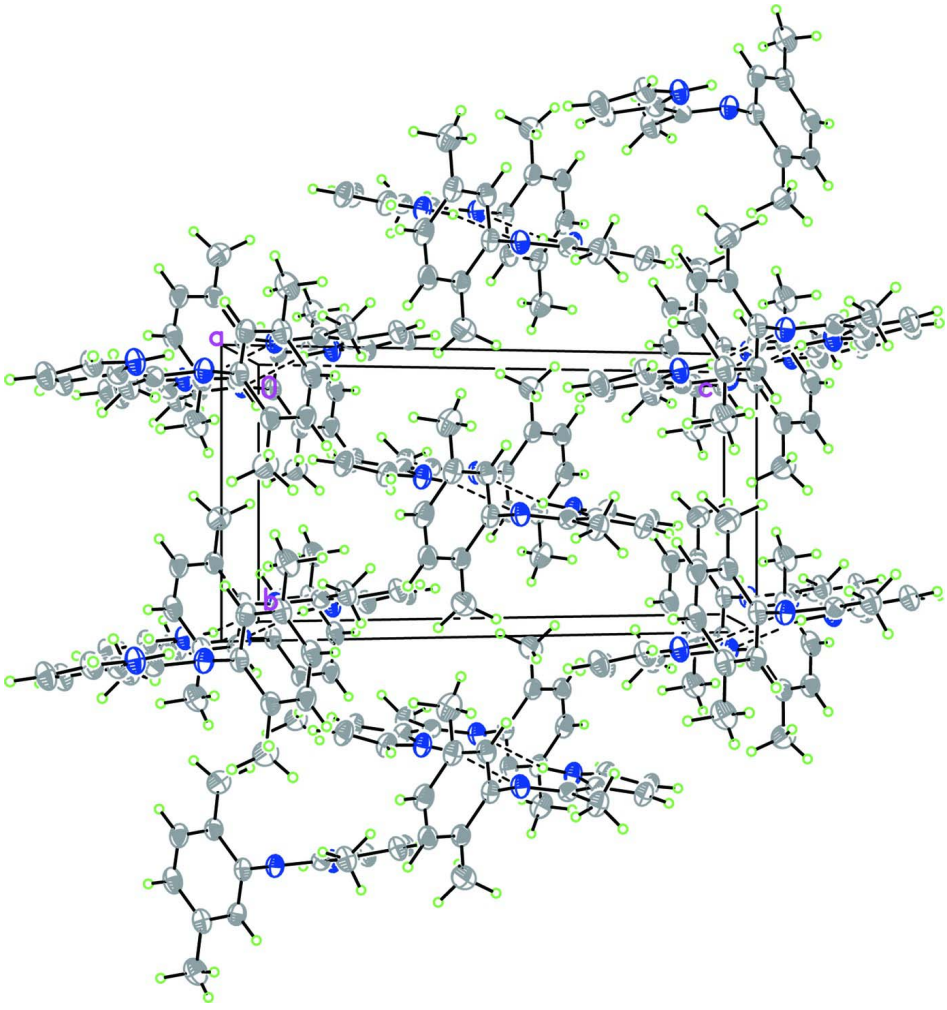

**Figure 2**

The crystal packing of the title compound viewed down the *a* axis, with hydrogen bond is shown as dashed lines.

### 2,5-Dimethyl-*N*-[1-(1*H*-pyrrol-2-yl)ethylidene]aniline

*Crystal data*

$C_{14}H_{16}N_2$
$M_r = 212.29$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.5894\ (17)$ Å
$b = 7.3109\ (10)$ Å
$c = 14.8425\ (19)$ Å
$\beta = 113.118\ (2)°$
$V = 1256.4\ (3)$ Å$^3$
$Z = 4$
$F(000) = 456$
$D_x = 1.122$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2093 reflections
$\theta = 2.7–26.0°$
$\mu = 0.07$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.37 × 0.28 × 0.15 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, 2008)
$T_{min}$ = 0.976, $T_{max}$ = 0.990
6463 measured reflections
2441 independent reflections
1885 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.021
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 2.7°
$h$ = −15→13
$k$ = −8→8
$l$ = −18→15

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.156
$S$ = 0.96
2441 reflections
149 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.1684P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.030 (5)

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.02765 (11) | 0.93936 (18) | 0.15136 (9) | 0.0509 (4) |
| H1 | −0.0111 | 0.9621 | 0.0903 | 0.061* |
| N2 | 0.16704 (11) | 0.92217 (17) | 0.04350 (9) | 0.0493 (4) |
| C1 | −0.01726 (14) | 0.9302 (2) | 0.22049 (12) | 0.0556 (5) |
| H1A | −0.0944 | 0.9481 | 0.2098 | 0.067* |
| C2 | 0.06832 (16) | 0.8908 (2) | 0.30727 (13) | 0.0606 (5) |
| H2 | 0.0608 | 0.8759 | 0.3667 | 0.073* |
| C3 | 0.17118 (15) | 0.8764 (2) | 0.29152 (12) | 0.0572 (5) |
| H3 | 0.2441 | 0.8510 | 0.3388 | 0.069* |
| C4 | 0.14446 (13) | 0.90679 (19) | 0.19355 (11) | 0.0447 (4) |
| C5 | 0.21617 (12) | 0.90262 (18) | 0.13711 (11) | 0.0429 (4) |
| C6 | 0.34366 (13) | 0.8754 (3) | 0.19343 (12) | 0.0584 (5) |
| H6A | 0.3790 | 0.8420 | 0.1491 | 0.088* |
| H6B | 0.3559 | 0.7799 | 0.2409 | 0.088* |
| H6C | 0.3774 | 0.9870 | 0.2263 | 0.088* |
| C7 | 0.23363 (12) | 0.9170 (2) | −0.01501 (11) | 0.0463 (4) |
| C8 | 0.29383 (12) | 1.0713 (2) | −0.02269 (11) | 0.0495 (4) |

| | | | | |
|---|---|---|---|---|
| H8 | 0.2956 | 1.1732 | 0.0154 | 0.059* |
| C9 | 0.35159 (13) | 1.0782 (2) | −0.08547 (12) | 0.0519 (4) |
| C10 | 0.34733 (15) | 0.9243 (2) | −0.14132 (12) | 0.0593 (5) |
| H10 | 0.3852 | 0.9247 | −0.1840 | 0.071* |
| C11 | 0.28748 (15) | 0.7705 (2) | −0.13432 (12) | 0.0596 (5) |
| H11 | 0.2865 | 0.6689 | −0.1723 | 0.072* |
| C12 | 0.22837 (14) | 0.7620 (2) | −0.07228 (11) | 0.0519 (4) |
| C13 | 0.41634 (15) | 1.2478 (3) | −0.09201 (14) | 0.0697 (6) |
| H13A | 0.4961 | 1.2359 | −0.0489 | 0.105* |
| H13B | 0.3837 | 1.3525 | −0.0733 | 0.105* |
| H13C | 0.4104 | 1.2630 | −0.1581 | 0.105* |
| C14 | 0.16000 (19) | 0.5964 (3) | −0.06737 (16) | 0.0763 (6) |
| H14A | 0.1561 | 0.5120 | −0.1181 | 0.115* |
| H14B | 0.0833 | 0.6330 | −0.0762 | 0.115* |
| H14C | 0.1969 | 0.5386 | −0.0047 | 0.115* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0432 (7) | 0.0719 (9) | 0.0400 (7) | 0.0059 (6) | 0.0191 (6) | 0.0070 (6) |
| N2 | 0.0423 (7) | 0.0664 (9) | 0.0424 (7) | 0.0002 (6) | 0.0202 (6) | −0.0022 (6) |
| C1 | 0.0489 (9) | 0.0738 (11) | 0.0523 (10) | 0.0075 (8) | 0.0288 (8) | 0.0091 (8) |
| C2 | 0.0652 (10) | 0.0790 (12) | 0.0473 (9) | 0.0149 (9) | 0.0326 (8) | 0.0163 (8) |
| C3 | 0.0541 (9) | 0.0734 (11) | 0.0453 (9) | 0.0149 (8) | 0.0209 (7) | 0.0138 (8) |
| C4 | 0.0438 (8) | 0.0480 (8) | 0.0448 (8) | 0.0050 (6) | 0.0201 (7) | 0.0048 (6) |
| C5 | 0.0433 (8) | 0.0435 (8) | 0.0443 (8) | 0.0028 (6) | 0.0199 (7) | 0.0018 (6) |
| C6 | 0.0464 (9) | 0.0780 (11) | 0.0532 (10) | 0.0155 (8) | 0.0224 (8) | 0.0126 (8) |
| C7 | 0.0386 (7) | 0.0633 (10) | 0.0379 (8) | 0.0077 (6) | 0.0160 (6) | 0.0014 (6) |
| C8 | 0.0434 (8) | 0.0631 (10) | 0.0434 (9) | 0.0018 (7) | 0.0186 (7) | −0.0037 (7) |
| C9 | 0.0407 (8) | 0.0717 (11) | 0.0447 (9) | 0.0111 (7) | 0.0182 (7) | 0.0096 (7) |
| C10 | 0.0574 (10) | 0.0814 (13) | 0.0470 (9) | 0.0206 (9) | 0.0290 (8) | 0.0107 (8) |
| C11 | 0.0686 (11) | 0.0677 (11) | 0.0442 (9) | 0.0206 (9) | 0.0240 (8) | −0.0019 (7) |
| C12 | 0.0515 (9) | 0.0592 (10) | 0.0417 (8) | 0.0093 (7) | 0.0146 (7) | 0.0018 (7) |
| C13 | 0.0578 (10) | 0.0887 (14) | 0.0699 (12) | −0.0006 (9) | 0.0330 (9) | 0.0152 (10) |
| C14 | 0.0877 (14) | 0.0680 (13) | 0.0735 (14) | −0.0043 (10) | 0.0318 (12) | −0.0063 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.3536 (19) | C7—C12 | 1.403 (2) |
| N1—C4 | 1.3742 (19) | C8—C9 | 1.390 (2) |
| N1—H1 | 0.8600 | C8—H8 | 0.9300 |
| N2—C5 | 1.288 (2) | C9—C10 | 1.386 (2) |
| N2—C7 | 1.4248 (18) | C9—C13 | 1.508 (2) |
| C1—C2 | 1.346 (2) | C10—C11 | 1.380 (2) |
| C1—H1A | 0.9300 | C10—H10 | 0.9300 |
| C2—C3 | 1.407 (2) | C11—C12 | 1.394 (2) |
| C2—H2 | 0.9300 | C11—H11 | 0.9300 |
| C3—C4 | 1.376 (2) | C12—C14 | 1.504 (2) |

| | | | |
|---|---|---|---|
| C3—H3 | 0.9300 | C13—H13A | 0.9600 |
| C4—C5 | 1.453 (2) | C13—H13B | 0.9600 |
| C5—C6 | 1.504 (2) | C13—H13C | 0.9600 |
| C6—H6A | 0.9600 | C14—H14A | 0.9600 |
| C6—H6B | 0.9600 | C14—H14B | 0.9600 |
| C6—H6C | 0.9600 | C14—H14C | 0.9600 |
| C7—C8 | 1.388 (2) | | |

| | | | |
|---|---|---|---|
| C1—N1—C4 | 109.68 (13) | C7—C8—C9 | 122.06 (14) |
| C1—N1—H1 | 125.2 | C7—C8—H8 | 119.0 |
| C4—N1—H1 | 125.2 | C9—C8—H8 | 119.0 |
| C5—N2—C7 | 120.42 (13) | C10—C9—C8 | 117.65 (15) |
| C2—C1—N1 | 108.68 (14) | C10—C9—C13 | 121.59 (15) |
| C2—C1—H1A | 125.7 | C8—C9—C13 | 120.75 (15) |
| N1—C1—H1A | 125.7 | C11—C10—C9 | 120.68 (15) |
| C1—C2—C3 | 107.46 (15) | C11—C10—H10 | 119.7 |
| C1—C2—H2 | 126.3 | C9—C10—H10 | 119.7 |
| C3—C2—H2 | 126.3 | C10—C11—C12 | 122.33 (15) |
| C4—C3—C2 | 107.72 (15) | C10—C11—H11 | 118.8 |
| C4—C3—H3 | 126.1 | C12—C11—H11 | 118.8 |
| C2—C3—H3 | 126.1 | C11—C12—C7 | 117.00 (15) |
| N1—C4—C3 | 106.46 (13) | C11—C12—C14 | 122.13 (15) |
| N1—C4—C5 | 122.47 (13) | C7—C12—C14 | 120.86 (14) |
| C3—C4—C5 | 131.04 (14) | C9—C13—H13A | 109.5 |
| N2—C5—C4 | 118.40 (13) | C9—C13—H13B | 109.5 |
| N2—C5—C6 | 124.76 (13) | H13A—C13—H13B | 109.5 |
| C4—C5—C6 | 116.83 (13) | C9—C13—H13C | 109.5 |
| C5—C6—H6A | 109.5 | H13A—C13—H13C | 109.5 |
| C5—C6—H6B | 109.5 | H13B—C13—H13C | 109.5 |
| H6A—C6—H6B | 109.5 | C12—C14—H14A | 109.5 |
| C5—C6—H6C | 109.5 | C12—C14—H14B | 109.5 |
| H6A—C6—H6C | 109.5 | H14A—C14—H14B | 109.5 |
| H6B—C6—H6C | 109.5 | C12—C14—H14C | 109.5 |
| C8—C7—C12 | 120.27 (14) | H14A—C14—H14C | 109.5 |
| C8—C7—N2 | 119.97 (13) | H14B—C14—H14C | 109.5 |
| C12—C7—N2 | 119.44 (13) | | |

| | | | |
|---|---|---|---|
| C4—N1—C1—C2 | −0.40 (19) | C5—N2—C7—C12 | 105.74 (16) |
| N1—C1—C2—C3 | 0.5 (2) | C12—C7—C8—C9 | −0.7 (2) |
| C1—C2—C3—C4 | −0.4 (2) | N2—C7—C8—C9 | −174.23 (13) |
| C1—N1—C4—C3 | 0.13 (17) | C7—C8—C9—C10 | 0.1 (2) |
| C1—N1—C4—C5 | 178.29 (13) | C7—C8—C9—C13 | −179.93 (15) |
| C2—C3—C4—N1 | 0.17 (18) | C8—C9—C10—C11 | 0.1 (2) |
| C2—C3—C4—C5 | −177.76 (15) | C13—C9—C10—C11 | −179.93 (15) |
| C7—N2—C5—C4 | −179.32 (12) | C9—C10—C11—C12 | 0.5 (3) |
| C7—N2—C5—C6 | 0.7 (2) | C10—C11—C12—C7 | −1.1 (2) |
| N1—C4—C5—N2 | −3.2 (2) | C10—C11—C12—C14 | 177.92 (16) |
| C3—C4—C5—N2 | 174.48 (16) | C8—C7—C12—C11 | 1.2 (2) |

| | | | |
|---|---|---|---|
| N1—C4—C5—C6 | 176.84 (14) | N2—C7—C12—C11 | 174.73 (13) |
| C3—C4—C5—C6 | −5.5 (2) | C8—C7—C12—C14 | −177.81 (15) |
| C5—N2—C7—C8 | −80.71 (18) | N2—C7—C12—C14 | −4.3 (2) |

*Hydrogen-bond geometry (Å, º)*

*Cg1* is the centroid of the C7–C12 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···N2$^{i}$ | 0.86 | 2.34 | 3.1354 (18) | 155 |
| C1—H1*A*···*Cg*1$^{i}$ | 0.93 | 2.65 | 3.4298 (16) | 142 |

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