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# 2-Amino-4-methylpyridinium 2-(3-methylphenyl)-acetate

P. Sivakumar,[a,b] S. Sudhahar,[c] S. Israel[d]* and G. Chakkaravarthi[b]*

[a]Research and Development Centre, Bharathiar University, Coimbatore 641 046, India, [b]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India, [c]Department of Physics, Alagappa University, Karaikkudi 630 003, India, and [d]Post graduate and Research Department of Physics, The American college, Madurai 625 002, India.
*Correspondence e-mail: israel.samuel@gmail.com, chakkaravarthi_2005@yahoo.com

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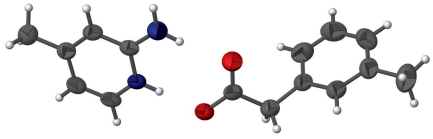
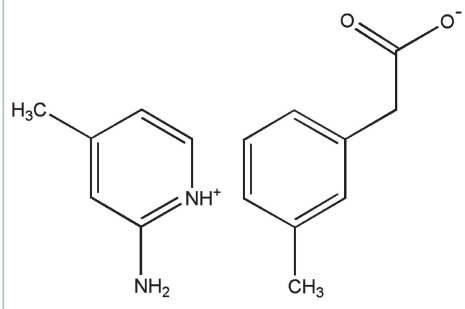
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title molecular salt, $C_6H_9N_2^+\cdot C_9H_9O_2^-$, the cation is protonated at the pyridine N atom and the anion is deprotonated at the hydroxy O atom. The dihedral angle between the benzene and pyridine rings is 66.58 (10)°. In the molecular structure, a pair of N—H···O hydrogen bonds links the anion and cation, generating an $R_2^2(8)$ ring motif. These ring motifs are connected to adjacent anions and cations *via* intermolecular N—H···O hydrogen bonding, generating a bifurcated $R_2^2(8)$ ring motif. C—H···O, C—H···$\pi$ and $\pi$–$\pi$ [centroid-to-centroid distances = 3.7053 (11) and 3.9547 (13) Å] interactions lead to the formation of a three-dimensional network.

**3D view**



**Chemical scheme**




## Structure description

Pyridine derivatives exhibit antifungal, anticancer and anti-inflammatory activities (Luo & Hu, 2006; Liu & Hu, 2002). We herein report the synthesis and the crystal structure of the title compound (Fig. 1). The geometric parameters are comparable with those reported for similar structures (Divya Bharathi *et al.*, 2015; Sivakumar *et al.*, 2016).

The asymmetric unit of (Fig. 1) consists of a 2-amino-4-methylpyridinium cation, which is protonated at atom N1, and a 3-methylphenylacetate anion, which is deprotonated at the hydroxy O atom. The dihedral angle between the benzene ring (C1–C6) and the pyridine ring (N2/C10–C14) is 66.58 (10)°. N1—H1···O1 and N2—H2*A*···O2 hydrogen bonds (Table 1) link the anion and cation, generating an $R_2^2(8)$ ring motif (Fig. 2). These ring motifs are connected with adjacent anions and cations *via* N2—H2*B*···O2$^{i}$ hydrogen bonds (Table 1), generating a bifurcated $R_2^2(8)$ ring motif (Fig. 2). Intermolecular C—H···O, C—H···$\pi$ (Table 1) and $\pi$–$\pi$ [*Cg*1···*Cg*1$^{i}$ = 3.9547 (13) Å; *Cg*2···*Cg*2 = 3.7053 (11) Å; symmetry odes: (i) $1-x, 2-y, 1-z$; (ii) $-x, 1-y, -z$; *Cg*1 and *Cg*2 are

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

*Cg*1 is the centroid of the C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1 | 0.88 (2) | 1.75 (2) | 2.627 (2) | 172 (2) |
| N2—H2*A*···O2 | 0.86 | 2.01 | 2.845 (2) | 163 |
| N2—H2*B*···O2$^{i}$ | 0.86 | 2.10 | 2.829 (2) | 142 |
| C14—H14···O1$^{ii}$ | 0.93 | 2.43 | 3.347 (2) | 168 |
| C11—H11···*Cg*1$^{i}$ | 0.93 | 2.81 | 3.706 (2) | 161 |

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

the centroids of the rings (C1–C6) and (N2/C10–C14), respectively] interactions lead to the formation of a three dimensional network (Fig. 3).

## Synthesis and crystallization

The title compound was synthesized using the raw materials *m*-tolylacetic acid (1.001 g) and 2-amino-4-methylpyridine (0.72 g) in an equimolar ratio. These reactants were dissolved in 15 ml acetone and kept for slow evaporation at room temperature. Crystals suitable for X-ray diffraction were harvested after two weeks.

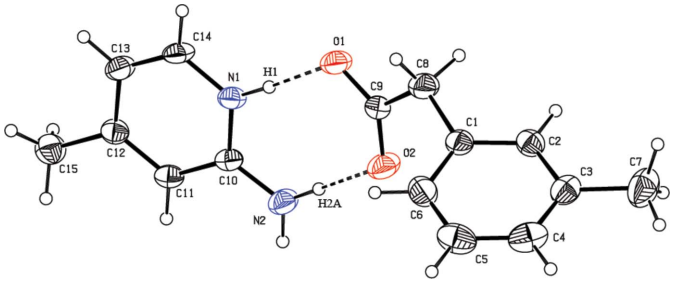



**Figure 1**
The molecular structure of the title molecular salt, showing the atom labelling and 30% probability displacement ellipsoids. Hydrogen bonds are shown as dashed lines.

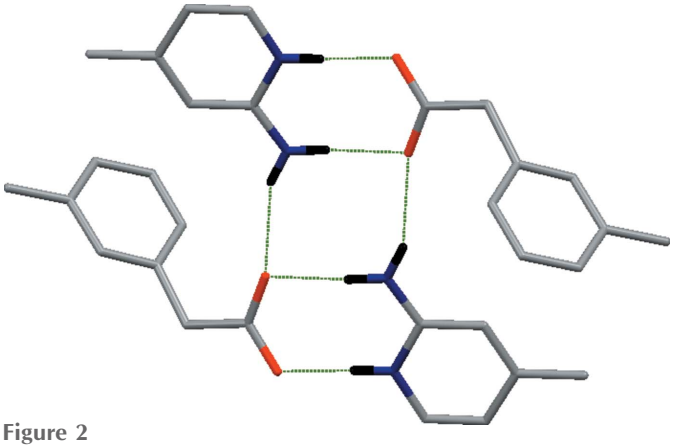


**Figure 2**
A partial view of the crystal packing of the title molecular salt, showing the ring graph-set motifs. Hydrogen bonds are shown as dashed lines and C-bound H atoms which are not involved in interactions have been omitted for clarity.

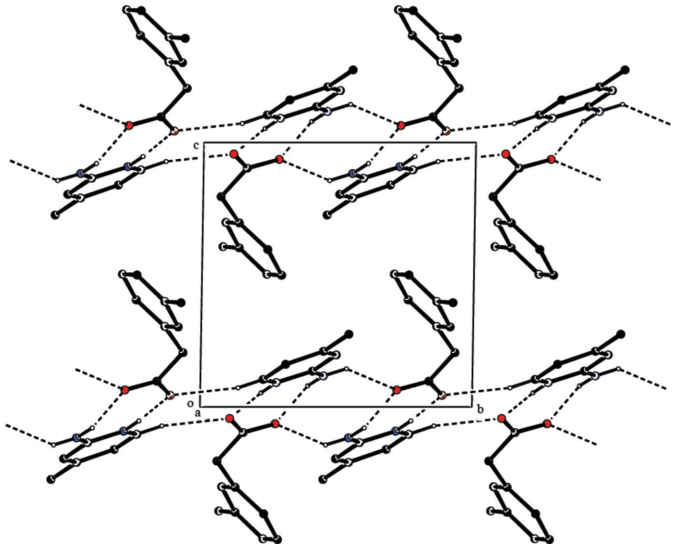



**Figure 3**
The crystal packing of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines and C-bound H atoms which are not involved in interactions have been omitted for clarity.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_6H_9N_2^+\cdot C_9H_9O_2^-$ |
| $M_r$ | 258.31 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 293 |
| *a*, *b*, *c* (Å) | 8.3253 (4), 9.5065 (5), 9.5909 (5) |
| $\alpha, \beta, \gamma$ (°) | 85.526 (3), 70.885 (3), 78.863 (3) |
| *V* (Å$^3$) | 703.62 (6) |
| *Z* | 2 |
| Radiation type | Mo *K*$\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.08 |
| Crystal size (mm) | 0.26 × 0.24 × 0.20 |
| | |
| Data collection | |
| Diffractometer | Bruker Kappa APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2004) |
| $T_{min}$, $T_{max}$ | 0.979, 0.984 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 15018, 3059, 1885 |
| $R_{int}$ | 0.035 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.641 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.050, 0.150, 1.02 |
| No. of reflections | 3059 |
| No. of parameters | 178 |
| No. of restraints | 2 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.22, −0.21 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

## Acknowledgements

The authors acknowledge the SAIF, IIT, Madras, for the data collection.

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# full crystallographic data

*IUCrData* (2016). **1**, x161098 [https://doi.org/10.1107/S2414314616010981]

## 2-Amino-4-methylpyridinium 2-(3-methylphenyl)acetate

**P. Sivakumar, S. Sudhahar, S. Israel and G. Chakkaravarthi**

### 2-Amino-4-methylpyridinium 2-(3-methylphenyl)acetate

*Crystal data*

$C_6H_9N_2^+·C_9H_9O_2^-$
$M_r$ = 258.31
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 8.3253 (4) Å
$b$ = 9.5065 (5) Å
$c$ = 9.5909 (5) Å
$\alpha$ = 85.526 (3)°
$\beta$ = 70.885 (3)°
$\gamma$ = 78.863 (3)°
$V$ = 703.62 (6) Å$^3$
$Z$ = 2
$F(000)$ = 276
$D_x$ = 1.219 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4380 reflections
$\theta$ = 2.2–27.0°
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 K
Block, colourless
0.26 × 0.24 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
$T_{min}$ = 0.979, $T_{max}$ = 0.984
15018 measured reflections
3059 independent reflections
1885 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035
$\theta_{max}$ = 27.1°, $\theta_{min}$ = 2.2°
$h$ = −10→10
$k$ = −12→12
$l$ = −12→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.150
$S$ = 1.02
3059 reflections
178 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
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.2177P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.4822 (2) | 0.8660 (2) | 0.3042 (2) | 0.0475 (5) |
| C2 | 0.6275 (3) | 0.9154 (2) | 0.3021 (2) | 0.0490 (5) |
| H2 | 0.6663 | 0.9857 | 0.2329 | 0.059* |
| C3 | 0.7182 (3) | 0.8647 (2) | 0.3985 (2) | 0.0558 (6) |
| C4 | 0.6600 (3) | 0.7610 (3) | 0.4989 (3) | 0.0699 (6) |
| H4 | 0.7180 | 0.7261 | 0.5659 | 0.084* |
| C5 | 0.5160 (4) | 0.7072 (3) | 0.5021 (3) | 0.0730 (7) |
| H5 | 0.4787 | 0.6356 | 0.5701 | 0.088* |
| C6 | 0.4279 (3) | 0.7596 (2) | 0.4047 (3) | 0.0619 (6) |
| H6 | 0.3312 | 0.7230 | 0.4069 | 0.074* |
| C7 | 0.8749 (3) | 0.9245 (3) | 0.3939 (3) | 0.0870 (9) |
| H7A | 0.8417 | 1.0247 | 0.4162 | 0.131* |
| H7B | 0.9586 | 0.9121 | 0.2973 | 0.131* |
| H7C | 0.9243 | 0.8747 | 0.4654 | 0.131* |
| C8 | 0.3800 (3) | 0.9344 (2) | 0.2050 (3) | 0.0600 (6) |
| H8A | 0.2665 | 0.9784 | 0.2672 | 0.072* |
| H8B | 0.4360 | 1.0111 | 0.1492 | 0.072* |
| C9 | 0.3557 (2) | 0.83992 (19) | 0.0971 (2) | 0.0458 (5) |
| C10 | 0.2100 (2) | 0.58859 (19) | −0.1350 (2) | 0.0409 (4) |
| C11 | 0.1335 (2) | 0.5018 (2) | −0.1964 (2) | 0.0443 (5) |
| H11 | 0.1923 | 0.4106 | −0.2283 | 0.053* |
| C12 | −0.0260 (2) | 0.5491 (2) | −0.2101 (2) | 0.0447 (5) |
| C13 | −0.1123 (3) | 0.6872 (2) | −0.1610 (2) | 0.0526 (5) |
| H13 | −0.2218 | 0.7217 | −0.1680 | 0.063* |
| C14 | −0.0352 (3) | 0.7693 (2) | −0.1038 (2) | 0.0524 (5) |
| H14 | −0.0921 | 0.8610 | −0.0720 | 0.063* |
| C15 | −0.1096 (3) | 0.4565 (2) | −0.2745 (3) | 0.0619 (6) |
| H15A | −0.0876 | 0.4791 | −0.3776 | 0.093* |
| H15B | −0.2320 | 0.4735 | −0.2246 | 0.093* |
| H15C | −0.0630 | 0.3575 | −0.2624 | 0.093* |
| N1 | 0.1233 (2) | 0.72080 (16) | −0.09179 (18) | 0.0446 (4) |
| N2 | 0.3643 (2) | 0.54781 (18) | −0.1174 (2) | 0.0547 (5) |
| H2A | 0.4059 | 0.6054 | −0.0794 | 0.066* |
| H2B | 0.4226 | 0.4638 | −0.1441 | 0.066* |
| O1 | 0.23722 (19) | 0.88996 (14) | 0.04377 (17) | 0.0591 (4) |

| | | | | |
|---|---|---|---|---|
| O2 | 0.45236 (18) | 0.72287 (15) | 0.06398 (18) | 0.0653 (5) |
| H1 | 0.170 (2) | 0.7762 (19) | −0.053 (2) | 0.056 (6)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0480 (11) | 0.0395 (10) | 0.0534 (12) | −0.0016 (9) | −0.0159 (9) | −0.0084 (9) |
| C2 | 0.0526 (11) | 0.0435 (11) | 0.0482 (12) | −0.0073 (9) | −0.0121 (9) | −0.0053 (9) |
| C3 | 0.0525 (12) | 0.0572 (13) | 0.0575 (14) | 0.0028 (10) | −0.0204 (10) | −0.0190 (11) |
| C4 | 0.0866 (15) | 0.0690 (16) | 0.0532 (14) | 0.0105 (12) | −0.0327 (13) | −0.0107 (12) |
| C5 | 0.0947 (17) | 0.0595 (14) | 0.0528 (14) | −0.0116 (12) | −0.0110 (13) | 0.0098 (12) |
| C6 | 0.0562 (13) | 0.0530 (13) | 0.0717 (16) | −0.0133 (10) | −0.0109 (11) | −0.0044 (12) |
| C7 | 0.0654 (15) | 0.096 (2) | 0.110 (2) | −0.0045 (14) | −0.0388 (15) | −0.0381 (17) |
| C8 | 0.0659 (13) | 0.0416 (11) | 0.0808 (16) | −0.0003 (10) | −0.0380 (12) | −0.0078 (11) |
| C9 | 0.0432 (10) | 0.0340 (10) | 0.0603 (13) | −0.0046 (8) | −0.0180 (10) | −0.0009 (9) |
| C10 | 0.0424 (10) | 0.0351 (10) | 0.0391 (10) | 0.0012 (8) | −0.0099 (8) | 0.0011 (8) |
| C11 | 0.0497 (11) | 0.0347 (10) | 0.0428 (11) | 0.0011 (8) | −0.0116 (9) | −0.0033 (8) |
| C12 | 0.0494 (11) | 0.0418 (11) | 0.0411 (11) | −0.0067 (9) | −0.0134 (9) | 0.0026 (8) |
| C13 | 0.0489 (11) | 0.0459 (11) | 0.0617 (14) | 0.0041 (9) | −0.0229 (10) | −0.0005 (10) |
| C14 | 0.0546 (12) | 0.0343 (10) | 0.0639 (14) | 0.0115 (9) | −0.0232 (10) | −0.0042 (9) |
| C15 | 0.0673 (14) | 0.0570 (13) | 0.0660 (15) | −0.0108 (11) | −0.0271 (12) | −0.0035 (11) |
| N1 | 0.0511 (9) | 0.0319 (8) | 0.0509 (10) | −0.0001 (7) | −0.0205 (8) | −0.0015 (7) |
| N2 | 0.0480 (9) | 0.0461 (10) | 0.0690 (12) | 0.0067 (7) | −0.0235 (9) | −0.0115 (8) |
| O1 | 0.0656 (9) | 0.0387 (8) | 0.0813 (11) | 0.0062 (7) | −0.0416 (8) | −0.0081 (7) |
| O2 | 0.0612 (9) | 0.0488 (9) | 0.0902 (12) | 0.0131 (7) | −0.0384 (8) | −0.0210 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.374 (3) | C9—O1 | 1.254 (2) |
| C1—C6 | 1.377 (3) | C10—N2 | 1.330 (2) |
| C1—C8 | 1.507 (3) | C10—N1 | 1.344 (2) |
| C2—C3 | 1.380 (3) | C10—C11 | 1.400 (3) |
| C2—H2 | 0.9300 | C11—C12 | 1.363 (2) |
| C3—C4 | 1.366 (3) | C11—H11 | 0.9300 |
| C3—C7 | 1.507 (3) | C12—C13 | 1.405 (3) |
| C4—C5 | 1.381 (4) | C12—C15 | 1.498 (3) |
| C4—H4 | 0.9300 | C13—C14 | 1.346 (3) |
| C5—C6 | 1.376 (3) | C13—H13 | 0.9300 |
| C5—H5 | 0.9300 | C14—N1 | 1.350 (2) |
| C6—H6 | 0.9300 | C14—H14 | 0.9300 |
| C7—H7A | 0.9600 | C15—H15A | 0.9600 |
| C7—H7B | 0.9600 | C15—H15B | 0.9600 |
| C7—H7C | 0.9600 | C15—H15C | 0.9600 |
| C8—C9 | 1.507 (3) | N1—H1 | 0.877 (9) |
| C8—H8A | 0.9700 | N2—H2A | 0.8600 |
| C8—H8B | 0.9700 | N2—H2B | 0.8600 |
| C9—O2 | 1.236 (2) | | |

| | | | |
|---|---|---|---|
| C2—C1—C6 | 118.3 (2) | O2—C9—O1 | 124.30 (18) |
| C2—C1—C8 | 120.02 (19) | O2—C9—C8 | 119.97 (17) |
| C6—C1—C8 | 121.54 (19) | O1—C9—C8 | 115.70 (16) |
| C1—C2—C3 | 122.6 (2) | N2—C10—N1 | 118.07 (17) |
| C1—C2—H2 | 118.7 | N2—C10—C11 | 123.63 (17) |
| C3—C2—H2 | 118.7 | N1—C10—C11 | 118.30 (16) |
| C4—C3—C2 | 118.0 (2) | C12—C11—C10 | 120.93 (17) |
| C4—C3—C7 | 121.4 (2) | C12—C11—H11 | 119.5 |
| C2—C3—C7 | 120.6 (2) | C10—C11—H11 | 119.5 |
| C3—C4—C5 | 120.9 (2) | C11—C12—C13 | 118.45 (18) |
| C3—C4—H4 | 119.6 | C11—C12—C15 | 121.33 (18) |
| C5—C4—H4 | 119.6 | C13—C12—C15 | 120.22 (18) |
| C6—C5—C4 | 120.0 (2) | C14—C13—C12 | 119.53 (18) |
| C6—C5—H5 | 120.0 | C14—C13—H13 | 120.2 |
| C4—C5—H5 | 120.0 | C12—C13—H13 | 120.2 |
| C5—C6—C1 | 120.2 (2) | C13—C14—N1 | 121.13 (18) |
| C5—C6—H6 | 119.9 | C13—C14—H14 | 119.4 |
| C1—C6—H6 | 119.9 | N1—C14—H14 | 119.4 |
| C3—C7—H7A | 109.5 | C12—C15—H15A | 109.5 |
| C3—C7—H7B | 109.5 | C12—C15—H15B | 109.5 |
| H7A—C7—H7B | 109.5 | H15A—C15—H15B | 109.5 |
| C3—C7—H7C | 109.5 | C12—C15—H15C | 109.5 |
| H7A—C7—H7C | 109.5 | H15A—C15—H15C | 109.5 |
| H7B—C7—H7C | 109.5 | H15B—C15—H15C | 109.5 |
| C9—C8—C1 | 117.78 (17) | C10—N1—C14 | 121.64 (17) |
| C9—C8—H8A | 107.9 | C10—N1—H1 | 119.1 (14) |
| C1—C8—H8A | 107.9 | C14—N1—H1 | 119.2 (13) |
| C9—C8—H8B | 107.9 | C10—N2—H2A | 120.0 |
| C1—C8—H8B | 107.9 | C10—N2—H2B | 120.0 |
| H8A—C8—H8B | 107.2 | H2A—N2—H2B | 120.0 |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −1.4 (3) | C1—C8—C9—O2 | −18.8 (3) |
| C8—C1—C2—C3 | 174.70 (19) | C1—C8—C9—O1 | 162.85 (19) |
| C1—C2—C3—C4 | 0.3 (3) | N2—C10—C11—C12 | 179.30 (18) |
| C1—C2—C3—C7 | −178.7 (2) | N1—C10—C11—C12 | −1.0 (3) |
| C2—C3—C4—C5 | 0.9 (3) | C10—C11—C12—C13 | 0.0 (3) |
| C7—C3—C4—C5 | 179.9 (2) | C10—C11—C12—C15 | −179.46 (18) |
| C3—C4—C5—C6 | −0.9 (4) | C11—C12—C13—C14 | 0.8 (3) |
| C4—C5—C6—C1 | −0.2 (4) | C15—C12—C13—C14 | −179.8 (2) |
| C2—C1—C6—C5 | 1.4 (3) | C12—C13—C14—N1 | −0.5 (3) |
| C8—C1—C6—C5 | −174.7 (2) | N2—C10—N1—C14 | −178.95 (18) |
| C2—C1—C8—C9 | 121.8 (2) | C11—C10—N1—C14 | 1.3 (3) |
| C6—C1—C8—C9 | −62.2 (3) | C13—C14—N1—C10 | −0.6 (3) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1 | 0.88 (2) | 1.75 (2) | 2.627 (2) | 172 (2) |
| N2—H2*A*···O2 | 0.86 | 2.01 | 2.845 (2) | 163 |
| N2—H2*B*···O2$^{i}$ | 0.86 | 2.10 | 2.829 (2) | 142 |
| C14—H14···O1$^{ii}$ | 0.93 | 2.43 | 3.347 (2) | 168 |
| C11—H11···*Cg*1$^{i}$ | 0.93 | 2.81 | 3.706 (2) | 161 |

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