# organic compounds

# N′-[(E)-1-(5-Chloro-2-hydroxyphenyl)-ethylidene]pyridine-3-carbohydrazide monohydrate

## Abid Hussain,[a] Zahid Shafiq,[a] M. Nawaz Tahir[b]* and Muhammad Yaqub[a]

[a]Department of Chemistry, Bahauddin Zakariya University, Multan 60800, Pakistan, and [b]Department of Physics, University of Sargodha, Sargodha, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

In the title compound, $C_{14}H_{12}ClN_3O_2 \cdot H_2O$, the benzene ring and the pyridine rings are oriented at a dihedral angle of 57.73 (12)° and an intramolecular O—H···N hydrogen bond generates an $S(6)$ ring. In the crystal, the water molecule forms O—H···O and O—H···N hydrogen bonds to the organic molecule, leading to chains containing $R_4^4(16)$ loops. In addition, weak aromatic $\pi$–$\pi$ stacking interactions between the centroids of pyridine rings [at distance of 3.864 (2) and 4.013 (2) Å] and C—H···$\pi$ interactions occur.

## Related literature

For background to Schiff bases and for related structures, see: Shafiq et al. (2009a,b): For graph-set notation, see: Bernstein et al. (1995).
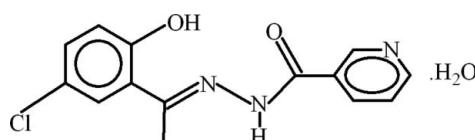


## Experimental

### Crystal data

| | |
|---|---|
| $C_{14}H_{12}ClN_3O_2 \cdot H_2O$ | $\gamma$ = 115.755 (2)° |
| $M_r$ = 307.73 | $V$ = 701.94 (8) Å³ |
| Triclinic, $P\bar{1}$ | $Z$ = 2 |
| $a$ = 7.1693 (5) Å | Mo $K\alpha$ radiation |
| $b$ = 7.4964 (4) Å | $\mu$ = 0.29 mm⁻¹ |
| $c$ = 14.5966 (9) Å | $T$ = 296 K |
| $\alpha$ = 90.138 (2)° | 0.28 × 0.18 × 0.14 mm |
| $\beta$ = 95.835 (1)° | |

### Data collection

| | |
|---|---|
| Bruker Kappa APEXII CCD diffractometer | 10105 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2005) | 2491 independent reflections |
| $T_{min}$ = 0.942, $T_{max}$ = 0.959 | 2151 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.027 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.047 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.135 | |
| $S$ = 1.17 | $\Delta\rho_{max}$ = 0.24 e Å⁻³ |
| 2491 reflections | $\Delta\rho_{min}$ = −0.35 e Å⁻³ |
| 198 parameters | |

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

$Cg2$ is the centroid of the C1–C6 phenyl ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.84 | 2.555 (3) | 144 |
| N2—H2···O3[i] | 0.86 | 2.06 | 2.898 (4) | 166 |
| O3—H3A···O2 | 0.89 (5) | 1.88 (5) | 2.760 (4) | 171 (3) |
| O3—H3B···N3[ii] | 0.91 (4) | 2.01 (4) | 2.885 (4) | 161 (4) |
| C8—H8A···$Cg2$[iii] | 0.96 | 2.99 | 3.763 (4) | 139 |

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); 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) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

## References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). Angew. Chem. Int. Ed. Engl. **34**, 1555–1573.
Bruker (2005). SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). J. Appl. Cryst. **30**, 565.
Farrugia, L. J. (1999). J. Appl. Cryst. **32**, 837–838.
Shafiq, Z., Yaqub, M., Tahir, M. N., Hussain, A. & Iqbal, M. S. (2009a). Acta Cryst. E**65**, o2496.
Shafiq, Z., Yaqub, M., Tahir, M. N., Hussain, A. & Iqbal, M. S. (2009b). Acta Cryst. E**65**, o2899.
Sheldrick, G. M. (2008). Acta Cryst. A**64**, 112–122.
Spek, A. L. (2009). Acta Cryst. D**65**, 148–155.

# supporting information

# *N*′-[(*E*)-1-(5-Chloro-2-hydroxyphenyl)ethylidene]pyridine-3-carbohydrazide monohydrate

## Abid Hussain, Zahid Shafiq, M. Nawaz Tahir and Muhammad Yaqub

### S1. Comment

We have reported crystal structures of Schiff bases containing pyridne (Shafiq *et al.*, 2009*a*, 2009*b*) and as a part of this project, we report herein the structure and synthesis of the title compound (I, Fig. 1).

In (I) the group A (C1–C8/O1/CL1) of 5-chloro-2-hydroxyacetophenone, the central group B (N1/N2/C9/O2) and the pyridine ring C (C10—C14/N3) are planar with r. m. s. deviation of 0.0330, 0.0182 and 0.0082 Å, respectively. The dihedral angle between A/B, A/C and B/C is 6.62 (11), 58.08 (10) and 52.98 (14)°, respectively. There exist intramolecular H-bonding of O—H···N type forming an S(6) ring motif (Bernstein *et al.*, 1995). The water molecule acts as donar as well as accepter and therefore interconnects three molecules. Due to intra as well as intermolecular H-bondings of O—H···O and O—H···N types (Table 1, Fig. 2), the title compound is stabilized in infinite one dimensional polymeric chains. In the polymeric chains $R_4^4(16)$ ring motifs are formed. The π–π interactions exist between the centroids of pyridine rings at distance of 3.864 (2) Å [symmetry: -*x*, -*y*, 1 - *z*] and at 4.013 (2) Å [symmetry: 1 - *x*, 1 - *y*, 1 - *z*]. The C—H···π interaction (Table 1) also plays an important role in stabilizing the structure.

### S2. Experimental

To a hot stirred solution of 5-chloro-2-hydroxyacetophenone (1.71 g, 0.01 mole) in ethanol, 25 ml nicotinic acid hydrazide (1.37 g, 0.01 mol) was added. The resultant mixture was then heated under reflux for 7–8 h. The reaction was monitored through TLC. The precipitate were formed were collected by suction filteration. The resultant crude material was dried and recrystalized in 1,4-dioxan:ethanol(1:2) to affaord light brown needles of (I).

### S3. Refinement

The coordinates of H-atoms of water molecule were refined. The H-atoms were positioned geometrically (O–H = 0.82, N–H = 0.86, C–H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C, N, O)$, where $x$ = 1.5 for methyl and $x$ = 1.2 for all other H-atoms.
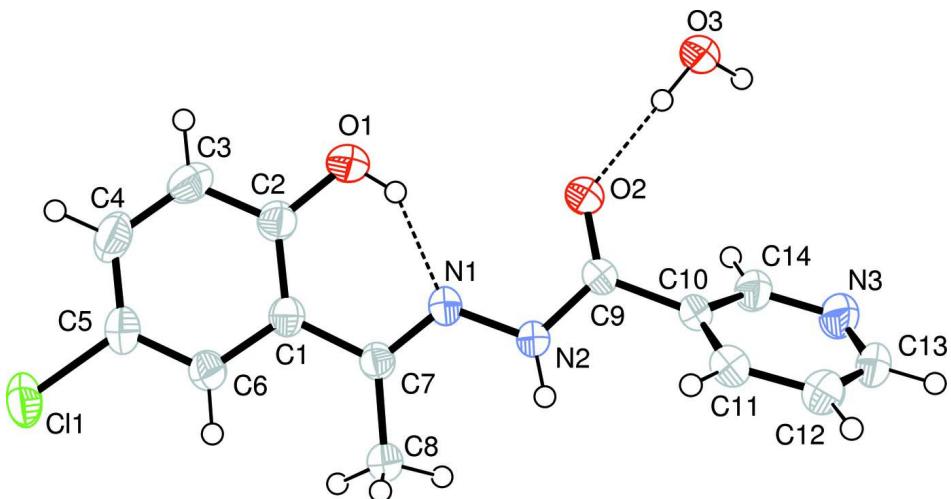
**Figure 1**

View of the title compound with displacement ellipsoids drawn at the 50% probability level. The dotted line shows the intramolecular H-bond.
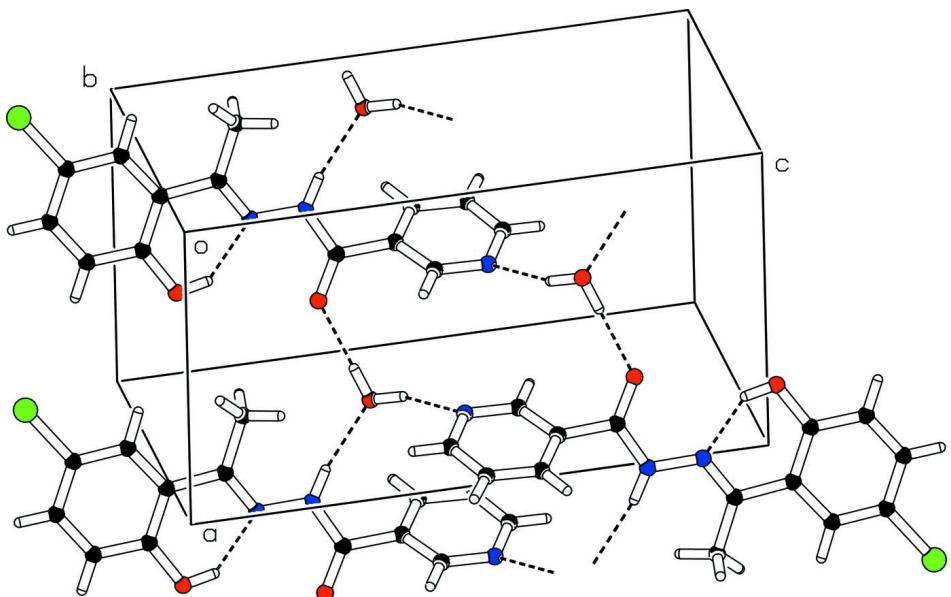


**Figure 2**

The partial packing of (I), which shows that molecules form infinite one dimensional polymeric chains with different ring motifs.

***N′*-[(*E*)-1-(5-Chloro-2-hydroxyphenyl)ethylidene]pyridine-3- carbohydrazide monohydrate**

*Crystal data*

| | |
|---|---|
| $C_{14}H_{12}ClN_3O_2 \cdot H_2O$ | $c = 14.5966$ (9) Å |
| $M_r = 307.73$ | $\alpha = 90.138$ (2)° |
| Triclinic, $P\overline{1}$ | $\beta = 95.835$ (1)° |
| Hall symbol: -P 1 | $\gamma = 115.755$ (2)° |
| $a = 7.1693$ (5) Å | $V = 701.94$ (8) Å³ |
| $b = 7.4964$ (4) Å | $Z = 2$ |

$F(000) = 320$
$D_x = 1.456$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1770 reflections
$\theta = 2.6–28.4°$

$\mu = 0.29$ mm$^{-1}$
$T = 296$ K
Needle, light brown
$0.28 \times 0.18 \times 0.14$ mm

*Data collection*

Bruker Kappa APEXII CCD
   diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.20 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan
   (*SADABS*; Bruker, 2005)
$T_{min} = 0.942$, $T_{max} = 0.959$

10105 measured reflections
2491 independent reflections
2151 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 25.3°$, $\theta_{min} = 2.8°$
$h = -8\rightarrow8$
$k = -8\rightarrow8$
$l = -16\rightarrow17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.135$
$S = 1.17$
2491 reflections
198 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 atoms treated by a mixture of independent
   and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 0.8617P]$
   where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å$^{-3}$
$\Delta\rho_{min} = -0.35$ e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | −0.33027 (14) | 0.26260 (13) | −0.24936 (5) | 0.0523 (3) |
| O1 | 0.3445 (3) | 0.2717 (4) | 0.01706 (15) | 0.0491 (8) |
| O2 | 0.4191 (3) | 0.2364 (4) | 0.25756 (15) | 0.0544 (8) |
| N1 | 0.1131 (3) | 0.2425 (3) | 0.14368 (15) | 0.0338 (7) |
| N2 | 0.0986 (4) | 0.2273 (4) | 0.23701 (15) | 0.0347 (7) |
| N3 | 0.2974 (4) | 0.0892 (5) | 0.53373 (18) | 0.0523 (10) |
| C1 | −0.0064 (4) | 0.2462 (4) | −0.01053 (18) | 0.0311 (8) |
| C2 | 0.1854 (4) | 0.2739 (4) | −0.04006 (19) | 0.0365 (9) |
| C3 | 0.2156 (5) | 0.3040 (5) | −0.1323 (2) | 0.0505 (11) |
| C4 | 0.0595 (6) | 0.3026 (5) | −0.1958 (2) | 0.0502 (11) |
| C5 | −0.1289 (5) | 0.2703 (4) | −0.16794 (19) | 0.0391 (9) |

| | | | | |
|---|---|---|---|---|
| C6 | −0.1630 (4) | 0.2451 (4) | −0.07681 (19) | 0.0347 (8) |
| C7 | −0.0461 (4) | 0.2199 (4) | 0.08716 (18) | 0.0306 (8) |
| C8 | −0.2576 (5) | 0.1709 (6) | 0.1141 (2) | 0.0476 (10) |
| C9 | 0.2671 (4) | 0.2336 (4) | 0.28988 (19) | 0.0343 (9) |
| C10 | 0.2551 (4) | 0.2337 (4) | 0.39173 (18) | 0.0341 (9) |
| C11 | 0.2132 (4) | 0.3709 (5) | 0.4384 (2) | 0.0398 (9) |
| C12 | 0.2188 (5) | 0.3679 (5) | 0.5328 (2) | 0.0500 (11) |
| C13 | 0.2599 (5) | 0.2246 (6) | 0.5769 (2) | 0.0537 (13) |
| C14 | 0.2966 (5) | 0.0971 (5) | 0.4425 (2) | 0.0421 (10) |
| O3 | 0.7770 (3) | 0.2277 (4) | 0.34221 (16) | 0.0478 (8) |
| H1 | 0.31433 | 0.26059 | 0.07012 | 0.0736* |
| H2 | −0.01187 | 0.21446 | 0.26025 | 0.0416* |
| H3 | 0.34320 | 0.32529 | −0.15140 | 0.0608* |
| H4 | 0.08174 | 0.32343 | −0.25733 | 0.0605* |
| H6 | −0.29067 | 0.22721 | −0.05904 | 0.0416* |
| H8A | −0.27145 | 0.29111 | 0.12362 | 0.0715* |
| H8B | −0.27573 | 0.10118 | 0.17002 | 0.0715* |
| H8C | −0.36158 | 0.08889 | 0.06588 | 0.0715* |
| H11 | 0.18180 | 0.46339 | 0.40644 | 0.0478* |
| H12 | 0.19538 | 0.46062 | 0.56616 | 0.0598* |
| H13 | 0.26161 | 0.22236 | 0.64064 | 0.0645* |
| H14 | 0.32550 | 0.00545 | 0.41125 | 0.0505* |
| H3A | 0.657 (6) | 0.217 (5) | 0.314 (3) | 0.0574* |
| H3B | 0.735 (6) | 0.139 (5) | 0.387 (3) | 0.0574* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0600 (5) | 0.0632 (5) | 0.0309 (4) | 0.0269 (4) | −0.0066 (3) | 0.0055 (3) |
| O1 | 0.0391 (12) | 0.0743 (16) | 0.0436 (12) | 0.0329 (12) | 0.0093 (10) | 0.0112 (12) |
| O2 | 0.0426 (12) | 0.1011 (19) | 0.0355 (12) | 0.0456 (13) | 0.0069 (10) | 0.0129 (12) |
| N1 | 0.0346 (12) | 0.0435 (14) | 0.0252 (12) | 0.0192 (11) | 0.0011 (9) | 0.0024 (10) |
| N2 | 0.0313 (12) | 0.0509 (14) | 0.0248 (12) | 0.0209 (11) | 0.0026 (9) | 0.0032 (10) |
| N3 | 0.0568 (17) | 0.079 (2) | 0.0347 (14) | 0.0416 (16) | 0.0083 (12) | 0.0156 (14) |
| C1 | 0.0344 (14) | 0.0286 (14) | 0.0287 (14) | 0.0127 (12) | 0.0015 (11) | 0.0001 (11) |
| C2 | 0.0393 (16) | 0.0394 (16) | 0.0347 (15) | 0.0204 (13) | 0.0056 (12) | 0.0032 (12) |
| C3 | 0.0509 (19) | 0.069 (2) | 0.0438 (18) | 0.0342 (18) | 0.0205 (15) | 0.0110 (16) |
| C4 | 0.067 (2) | 0.063 (2) | 0.0297 (16) | 0.0352 (19) | 0.0135 (15) | 0.0081 (14) |
| C5 | 0.0493 (18) | 0.0391 (16) | 0.0281 (14) | 0.0199 (14) | −0.0012 (12) | 0.0013 (12) |
| C6 | 0.0338 (14) | 0.0366 (15) | 0.0316 (15) | 0.0141 (12) | 0.0012 (11) | 0.0001 (12) |
| C7 | 0.0314 (14) | 0.0326 (14) | 0.0282 (14) | 0.0148 (12) | 0.0015 (11) | 0.0004 (11) |
| C8 | 0.0356 (16) | 0.079 (2) | 0.0296 (15) | 0.0264 (16) | 0.0031 (12) | 0.0055 (15) |
| C9 | 0.0307 (14) | 0.0450 (17) | 0.0301 (14) | 0.0197 (13) | 0.0014 (11) | 0.0039 (12) |
| C10 | 0.0270 (13) | 0.0469 (17) | 0.0267 (14) | 0.0153 (12) | −0.0004 (11) | 0.0020 (12) |
| C11 | 0.0356 (15) | 0.0473 (17) | 0.0368 (16) | 0.0192 (14) | 0.0000 (12) | 0.0014 (13) |
| C12 | 0.0470 (18) | 0.068 (2) | 0.0382 (17) | 0.0284 (17) | 0.0032 (14) | −0.0074 (16) |
| C13 | 0.053 (2) | 0.092 (3) | 0.0261 (16) | 0.041 (2) | 0.0038 (14) | 0.0042 (16) |
| C14 | 0.0458 (17) | 0.057 (2) | 0.0322 (16) | 0.0302 (16) | 0.0057 (13) | 0.0064 (14) |

| O3 | 0.0364 (12) | 0.0757 (17) | 0.0380 (12) | 0.0304 (12) | 0.0052 (9) | 0.0118 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C5 | 1.755 (4) | C5—C6 | 1.376 (4) |
| O1—C2 | 1.349 (4) | C7—C8 | 1.492 (5) |
| O2—C9 | 1.223 (4) | C9—C10 | 1.498 (4) |
| O1—H1 | 0.8200 | C10—C11 | 1.385 (4) |
| O3—H3A | 0.89 (5) | C10—C14 | 1.382 (4) |
| O3—H3B | 0.91 (4) | C11—C12 | 1.375 (4) |
| N1—N2 | 1.378 (3) | C12—C13 | 1.377 (5) |
| N1—C7 | 1.285 (4) | C3—H3 | 0.9300 |
| N2—C9 | 1.348 (4) | C4—H4 | 0.9300 |
| N3—C14 | 1.333 (4) | C6—H6 | 0.9300 |
| N3—C13 | 1.330 (5) | C8—H8C | 0.9600 |
| N2—H2 | 0.8600 | C8—H8A | 0.9600 |
| C1—C7 | 1.479 (4) | C8—H8B | 0.9600 |
| C1—C6 | 1.403 (4) | C11—H11 | 0.9300 |
| C1—C2 | 1.412 (4) | C12—H12 | 0.9300 |
| C2—C3 | 1.389 (4) | C13—H13 | 0.9300 |
| C3—C4 | 1.375 (5) | C14—H14 | 0.9300 |
| C4—C5 | 1.370 (6) | | |
| | | | |
| C2—O1—H1 | 109.00 | C9—C10—C14 | 119.0 (3) |
| H3A—O3—H3B | 102 (4) | C9—C10—C11 | 122.9 (3) |
| N2—N1—C7 | 120.6 (3) | C10—C11—C12 | 118.8 (3) |
| N1—N2—C9 | 116.3 (3) | C11—C12—C13 | 118.5 (3) |
| C13—N3—C14 | 116.9 (3) | N3—C13—C12 | 123.9 (3) |
| N1—N2—H2 | 122.00 | N3—C14—C10 | 123.7 (3) |
| C9—N2—H2 | 122.00 | C2—C3—H3 | 120.00 |
| C2—C1—C6 | 118.2 (2) | C4—C3—H3 | 120.00 |
| C2—C1—C7 | 122.3 (3) | C5—C4—H4 | 120.00 |
| C6—C1—C7 | 119.5 (3) | C3—C4—H4 | 120.00 |
| C1—C2—C3 | 119.6 (3) | C1—C6—H6 | 120.00 |
| O1—C2—C3 | 117.1 (3) | C5—C6—H6 | 120.00 |
| O1—C2—C1 | 123.3 (3) | C7—C8—H8B | 109.00 |
| C2—C3—C4 | 120.9 (3) | C7—C8—H8C | 109.00 |
| C3—C4—C5 | 119.7 (3) | H8A—C8—H8B | 110.00 |
| Cl1—C5—C6 | 119.2 (3) | H8A—C8—H8C | 109.00 |
| Cl1—C5—C4 | 119.7 (2) | H8B—C8—H8C | 109.00 |
| C4—C5—C6 | 121.1 (3) | C7—C8—H8A | 109.00 |
| C1—C6—C5 | 120.4 (3) | C10—C11—H11 | 121.00 |
| N1—C7—C8 | 124.7 (2) | C12—C11—H11 | 121.00 |
| C1—C7—C8 | 120.6 (3) | C13—C12—H12 | 121.00 |
| N1—C7—C1 | 114.7 (3) | C11—C12—H12 | 121.00 |
| O2—C9—N2 | 122.8 (3) | N3—C13—H13 | 118.00 |
| O2—C9—C10 | 121.7 (3) | C12—C13—H13 | 118.00 |
| N2—C9—C10 | 115.5 (3) | N3—C14—H14 | 118.00 |

| C11—C10—C14 | 118.1 (3) | C10—C14—H14 | 118.00 |
|---|---|---|---|
| | | | |
| C7—N1—N2—C9 | 173.6 (3) | O1—C2—C3—C4 | 178.1 (3) |
| N2—N1—C7—C1 | 178.2 (2) | C1—C2—C3—C4 | −1.5 (5) |
| N2—N1—C7—C8 | −1.8 (4) | C2—C3—C4—C5 | −0.3 (5) |
| N1—N2—C9—O2 | −5.8 (4) | C3—C4—C5—Cl1 | −178.5 (3) |
| N1—N2—C9—C10 | 175.2 (2) | C3—C4—C5—C6 | 2.0 (5) |
| C14—N3—C13—C12 | 0.8 (6) | Cl1—C5—C6—C1 | 178.6 (2) |
| C13—N3—C14—C10 | −1.4 (6) | C4—C5—C6—C1 | −1.9 (4) |
| C6—C1—C2—O1 | −178.0 (3) | O2—C9—C10—C11 | 126.3 (3) |
| C6—C1—C2—C3 | 1.6 (4) | O2—C9—C10—C14 | −50.7 (4) |
| C7—C1—C2—O1 | 2.4 (4) | N2—C9—C10—C11 | −54.6 (4) |
| C7—C1—C2—C3 | −178.0 (3) | N2—C9—C10—C14 | 128.4 (3) |
| C2—C1—C6—C5 | 0.1 (4) | C9—C10—C11—C12 | −175.7 (3) |
| C7—C1—C6—C5 | 179.7 (3) | C14—C10—C11—C12 | 1.3 (5) |
| C2—C1—C7—N1 | 6.1 (4) | C9—C10—C14—N3 | 177.6 (3) |
| C2—C1—C7—C8 | −173.9 (3) | C11—C10—C14—N3 | 0.4 (5) |
| C6—C1—C7—N1 | −173.5 (2) | C10—C11—C12—C13 | −1.9 (5) |
| C6—C1—C7—C8 | 6.6 (4) | C11—C12—C13—N3 | 0.9 (6) |

*Hydrogen-bond geometry (Å, º)*

Cg2 is the centroid of the C1–C6 phenyl ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.84 | 2.555 (3) | 144 |
| N2—H2···O3[i] | 0.86 | 2.06 | 2.898 (4) | 166 |
| O3—H3*A*···O2 | 0.89 (5) | 1.88 (5) | 2.760 (4) | 171 (3) |
| O3—H3*B*···N3[ii] | 0.91 (4) | 2.01 (4) | 2.885 (4) | 161 (4) |
| C8—H8*A*···*Cg*2[iii] | 0.96 | 2.99 | 3.763 (4) | 139 |

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