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

# 10′-Chloro-3′,4′-dihydro-2′*H*-spiro[cyclopropane-1,7′(6′*H*)-pyrimido[2,1-*a*]isoquinolin]-6′-one

**Kensuke Okuda,[a]* Takashi Hirota,[b] Yuta Nishina[c] and Hiroyuki Ishida[d]***

[a]Laboratory of Medicinal and Pharmaceutical Chemistry, Gifu Pharmaceutical University, Gifu 501-1196, Japan, [b]Laboratory of Pharmaceutical Chemistry, Faculty of Pharmaceutical Sciences, Okayama University, Okayama 700-8530, Japan, [c]Research Core for Interdisciplinary Sciences, Okayama University, Okayama 700-8530, Japan, and [d]Department of Chemistry, Faculty of Science, Okayama University, Okayama 700-8530, Japan
Correspondence e-mail: okuda@gifu-pu.ac.jp, ishidah@cc.okayama-u.ac.jp

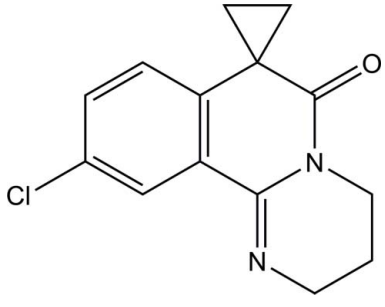
Received 14 October 2012; accepted 25 October 2012

Key indicators: single-crystal X-ray study; $T$ = 180 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.031; $wR$ factor = 0.079; data-to-parameter ratio = 20.6.

In the title compound, $C_{14}H_{13}ClN_2O$, the fused hydropyrimidine ring adopts an envelope conformation with one of the methylene C atoms at the flap. The three-membered ring is approximately perpendicular to the attached isoquinoline ring system, with a dihedral angle of 89.44 (11)°. In the crystal, molecules are linked by a weak C—H$\cdots\pi$ interaction, forming a helical chain along the $c$ axis.

## Related literature

For recent reports on the development of complex heterocyclic skeletons for potential pharmaceutics in one step using the Truce–Smiles rearrangement, see: Okuda *et al.* (2010, 2011). For the synthesis of the title compound, see: Okuda *et al.* (2012).




## Experimental

### Crystal data

$C_{14}H_{13}ClN_2O$
$M_r$ = 260.72
Orthorhombic, $Pca2_1$
$a$ = 8.8746 (5) Å
$b$ = 13.3273 (7) Å
$c$ = 9.8331 (6) Å
$V$ = 1163.01 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.32 mm$^{-1}$
$T$ = 180 K
0.25 × 0.21 × 0.03 mm

### Data collection

Rigaku R-AXIS RAPIDII diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
$T_{min}$ = 0.931, $T_{max}$ = 0.991
17373 measured reflections
3359 independent reflections
3095 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.079
$S$ = 1.05
3359 reflections
163 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$
Absolute structure: Flack (1983), 1571 Friedel pairs
Flack parameter: 0.01 (5)

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

*Cg*1 is the centroid of the C1/N1/C2–C4/C9 ring.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C12—H12*B*$\cdots$*Cg*1$^{i}$ | 0.99 | 2.72 | 3.6000 (15) | 148 |

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

Data collection: *PROCESS-AUTO* (Rigaku/MSC, 2004); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); 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).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2085).

## References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Higashi, T. (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
Okuda, K., Takechi, H., Hirota, T. & Sasaki, K. (2011). *Heterocycles*, **83**, 1315–1328.
Okuda, K., Yoshida, M., Hirota, T. & Sasaki, K. (2010). *Chem. Pharm. Bull.* **58**, 363–368.
Okuda, K., Yoshida, M., Hirota, T. & Sasaki, K. (2012). *Synth. Commun.* **42**, 865–871.
Rigaku/MSC (2004). *PROCESS-AUTO* and *CrystalStructure*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supporting information

*Acta Cryst.* (2012). E**68**, o3252 [doi:10.1107/S1600536812044261]

## 10′-Chloro-3′,4′-dihydro-2′*H*-spiro[cyclopropane-1,7′(6′*H*)-pyrimido[2,1-*a*]isoquinolin]-6′-one

**Kensuke Okuda, Takashi Hirota, Yuta Nishina and Hiroyuki Ishida**

### S1. Comment

As an extension of our work to develop complex heterocyclic skeletons as leads for potential pharmaceutical agents (Okuda *et al.*, 2011), we found that tricyclic 5-amino-1,2-dihydrofuro[2,3-*c*]isoquinolines (Okuda *et al.*, 2010), easily accessible by a one step base-induced Truce-Smiles rearrangement of 2-(3-cyanopropoxy)benzonitriles, showed bronchodilator activity (unpublished results). In the pursuit of more potent analogs, we have explored preparation of additional new ring-fused tetracyclic heterocycles. Herein we report that reaction of 5-amino-7-chloro-1,2-dihydrofuro[2,3-*c*]isoquinoline with 1,3-dibromopropane in the presence of calcium oxide afforded the title compound (Okuda *et al.*, 2012) *via* rearrangement instead of the anticipated 10-chloro-2,3,6,7-tetrahydrofuro[2,3-*c*]imidazo[2,1-*a*]isoquinoline.

In the title compound, the fused hydropyrimidine N1/C1/N2/C12–C14 ring adopts an envelope conformation with atom C13 at the flap. The isoquinoline C1/N1/C2–C9 ring system is planar with an *r.m.s.* deviation of 0.044 (1) Å. The three-membered C3/C10/C11 ring is approximately perpendicular to the attached isoquinoline ring system with a dihedral angle of 89.44 (11)°. In the crystal, molecules are linked by a weak C—H···$\pi$ interaction (Table 1), forming a helical chain along the *c* axis.

### S2. Experimental

The detailed experimental procedure for the synthesis of 10′-chloro-3′,4′-dihydro-2′*H*-spiro[cyclopropane-1,7′(6′*H*)-pyrimido[2,1-*a*]isoquinolin]-6′-one (m.p. 424–425 K from *n*-hexane) from 5-amino-7-chloro-1,2-dihydrofuro[2,3-*c*]isoquinoline was described in our previous paper (Okuda *et al.*, 2012). Single crystals suitable for X-ray diffraction were obtained from an acetonitrile/water solution. The title compound was dissolved in hot acetonitrile, then water was added dropwise until the solution became turbid. Slow evaporation at room temperature gave the colourless crystals

### S3. Refinement

H atoms were located in a difference Fourier map and then were positioned geometrically (C—H = 0.95 or 0.99 Å) and refined as riding, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

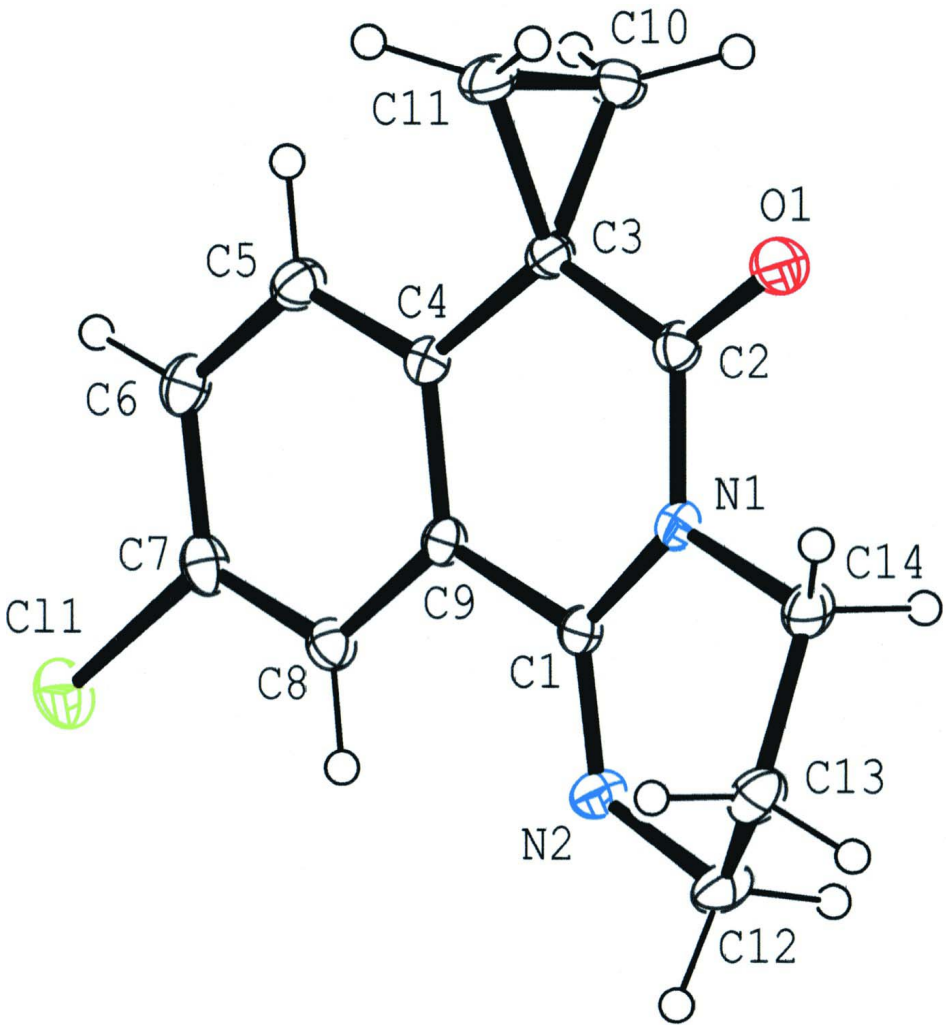



**Figure 1**

The molecular structure of the title compound, with the atom-labeling. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

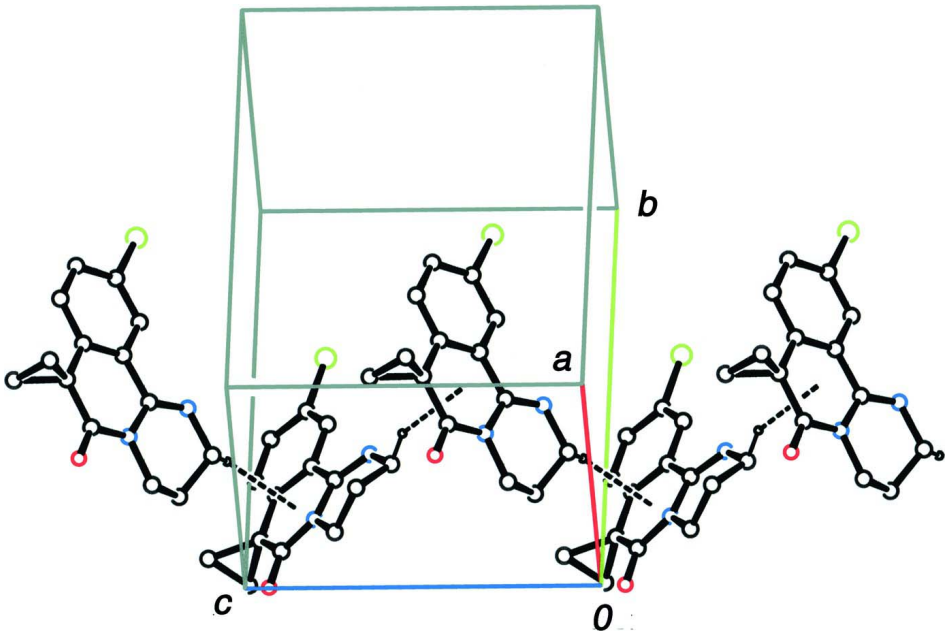



**Figure 2**

A packing diagram of the title compound, showing a chain structure formed by C—H···$\pi$ interactions (dashed lines).

**10′-Chloro-3′,4′-dihydro-2′*H*-spiro[cyclopropane- 1,7′(6′*H*)-pyrimido[2,1-*a*]isoquinolin]-6′-one**

*Crystal data*

$C_{14}H_{13}ClN_2O$
$M_r = 260.72$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 8.8746$ (5) Å
$b = 13.3273$ (7) Å
$c = 9.8331$ (6) Å
$V = 1163.01$ (11) Å$^3$
$Z = 4$
$F(000) = 544.00$
$D_x = 1.489$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 15021 reflections
$\theta = 3.1$–$30.0°$
$\mu = 0.32$ mm$^{-1}$
$T = 180$ K
Platelet, colourless
0.25 × 0.21 × 0.03 mm

*Data collection*

Rigaku R-AXIS RAPIDII diffractometer
Detector resolution: 10.00 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: numerical (*NUMABS*; Higashi, 1999)
$T_{min} = 0.931$, $T_{max} = 0.991$
17373 measured reflections
3359 independent reflections
3095 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 30.0°$
$h = -12 \rightarrow 12$
$k = -18 \rightarrow 18$
$l = -13 \rightarrow 13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.079$
$S = 1.05$
3359 reflections
163 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
$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 0.1225P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{min} = -0.15$ e Å$^{-3}$
Absolute structure: Flack (1983), 1571 Friedel pairs
Absolute structure parameter: 0.01 (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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.55266 (4) | 0.63700 (2) | 0.30542 (5) | 0.03531 (10) |
| O1 | 0.57503 (12) | 0.04186 (7) | 0.43848 (12) | 0.0307 (2) |
| N1 | 0.45976 (11) | 0.15982 (7) | 0.31067 (13) | 0.01989 (19) |
| N2 | 0.36794 (13) | 0.28236 (8) | 0.15502 (12) | 0.0249 (2) |
| C1 | 0.44659 (13) | 0.25802 (10) | 0.25827 (13) | 0.0189 (2) |
| C2 | 0.56200 (15) | 0.13087 (10) | 0.40789 (14) | 0.0211 (2) |
| C3 | 0.65462 (14) | 0.20982 (9) | 0.47518 (13) | 0.0205 (2) |
| C4 | 0.63116 (14) | 0.31618 (9) | 0.43507 (12) | 0.0191 (2) |
| C5 | 0.70816 (15) | 0.39510 (11) | 0.49866 (14) | 0.0259 (3) |
| H5 | 0.7774 | 0.3806 | 0.5697 | 0.031* |
| C6 | 0.68510 (16) | 0.49385 (10) | 0.45973 (15) | 0.0260 (3) |
| H6 | 0.7372 | 0.5470 | 0.5038 | 0.031* |
| C7 | 0.58418 (16) | 0.51363 (10) | 0.35496 (15) | 0.0242 (3) |
| C8 | 0.50749 (14) | 0.43794 (9) | 0.28990 (14) | 0.0226 (2) |
| H8 | 0.4391 | 0.4531 | 0.2185 | 0.027* |
| C9 | 0.53128 (13) | 0.33791 (9) | 0.33006 (13) | 0.0187 (2) |
| C10 | 0.81354 (17) | 0.17547 (12) | 0.51350 (16) | 0.0301 (3) |
| H10A | 0.8443 | 0.1069 | 0.4865 | 0.036* |
| H10B | 0.8952 | 0.2260 | 0.5108 | 0.036* |
| C11 | 0.69779 (19) | 0.18535 (11) | 0.62195 (15) | 0.0293 (3) |
| H11A | 0.7079 | 0.2420 | 0.6864 | 0.035* |
| H11B | 0.6570 | 0.1229 | 0.6621 | 0.035* |
| C12 | 0.27594 (16) | 0.20671 (11) | 0.08694 (15) | 0.0297 (3) |
| H12A | 0.3328 | 0.1794 | 0.0086 | 0.036* |
| H12B | 0.1836 | 0.2390 | 0.0513 | 0.036* |
| C13 | 0.23159 (15) | 0.12115 (11) | 0.17992 (16) | 0.0289 (3) |
| H13A | 0.1610 | 0.1456 | 0.2505 | 0.035* |
| H13B | 0.1802 | 0.0681 | 0.1268 | 0.035* |
| C14 | 0.37139 (16) | 0.07873 (10) | 0.24647 (16) | 0.0267 (3) |
| H14A | 0.3421 | 0.0288 | 0.3162 | 0.032* |

| | | | | |
|---|---|---|---|---|
| H14B | 0.4338 | 0.0443 | 0.1773 | 0.032* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.04450 (18) | 0.01793 (13) | 0.0435 (2) | −0.00198 (13) | 0.00151 (18) | 0.00384 (15) |
| O1 | 0.0391 (5) | 0.0195 (5) | 0.0334 (6) | −0.0010 (4) | −0.0080 (5) | 0.0010 (4) |
| N1 | 0.0222 (4) | 0.0189 (4) | 0.0186 (5) | −0.0024 (3) | −0.0003 (4) | −0.0022 (5) |
| N2 | 0.0257 (5) | 0.0269 (5) | 0.0221 (5) | −0.0025 (4) | −0.0051 (4) | 0.0002 (4) |
| C1 | 0.0193 (5) | 0.0197 (5) | 0.0177 (5) | 0.0001 (4) | 0.0020 (4) | −0.0015 (4) |
| C2 | 0.0244 (5) | 0.0197 (6) | 0.0190 (6) | −0.0007 (4) | 0.0012 (4) | 0.0000 (4) |
| C3 | 0.0227 (5) | 0.0201 (5) | 0.0187 (5) | −0.0006 (4) | −0.0026 (4) | −0.0005 (4) |
| C4 | 0.0205 (5) | 0.0185 (5) | 0.0184 (5) | −0.0011 (4) | 0.0005 (4) | −0.0012 (4) |
| C5 | 0.0280 (6) | 0.0252 (6) | 0.0245 (6) | −0.0031 (5) | −0.0051 (5) | −0.0013 (5) |
| C6 | 0.0295 (6) | 0.0215 (6) | 0.0270 (7) | −0.0065 (5) | 0.0022 (5) | −0.0046 (5) |
| C7 | 0.0279 (6) | 0.0176 (5) | 0.0272 (6) | −0.0009 (5) | 0.0069 (5) | 0.0009 (5) |
| C8 | 0.0239 (5) | 0.0209 (5) | 0.0231 (6) | 0.0005 (4) | 0.0005 (5) | 0.0008 (5) |
| C9 | 0.0193 (5) | 0.0194 (5) | 0.0174 (6) | −0.0005 (4) | 0.0020 (4) | −0.0013 (4) |
| C10 | 0.0273 (7) | 0.0278 (7) | 0.0351 (8) | 0.0024 (6) | −0.0106 (6) | −0.0001 (6) |
| C11 | 0.0407 (8) | 0.0257 (6) | 0.0214 (6) | −0.0004 (6) | −0.0089 (6) | 0.0032 (5) |
| C12 | 0.0302 (7) | 0.0331 (7) | 0.0259 (7) | −0.0057 (6) | −0.0092 (6) | −0.0028 (5) |
| C13 | 0.0256 (6) | 0.0330 (7) | 0.0281 (7) | −0.0072 (5) | −0.0040 (5) | −0.0051 (6) |
| C14 | 0.0321 (6) | 0.0200 (6) | 0.0282 (6) | −0.0051 (5) | −0.0052 (5) | −0.0039 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C7 | 1.7376 (14) | C6—H6 | 0.9500 |
| O1—C2 | 1.2292 (16) | C7—C8 | 1.3748 (19) |
| N1—C2 | 1.3733 (17) | C8—C9 | 1.4063 (17) |
| N1—C1 | 1.4113 (16) | C8—H8 | 0.9500 |
| N1—C14 | 1.4769 (16) | C10—C11 | 1.486 (2) |
| N2—C1 | 1.2740 (17) | C10—H10A | 0.9900 |
| N2—C12 | 1.4599 (17) | C10—H10B | 0.9900 |
| C1—C9 | 1.4822 (17) | C11—H11A | 0.9900 |
| C2—C3 | 1.4902 (18) | C11—H11B | 0.9900 |
| C3—C4 | 1.4859 (17) | C12—C13 | 1.514 (2) |
| C3—C11 | 1.5284 (19) | C12—H12A | 0.9900 |
| C3—C10 | 1.5299 (19) | C12—H12B | 0.9900 |
| C4—C9 | 1.3913 (17) | C13—C14 | 1.512 (2) |
| C4—C5 | 1.4015 (18) | C13—H13A | 0.9900 |
| C5—C6 | 1.3859 (19) | C13—H13B | 0.9900 |
| C5—H5 | 0.9500 | C14—H14A | 0.9900 |
| C6—C7 | 1.390 (2) | C14—H14B | 0.9900 |
| | | | |
| C2—N1—C1 | 124.71 (10) | C4—C9—C1 | 121.81 (11) |
| C2—N1—C14 | 116.28 (10) | C8—C9—C1 | 118.10 (11) |
| C1—N1—C14 | 118.59 (11) | C11—C10—C3 | 60.87 (9) |
| C1—N2—C12 | 119.73 (12) | C11—C10—H10A | 117.7 |

| | | | |
|---|---|---|---|
| N2—C1—N1 | 124.92 (12) | C3—C10—H10A | 117.7 |
| N2—C1—C9 | 118.32 (12) | C11—C10—H10B | 117.7 |
| N1—C1—C9 | 116.76 (11) | C3—C10—H10B | 117.7 |
| O1—C2—N1 | 120.24 (12) | H10A—C10—H10B | 114.8 |
| O1—C2—C3 | 121.39 (12) | C10—C11—C3 | 60.97 (9) |
| N1—C2—C3 | 118.37 (11) | C10—C11—H11A | 117.7 |
| C4—C3—C2 | 118.58 (11) | C3—C11—H11A | 117.7 |
| C4—C3—C11 | 119.30 (11) | C10—C11—H11B | 117.7 |
| C2—C3—C11 | 114.01 (11) | C3—C11—H11B | 117.7 |
| C4—C3—C10 | 118.68 (11) | H11A—C11—H11B | 114.8 |
| C2—C3—C10 | 113.99 (11) | N2—C12—C13 | 112.88 (12) |
| C11—C3—C10 | 58.16 (9) | N2—C12—H12A | 109.0 |
| C9—C4—C5 | 119.05 (11) | C13—C12—H12A | 109.0 |
| C9—C4—C3 | 119.00 (11) | N2—C12—H12B | 109.0 |
| C5—C4—C3 | 121.94 (11) | C13—C12—H12B | 109.0 |
| C6—C5—C4 | 121.16 (12) | H12A—C12—H12B | 107.8 |
| C6—C5—H5 | 119.4 | C14—C13—C12 | 109.24 (11) |
| C4—C5—H5 | 119.4 | C14—C13—H13A | 109.8 |
| C5—C6—C7 | 118.68 (12) | C12—C13—H13A | 109.8 |
| C5—C6—H6 | 120.7 | C14—C13—H13B | 109.8 |
| C7—C6—H6 | 120.7 | C12—C13—H13B | 109.8 |
| C8—C7—C6 | 121.64 (12) | H13A—C13—H13B | 108.3 |
| C8—C7—Cl1 | 118.96 (11) | N1—C14—C13 | 110.31 (11) |
| C6—C7—Cl1 | 119.40 (10) | N1—C14—H14A | 109.6 |
| C7—C8—C9 | 119.38 (12) | C13—C14—H14A | 109.6 |
| C7—C8—H8 | 120.3 | N1—C14—H14B | 109.6 |
| C9—C8—H8 | 120.3 | C13—C14—H14B | 109.6 |
| C4—C9—C8 | 120.09 (11) | H14A—C14—H14B | 108.1 |

| | | | |
|---|---|---|---|
| C12—N2—C1—N1 | 3.66 (19) | C4—C5—C6—C7 | −0.4 (2) |
| C12—N2—C1—C9 | −176.29 (11) | C5—C6—C7—C8 | 0.0 (2) |
| C2—N1—C1—N2 | 169.27 (13) | C5—C6—C7—Cl1 | 179.55 (11) |
| C14—N1—C1—N2 | −2.93 (19) | C6—C7—C8—C9 | 0.1 (2) |
| C2—N1—C1—C9 | −10.78 (18) | Cl1—C7—C8—C9 | −179.46 (10) |
| C14—N1—C1—C9 | 177.02 (11) | C5—C4—C9—C8 | −0.63 (18) |
| C1—N1—C2—O1 | −173.21 (13) | C3—C4—C9—C8 | −179.79 (11) |
| C14—N1—C2—O1 | −0.84 (19) | C5—C4—C9—C1 | 179.82 (11) |
| C1—N1—C2—C3 | 7.29 (19) | C3—C4—C9—C1 | 0.66 (17) |
| C14—N1—C2—C3 | 179.66 (12) | C7—C8—C9—C4 | 0.24 (18) |
| O1—C2—C3—C4 | −178.91 (12) | C7—C8—C9—C1 | 179.81 (11) |
| N1—C2—C3—C4 | 0.58 (18) | N2—C1—C9—C4 | −173.56 (12) |
| O1—C2—C3—C11 | −30.41 (18) | N1—C1—C9—C4 | 6.49 (17) |
| N1—C2—C3—C11 | 149.08 (13) | N2—C1—C9—C8 | 6.88 (17) |
| O1—C2—C3—C10 | 33.87 (19) | N1—C1—C9—C8 | −173.07 (11) |
| N1—C2—C3—C10 | −146.63 (13) | C4—C3—C10—C11 | 108.47 (14) |
| C2—C3—C4—C9 | −4.26 (17) | C2—C3—C10—C11 | −104.35 (13) |
| C11—C3—C4—C9 | −151.08 (12) | C4—C3—C11—C10 | −107.42 (14) |
| C10—C3—C4—C9 | 141.41 (12) | C2—C3—C11—C10 | 104.32 (13) |

| | | | |
|---|---|---|---|
| C2—C3—C4—C5 | 176.60 (12) | C1—N2—C12—C13 | 25.27 (18) |
| C11—C3—C4—C5 | 29.78 (18) | N2—C12—C13—C14 | −52.69 (16) |
| C10—C3—C4—C5 | −37.73 (18) | C2—N1—C14—C13 | 160.89 (12) |
| C9—C4—C5—C6 | 0.73 (19) | C1—N1—C14—C13 | −26.25 (17) |
| C3—C4—C5—C6 | 179.87 (13) | C12—C13—C14—N1 | 51.96 (16) |

*Hydrogen-bond geometry (Å, º)*

*Cg*1 is the centroid of the C1/N1/C2–C4/C9 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12*B*···*Cg*1$^{i}$ | 0.99 | 2.72 | 3.6000 (15) | 148 |

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