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# 5-(4-Chlorophenyl)-6-isopropyl-5,6-dihydro-4*H*-pyrrolo[3,4-*c*]isoxazole

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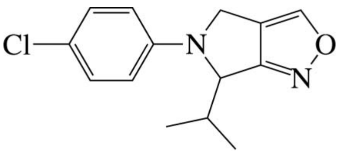
Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.044; $wR$ factor = 0.117; data-to-parameter ratio = 19.5.

The title compound, $C_{14}H_{15}ClN_2O$, contains an eight-membered 5,5-fused bicycle with two substituents. The dihedral angle between the nearly planar eight-membered ring [maximum deviation = 0.033 (2) Å] and the benzene ring is 25.0 (1)°. In the crystal structure, molecules are stacked in columns along the $b$ axis and C—H$\cdots\pi$ interactions are observed between the columns.

## Related literature

For the synthesis of the title compound, see: Kim & Lee (1994). For the biological activity of isoxazoles, see: Boyd (1991); Kim *et al.* (1994, 1997, 1999); Lang & Lin (1984); Sutharchanadevi & Murugan (1996).



## Experimental

*Crystal data*

$C_{14}H_{15}ClN_2O$
$M_r$ = 262.73
Monoclinic, $P2_1/c$
$a$ = 15.0037 (9) Å
$b$ = 6.2364 (4) Å
$c$ = 15.5801 (9) Å
$\beta$ = 117.238 (1)°
$V$ = 1296.16 (14) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 200 K
0.35 × 0.28 × 0.12 mm

*Data collection*

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000) $T_{\min}$ = 0.861, $T_{\max}$ = 0.966
9224 measured reflections
3211 independent reflections
1907 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.043

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.117
$S$ = 1.07
3211 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.44 e Å$^{-3}$

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

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C5—H5$\cdots Cg1^{\rm i}$ | 0.95 | 2.65 | 3.405 (3) | 136 |
| C9—H9$\cdots Cg1^{\rm ii}$ | 0.95 | 2.62 | 3.392 (3) | 138 |

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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: *SHELXL97*.

This study was supported by financially Chonnam National University (2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2594).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, o2483 [ **doi:10.1107/S1600536810034872** ]

# 5-(4-Chlorophenyl)-6-isopropyl-5,6-dihydro-4*H*-pyrrolo[3,4-*c*]isoxazole

**K. Ha**, **H. S. Lim** and **H. J. Kim**

## Comment

Isoxazole derivatives bearing various substituents are known to have diverse biological activities in pharmaceutical and agricultural areas (Lang & Lin, 1984; Boyd, 1991). Dihydropyrrolo[3,4-*c*]isoxazole, a fused bicyclic isoxazole, is interesting to develop a new lead compound as a plant fungicide because bicyclic isoxazoles such as dihydrofuro[3,4-*c*]isoxazole and dihydropyrano[3,4-*c*]isoxazole derivatives particularly have fungicidal activities against some plant pathogens (Kim *et al.*, 1994, 1997, 1999). The title compound was prepared by the known method (Kim & Lee, 1994) with a minor modification.

The title compound, $C_{14}H_{15}ClN_2O$, is an 8-membered 5,5-fused bicycle with two substituents (Fig. 1). The dihedral angle between the nearly planar 8-membered ring [maximum deviation of 0.033 (2) Å for C7] and the benzene ring [maximum deviation of 0.023 (2) Å for C1] is 25.0 (1)°. In the crystal structure, the molecules are stacked in columns along the *b* axis (Fig. 2), and display C—H···*Cg*1 (the centroid of ring C1–C6) interactions (Table 1).

## Experimental

A mixture of 3-methyl-1-nitrobutan-2-yl acetate (1.23 g, 7 mmol), 4-chloro-*N*-(prop-2-ynyl)aniline (3.48 g, 21 mmol) and $K_2CO_3$ (1.16 g, 8.4 mmol) in THF (20 ml) was stirred for 12 h at 25 °C. The mixture was concentrated *in vacuo* and column chromatographed ($SiO_2$) by eluting with a mixture of n-hexane/EtOAc (5:1) to afford 4-chloro-*N*-(3-methyl-1-nitrobutan-2-yl)-*N*-(prop-2-ynyl)aniline (0.49 g, 25%). The title compound was prepared by the intramolecular nitrile oxide-alkyne cycloaddition of 4-chloro-*N*-(3-methyl-1-nitrobutan-2-yl)-*N*-(prop-2-ynyl)aniline in the presence of 4-chlorophenylisocyanate and triethylamine (Kim & Lee, 1994). Crystals suitable for X-ray analysis were obtained by slow evaporation from an n-hexane/$CHCl_3$ solution.

## Refinement

H atoms were positioned geometrically and allowed to ride on their respective parent atoms [C—H = 0.95 (CH, *sp*$^2$), 1.00 (CH, *sp*$^3$), 0.99 ($CH_2$) or 0.98 Å ($CH_3$), and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C)].

## Figures

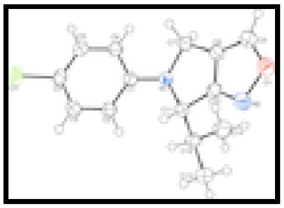

Fig. 1. The structure of the title compound, with displacement ellipsoids drawn at the 50% probability level for non-H atoms.

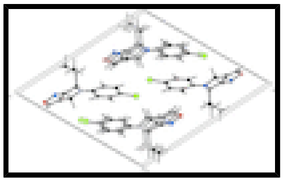

Fig. 2. View of the unit-cell contents of the title compound.

## 5-(4-Chlorophenyl)-6-isopropyl-5,6-dihydro-4*H*- pyrrolo[3,4-*c*]isoxazole

### *Crystal data*

$C_{14}H_{15}ClN_2O$

$M_r = 262.73$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 15.0037$ (9) Å

$b = 6.2364$ (4) Å

$c = 15.5801$ (9) Å

$\beta = 117.238$ (1)°

$V = 1296.16$ (14) Å$^3$

$Z = 4$

$F(000) = 552$

$D_x = 1.346$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2659 reflections

$\theta = 2.6$–27.1°

$\mu = 0.28$ mm$^{-1}$

$T = 200$ K

Stick, pale yellow

0.35 × 0.28 × 0.12 mm

### *Data collection*

Bruker SMART 1000 CCD diffractometer

Radiation source: fine-focus sealed tube

graphite

$\varphi$ and $\omega$ scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2000)

$T_{min} = 0.861$, $T_{max} = 0.966$

9224 measured reflections

3211 independent reflections

1907 reflections with $I > 2\sigma(I)$

$R_{int} = 0.043$

$\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$

$h = -19 \rightarrow 20$

$k = -8 \rightarrow 8$

$l = -18 \rightarrow 20$

### *Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.117$

$S = 1.07$

3211 reflections

165 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

$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2 + 0.6269P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.36$ e Å$^{-3}$

$\Delta\rho_{min} = -0.44$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{\rm iso}$*/$U_{\rm eq}$ |
|---|---|---|---|---|
| Cl1 | 0.53029 (5) | 0.72970 (11) | 0.07428 (5) | 0.0460 (2) |
| O1 | 0.17957 (13) | 1.1528 (3) | 0.45555 (12) | 0.0468 (5) |
| N1 | 0.25711 (13) | 0.8986 (3) | 0.24578 (13) | 0.0292 (4) |
| N2 | 0.17208 (15) | 1.2612 (3) | 0.37156 (14) | 0.0400 (5) |
| C1 | 0.31613 (16) | 0.8552 (4) | 0.20076 (15) | 0.0284 (5) |
| C2 | 0.32447 (17) | 1.0003 (4) | 0.13595 (16) | 0.0317 (5) |
| H2 | 0.2857 | 1.1280 | 0.1193 | 0.038* |
| C3 | 0.38835 (17) | 0.9599 (4) | 0.09593 (16) | 0.0341 (5) |
| H3 | 0.3940 | 1.0608 | 0.0530 | 0.041* |
| C4 | 0.44355 (17) | 0.7739 (4) | 0.11838 (16) | 0.0327 (5) |
| C5 | 0.43342 (16) | 0.6228 (4) | 0.17806 (16) | 0.0333 (5) |
| H5 | 0.4696 | 0.4918 | 0.1911 | 0.040* |
| C6 | 0.37017 (16) | 0.6630 (4) | 0.21896 (16) | 0.0316 (5) |
| H6 | 0.3634 | 0.5586 | 0.2600 | 0.038* |
| C7 | 0.27190 (18) | 0.7731 (4) | 0.33222 (17) | 0.0341 (5) |
| H7A | 0.3437 | 0.7411 | 0.3738 | 0.041* |
| H7B | 0.2335 | 0.6372 | 0.3140 | 0.041* |
| C8 | 0.23192 (17) | 0.9227 (4) | 0.38036 (16) | 0.0322 (5) |
| C9 | 0.21539 (18) | 0.9522 (4) | 0.45747 (17) | 0.0412 (6) |
| H9 | 0.2271 | 0.8481 | 0.5060 | 0.049* |
| C10 | 0.20329 (16) | 1.1175 (4) | 0.33080 (16) | 0.0298 (5) |
| C11 | 0.21313 (16) | 1.1144 (4) | 0.23924 (15) | 0.0279 (5) |
| H11 | 0.2625 | 1.2261 | 0.2426 | 0.034* |
| C12 | 0.11400 (17) | 1.1478 (4) | 0.14745 (16) | 0.0325 (5) |
| H12 | 0.1255 | 1.1103 | 0.0909 | 0.039* |
| C13 | 0.0833 (2) | 1.3827 (4) | 0.13769 (19) | 0.0464 (7) |
| H13A | 0.0713 | 1.4239 | 0.1922 | 0.070* |
| H13B | 0.0218 | 1.4036 | 0.0772 | 0.070* |
| H13C | 0.1369 | 1.4716 | 0.1373 | 0.070* |
| C14 | 0.03096 (18) | 1.0035 (4) | 0.14450 (19) | 0.0488 (7) |
| H14A | 0.0132 | 1.0470 | 0.1951 | 0.073* |
| H14B | 0.0542 | 0.8544 | 0.1551 | 0.073* |
| H14C | −0.0280 | 1.0161 | 0.0813 | 0.073* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0449 (4) | 0.0560 (4) | 0.0462 (4) | 0.0075 (3) | 0.0287 (3) | −0.0022 (3) |
| O1 | 0.0517 (11) | 0.0585 (12) | 0.0343 (10) | 0.0084 (9) | 0.0233 (9) | −0.0015 (9) |
| N1 | 0.0326 (10) | 0.0275 (10) | 0.0298 (10) | 0.0036 (8) | 0.0164 (8) | 0.0050 (8) |
| N2 | 0.0474 (12) | 0.0423 (12) | 0.0348 (11) | 0.0057 (10) | 0.0226 (10) | 0.0010 (10) |
| C1 | 0.0285 (12) | 0.0294 (12) | 0.0256 (12) | −0.0007 (10) | 0.0109 (9) | −0.0007 (9) |
| C2 | 0.0340 (13) | 0.0306 (12) | 0.0314 (13) | 0.0048 (10) | 0.0158 (10) | 0.0041 (10) |
| C3 | 0.0370 (13) | 0.0362 (14) | 0.0310 (13) | −0.0029 (11) | 0.0172 (11) | 0.0018 (10) |
| C4 | 0.0322 (12) | 0.0364 (13) | 0.0315 (13) | 0.0016 (11) | 0.0163 (10) | −0.0042 (10) |
| C5 | 0.0312 (12) | 0.0306 (13) | 0.0340 (13) | 0.0033 (10) | 0.0115 (10) | −0.0008 (10) |
| C6 | 0.0300 (12) | 0.0314 (12) | 0.0308 (12) | 0.0003 (10) | 0.0117 (10) | 0.0027 (10) |
| C7 | 0.0414 (13) | 0.0312 (13) | 0.0331 (13) | 0.0030 (11) | 0.0199 (11) | 0.0064 (10) |
| C8 | 0.0317 (12) | 0.0369 (13) | 0.0291 (12) | −0.0003 (11) | 0.0148 (10) | 0.0034 (10) |
| C9 | 0.0400 (14) | 0.0509 (16) | 0.0330 (14) | 0.0066 (12) | 0.0171 (11) | 0.0067 (12) |
| C10 | 0.0264 (11) | 0.0332 (13) | 0.0294 (12) | −0.0006 (10) | 0.0124 (10) | −0.0002 (10) |
| C11 | 0.0275 (11) | 0.0290 (12) | 0.0286 (12) | −0.0002 (10) | 0.0139 (9) | 0.0017 (9) |
| C12 | 0.0322 (13) | 0.0359 (13) | 0.0283 (12) | 0.0036 (10) | 0.0128 (10) | 0.0030 (10) |
| C13 | 0.0456 (15) | 0.0455 (16) | 0.0449 (16) | 0.0111 (13) | 0.0180 (13) | 0.0129 (13) |
| C14 | 0.0350 (14) | 0.0522 (17) | 0.0492 (16) | −0.0046 (13) | 0.0106 (12) | 0.0032 (13) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cl1—C4 | 1.749 (2) | C7—H7A | 0.9900 |
| O1—C9 | 1.356 (3) | C7—H7B | 0.9900 |
| O1—N2 | 1.431 (2) | C8—C9 | 1.346 (3) |
| N1—C1 | 1.385 (3) | C8—C10 | 1.398 (3) |
| N1—C11 | 1.482 (3) | C9—H9 | 0.9500 |
| N1—C7 | 1.484 (3) | C10—C11 | 1.500 (3) |
| N2—C10 | 1.303 (3) | C11—C12 | 1.534 (3) |
| C1—C6 | 1.401 (3) | C11—H11 | 1.0000 |
| C1—C2 | 1.403 (3) | C12—C14 | 1.521 (3) |
| C2—C3 | 1.385 (3) | C12—C13 | 1.522 (3) |
| C2—H2 | 0.9500 | C12—H12 | 1.0000 |
| C3—C4 | 1.374 (3) | C13—H13A | 0.9800 |
| C3—H3 | 0.9500 | C13—H13B | 0.9800 |
| C4—C5 | 1.380 (3) | C13—H13C | 0.9800 |
| C5—C6 | 1.387 (3) | C14—H14A | 0.9800 |
| C5—H5 | 0.9500 | C14—H14B | 0.9800 |
| C6—H6 | 0.9500 | C14—H14C | 0.9800 |
| C7—C8 | 1.485 (3) | | |
| C9—O1—N2 | 108.68 (17) | C10—C8—C7 | 111.13 (19) |
| C1—N1—C11 | 120.72 (17) | C8—C9—O1 | 109.8 (2) |
| C1—N1—C7 | 119.44 (18) | C8—C9—H9 | 125.1 |
| C11—N1—C7 | 114.75 (16) | O1—C9—H9 | 125.1 |
| C10—N2—O1 | 103.03 (18) | N2—C10—C8 | 114.6 (2) |

| | | | |
|---|---|---|---|
| N1—C1—C6 | 120.6 (2) | N2—C10—C11 | 133.3 (2) |
| N1—C1—C2 | 121.8 (2) | C8—C10—C11 | 112.02 (19) |
| C6—C1—C2 | 117.59 (19) | N1—C11—C10 | 100.43 (17) |
| C3—C2—C1 | 121.0 (2) | N1—C11—C12 | 113.51 (18) |
| C3—C2—H2 | 119.5 | C10—C11—C12 | 114.16 (17) |
| C1—C2—H2 | 119.5 | N1—C11—H11 | 109.5 |
| C4—C3—C2 | 120.0 (2) | C10—C11—H11 | 109.5 |
| C4—C3—H3 | 120.0 | C12—C11—H11 | 109.5 |
| C2—C3—H3 | 120.0 | C14—C12—C13 | 111.1 (2) |
| C3—C4—C5 | 120.6 (2) | C14—C12—C11 | 112.28 (19) |
| C3—C4—Cl1 | 120.21 (18) | C13—C12—C11 | 110.13 (19) |
| C5—C4—Cl1 | 119.21 (18) | C14—C12—H12 | 107.7 |
| C4—C5—C6 | 119.7 (2) | C13—C12—H12 | 107.7 |
| C4—C5—H5 | 120.1 | C11—C12—H12 | 107.7 |
| C6—C5—H5 | 120.1 | C12—C13—H13A | 109.5 |
| C5—C6—C1 | 121.0 (2) | C12—C13—H13B | 109.5 |
| C5—C6—H6 | 119.5 | H13A—C13—H13B | 109.5 |
| C1—C6—H6 | 119.5 | C12—C13—H13C | 109.5 |
| N1—C7—C8 | 101.51 (17) | H13A—C13—H13C | 109.5 |
| N1—C7—H7A | 111.5 | H13B—C13—H13C | 109.5 |
| C8—C7—H7A | 111.5 | C12—C14—H14A | 109.5 |
| N1—C7—H7B | 111.5 | C12—C14—H14B | 109.5 |
| C8—C7—H7B | 111.5 | H14A—C14—H14B | 109.5 |
| H7A—C7—H7B | 109.3 | C12—C14—H14C | 109.5 |
| C9—C8—C10 | 103.8 (2) | H14A—C14—H14C | 109.5 |
| C9—C8—C7 | 145.0 (2) | H14B—C14—H14C | 109.5 |

| | | | |
|---|---|---|---|
| C9—O1—N2—C10 | 0.3 (2) | C7—C8—C9—O1 | 175.2 (3) |
| C11—N1—C1—C6 | 170.09 (19) | N2—O1—C9—C8 | 0.1 (3) |
| C7—N1—C1—C6 | 16.6 (3) | O1—N2—C10—C8 | −0.5 (3) |
| C11—N1—C1—C2 | −9.7 (3) | O1—N2—C10—C11 | 177.8 (2) |
| C7—N1—C1—C2 | −163.2 (2) | C9—C8—C10—N2 | 0.6 (3) |
| N1—C1—C2—C3 | 176.2 (2) | C7—C8—C10—N2 | −176.7 (2) |
| C6—C1—C2—C3 | −3.7 (3) | C9—C8—C10—C11 | −178.10 (19) |
| C1—C2—C3—C4 | 1.0 (3) | C7—C8—C10—C11 | 4.6 (3) |
| C2—C3—C4—C5 | 2.2 (3) | C1—N1—C11—C10 | −153.36 (19) |
| C2—C3—C4—Cl1 | −175.91 (18) | C7—N1—C11—C10 | 1.3 (2) |
| C3—C4—C5—C6 | −2.7 (3) | C1—N1—C11—C12 | 84.4 (2) |
| Cl1—C4—C5—C6 | 175.43 (17) | C7—N1—C11—C12 | −121.0 (2) |
| C4—C5—C6—C1 | 0.0 (3) | N2—C10—C11—N1 | 178.2 (2) |
| N1—C1—C6—C5 | −176.7 (2) | C8—C10—C11—N1 | −3.5 (2) |
| C2—C1—C6—C5 | 3.2 (3) | N2—C10—C11—C12 | −60.0 (3) |
| C1—N1—C7—C8 | 156.14 (19) | C8—C10—C11—C12 | 118.3 (2) |
| C11—N1—C7—C8 | 1.2 (2) | N1—C11—C12—C14 | 65.4 (2) |
| N1—C7—C8—C9 | −178.9 (3) | C10—C11—C12—C14 | −48.9 (3) |
| N1—C7—C8—C10 | −3.4 (2) | N1—C11—C12—C13 | −170.28 (18) |
| C10—C8—C9—O1 | −0.4 (3) | C10—C11—C12—C13 | 75.4 (2) |

*Hydrogen-bond geometry (Å, °)*

Cg1 is the centroid of the C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5···Cg1$^{i}$ | 0.95 | 2.65 | 3.405 (3) | 136 |
| C9—H9···Cg1$^{ii}$ | 0.95 | 2.62 | 3.392 (3) | 138 |

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) *x*, −*y*+3/2, *z*+1/2.

**Fig. 1**

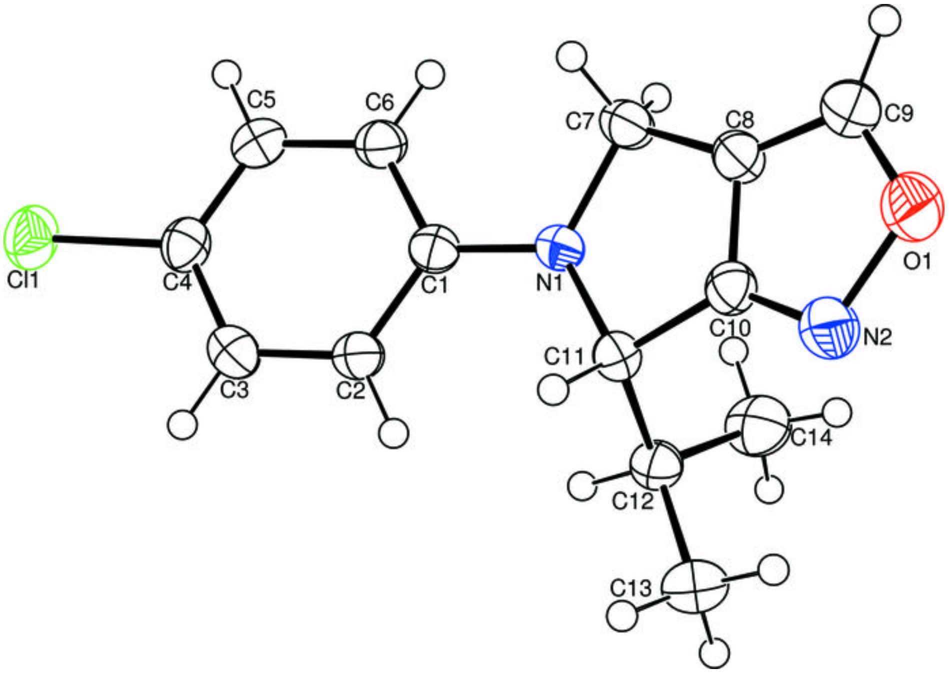

Fig. 2