

## 5-(3-Chlorophenyl)-2-phenyl-3,4-dihydro-2H-pyrrole

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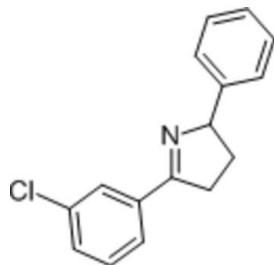
Received 25 September 2010; accepted 26 September 2010

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.033;  $wR$  factor = 0.091; data-to-parameter ratio = 14.4.

In the title compound,  $\text{C}_{16}\text{H}_{14}\text{ClN}$ , the conformation of the five-membered ring approximates to an envelope with a C atom as the flap. The dihedral angle between the aromatic rings is  $78.71$  ( $9$ )°.

### Related literature

For chemical background to pyrrolines, see: Tsuge *et al.* (1987).



### Experimental

#### Crystal data

$\text{C}_{16}\text{H}_{14}\text{ClN}$	$V = 1329.0$ (2) Å <sup>3</sup>
$M_r = 255.73$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 18.2543$ (18) Å	$\mu = 0.27$ mm <sup>-1</sup>
$b = 5.6398$ (5) Å	$T = 296$ K
$c = 13.0095$ (13) Å	$0.38 \times 0.32 \times 0.20$ mm
$\beta = 97.129$ (2)°	

#### Data collection

Bruker SMART CCD diffractometer	6409 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	2344 independent reflections
$T_{\min} = 0.905$ , $T_{\max} = 0.948$	1856 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.017$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$	163 parameters
$wR(F^2) = 0.091$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\max} = 0.13$ e Å <sup>-3</sup>
2344 reflections	$\Delta\rho_{\min} = -0.18$ e Å <sup>-3</sup>

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); 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: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5651).

### References

- Bruker (2001). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Tsuge, O., Ueno, K., Kanemasa, S. & Yorozu, K. (1987). *Bull. Chem. Soc. Jpn.*, **60**, 3347–3358.

**supplementary materials**

*Acta Cryst.* (2010). E66, o2782 [ doi:10.1107/S160053681003847X ]

## 5-(3-Chlorophenyl)-2-phenyl-3,4-dihydro-2H-pyrrole

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### Experimental

To a 500 ml flask *N*-(4-(3-chlorophenyl)-4-oxo-1-phenylbutyl)acetamide (6.25 g, 19.79 mmol), 40 mL 6*M* Hydrochloric acid aqueous solution and 120 ml ethanol were added sequentially. The reaction mixture was heated to reflux and reacted for 20 h. After separation through silica gel column chromatography (fluent: ethyl acetate/petroleum ether=1/20), The title product compound was gained as a pale yellow solid (3.50 g, 69%) and recrystallised from methylene chloride to yield colourless blocks of (I).

Anal. Calcd for C<sub>16</sub>H<sub>14</sub>ClN: C, 75.14; H, 5.52; Cl, 13.86; N, 5.48. Found: C, 75.22; H, 5.50; N, 5.45. <sup>1</sup>H NMR(CDCl<sub>3</sub>): 1.94(m,1H, N—CH—CH<sub>1</sub>), 2.83 (m,1H, N—CH—CH<sub>1</sub>), 3.02(m, 1H, N=C—CH<sub>1</sub>), 3.15 (m, 1H, N=C—CH<sub>1</sub>), 5.33 (t, 1H,C=N—CH<sub>1</sub>), 7.28–7.88(m, 9H, Ph—H).

### Refinement

Although all H atoms were visible in difference maps, they were finally placed in geometrically calculated positions, with C—H distances in the range 0.93–0.98 Å, and included in the final refinement in the riding model approximation, with  $U_{\text{iso}}(\text{H}) = 1.1U_{\text{eq}}(\text{C}, \text{N})$  and  $U_{\text{iso}}(\text{H}) = 1.1U_{\text{eq}}(\text{C})$ .

### Figures

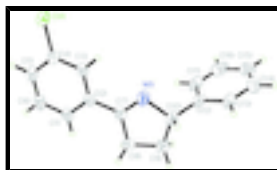


Fig. 1. The molecular structure of (I), with 30% probability displacement ellipsoids.

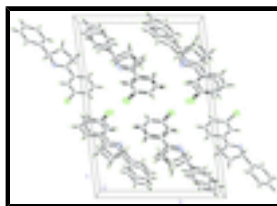


Fig. 2. Crystal packing of (I).

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### Crystal data

C<sub>16</sub>H<sub>14</sub>ClN  
 $M_r = 255.73$

$F(000) = 536$   
 $D_x = 1.278 \text{ Mg m}^{-3}$

# supplementary materials

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Monoclinic,  $P2_1/c$   
Hall symbol: -P 2ybc  
 $a = 18.2543$  (18) Å  
 $b = 5.6398$  (5) Å  
 $c = 13.0095$  (13) Å  
 $\beta = 97.129$  (2)°  
 $V = 1329.0$  (2) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å  
Cell parameters from 2445 reflections  
 $\theta = 3.2$ – $25.0$ °  
 $\mu = 0.27$  mm<sup>-1</sup>  
 $T = 296$  K  
Block, colourless  
 $0.38 \times 0.32 \times 0.20$  mm

## Data collection

Bruker SMART CCD  
diffractometer  
Radiation source: fine-focus sealed tube  
graphite  
phi and  $\omega$  scans  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 2001)  
 $T_{\min} = 0.905$ ,  $T_{\max} = 0.948$   
6409 measured reflections

2344 independent reflections  
1856 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.017$   
 $\theta_{\max} = 25.0$ °,  $\theta_{\min} = 3.2$ °  
 $h = -21 \rightarrow 21$   
 $k = -6 \rightarrow 4$   
 $l = -14 \rightarrow 15$

## Refinement

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.033$   
 $wR(F^2) = 0.091$   
 $S = 1.06$   
2344 reflections  
163 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.239P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.13$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.18$  e Å<sup>-3</sup>

## 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.

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.46600 (3)	-0.37904 (9)	0.67127 (4)	0.07239 (19)
N1	0.26607 (7)	0.2985 (3)	0.70282 (10)	0.0606 (4)
C1	0.36885 (8)	-0.0215 (3)	0.63059 (11)	0.0477 (4)

H1	0.3644	-0.0242	0.7010	0.057*
C2	0.41540 (8)	-0.1765 (3)	0.59008 (12)	0.0514 (4)
C3	0.42310 (9)	-0.1765 (4)	0.48568 (13)	0.0625 (5)
H3	0.4547	-0.2834	0.4591	0.075*
C4	0.38333 (9)	-0.0163 (4)	0.42214 (13)	0.0669 (5)
H4	0.3883	-0.0140	0.3518	0.080*
C5	0.33616 (9)	0.1414 (3)	0.46108 (12)	0.0573 (4)
H5	0.3096	0.2492	0.4170	0.069*
C6	0.32813 (8)	0.1401 (3)	0.56578 (11)	0.0462 (4)
C7	0.27682 (8)	0.3056 (3)	0.60801 (11)	0.0480 (4)
C8	0.23478 (9)	0.4944 (3)	0.54365 (13)	0.0548 (4)
H8A	0.2677	0.6161	0.5233	0.066*
H8B	0.2070	0.4274	0.4820	0.066*
C9	0.18419 (12)	0.5915 (4)	0.61625 (14)	0.0760 (6)
H9A	0.1337	0.5408	0.5957	0.091*
H9B	0.1857	0.7635	0.6174	0.091*
C10	0.21413 (9)	0.4885 (3)	0.72331 (13)	0.0589 (4)
H10	0.2420	0.6131	0.7636	0.071*
C11	0.15575 (8)	0.3978 (3)	0.78499 (12)	0.0505 (4)
C12	0.13832 (10)	0.5176 (3)	0.87106 (13)	0.0601 (5)
H12	0.1635	0.6565	0.8916	0.072*
C13	0.08427 (11)	0.4353 (4)	0.92721 (16)	0.0761 (6)
H13	0.0735	0.5184	0.9852	0.091*
C14	0.04680 (11)	0.2338 (4)	0.89818 (18)	0.0795 (6)
H14	0.0102	0.1793	0.9360	0.095*
C15	0.06289 (12)	0.1112 (4)	0.8137 (2)	0.0839 (6)
H15	0.0373	-0.0272	0.7937	0.101*
C16	0.11725 (11)	0.1926 (4)	0.75748 (16)	0.0719 (5)
H16	0.1281	0.1073	0.7001	0.086*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cl1	0.0734 (3)	0.0730 (3)	0.0733 (3)	0.0237 (2)	0.0194 (2)	0.0061 (2)
N1	0.0599 (8)	0.0775 (10)	0.0437 (8)	0.0241 (8)	0.0038 (6)	-0.0048 (7)
C1	0.0469 (8)	0.0571 (10)	0.0401 (8)	-0.0006 (7)	0.0087 (6)	-0.0050 (7)
C2	0.0442 (8)	0.0575 (10)	0.0536 (9)	-0.0003 (7)	0.0105 (7)	-0.0047 (8)
C3	0.0532 (9)	0.0790 (13)	0.0581 (10)	0.0053 (9)	0.0177 (8)	-0.0161 (10)
C4	0.0605 (10)	0.1011 (15)	0.0413 (9)	0.0014 (10)	0.0155 (8)	-0.0081 (10)
C5	0.0534 (9)	0.0760 (12)	0.0425 (9)	0.0009 (9)	0.0064 (7)	0.0010 (8)
C6	0.0426 (8)	0.0557 (10)	0.0402 (8)	-0.0028 (7)	0.0046 (6)	-0.0057 (7)
C7	0.0467 (8)	0.0550 (10)	0.0415 (8)	0.0014 (7)	0.0019 (6)	-0.0047 (7)
C8	0.0580 (9)	0.0512 (10)	0.0542 (9)	-0.0003 (8)	0.0031 (8)	0.0030 (8)
C9	0.0848 (13)	0.0769 (14)	0.0667 (12)	0.0310 (11)	0.0118 (10)	0.0077 (10)
C10	0.0606 (10)	0.0617 (11)	0.0543 (10)	0.0154 (9)	0.0061 (8)	-0.0110 (9)
C11	0.0526 (9)	0.0463 (9)	0.0503 (9)	0.0123 (7)	-0.0026 (7)	-0.0103 (7)
C12	0.0645 (10)	0.0562 (11)	0.0597 (10)	0.0026 (9)	0.0080 (8)	-0.0168 (9)
C13	0.0760 (13)	0.0863 (15)	0.0690 (12)	0.0065 (11)	0.0213 (10)	-0.0087 (11)

## supplementary materials

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C14	0.0666 (12)	0.0777 (15)	0.0946 (16)	0.0033 (11)	0.0111 (11)	0.0177 (13)
C15	0.0753 (13)	0.0512 (12)	0.1202 (19)	-0.0043 (10)	-0.0082 (13)	-0.0044 (12)
C16	0.0749 (12)	0.0584 (12)	0.0803 (13)	0.0084 (10)	0.0011 (10)	-0.0247 (10)

### *Geometric parameters (Å, °)*

C11—C2	1.7410 (17)	C8—H8B	0.9700
N1—C7	1.2733 (19)	C9—C10	1.545 (2)
N1—C10	1.477 (2)	C9—H9A	0.9700
C1—C2	1.369 (2)	C9—H9B	0.9700
C1—C6	1.392 (2)	C10—C11	1.501 (2)
C1—H1	0.9300	C10—H10	0.9800
C2—C3	1.383 (2)	C11—C16	1.378 (2)
C3—C4	1.370 (3)	C11—C12	1.378 (2)
C3—H3	0.9300	C12—C13	1.379 (3)
C4—C5	1.377 (2)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.356 (3)
C5—C6	1.388 (2)	C13—H13	0.9300
C5—H5	0.9300	C14—C15	1.361 (3)
C6—C7	1.476 (2)	C14—H14	0.9300
C7—C8	1.505 (2)	C15—C16	1.382 (3)
C8—C9	1.504 (2)	C15—H15	0.9300
C8—H8A	0.9700	C16—H16	0.9300
C7—N1—C10	109.37 (14)	C8—C9—H9A	110.8
C2—C1—C6	119.66 (14)	C10—C9—H9A	110.8
C2—C1—H1	120.2	C8—C9—H9B	110.8
C6—C1—H1	120.2	C10—C9—H9B	110.8
C1—C2—C3	121.45 (16)	H9A—C9—H9B	108.9
C1—C2—C11	119.55 (12)	N1—C10—C11	111.31 (15)
C3—C2—C11	119.01 (13)	N1—C10—C9	105.86 (13)
C4—C3—C2	118.80 (16)	C11—C10—C9	114.51 (14)
C4—C3—H3	120.6	N1—C10—H10	108.3
C2—C3—H3	120.6	C11—C10—H10	108.3
C3—C4—C5	120.82 (15)	C9—C10—H10	108.3
C3—C4—H4	119.6	C16—C11—C12	117.45 (17)
C5—C4—H4	119.6	C16—C11—C10	121.35 (15)
C4—C5—C6	120.29 (16)	C12—C11—C10	121.19 (16)
C4—C5—H5	119.9	C11—C12—C13	121.18 (18)
C6—C5—H5	119.9	C11—C12—H12	119.4
C5—C6—C1	118.98 (15)	C13—C12—H12	119.4
C5—C6—C7	120.74 (15)	C14—C13—C12	120.27 (19)
C1—C6—C7	120.28 (13)	C14—C13—H13	119.9
N1—C7—C6	121.47 (14)	C12—C13—H13	119.9
N1—C7—C8	115.58 (14)	C13—C14—C15	119.9 (2)
C6—C7—C8	122.94 (13)	C13—C14—H14	120.0
C9—C8—C7	102.64 (14)	C15—C14—H14	120.0
C9—C8—H8A	111.2	C14—C15—C16	120.0 (2)
C7—C8—H8A	111.2	C14—C15—H15	120.0
C9—C8—H8B	111.2	C16—C15—H15	120.0

C7—C8—H8B	111.2	C11—C16—C15	121.21 (18)
H8A—C8—H8B	109.2	C11—C16—H16	119.4
C8—C9—C10	104.67 (14)	C15—C16—H16	119.4
C6—C1—C2—C3	0.0 (2)	C7—C8—C9—C10	12.4 (2)
C6—C1—C2—C11	-179.78 (12)	C7—N1—C10—C11	134.21 (15)
C1—C2—C3—C4	0.4 (3)	C7—N1—C10—C9	9.2 (2)
C11—C2—C3—C4	-179.80 (14)	C8—C9—C10—N1	-13.5 (2)
C2—C3—C4—C5	-0.4 (3)	C8—C9—C10—C11	-136.50 (16)
C3—C4—C5—C6	-0.1 (3)	N1—C10—C11—C16	-48.5 (2)
C4—C5—C6—C1	0.5 (2)	C9—C10—C11—C16	71.5 (2)
C4—C5—C6—C7	-178.99 (16)	N1—C10—C11—C12	131.90 (16)
C2—C1—C6—C5	-0.5 (2)	C9—C10—C11—C12	-108.09 (19)
C2—C1—C6—C7	179.01 (14)	C16—C11—C12—C13	-0.2 (3)
C10—N1—C7—C6	178.25 (14)	C10—C11—C12—C13	179.46 (17)
C10—N1—C7—C8	-1.0 (2)	C11—C12—C13—C14	-0.3 (3)
C5—C6—C7—N1	176.41 (16)	C12—C13—C14—C15	0.4 (3)
C1—C6—C7—N1	-3.0 (2)	C13—C14—C15—C16	-0.1 (3)
C5—C6—C7—C8	-4.4 (2)	C12—C11—C16—C15	0.5 (3)
C1—C6—C7—C8	176.10 (14)	C10—C11—C16—C15	-179.16 (17)
N1—C7—C8—C9	-7.8 (2)	C14—C15—C16—C11	-0.3 (3)
C6—C7—C8—C9	173.00 (15)		

Fig. 1

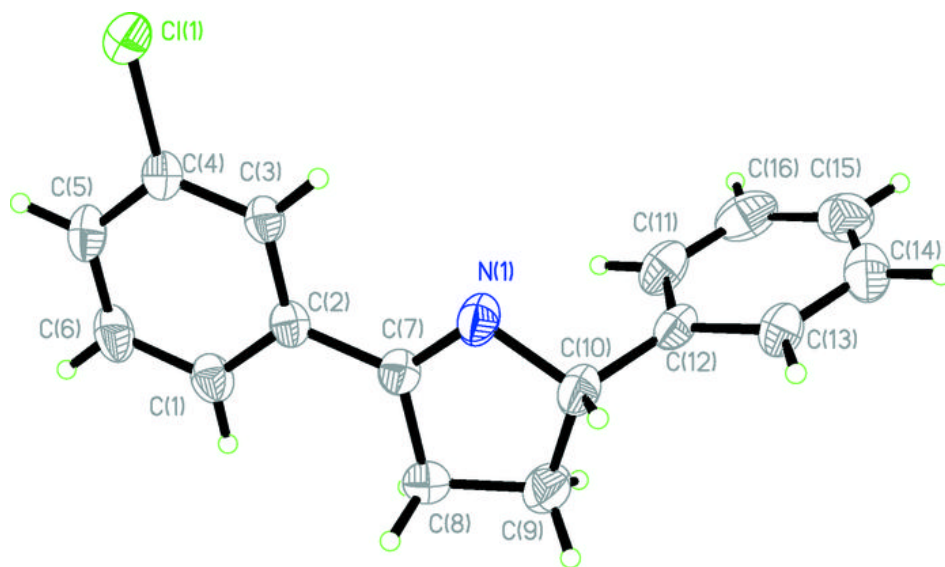




Fig. 2

