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# 3-(4-Chlorobutyl)-3*H*-indole-5-carbonitrile. Corrigendum

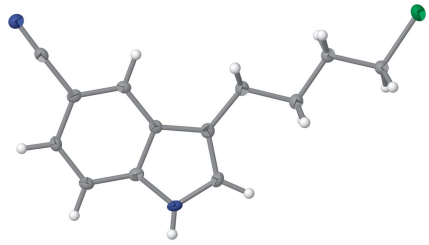
Devakumar Manikandan,[a] Sundaramoorthy Gomathi,[a] Jeyaraman Selvaraj Nirmalram,[b] Sadasivam Sharmila Tagore,[a] Velusamy Sethuraman,[a]* Joseph Agim[c] and Ray Butcher[c]

[a]Department of Chemistry, Periyar Maniammai University, Thanjavur 613 403, Tamil Nadu, India, [b]Centre for Research and Development, PRIST University, Thanjavur 613 403, Tamil Nadu, India, and [c]Inorganic & Structural Chemistry, Howard University, Washington, DC 20059, USA. *Correspondence e-mail: lvsethu13@gmail.com

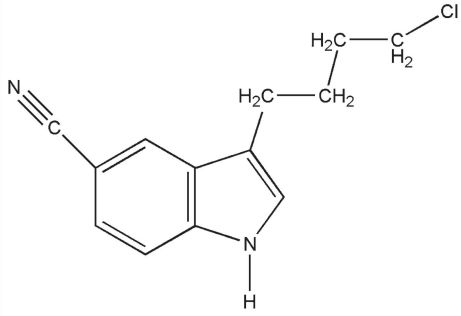
CCDC references: 1573008-1573009;

In the paper by Manikandan *et al.* [*IUCrData* (2017). **2**, x170376], a proton on the indole N was missed in the structure solution. The proton is now added and the changes are reported here. The title, scheme, Figs. 1 and 2, the hydrogen-bonding table, the crystallographic data table and description of the supramolecular architectures are corrected.

3D view



Chemical scheme




## Structure description

In the paper by Manikandan *et al.* (2017), a proton on the indole N atom was missed in the structure solution. The proton has been added and the changes are reported here. The title and the chemical name of the compound should be '3-(4-Chlorobutyl)-1*H*-indole-5-carbonitrile'.

The proton on the indole nitrogen (N1) is involved in an N—H···N hydrogen bond with symmetry-related neighboring molecules and forms an $R_3^3(23)$ ring motif instead of a chain with a $C(9)$ graph set.

The figure caption of Fig. 2, the hydrogen-bonding table and the crystallographic data table are updated. In the structure description section, the sentence 'In the crystal,

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···N2$^{i}$ | 0.787 (19) | 2.263 (19) | 3.039 (2) | 168.7 (19) |
| C4—H4···Cl1$^{ii}$ | 0.95 | 2.80 | 3.7497 (18) | 178 |

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

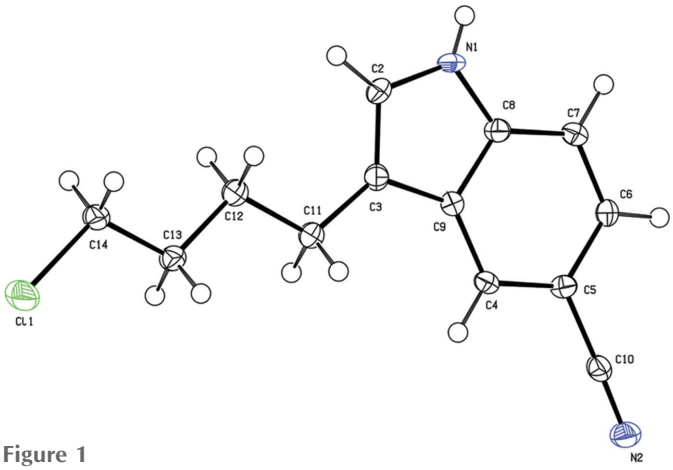



**Figure 1**
The asymmetric unit of (I), shown with 50% probability displacement ellipsoids.

neighboring molecules self-assemble through weak C—H···Cl interactions (Table 1), forming zigzag supramolecular *C*(9) chains extending along the *b*-axis direction, as shown in Fig. 2*a*.' should be replaced by 'In the crystal, neighboring molecules self-assemble through N—H···N and weak C—H···Cl interactions (Table 1), resulting in an $R_3^3(23)$ ring motif, which forms a supramolecular sheet extending along the *b* axis, as shown in Fig. 2*a*.' Revised experimental details are given in Table 2.

**Table 2**
Updated experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{13}H_{13}ClN_2$ |
| $M_r$ | 232.70 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.034, 0.097, 1.05 |
| No. of parameters | 149 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.29, −0.24 |

## References

Manikandan, D., Gomathi, S., Nirmalram, J. S., Tagore, S. S., Sethuraman, V., Agim, J. & Butcher, R. J. (2017). *IUCrData*, **2**, x170376.

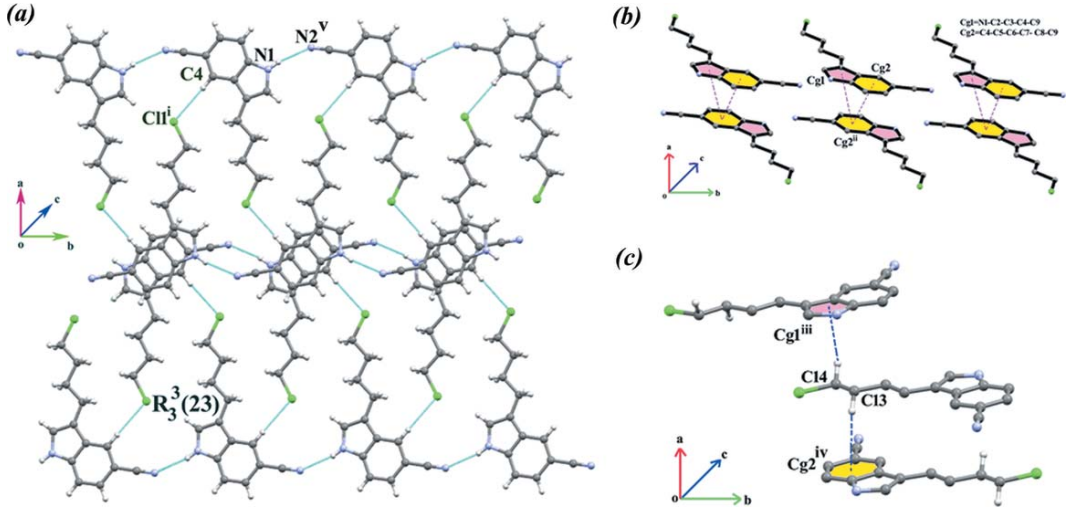



**Figure 2**
A view of two-dimensional supramolecular sheet *via* N—H···N and weak intermolecular C—H···Cl hydrogen bonding, aromatic $\pi$–$\pi$ and weak C—H···$\pi$ interactions. [Symmetry codes: (i) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (ii) $-x, 1-y, 1-z$; (iii) $1-x, 1-y, 1-z$; (iv) $x, \frac{3}{2}-y, -\frac{1}{2}+z$; (v) $x, 1+y, z$.]

# full crystallographic data

*IUCrData* (2017). **2**, x171132 [https://doi.org/10.1107/S2414314617011324]

## 3-(4-Chlorobutyl)-3*H*-indole-5-carbonitrile. Corrigendum

**Devakumar Manikandan, Sundaramoorthy Gomathi, Jeyaraman Selvaraj Nirmalram, Sadasivam Sharmila Tagore, Velusamy Sethuraman, Joseph Agim and Ray Butcher**

### 3-(4-Chlorobutyl)-1*H*-indole-5-carbonitrile

*Crystal data*

$C_{13}H_{13}ClN_2$
$M_r$ = 232.70
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 8.870 (2) Å
$b$ = 9.271 (2) Å
$c$ = 14.498 (3) Å
$\beta$ = 100.236 (4)°
$V$ = 1173.3 (4) Å$^3$
$Z$ = 4
$F(000)$ = 488
$D_x$ = 1.317 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1952 reflections
$\theta$ = 2.6–24.6°
$\mu$ = 0.30 mm$^{-1}$
$T$ = 100 K
Block, colourless
0.18 × 0.17 × 0.15 mm

*Data collection*

Bruker APEXII diffractometer
Detector resolution: 18.4 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2008)
$T_{min}$ = 0.618, $T_{max}$ = 0.745
7342 measured reflections
1952 independent reflections
1632 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039
$\theta_{max}$ = 24.6°, $\theta_{min}$ = 2.6°
$h$ = −10→10
$k$ = −10→10
$l$ = −17→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
$S$ = 1.05
1952 reflections
149 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\Sigma^2(FO^2) + (0.0615P)^2 + 0.1055P]$ where $P = (FO^2 + 2FC^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 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 esds are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 | 0.64036 (6) | 0.62781 (5) | 0.10556 (3) | 0.0373 (2) |
| N1 | 0.17181 (16) | 0.77684 (15) | 0.56118 (10) | 0.0202 (4) |
| N2 | 0.10999 (16) | 0.07038 (15) | 0.64000 (9) | 0.0248 (5) |
| C2 | 0.24682 (17) | 0.77009 (16) | 0.48566 (10) | 0.0193 (5) |
| C3 | 0.27344 (17) | 0.62953 (17) | 0.46452 (11) | 0.0177 (5) |
| C4 | 0.19953 (17) | 0.39623 (17) | 0.54478 (10) | 0.0160 (5) |
| C5 | 0.12918 (17) | 0.34723 (16) | 0.61736 (10) | 0.0170 (5) |
| C6 | 0.07019 (17) | 0.44431 (16) | 0.67723 (10) | 0.0180 (5) |
| C7 | 0.07908 (18) | 0.59143 (17) | 0.66461 (11) | 0.0190 (5) |
| C8 | 0.14877 (17) | 0.64002 (16) | 0.59099 (11) | 0.0175 (5) |
| C9 | 0.21099 (16) | 0.54435 (17) | 0.53130 (10) | 0.0154 (4) |
| C10 | 0.11661 (17) | 0.19387 (17) | 0.63039 (11) | 0.0187 (5) |
| C11 | 0.34895 (17) | 0.56971 (18) | 0.38827 (10) | 0.0185 (5) |
| C12 | 0.40919 (18) | 0.68138 (17) | 0.32640 (11) | 0.0200 (5) |
| C13 | 0.48445 (18) | 0.60781 (16) | 0.25127 (10) | 0.0189 (5) |
| C14 | 0.54689 (19) | 0.71647 (17) | 0.19063 (11) | 0.0212 (5) |
| H1 | 0.147 (2) | 0.847 (2) | 0.5852 (15) | 0.033 (6)* |
| H2 | 0.27584 | 0.85143 | 0.45299 | 0.0230* |
| H4 | 0.23903 | 0.32991 | 0.50516 | 0.0190* |
| H6 | 0.02389 | 0.40786 | 0.72672 | 0.0220* |
| H7 | 0.03936 | 0.65728 | 0.70443 | 0.0230* |
| H11A | 0.27441 | 0.50716 | 0.34779 | 0.0220* |
| H11B | 0.43558 | 0.50800 | 0.41731 | 0.0220* |
| H12A | 0.32349 | 0.74283 | 0.29573 | 0.0240* |
| H12B | 0.48506 | 0.74413 | 0.36573 | 0.0240* |
| H13A | 0.40795 | 0.54624 | 0.21146 | 0.0230* |
| H13B | 0.56878 | 0.54494 | 0.28208 | 0.0230* |
| H14A | 0.46214 | 0.77713 | 0.15787 | 0.0250* |
| H14B | 0.62099 | 0.78019 | 0.23049 | 0.0250* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0598 (4) | 0.0245 (3) | 0.0364 (3) | 0.0068 (2) | 0.0329 (2) | 0.0054 (2) |
| N1 | 0.0273 (8) | 0.0099 (7) | 0.0255 (7) | 0.0006 (6) | 0.0108 (6) | −0.0031 (6) |
| N2 | 0.0349 (8) | 0.0165 (8) | 0.0256 (8) | 0.0013 (6) | 0.0125 (6) | 0.0011 (6) |
| C2 | 0.0227 (8) | 0.0148 (8) | 0.0217 (8) | −0.0020 (6) | 0.0077 (7) | 0.0029 (6) |
| C3 | 0.0163 (8) | 0.0183 (9) | 0.0191 (8) | −0.0002 (6) | 0.0046 (6) | 0.0012 (6) |
| C4 | 0.0172 (8) | 0.0146 (8) | 0.0169 (8) | 0.0019 (6) | 0.0049 (6) | −0.0018 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0191 (8) | 0.0136 (8) | 0.0182 (8) | 0.0003 (6) | 0.0032 (6) | −0.0002 (6) |
| C6 | 0.0198 (8) | 0.0184 (8) | 0.0178 (8) | −0.0011 (7) | 0.0085 (6) | 0.0012 (6) |
| C7 | 0.0221 (8) | 0.0156 (8) | 0.0210 (8) | 0.0012 (7) | 0.0082 (7) | −0.0029 (6) |
| C8 | 0.0177 (8) | 0.0145 (9) | 0.0202 (8) | 0.0007 (6) | 0.0035 (6) | −0.0008 (6) |
| C9 | 0.0150 (8) | 0.0155 (8) | 0.0161 (7) | 0.0001 (6) | 0.0040 (6) | −0.0002 (6) |
| C10 | 0.0203 (8) | 0.0191 (9) | 0.0184 (8) | 0.0019 (7) | 0.0079 (7) | 0.0000 (7) |
| C11 | 0.0207 (9) | 0.0166 (8) | 0.0194 (8) | 0.0004 (6) | 0.0066 (7) | 0.0020 (6) |
| C12 | 0.0224 (9) | 0.0177 (8) | 0.0211 (8) | 0.0006 (7) | 0.0072 (7) | 0.0025 (7) |
| C13 | 0.0234 (9) | 0.0159 (8) | 0.0185 (8) | −0.0007 (7) | 0.0066 (7) | 0.0005 (6) |
| C14 | 0.0278 (9) | 0.0171 (8) | 0.0214 (8) | 0.0007 (7) | 0.0114 (7) | −0.0001 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C14 | 1.8021 (17) | C11—C12 | 1.527 (2) |
| N1—C2 | 1.380 (2) | C12—C13 | 1.535 (2) |
| N1—C8 | 1.367 (2) | C13—C14 | 1.506 (2) |
| N2—C10 | 1.156 (2) | C2—H2 | 0.9500 |
| N1—H1 | 0.787 (19) | C4—H4 | 0.9500 |
| C2—C3 | 1.369 (2) | C6—H6 | 0.9500 |
| C3—C9 | 1.435 (2) | C7—H7 | 0.9500 |
| C3—C11 | 1.497 (2) | C11—H11A | 0.9900 |
| C4—C9 | 1.393 (2) | C11—H11B | 0.9900 |
| C4—C5 | 1.392 (2) | C12—H12A | 0.9900 |
| C5—C6 | 1.414 (2) | C12—H12B | 0.9900 |
| C5—C10 | 1.441 (2) | C13—H13A | 0.9900 |
| C6—C7 | 1.380 (2) | C13—H13B | 0.9900 |
| C7—C8 | 1.400 (2) | C14—H14A | 0.9900 |
| C8—C9 | 1.418 (2) | C14—H14B | 0.9900 |
| | | | |
| C2—N1—C8 | 109.21 (13) | C5—C4—H4 | 121.00 |
| C8—N1—H1 | 123.9 (14) | C9—C4—H4 | 121.00 |
| C2—N1—H1 | 126.9 (14) | C5—C6—H6 | 120.00 |
| N1—C2—C3 | 110.34 (13) | C7—C6—H6 | 120.00 |
| C2—C3—C11 | 129.47 (14) | C6—C7—H7 | 121.00 |
| C2—C3—C9 | 105.68 (13) | C8—C7—H7 | 121.00 |
| C9—C3—C11 | 124.85 (14) | C3—C11—H11A | 108.00 |
| C5—C4—C9 | 118.78 (14) | C3—C11—H11B | 108.00 |
| C4—C5—C6 | 121.40 (14) | C12—C11—H11A | 108.00 |
| C6—C5—C10 | 120.12 (13) | C12—C11—H11B | 108.00 |
| C4—C5—C10 | 118.47 (14) | H11A—C11—H11B | 107.00 |
| C5—C6—C7 | 120.77 (14) | C11—C12—H12A | 109.00 |
| C6—C7—C8 | 117.55 (14) | C11—C12—H12B | 109.00 |
| N1—C8—C7 | 130.61 (14) | C13—C12—H12A | 109.00 |
| N1—C8—C9 | 106.93 (13) | C13—C12—H12B | 109.00 |
| C7—C8—C9 | 122.46 (14) | H12A—C12—H12B | 108.00 |
| C3—C9—C4 | 133.13 (14) | C12—C13—H13A | 109.00 |
| C4—C9—C8 | 119.01 (13) | C12—C13—H13B | 109.00 |
| C3—C9—C8 | 107.84 (13) | C14—C13—H13A | 109.00 |

| | | | |
|---|---|---|---|
| N2—C10—C5 | 178.25 (17) | C14—C13—H13B | 109.00 |
| C3—C11—C12 | 115.58 (14) | H13A—C13—H13B | 108.00 |
| C11—C12—C13 | 110.93 (13) | Cl1—C14—H14A | 109.00 |
| C12—C13—C14 | 111.62 (13) | Cl1—C14—H14B | 109.00 |
| Cl1—C14—C13 | 110.86 (11) | C13—C14—H14A | 109.00 |
| N1—C2—H2 | 125.00 | C13—C14—H14B | 109.00 |
| C3—C2—H2 | 125.00 | H14A—C14—H14B | 108.00 |
| | | | |
| C8—N1—C2—C3 | 0.28 (18) | C5—C4—C9—C8 | −0.9 (2) |
| C2—N1—C8—C7 | 179.69 (16) | C4—C5—C6—C7 | 0.8 (2) |
| C2—N1—C8—C9 | −0.39 (17) | C10—C5—C6—C7 | −178.90 (14) |
| N1—C2—C3—C9 | −0.05 (18) | C5—C6—C7—C8 | −0.2 (2) |
| N1—C2—C3—C11 | 179.18 (15) | C6—C7—C8—N1 | 179.00 (16) |
| C2—C3—C9—C4 | 178.35 (16) | C6—C7—C8—C9 | −0.9 (2) |
| C2—C3—C9—C8 | −0.19 (17) | N1—C8—C9—C3 | 0.35 (17) |
| C11—C3—C9—C4 | −0.9 (3) | N1—C8—C9—C4 | −178.43 (14) |
| C11—C3—C9—C8 | −179.47 (14) | C7—C8—C9—C3 | −179.72 (14) |
| C2—C3—C11—C12 | 1.8 (2) | C7—C8—C9—C4 | 1.5 (2) |
| C9—C3—C11—C12 | −179.05 (14) | C3—C11—C12—C13 | 179.79 (13) |
| C9—C4—C5—C6 | −0.2 (2) | C11—C12—C13—C14 | −179.04 (13) |
| C9—C4—C5—C10 | 179.49 (14) | C12—C13—C14—Cl1 | 178.05 (11) |
| C5—C4—C9—C3 | −179.31 (16) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···N2$^{i}$ | 0.787 (19) | 2.263 (19) | 3.039 (2) | 168.7 (19) |
| C4—H4···Cl1$^{ii}$ | 0.95 | 2.80 | 3.7497 (18) | 178 |

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