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# Corrigenda for three related articles

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The schemes and chemical names are corrected in three related papers: Vishnupriya, Suresh, Bharkavi *et al.* [*Acta Cryst.* (2014), E**70**, o968–o969], Vishnupriya, Suresh, Gunasekaran *et al.* [*Acta Cryst.* (2014), E**70**, o978], and Vishnupriya, Suresh, Sakthi *et al.* [*Acta Cryst.* (2014), E**70**, o1120–o1121].

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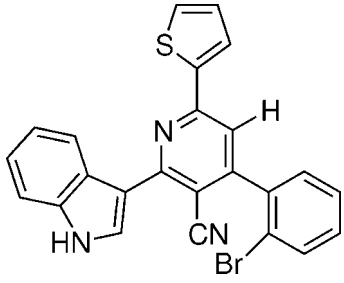
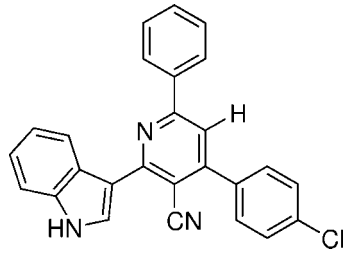
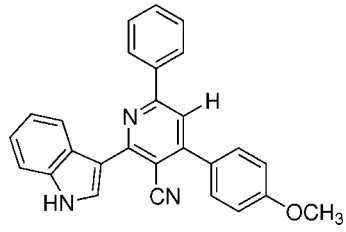
In the paper by Vishnupriya, Suresh, Bharkavi *et al.* (2014), the chemical name in the title should be given as '4-(2-bromophenyl)-2-(1*H*-indol-3-yl)-6-(thiophen-2-yl)pyridine-3-carbonitrile' and the correct scheme is shown below.




In the paper by Vishnupriya, Suresh, Gunasekaran *et al.* (2014), the chemical name in the title should be given as '4-(4-chlorophenyl)-2-(1*H*-indol-3-yl)-6-phenylpyridine-3-carbonitrile' and the correct scheme is shown below.




In the paper by Vishnupriya, Suresh, Sakthi *et al.* (2014), the chemical name in the title should be given as '2-(1*H*-indol-3-yl)-4-(4-methoxyphenyl)-6-phenylpyridine-3-carbonitrile' and the correct scheme is shown below.

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Vishnupriya, R., Suresh, J., Bharkavi, S., Perumal, S. & Lakshman, P. L. N. (2014). *Acta Cryst.* E**70**, o968–o969.

Vishnupriya, R., Suresh, J., Gunasekaran, P., Perumal, S. & Lakshman, P. L. N. (2014). *Acta Cryst.* E**70**, o978.

Vishnupriya, R., Suresh, J., Sakthi, M., Perumal, S. & Lakshman, P. L. N. (2014). *Acta Cryst.* E**70**, o1120–o1121.

Acta Cryst E STRUCTURE REPORTS

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# Crystal structure of 4-(1*H*-indol-3-yl)-2-(4-methoxyphenyl)-6-phenylpyridine-3-carbonitrile

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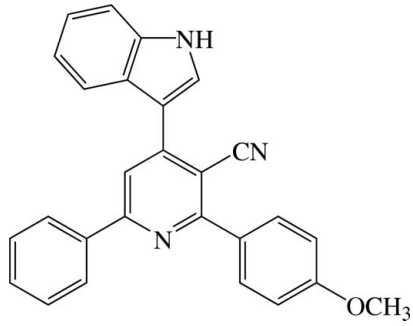
In the title compound, $C_{27}H_{19}N_3O$, the dihedral angles between the plane of the pyridine ring and those of the indole (r.m.s. deviation = 0.018 Å), phenyl and methoxybenzene substituents are 33.60 (6), 25.28 (7) and 49.31 (7)°, respectively. The N atom of the carbonitrile group is significantly displaced [0.288 (2) Å] from the plane of the pyridine ring, perhaps due to steric crowding. In the crystal, inversion dimers linked by pairs of N—H···$N_n$ (n = nitrile) hydrogen bonds generate $R_2^2(16)$ loops. Aromatic $\pi$–$\pi$ stacking [centroid–centroid separation = 3.6906 (7) Å] and very weak C—H···$\pi$ interactions are also observed".

**Keywords:** crystal structure; pyridine-3-carbonitrile; heterocyclic compounds; hydrogen bonding.

**CCDC reference**: 1023204

## 1. Related literature

For the use of 2-amino-3-cyanopyridines as intermediates in the preparation of heterocyclic compounds, see: Shishoo *et al.* (1983).




## 2. Experimental

### 2.1. Crystal data

$C_{27}H_{19}N_3O$
$M_r$ = 401.45
Orthorhombic, *Pbca*
$a$ = 15.7102 (5) Å
$b$ = 10.7491 (3) Å
$c$ = 24.3648 (7) Å
$V$ = 4114.5 (2) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 K
0.30 × 0.28 × 0.25 mm

### 2.2. Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.976, $T_{max}$ = 0.980
27554 measured reflections
4486 independent reflections
3331 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.104
$S$ = 1.01
4486 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

*Cg*1 is the centroid of the pyrrole ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3···N2$^{i}$ | 0.86 | 2.15 | 2.9693 (19) | 159 |
| C32—H32···*Cg*1$^{ii}$ | 0.93 | 3.00 | 3.9157 (19) | 170 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

## Acknowledgements

JS and RV thank the management of Madura College for their encouragement and support. SP thanks the Department of Science and Technology, New Delhi, for a major research project (SR/S1/OC/-50/2011) and the University Grants

Commission, New Delhi, for the award of a BSR Faculty Fellowship

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7280).

## References

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Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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Shishoo, C. J., Devani, M. B., Bhadti, V. S., Ananthan, S. & Ullas, G. V. (1983). *Tetrahedron Lett.* pp. 4611–4612.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supporting information

*Acta Cryst.* (2014). E**70**, o1120–o1121 [doi:10.1107/S1600536814020170]

# Crystal structure of 4-(1*H*-indol-3-yl)-2-(4-methoxyphenyl)-6-phenylpyridine-3-carbonitrile

**R. Vishnupriya, J. Suresh, Marimuthu Sakthi, Subbu Perumal and P. L. Nilantha Lakshman**

## S1. Comment

Derivatives of 3-cyanopyridine are important and useful intermediates in preparing a varity of heterocyclic compounds (Shishoo *et al.*, 1983). Therefore, the synthesis of 3-cyanopyridine derivatives attracts much interest in organic chemistry. It was in this context that the title compound, was investigated.

The deviation of the nitrile atoms (C41,N2) from the mean plane of the pyridine ring system is -0.1497 (1) Å and -0.2886 (5) Å. The shortening of the C—N distances [1.337 (3) and 1.341 Å] and the opening of the N1–C11–C10 angle [121.15 (2)°] may be attributed to the size of the substituent at C1, correlating well with the values observed in the *ortho*-substituted derivative. The dihedral angle between the pseudo-axial phenyl substituent and the plane of the pyridine ring is 69.13 (8)°.

The crystal structure features an N—H···N interaction between inverse related molecules generating a graph set ring motif $R_2^2$ (16) which are linked into chains through C—H···*Cg*1 interation (*Cg*1 is the centroid of the pyrrole ring of the indole moiety) and by $\pi\cdots\pi$ stacking interaction involving adjacent pyridine rings of the symmetry related molecule at (1-*X*,1-Y,-*Z*), with a centroid-to-centroid distance of 3.6906 (7) Å·(Fig 2).

## S2. Experimental

A mixture of 3-(1*H*-indol-3-yl)-3-oxopropanenitrile 1 (1 mmol), 4,4,4-trifluoro-1- phenylbutane-1,3-dione 2 (1 mmol) and 4-methoxy benzaldehyde 3 (1 mmol) in the presence of ammonium acetate (400 mmol) under solvent-free condition was heated at 110°C for 7 h. After completion of the reaction (TLC), the reaction mixture was poured into water and extracted with dichloromethane. After removal of the solvent, the residue was chromatographed over $\sigma$ilica gel (230–400 mesh) using petroleum ether-ethyl acetate mixture (7:3 *v*/*v*), which afforded the pure compound.

Melting point:265 °C, Yield: 72%.

## S3. Refinement

H atoms were placed at calculated positions and allowed to ride on their carrier atoms with C—H = 0.93–0.98 Å and with $U_{iso}$ = 1.2$U_{eq}$(C, N) for N, $CH_2$ and CH atoms and $U_{iso}$ = 1.5$U_{eq}$(C) for $CH_3$ atoms.

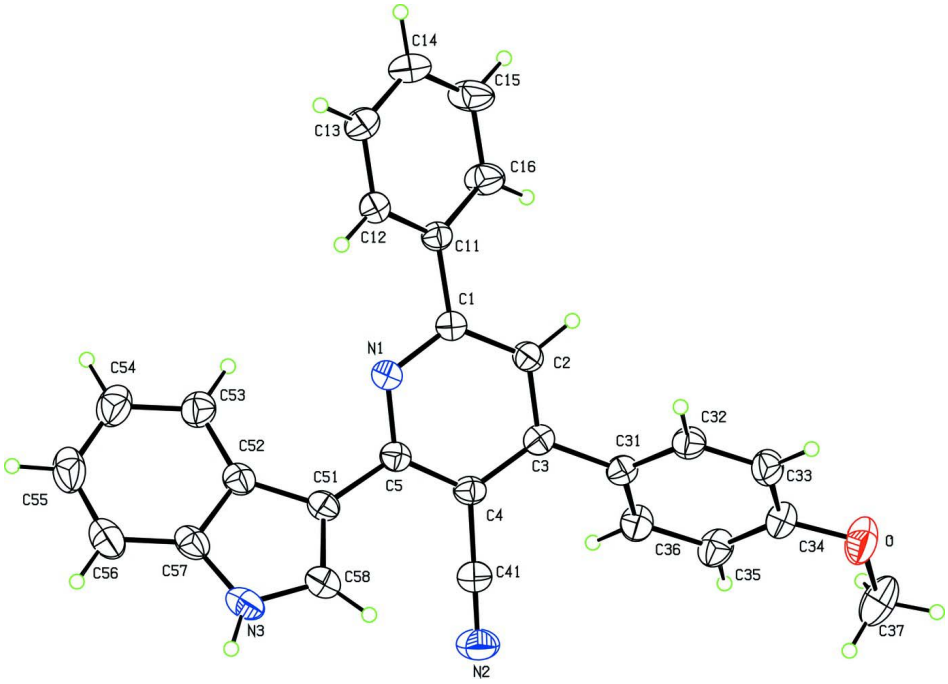


**Figure 1**

The molecular structure of compound showing 30% probability displacement ellipsoids.

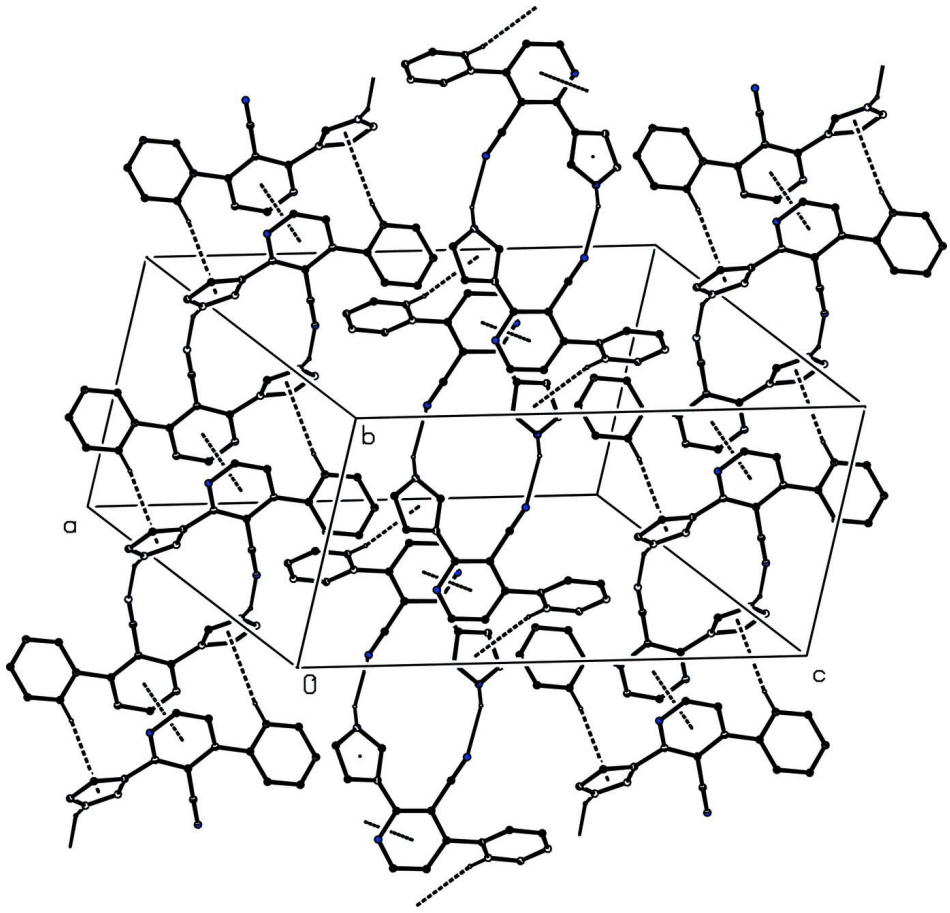


**Figure 2**

partial packing view of the compound showing molecules interconnected through a C—H···$\pi$ and $\pi$···$\pi$ stacking interaction (dotted lines; symmetry code: (i) (1-*x*, 1-*y*,-*z*)

### 4-(1*H*-Indol-3-yl)-2-(4-methoxyphenyl)-6-phenylpyridine-3-carbonitrile

*Crystal data*

$C_{27}H_{19}N_3O$
$M_r$ = 401.45
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
*a* = 15.7102 (5) Å
*b* = 10.7491 (3) Å
*c* = 24.3648 (7) Å
*V* = 4114.5 (2) Å$^3$
*Z* = 8
*F*(000) = 1680
$D_x$ = 1.296 Mg m$^{-3}$
Mo *K*$\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2000 reflections
$\theta$ = 2–27°
$\mu$ = 0.08 mm$^{-1}$
*T* = 293 K
Block, colourless
0.30 × 0.28 × 0.25 mm

*Data collection*

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.976, $T_{max}$ = 0.980
27554 measured reflections
4486 independent reflections
3331 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.025
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.1°
$h$ = −20→20
$k$ = −13→8
$l$ = −31→31

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.104
$S$ = 1.01
4486 reflections
282 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
$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 1.0149P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0027 (4)

*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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.11716 (8) | 1.07304 (12) | 0.96916 (5) | 0.0400 (3) |
| C2 | 0.14114 (9) | 1.06339 (12) | 1.02373 (5) | 0.0436 (3) |
| H2 | 0.1574 | 1.1344 | 1.0428 | 0.052* |
| C3 | 0.14124 (8) | 0.94978 (12) | 1.05007 (5) | 0.0416 (3) |
| C4 | 0.11465 (8) | 0.84683 (11) | 1.01907 (5) | 0.0416 (3) |
| C5 | 0.08413 (8) | 0.86400 (11) | 0.96531 (5) | 0.0407 (3) |
| C11 | 0.12231 (8) | 1.19255 (12) | 0.93922 (5) | 0.0402 (3) |
| C12 | 0.07016 (9) | 1.21553 (12) | 0.89470 (5) | 0.0465 (3) |
| H12 | 0.0316 | 1.1552 | 0.8833 | 0.056* |
| C13 | 0.07492 (11) | 1.32728 (14) | 0.86716 (6) | 0.0559 (4) |
| H13 | 0.0391 | 1.3420 | 0.8375 | 0.067* |
| C14 | 0.13180 (11) | 1.41679 (14) | 0.88303 (7) | 0.0605 (4) |
| H14 | 0.1350 | 1.4917 | 0.8641 | 0.073* |
| C15 | 0.18372 (11) | 1.39515 (15) | 0.92690 (8) | 0.0711 (5) |
| H15 | 0.2223 | 1.4558 | 0.9380 | 0.085* |
| C16 | 0.17937 (10) | 1.28396 (14) | 0.95483 (7) | 0.0614 (4) |
| H16 | 0.2152 | 1.2701 | 0.9846 | 0.074* |
| C31 | 0.16647 (9) | 0.94381 (12) | 1.10856 (5) | 0.0430 (3) |
| C32 | 0.13218 (10) | 1.03013 (13) | 1.14465 (6) | 0.0515 (4) |
| H32 | 0.0935 | 1.0886 | 1.1317 | 0.062* |

| | | | | |
|---|---|---|---|---|
| C33 | 0.15425 (11) | 1.03077 (14) | 1.19904 (6) | 0.0576 (4) |
| H33 | 0.1301 | 1.0888 | 1.2227 | 0.069* |
| C34 | 0.21220 (10) | 0.94553 (14) | 1.21888 (6) | 0.0547 (4) |
| C35 | 0.24701 (10) | 0.85934 (15) | 1.18375 (6) | 0.0586 (4) |
| H35 | 0.2862 | 0.8015 | 1.1968 | 0.070* |
| C36 | 0.22377 (10) | 0.85875 (14) | 1.12909 (6) | 0.0532 (4) |
| H36 | 0.2473 | 0.7997 | 1.1057 | 0.064* |
| C37 | 0.28200 (13) | 0.8619 (2) | 1.29741 (7) | 0.0858 (6) |
| H37A | 0.2574 | 0.7814 | 1.2910 | 0.129* |
| H37B | 0.2861 | 0.8763 | 1.3362 | 0.129* |
| H37C | 0.3378 | 0.8651 | 1.2814 | 0.129* |
| C41 | 0.11876 (9) | 0.72404 (13) | 1.04200 (6) | 0.0492 (3) |
| C51 | 0.04591 (9) | 0.76538 (12) | 0.93237 (6) | 0.0441 (3) |
| C52 | 0.04502 (9) | 0.75788 (12) | 0.87349 (6) | 0.0462 (3) |
| C53 | 0.08391 (10) | 0.82422 (15) | 0.83125 (6) | 0.0572 (4) |
| H53 | 0.1182 | 0.8925 | 0.8390 | 0.069* |
| C54 | 0.07081 (13) | 0.78724 (17) | 0.77795 (7) | 0.0721 (5) |
| H54 | 0.0967 | 0.8311 | 0.7496 | 0.087* |
| C55 | 0.01956 (14) | 0.68547 (18) | 0.76559 (8) | 0.0784 (6) |
| H55 | 0.0120 | 0.6623 | 0.7291 | 0.094* |
| C56 | −0.01989 (12) | 0.61900 (15) | 0.80601 (8) | 0.0704 (5) |
| H56 | −0.0543 | 0.5511 | 0.7977 | 0.085* |
| C57 | −0.00692 (10) | 0.65614 (13) | 0.85977 (7) | 0.0533 (4) |
| C58 | −0.00419 (10) | 0.66969 (13) | 0.95069 (6) | 0.0529 (4) |
| H58 | −0.0145 | 0.6513 | 0.9874 | 0.063* |
| N1 | 0.08729 (7) | 0.97572 (9) | 0.94093 (4) | 0.0419 (3) |
| N2 | 0.12503 (10) | 0.62657 (12) | 1.05973 (6) | 0.0694 (4) |
| N3 | −0.03648 (9) | 0.60601 (11) | 0.90767 (6) | 0.0597 (4) |
| H3 | −0.0704 | 0.5435 | 0.9101 | 0.072* |
| O | 0.22989 (9) | 0.95450 (12) | 1.27328 (4) | 0.0808 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0366 (7) | 0.0401 (7) | 0.0433 (7) | 0.0005 (5) | 0.0008 (5) | 0.0017 (5) |
| C2 | 0.0461 (8) | 0.0390 (7) | 0.0457 (7) | −0.0014 (6) | −0.0031 (6) | −0.0012 (6) |
| C3 | 0.0385 (7) | 0.0436 (7) | 0.0427 (7) | 0.0036 (5) | 0.0014 (5) | 0.0027 (6) |
| C4 | 0.0398 (7) | 0.0374 (7) | 0.0477 (7) | 0.0027 (5) | 0.0046 (6) | 0.0030 (6) |
| C5 | 0.0383 (7) | 0.0384 (7) | 0.0453 (7) | 0.0021 (5) | 0.0043 (6) | −0.0007 (6) |
| C11 | 0.0390 (7) | 0.0396 (7) | 0.0420 (7) | 0.0000 (5) | 0.0025 (5) | 0.0025 (5) |
| C12 | 0.0513 (8) | 0.0437 (7) | 0.0444 (7) | −0.0006 (6) | −0.0023 (6) | −0.0008 (6) |
| C13 | 0.0626 (10) | 0.0533 (8) | 0.0518 (9) | 0.0050 (7) | −0.0070 (7) | 0.0100 (7) |
| C14 | 0.0608 (10) | 0.0472 (8) | 0.0736 (11) | 0.0003 (7) | 0.0047 (8) | 0.0200 (8) |
| C15 | 0.0608 (10) | 0.0561 (9) | 0.0963 (13) | −0.0219 (8) | −0.0149 (9) | 0.0197 (9) |
| C16 | 0.0568 (9) | 0.0567 (9) | 0.0706 (10) | −0.0151 (7) | −0.0196 (8) | 0.0164 (8) |
| C31 | 0.0436 (7) | 0.0424 (7) | 0.0429 (7) | 0.0017 (6) | 0.0001 (6) | 0.0037 (6) |
| C32 | 0.0586 (9) | 0.0455 (8) | 0.0504 (8) | 0.0109 (7) | −0.0023 (7) | 0.0032 (6) |
| C33 | 0.0707 (10) | 0.0544 (9) | 0.0477 (8) | 0.0103 (8) | 0.0017 (7) | −0.0055 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C34 | 0.0593 (9) | 0.0642 (9) | 0.0407 (7) | 0.0013 (8) | −0.0038 (7) | 0.0020 (7) |
| C35 | 0.0568 (9) | 0.0660 (10) | 0.0528 (8) | 0.0164 (7) | −0.0072 (7) | 0.0068 (7) |
| C36 | 0.0550 (9) | 0.0555 (8) | 0.0490 (8) | 0.0152 (7) | −0.0012 (7) | −0.0019 (7) |
| C37 | 0.0742 (12) | 0.1313 (17) | 0.0517 (10) | 0.0134 (12) | −0.0137 (9) | 0.0174 (11) |
| C41 | 0.0482 (8) | 0.0456 (8) | 0.0539 (8) | 0.0005 (6) | 0.0004 (6) | 0.0042 (6) |
| C51 | 0.0444 (7) | 0.0367 (7) | 0.0511 (8) | 0.0035 (6) | −0.0004 (6) | −0.0023 (6) |
| C52 | 0.0466 (7) | 0.0389 (7) | 0.0531 (8) | 0.0107 (6) | −0.0068 (6) | −0.0024 (6) |
| C53 | 0.0616 (10) | 0.0562 (9) | 0.0537 (9) | 0.0091 (7) | −0.0037 (7) | 0.0016 (7) |
| C54 | 0.0878 (13) | 0.0767 (12) | 0.0519 (9) | 0.0216 (10) | −0.0066 (9) | 0.0040 (9) |
| C55 | 0.1021 (15) | 0.0748 (12) | 0.0582 (11) | 0.0315 (11) | −0.0277 (10) | −0.0137 (9) |
| C56 | 0.0829 (13) | 0.0511 (9) | 0.0773 (12) | 0.0176 (9) | −0.0367 (10) | −0.0141 (9) |
| C57 | 0.0554 (9) | 0.0389 (7) | 0.0655 (10) | 0.0110 (6) | −0.0160 (7) | −0.0060 (7) |
| C58 | 0.0548 (9) | 0.0423 (7) | 0.0616 (9) | −0.0015 (6) | 0.0010 (7) | −0.0032 (7) |
| N1 | 0.0427 (6) | 0.0382 (6) | 0.0447 (6) | −0.0008 (5) | 0.0002 (5) | −0.0003 (5) |
| N2 | 0.0780 (10) | 0.0480 (8) | 0.0823 (10) | −0.0025 (7) | −0.0103 (8) | 0.0158 (7) |
| N3 | 0.0606 (8) | 0.0397 (6) | 0.0787 (10) | −0.0065 (6) | −0.0109 (7) | −0.0045 (6) |
| O | 0.0949 (10) | 0.1018 (10) | 0.0457 (6) | 0.0184 (8) | −0.0140 (6) | −0.0034 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.3370 (16) | C33—H33 | 0.9300 |
| C1—C2 | 1.3857 (18) | C34—O | 1.3577 (17) |
| C1—C11 | 1.4795 (17) | C34—C35 | 1.375 (2) |
| C2—C3 | 1.3796 (18) | C35—C36 | 1.381 (2) |
| C2—H2 | 0.9300 | C35—H35 | 0.9300 |
| C3—C4 | 1.4035 (18) | C36—H36 | 0.9300 |
| C3—C31 | 1.4806 (18) | C37—O | 1.417 (2) |
| C4—C5 | 1.4069 (18) | C37—H37A | 0.9600 |
| C4—C41 | 1.4347 (18) | C37—H37B | 0.9600 |
| C5—N1 | 1.3406 (16) | C37—H37C | 0.9600 |
| C5—C51 | 1.4590 (18) | C41—N2 | 1.1375 (17) |
| C11—C12 | 1.3817 (18) | C51—C58 | 1.3700 (19) |
| C11—C16 | 1.3833 (19) | C51—C52 | 1.4368 (19) |
| C12—C13 | 1.3780 (19) | C52—C53 | 1.393 (2) |
| C12—H12 | 0.9300 | C52—C57 | 1.405 (2) |
| C13—C14 | 1.369 (2) | C53—C54 | 1.374 (2) |
| C13—H13 | 0.9300 | C53—H53 | 0.9300 |
| C14—C15 | 1.365 (2) | C54—C55 | 1.391 (3) |
| C14—H14 | 0.9300 | C54—H54 | 0.9300 |
| C15—C16 | 1.377 (2) | C55—C56 | 1.365 (3) |
| C15—H15 | 0.9300 | C55—H55 | 0.9300 |
| C16—H16 | 0.9300 | C56—C57 | 1.384 (2) |
| C31—C36 | 1.3771 (19) | C56—H56 | 0.9300 |
| C31—C32 | 1.3872 (19) | C57—N3 | 1.367 (2) |
| C32—C33 | 1.370 (2) | C58—N3 | 1.3507 (19) |
| C32—H32 | 0.9300 | C58—H58 | 0.9300 |
| C33—C34 | 1.379 (2) | N3—H3 | 0.8600 |

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|---|---|---|---|
| N1—C1—C2 | 122.03 (12) | C35—C34—C33 | 119.47 (13) |
| N1—C1—C11 | 116.42 (11) | C34—C35—C36 | 119.89 (14) |
| C2—C1—C11 | 121.55 (12) | C34—C35—H35 | 120.1 |
| C3—C2—C1 | 120.85 (12) | C36—C35—H35 | 120.1 |
| C3—C2—H2 | 119.6 | C31—C36—C35 | 121.33 (14) |
| C1—C2—H2 | 119.6 | C31—C36—H36 | 119.3 |
| C2—C3—C4 | 116.57 (12) | C35—C36—H36 | 119.3 |
| C2—C3—C31 | 119.10 (12) | O—C37—H37A | 109.5 |
| C4—C3—C31 | 124.31 (11) | O—C37—H37B | 109.5 |
| C3—C4—C5 | 119.94 (11) | H37A—C37—H37B | 109.5 |
| C3—C4—C41 | 120.15 (12) | O—C37—H37C | 109.5 |
| C5—C4—C41 | 119.91 (12) | H37A—C37—H37C | 109.5 |
| N1—C5—C4 | 121.15 (12) | H37B—C37—H37C | 109.5 |
| N1—C5—C51 | 114.99 (12) | N2—C41—C4 | 177.55 (17) |
| C4—C5—C51 | 123.85 (12) | C58—C51—C52 | 106.12 (12) |
| C12—C11—C16 | 118.24 (12) | C58—C51—C5 | 127.06 (13) |
| C12—C11—C1 | 120.66 (12) | C52—C51—C5 | 126.44 (12) |
| C16—C11—C1 | 121.11 (12) | C53—C52—C57 | 118.51 (14) |
| C13—C12—C11 | 120.40 (13) | C53—C52—C51 | 134.80 (14) |
| C13—C12—H12 | 119.8 | C57—C52—C51 | 106.67 (13) |
| C11—C12—H12 | 119.8 | C54—C53—C52 | 118.99 (16) |
| C14—C13—C12 | 120.70 (14) | C54—C53—H53 | 120.5 |
| C14—C13—H13 | 119.6 | C52—C53—H53 | 120.5 |
| C12—C13—H13 | 119.6 | C53—C54—C55 | 121.26 (18) |
| C15—C14—C13 | 119.45 (14) | C53—C54—H54 | 119.4 |
| C15—C14—H14 | 120.3 | C55—C54—H54 | 119.4 |
| C13—C14—H14 | 120.3 | C56—C55—C54 | 121.20 (16) |
| C14—C15—C16 | 120.36 (15) | C56—C55—H55 | 119.4 |
| C14—C15—H15 | 119.8 | C54—C55—H55 | 119.4 |
| C16—C15—H15 | 119.8 | C55—C56—C57 | 117.69 (17) |
| C15—C16—C11 | 120.85 (14) | C55—C56—H56 | 121.2 |
| C15—C16—H16 | 119.6 | C57—C56—H56 | 121.2 |
| C11—C16—H16 | 119.6 | N3—C57—C56 | 130.11 (16) |
| C36—C31—C32 | 117.89 (13) | N3—C57—C52 | 107.52 (13) |
| C36—C31—C3 | 123.59 (12) | C56—C57—C52 | 122.35 (16) |
| C32—C31—C3 | 118.50 (12) | N3—C58—C51 | 110.08 (14) |
| C33—C32—C31 | 121.22 (13) | N3—C58—H58 | 125.0 |
| C33—C32—H32 | 119.4 | C51—C58—H58 | 125.0 |
| C31—C32—H32 | 119.4 | C1—N1—C5 | 119.08 (11) |
| C32—C33—C34 | 120.19 (14) | C58—N3—C57 | 109.59 (13) |
| C32—C33—H33 | 119.9 | C58—N3—H3 | 125.2 |
| C34—C33—H33 | 119.9 | C57—N3—H3 | 125.2 |
| O—C34—C35 | 125.05 (14) | C34—O—C37 | 118.26 (14) |
| O—C34—C33 | 115.48 (14) | | |

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| N1—C1—C2—C3 | 5.0 (2) | C33—C34—C35—C36 | 0.0 (3) |
| C11—C1—C2—C3 | −175.75 (12) | C32—C31—C36—C35 | −0.4 (2) |
| C1—C2—C3—C4 | −1.04 (19) | C3—C31—C36—C35 | 178.13 (14) |

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|---|---|---|---|
| C1—C2—C3—C31 | −179.38 (12) | C34—C35—C36—C31 | 0.5 (3) |
| C2—C3—C4—C5 | −4.40 (19) | N1—C5—C51—C58 | −143.80 (14) |
| C31—C3—C4—C5 | 173.84 (12) | C4—C5—C51—C58 | 35.2 (2) |
| C2—C3—C4—C41 | 175.41 (13) | N1—C5—C51—C52 | 28.20 (19) |
| C31—C3—C4—C41 | −6.3 (2) | C4—C5—C51—C52 | −152.85 (13) |
| C3—C4—C5—N1 | 6.38 (19) | C58—C51—C52—C53 | −178.06 (16) |
| C41—C4—C5—N1 | −173.43 (12) | C5—C51—C52—C53 | 8.6 (3) |
| C3—C4—C5—C51 | −172.52 (12) | C58—C51—C52—C57 | 0.18 (15) |
| C41—C4—C5—C51 | 7.7 (2) | C5—C51—C52—C57 | −173.18 (13) |
| N1—C1—C11—C12 | 24.87 (18) | C57—C52—C53—C54 | −0.6 (2) |
| C2—C1—C11—C12 | −154.39 (13) | C51—C52—C53—C54 | 177.47 (15) |
| N1—C1—C11—C16 | −154.96 (14) | C52—C53—C54—C55 | 0.1 (2) |
| C2—C1—C11—C16 | 25.8 (2) | C53—C54—C55—C56 | 0.3 (3) |
| C16—C11—C12—C13 | −0.5 (2) | C54—C55—C56—C57 | −0.2 (3) |
| C1—C11—C12—C13 | 179.65 (13) | C55—C56—C57—N3 | −178.46 (16) |
| C11—C12—C13—C14 | 0.6 (2) | C55—C56—C57—C52 | −0.3 (2) |
| C12—C13—C14—C15 | −0.6 (3) | C53—C52—C57—N3 | 179.24 (13) |
| C13—C14—C15—C16 | 0.4 (3) | C51—C52—C57—N3 | 0.66 (15) |
| C14—C15—C16—C11 | −0.3 (3) | C53—C52—C57—C56 | 0.7 (2) |
| C12—C11—C16—C15 | 0.3 (2) | C51—C52—C57—C56 | −177.84 (14) |
| C1—C11—C16—C15 | −179.83 (15) | C52—C51—C58—N3 | −0.98 (16) |
| C2—C3—C31—C36 | −132.13 (15) | C5—C51—C58—N3 | 172.33 (13) |
| C4—C3—C31—C36 | 49.7 (2) | C2—C1—N1—C5 | −3.18 (19) |
| C2—C3—C31—C32 | 46.38 (19) | C11—C1—N1—C5 | 177.56 (11) |
| C4—C3—C31—C32 | −131.82 (14) | C4—C5—N1—C1 | −2.49 (18) |
| C36—C31—C32—C33 | −0.2 (2) | C51—C5—N1—C1 | 176.49 (11) |
| C3—C31—C32—C33 | −178.80 (14) | C51—C58—N3—C57 | 1.44 (17) |
| C31—C32—C33—C34 | 0.7 (2) | C56—C57—N3—C58 | 177.06 (16) |
| C32—C33—C34—O | 179.74 (15) | C52—C57—N3—C58 | −1.28 (16) |
| C32—C33—C34—C35 | −0.6 (3) | C35—C34—O—C37 | −6.1 (3) |
| O—C34—C35—C36 | 179.65 (16) | C33—C34—O—C37 | 173.55 (16) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the pyrrole ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···N2$^{i}$ | 0.86 | 2.15 | 2.9693 (19) | 159 |
| C32—H32···*Cg*1$^{ii}$ | 0.93 | 3.00 | 3.9157 (19) | 170 |

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