Crystal structure of \(N-(1H\text{-}\text{indol}-2\text{-}ylmethylidene})\)-4-methoxyaniline

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The molecule of the title compound, \(C_{16}H_{14}N_{2}O\), contains an essentially planar indole ring system and a phenyl ring. In the crystal, the molecules are linked by a weak intermolecular \(C-H\cdots O\) hydrogen bond and \(C-H\cdots \pi\) interactions, forming a one-dimensional column structure along the \(b\)-axis direction. These columns are linked by other \(C-H\cdots \pi\) interactions, forming a two-dimensional network structure.

1. Chemical context

Indole and its derivatives are useful starting compounds to derive pharmaceutical (Nalli \textit{et al.}, 2020) and biological materials (Arumugam \textit{et al.}, 2021). Indole can function as a hydrogen-bond donor because of the high acidity of the hydrogen atom at position 1. The introduction of a hydrogen-bond acceptor to position 2 of the indole ring forms a five-to-seven-membered intramolecular hydrogen-bonded ring (Nosenko, \textit{et al.}, 2008). In this work, a Schiff base including an indole ring, \(N-(\text{indol}-2\text{-}ylmethylidene})\)-4-methoxyaniline, was newly synthesized. Similar Schiff bases such as salicylideneamines often function as bidentate ligands (Wang \textit{et al.}, 2018). Whereas salicylideneamines form intramolecular hydrogen bonds between coordination site atoms, such intramolecular interactions are absent from the crystal structure of the title compound. We report herein on its molecular and crystal structure.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The \(C=\text{N}\) double bond adopts an \(E\) configuration. The indole moiety is almost planar with an r.m.s. deviation of 0.009 (1) \(\text{Å}\). The bond lengths and angles in the title molecule are normal and agree with those in other indole imine compounds (IWIGUS; Suresh \textit{et al.}, 2016; KEVLON; Ho \textit{et al.},...
The dihedral angle between the indole system and the benzene ring is 9.89(5)°. In the related compound IWIGUS, the dihedral angles between the indole system and the benzene ring disordered over two sets of sites are widened to 81.8(3) and 85.2(3)° due to two isopropyl substituents in the benzene ring. There is no intramolecular hydrogen bond in the title compound, because the N2—H2/C1/C1/C1/N3 angle is as small as 94.4(10)°; however, the N2/C1/C1/C1/N3 distance is 2.8633(16) Å, and the N2—C4—C12—N3 torsion angle is 3.94(19)°.

Although no intramolecular hydrogen bond is observed, a broad peak assigned for the N—H proton is seen in the 1H NMR spectrum of the title compound in a CDCl3 medium and this suggests that the compound forms an intramolecular hydrogen bond in solution (see Synthesis and crystallization).

3. Supramolecular features

The title compound contains an N—H group, which is a hydrogen-bond donor, and an imino group, which is a hydrogen-bond acceptor, but neither of them forms an intermolecular hydrogen bond in the crystal. Compounds containing a similar indol-2-ylmethylidene-aniline fragment with a cis-conformation of the C—C single bond between the N atoms often form dimers by intermolecular N—H/C1/C1/C1/N hydrogen bonds (see Database survey). However, in the crystal the molecules of the title compound are linked by a weak intermolecular C10—H10···O1i hydrogen bond and C—H···π interactions [C17—H17···Cg1i and C19—H19C···Cg2i; Cg1 is the centroid of the N2/C4–C6/C11 ring and Cg2 is the centroid of the C6–C11 ring; symmetry code: (i) −x+1/2, y+1/2, −z+1/2; (ii) −x+1/2, y−1/2, −z+1/2] (Fig. 2, Table 1). Besides this, the molecules belonging to different columns are joined by other C—H/C1/C1/C1/C25 interactions [C14—H14/C1/C1/C1/Cg1ii and C15—H15/C1/C1/C1/Cg2ii; symmetry code: (ii) 3/2−x, −1/2+y, 3/2−z] (Fig. 3, Table 1). As a result, the intermolecular C—H···O hydrogen bonds and C—H···π interactions form a two-dimensional network structure (Fig. 4).
4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.42, update of May 2021; Groom et al., 2016) using ConQuest (Bruno et al., 2002) for indole derivatives gave 5272 hits, and for the (1H-indol-2-yl)methanimine skeleton gave 86 hits. Among these, the imino N atom bonded to an H atom gave one hit, to an N atom gave 24 hits, and to a C atom gave 61 hits. A search for the indol-2-ylmethylene-aniline fragment gave 30 hits, and those containing a (1H-indol-2-yl)methanimine fragment with a cis-conformation of the C—C single bond gave seven hits. These seven compounds include five examples of dimers linked by complementary N—H or the imino groups. Of these structures, the compounds most closely related to the title compound are N—H···N hydrogen bonds (FORJAA; Li et al., 2019; IWIGUS; Suresh et al., 2016; KEZCUJ; Ariyasu et al., 2016; VACKES; Gadekar et al., 2016; WAGCEP; Tian et al., 2016), one example of a one-dimensional-chain structure (UWUSAI; Kalalbandi & Seetharamappa, 2016), and one example of a monomer protected from hydrogen bonding by steric hindrance (KEVLO; Ho et al., 2006). These structures contain intermolecular or intramolecular hydrogen bonds involving the N—H or the imino groups. Of these structures, the compounds most closely related to the title compound are N-(2,6-diisopropylphenyl)-1-(1H-indol-2-yl)methanimine (IWIGUS; Suresh et al., 2016), 4,6-dimethoxy-3-methyl-2,7-bis[(phenylimino)methyl]indole (KEVLO; Ho et al., 2006) and 2-(phenyl-N-oxidoiminomethyl)-3-phenylaminoindole (CIP-WED; Greci & Sgarbotto, 1984). In the crystal of IWIGUS, which features a large dihedral angle between the indole and benzene rings, two neighbouring molecules are associated through pairs of N—H···N intermolecular hydrogen bonds, forming a centrosymmetric dimer. The crystal structure of an indol-2-ylmethylene-aniline compound without a hydrogen bond between the N—H and imino groups has not yet been reported. In an almost planar molecule without a bulky substituent such as the tile compound, the formation of a dimer by intermolecular N—H···N hydrogen bonding is probably not appropriate for the crystal packing.

Table 2

| Crystal data               | C16H14N2O       |
|----------------------------|-----------------|
| Chemical formula           | C2H2N2O         |
| M_r                        | 250.29          |
| Crystal system, space group| Monoclinic, P2_1/n |
| Temperature (K)            | 123             |
| a, b, c (Å)                | 5.87685 (19), 7.5999 (3), 28.4578 (11) |
| β (°)                      | 90.604 (3)      |
| V (Å³)                     | 1270.95 (8)     |
| Z                          | 4               |
| Radiation type             | Mo K            |
| μ (mm⁻¹)                   | 0.08            |
| Crystal size (mm)          | 0.30 × 0.20 × 0.10 |

Data collection

| Diffractometer             | Rigaku AFC10 Saturn70 area detector |
|----------------------------|------------------------------------|
| Absorption correction      | Multi-scan CrysAlis PRO; Rigaku OD, 2018 |
| T_min, T_max               | 0.608, 0.592                      |
| No. of measured, independent and observed | 11128, 2907, 2525 |
| No. of reflections          | 2907                             |
| No. of parameters           | 178                              |
| H-atom treatment           | H atoms treated by a mixture of independent and constrained refinement |
| Δρ_max, Δρ_min (e Å⁻³)      | 0.39, –0.29                      |

Computer programs: CrysAlis PRO (Rigaku OD, 2018), SIR92 (Altomare et al., 1993), SHELXL2018/3 (Sheldrick, 2015), PLATON (Spek, 2020) and CrystalStructure (Rigaku, 2019).

5. Synthesis and crystallization

Indole-2-carbaldehyde (145 mg, 1.00 mmol) and p-anisidine (148 mg, 1.20 mmol) were dissolved in toluene (20 mL), and the solution was refluxed under inert gas for 6 h, followed by evaporation. The residue was purified by recrystallization from a solvent mixture of acetone and n-hexane (1:1), and the title compound was then obtained (212 mg, 0.848 mmol, 84.8%) as a pale-red powder. The recrystallization of the title compound from a mixture of acetone and methanol afforded single crystals suitable for X-ray structure analysis.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atom attached to N2 was located in a difference-Fourier map and freely refined. The C-bound H atoms were positioned geometrically and refined using a riding model: C—H = 0.93–0.96 Å with Uiso(H) = 1.2Ueq(C).
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Crystal structure of N-(1H-indol-2-ylmethylidene)-4-methoxyaniline

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Computing details

Data collection: CrysAlis PRO (Rigaku OD, 2018); cell refinement: CrysAlis PRO (Rigaku OD, 2018); data reduction: CrysAlis PRO (Rigaku OD, 2018); program(s) used to solve structure: SIR92 (Altomare et al., 1993); program(s) used to refine structure: SHELXL2018/3 (Sheldrick, 2015); molecular graphics: PLATON (Spek, 2020); software used to prepare material for publication: CrystalStructure (Rigaku, 2019).

N-(1H-Indol-2-ylmethylidene)-4-methoxyaniline

Crystal data

C\textsubscript{16}H\textsubscript{14}N\textsubscript{2}O  
Mr = 250.29 
Monoclinic, \textit{P}2_1/n  
a = 5.87685 (19) Å  
b = 7.5999 (3) Å  
c = 28.4578 (11) Å  
β = 90.604 (3)°  
V = 1270.95 (8) Å\textsuperscript{3}  
Z = 4

\begin{align*}
F(000) & = 528.00 
D_\text{c} & = 1.308 \text{ Mg m}^{-3} 
\text{Mo } K\alpha \text{ radiation, } \lambda = 0.71073 \text{ Å} 
\text{Cell parameters from 6329 reflections} 
\theta & = 2.8–30.8° 
\mu & = 0.08 \text{ mm}^{-1} 
T & = 123 \text{ K} 
\text{Prism, colourless} 
0.30 \times 0.20 \times 0.10 \text{ mm}
\end{align*}

Data collection

\begin{align*}
\text{Rigaku AFC10 Saturn70 area detector} 
\text{Radiation source: rotating anode X-ray generator, micromax007} 
\text{Multi-layer mirror optics monochromator} 
\text{Detector resolution: 28.5714 pixels mm}^{-1} 
\text{ω scans} 
\text{Absorption correction: multi-scan} 
\text{CrysAlisPro; Rigaku OD, 2018)} 
\end{align*}

\begin{align*}
T_{\text{min}} & = 0.608, T_{\text{max}} = 0.992 
11128 \text{ measured reflections} 
2907 \text{ independent reflections} 
2525 \text{ reflections with } F^2 > 2.0\sigma(F^2) 
R_{\text{int}} & = 0.056 
\theta_{\text{max}} & = 27.5°, \theta_{\text{min}} = 2.8° 
h = -7→7 
k = -8→9 
l = -36→35
\end{align*}

Refinement

\begin{align*}
\text{Refinement on } F^2 
R[F^2 > 2\sigma(F^2)] & = 0.049 
wR(F^2) & = 0.127 
S & = 1.05 
2907 \text{ reflections} 
178 \text{ parameters} 
0 \text{ restraints} 
\end{align*}

Primary atom site location: structure-invariant direct methods  
Secondary atom site location: difference Fourier map

\begin{align*}
\text{Hydrogen site location: inferred from} 
\text{neighbouring sites} 
\text{H atoms treated by a mixture of independent} 
\text{and constrained refinement} 
w & = 1/[\sigma(F_c^2) + (0.0686P)^2 + 0.3253P] 
\text{where } P = (F_c^2 + 2F_s^2)/3 
(\Delta{\sigma})_{\text{max}} & = 0.001 
\Delta p_{\text{max}} & = 0.39 \text{ e Å}^{-3} 
\Delta p_{\text{min}} & = -0.29 \text{ e Å}^{-3} 
\text{Extinction correction: SHELXL} 
\text{Extinction coefficient: 0.259 (14)}
\end{align*}
**Special details**

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F². R-factor (gt) are based on F. The threshold expression of F² > 2.0 sigma(F²) is used only for calculating R-factor (gt).

| Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²) |
|---|---|---|---|
| x  | y  | z  | Uiso*/Ueq |
| O1  | 0.06455 (16) | 0.60985 (13) | 0.93970 (3) | 0.0292 (3) |
| N2  | 0.57779 (18) | 0.68608 (14) | 0.66418 (4) | 0.0237 (3) |
| N3  | 0.40410 (18) | 0.64748 (14) | 0.75724 (4) | 0.0248 (3) |
| C4  | 0.7005 (2) | 0.61479 (16) | 0.70151 (4) | 0.0240 (3) |
| C5  | 0.9058 (2) | 0.55340 (17) | 0.68542 (5) | 0.0249 (3) |
| H5  | 1.0199 | 0.5007 | 0.7034 | 0.030* |
| C6  | 0.9115 (2) | 0.58536 (16) | 0.63609 (4) | 0.0221 (3) |
| C7  | 1.0717 (2) | 0.55168 (17) | 0.60070 (5) | 0.0253 (3) |
| H7  | 1.2079 | 0.4950 | 0.6079 | 0.030* |
| C8  | 1.0237 (2) | 0.60388 (17) | 0.55530 (5) | 0.0272 (3) |
| H8  | 1.1287 | 0.5822 | 0.5318 | 0.033* |
| C9  | 0.8174 (2) | 0.68975 (17) | 0.54398 (5) | 0.0266 (3) |
| H9  | 0.7899 | 0.7250 | 0.5131 | 0.032* |
| C10 | 0.6548 (2) | 0.72278 (17) | 0.57776 (4) | 0.0253 (3) |
| H10 | 0.5182 | 0.7780 | 0.5701 | 0.030* |
| C11 | 0.7037 (2) | 0.67011 (16) | 0.62387 (4) | 0.0219 (3) |
| C12 | 0.6095 (2) | 0.60207 (17) | 0.74822 (4) | 0.0245 (3) |
| H12 | 0.7019 | 0.5599 | 0.7724 | 0.029* |
| C13 | 0.3193 (2) | 0.62794 (16) | 0.80344 (4) | 0.0231 (3) |
| C14 | 0.4210 (2) | 0.52631 (17) | 0.83908 (5) | 0.0264 (3) |
| H14 | 0.5511 | 0.4612 | 0.8327 | 0.032* |
| C15 | 0.3296 (2) | 0.52215 (17) | 0.88355 (5) | 0.0266 (3) |
| H15 | 0.3993 | 0.4548 | 0.9069 | 0.032* |
| C16 | 0.1332 (2) | 0.61828 (16) | 0.89388 (4) | 0.0233 (3) |
| C17 | 0.0233 (2) | 0.71292 (17) | 0.85845 (5) | 0.0253 (3) |
| H17 | −0.1111 | 0.7729 | 0.8645 | 0.030* |
| C18 | 0.1179 (2) | 0.71653 (17) | 0.81370 (5) | 0.0247 (3) |
| H18 | 0.0446 | 0.7798 | 0.7900 | 0.030* |
| C19 | −0.1427 (3) | 0.6969 (2) | 0.95149 (5) | 0.0367 (4) |
| H19A | −0.1793 | 0.6722 | 0.9836 | 0.044* |
| H19B | −0.2632 | 0.6554 | 0.9313 | 0.044* |
| H19C | −0.1247 | 0.8215 | 0.9474 | 0.044* |
| H2  | 0.438 (3) | 0.737 (2) | 0.6678 (5) | 0.032 (4)* |
Atomic displacement parameters (Å²)

|   | U¹¹  | U¹²  | U¹³  | U²²  | U²³  | U³³  |
|---|------|------|------|------|------|------|
| O1 | 0.0294 (5) | 0.0304 (5) | 0.0279 (5) | 0.0010 (4) | 0.0024 (4) | −0.0028 (4) |
| N2 | 0.0196 (5) | 0.0258 (6) | 0.0258 (5) | 0.0019 (4) | −0.0007 (4) | −0.0004 (4) |
| N3 | 0.0257 (5) | 0.0218 (6) | 0.0270 (6) | −0.0006 (4) | −0.0012 (4) | 0.0001 (4) |
| C4 | 0.0223 (6) | 0.0226 (6) | 0.0270 (7) | −0.0032 (5) | −0.0028 (5) | −0.0007 (5) |
| C5 | 0.0216 (6) | 0.0242 (6) | 0.0288 (7) | −0.0008 (5) | −0.0046 (5) | 0.0014 (5) |
| C6 | 0.0194 (6) | 0.0180 (6) | 0.0289 (7) | −0.0027 (4) | −0.0030 (5) | −0.0015 (5) |
| C7 | 0.0192 (6) | 0.0228 (6) | 0.0339 (7) | 0.0008 (5) | −0.0006 (5) | −0.0029 (5) |
| C8 | 0.0247 (6) | 0.0259 (7) | 0.0310 (7) | −0.0034 (5) | 0.0029 (5) | −0.0056 (5) |
| C9 | 0.0289 (6) | 0.0249 (7) | 0.0258 (6) | −0.0022 (5) | −0.0032 (5) | −0.0005 (5) |
| C10 | 0.0235 (6) | 0.0238 (6) | 0.0283 (7) | 0.0021 (5) | −0.0040 (5) | 0.0000 (5) |
| C11 | 0.0194 (6) | 0.0189 (6) | 0.0273 (6) | −0.0015 (5) | −0.0009 (4) | −0.0023 (5) |
| C12 | 0.0237 (6) | 0.0239 (7) | 0.0259 (6) | −0.0032 (5) | −0.0042 (5) | −0.0007 (5) |
| C13 | 0.0221 (6) | 0.0200 (6) | 0.0270 (6) | −0.0023 (5) | −0.0017 (5) | −0.0005 (5) |
| C14 | 0.0216 (6) | 0.0242 (7) | 0.0335 (7) | 0.0047 (5) | 0.0029 (5) | 0.0042 (5) |
| C15 | 0.0250 (6) | 0.0243 (7) | 0.0305 (7) | 0.0019 (5) | −0.0022 (5) | 0.0053 (5) |
| C16 | 0.0239 (6) | 0.0192 (6) | 0.0266 (6) | −0.0043 (5) | −0.0009 (5) | −0.0025 (5) |
| C17 | 0.0206 (6) | 0.0212 (6) | 0.0340 (7) | 0.0012 (5) | −0.0017 (5) | −0.0023 (5) |
| C18 | 0.0227 (6) | 0.0222 (6) | 0.0289 (7) | 0.0009 (5) | −0.0054 (5) | 0.0016 (5) |
| C19 | 0.0341 (8) | 0.0398 (9) | 0.0364 (8) | 0.0040 (6) | 0.0069 (6) | −0.0064 (7) |

Geometric parameters (Å, °)

|   |   | C9—H9  | O1—C19 | C9—C10—C11 |
|---|---|--------|--------|-------------|
| O1—C16 | 1.3705 (15) | 0.9300 |
| O1—C19 | 1.4287 (17) | 1.3989 (17) |
| N2—C11 | 1.3769 (16) | 0.9300 |
| N2—C4 | 1.3876 (16) | 0.9300 |
| N2—H2 | 0.912 (17) | 1.3950 (17) |
| N3—C12 | 1.2840 (17) | 1.4035 (18) |
| N3—C13 | 1.4189 (17) | 1.3803 (18) |
| C4—C5 | 1.3768 (18) | 0.9300 |
| C4—C12 | 1.4413 (18) | 1.4000 (18) |
| C5—C6 | 1.4252 (18) | 0.9300 |
| C5—H5 | 0.9300 | 1.3918 (18) |
| C6—C7 | 1.4094 (18) | 1.3950 (18) |
| C6—C11 | 1.4205 (17) | 0.9300 |
| C7—C8 | 1.3781 (19) | 0.9300 |
| C7—H7 | 0.9300 | 0.9600 |
| C8—C9 | 1.4111 (18) | 0.9600 |
| C8—H8 | 0.9300 | 0.9600 |
| C9—C10 | 1.3852 (19) | 1.3852 (19) |
| C16—O1—C19 | 117.50 (11) | C10—C11—C6 |
| C11—N2—C4 | 108.89 (10) | N3—C12—C4 |
| C11—N2—H2 | 128.4 (10) | N3—C12—H12 |
| C4—N2—H2 | 122.7 (10) | C4—C12—H12 |
| Bond                  | Value   | Bond                  | Value   |
|-----------------------|---------|-----------------------|---------|
| C12—N3—C13           | 119.83  | C18—C13—C14          | 118.05  |
| C5—C4—N2             | 109.15  | C18—C13—N3           | 116.78  |
| C5—C4—C12            | 128.24  | C14—C13—N3           | 125.17  |
| N2—C4—C12            | 122.51  | C15—C14—C13          | 120.54  |
| C4—C5—C6             | 107.42  | C15—C14—H14          | 119.7   |
| C4—C5—H5             | 126.3   | C13—C14—H14          | 119.7   |
| C6—C5—H5             | 126.3   | C14—C15—C16          | 120.68  |
| C7—C6—C11            | 119.10  | C14—C15—H15          | 119.7   |
| C7—C6—C5             | 134.07  | C16—C15—H15          | 119.7   |
| C11—C6—C5            | 106.83  | O1—C16—C17           | 125.06  |
| C8—C7—C6             | 119.08  | O1—C16—C15           | 115.28  |
| C8—C7—H7             | 120.5   | C17—C16—C15          | 119.65  |
| C6—C7—H7             | 120.5   | C16—C17—C18          | 119.03  |
| C7—C8—C9             | 120.94  | C16—C17—H17          | 120.5   |
| C7—C8—H8             | 119.5   | C18—C17—H17          | 120.5   |
| C9—C8—H8             | 119.5   | C13—C18—C17          | 121.91  |
| C10—C9—C8            | 121.49  | C13—C18—H18          | 119.0   |
| C10—C9—H9            | 119.3   | C17—C18—H18          | 119.0   |
| C8—C9—H9             | 119.3   | O1—C19—H19A          | 109.5   |
| C9—C10—C11           | 117.58  | O1—C19—H19B          | 109.5   |
| C9—C10—H10           | 121.2   | H19A—C19—H19B        | 109.5   |
| N2—C11—C10           | 130.50  | O1—C19—H19C          | 109.5   |
| N2—C11—C6            | 107.71  | H19B—C19—H19C        | 109.5   |
| C11—N2—C4—C5         | 0.24 (14)| C5—C6—C11—C10       | 179.05  |
| C11—N2—C4—C12        | −176.34 (11)| C13—N3—C12—C4     | 178.13  |
| N2—C4—C5—C6          | −0.69 (14)| C5—C4—C12—N3       | −171.94 (13)|
| C12—C4—C5—C6         | 175.63 (12)| N2—C4—C12—N3     | 3.94 (19) |
| C4—C5—C6—C7          | −179.42 (14)| C12—N3—C13—C18   | 165.19 (12)|
| C4—C5—C6—C11         | 0.87 (14)  | C12—N3—C13—C14     | −15.23 (19)|
| C11—C6—C7—C8         | 0.81 (18)  | C18—C13—C14—C15    | −3.23 (19)|
| C5—C6—C7—C8          | −178.88 (13)| N3—C13—C14—C15   | 177.21 (12)|
| C6—C7—C8—C9          | −0.08 (19)  | C13—C14—C15—C16    | 0.4 (2)   |
| C7—C8—C9—C10         | −0.8 (2)   | C19—O1—C16—C17     | 3.66 (18) |
| C8—C9—C10—C11        | 0.89 (19)   | C19—O1—C16—C15     | −176.29 (12)|
| C4—N2—C11—C10        | −179.44 (13)| C14—C15—C16—O1    | −177.25 (11)|
| C4—N2—C11—C6         | 0.32 (14)   | C14—C15—C16—C17    | 2.80 (19) |
| C9—C10—C11—N2        | 179.59 (12)| O1—C16—C17—C18    | 177.07 (11)|
| C9—C10—C11—C6        | −0.14 (19)  | C15—C16—C17—C18    | −2.98 (18)|
| C7—C6—C11—N2         | 179.51 (11)| C14—C13—C18—C17    | 3.04 (19)|
| C5—C6—C11—N2         | −0.73 (13)  | N3—C13—C18—C17    | −177.36 (11)|
| C7—C6—C11—C10        | −0.71 (19)  | C16—C17—C18—C13    | 0.05 (19) |
**Hydrogen-bond geometry (Å, °)**

$C_{g1}$ and $C_{g2}$ are the centroids of the N2/C4–C6/C11 and C6–C11 rings, respectively.

| D—H···A           | D—H | H···A | D···A     | D—H···A |
|-------------------|------|-------|-----------|---------|
| C10—H10···O1$^i$  | 0.93 | 2.58  | 3.2479 (16) | 129     |
| C14—H14···Cg1$^i$| 0.93 | 2.81  | 3.6006 (14) | 143     |
| C15—H15···Cg2$^i$| 0.93 | 2.79  | 3.5153 (14) | 136     |
| C17—H17···Cg1$^i$| 0.93 | 2.89  | 3.5718 (14) | 131     |
| C19—H19C···Cg2$^i$| 0.96 | 2.97  | 3.7716 (16) | 142     |

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

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