



Crystal structure of 4,5,6,7,8,8-hexachloro-2-(3,4-dimethoxyphenethyl)-3a,4,7,7a-tetrahydro-1H-4,7-methanoisoindole-1,3(2H)-dione [+solvent]

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Keywords: crystal structure; norbornene; hexachloro; isoindolene; hydrogen bonding; offset π - π interaction; C—Cl $\cdots\pi$ interaction.

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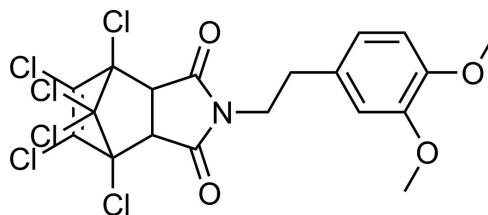
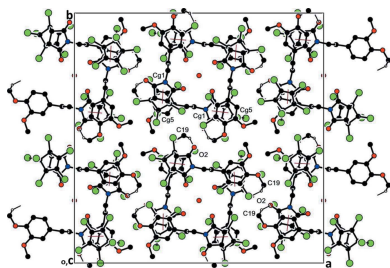
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In the title compound, C₁₉H₁₅Cl₆NO₄ [+solvent], the six-membered ring of the norbornene moiety adopts a boat conformation and the two five-membered rings have envelope conformations. The pyrrolidine ring makes a dihedral angle of 14.83 (12)° with the 3,4-dimethoxyphenyl ring, which are attached to each other by an extended N—CH₂—CH₂—C_{ar} bridge. In the crystal, the structure features C—H \cdots O intermolecular hydrogen bonds, an offset π - π interaction [intercentroid distance = 3.564 (1) Å] and a C—Cl $\cdots\pi$ interaction. The contribution of some disordered solvent to the scattering was removed using the SQUEEZE routine [Spek (2015). *Acta Cryst.* C71, 9–18] of PLATON. The solvent contribution was not included in the reported molecular weight and density.

1. Chemical context

One of the fundamental objectives of organic and medicinal chemistry is the design and synthesis of molecules having value as human therapeutic agents (Patil & Rajput, 2014). Succinimide derivatives are significant compounds found in various natural products, and have outstanding biological and pharmaceutical activity (Ahire & Mhaske, 2017). Cyclic imides and their derivatives contain an imide ring and the general structure —CO—N(R)—CO—, and can cross biological membranes *in vivo* (Hargreaves *et al.*, 1970). The variety of biological activities and pharmaceutical uses of compounds containing a succinimide moiety is considerable. They include activities such as antifungal (Hazra *et al.*, 2004), anti-tubercular (Isaka *et al.*, 2006), CNS depressant (Aeberli *et al.*, 1976), antispasmodic (Nunes *et al.*, 1995), cytostatic (Crider *et al.*, 1980), analgesic (Correa *et al.*, 1997), antibacterial (Zentz *et al.*, 2002), anticancer (Hall *et al.*, 1995), anorectic (Rich & Gardner, 1983), hypotensive (Coram & Brezenoff, 1983), nerve conduction blocking (Kaczorowski *et al.*, 2008), bacteriostatic (Piper *et al.*, 1971), anti-convulsant (Kornet *et al.*, 1977) and muscle relaxant (Musso *et al.*, 2003).



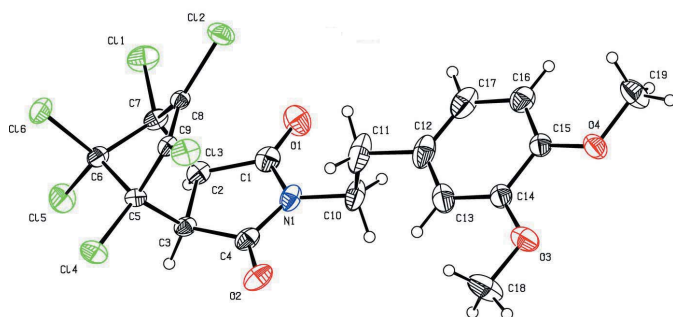


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at 30% probability level.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The six-membered ring of the norbornene moiety (C2/C3/C5/C7–C9) adopts a boat conformation [puckering parameters: amplitude $Q = 0.939(2) \text{ \AA}$, $\theta = 90.00(12)^\circ$, $\varphi = 299.27(14)^\circ$]. The two five-membered rings, *A* (C2/C3/C5–C7) and *B* (C5–C9), have envelope conformations with atom C6 as the flap: puckering parameters and the smallest displacement asymmetric parameters are $Q_2 = 0.619(2) \text{ \AA}$, $\varphi_2 = 108.6(2)^\circ$ and $\Delta s = 1.09^\circ$ for ring *A*, and $Q_2 = 0.582(2) \text{ \AA}$, $\varphi_2 = 215.5(2)^\circ$ and $\Delta s = 0.74^\circ$ for ring *B*. Atom C6 is displaced from the mean plane through the other four atoms by $0.908(2) \text{ \AA}$ in ring *A* and $0.875(2) \text{ \AA}$ in ring *B*. The dihedral angle between the pyrrolidine ring (N1/C1–C4) and the benzene ring (C12–C17) is $14.83(12)^\circ$, with the torsion angle N1–C10–C11–C12 being $175.8(3)^\circ$. The lengths of the C–Cl bonds involving the chlorine atoms attached to the C8=C9 double bond are $1.692(2) \text{ \AA}$ for C8–Cl2 and $1.692(2) \text{ \AA}$ for C9–Cl3. The lengths of the bonds to chlorine atoms attached to the single C–C bonds vary from $1.744(2)$ to $1.768(2) \text{ \AA}$. These value

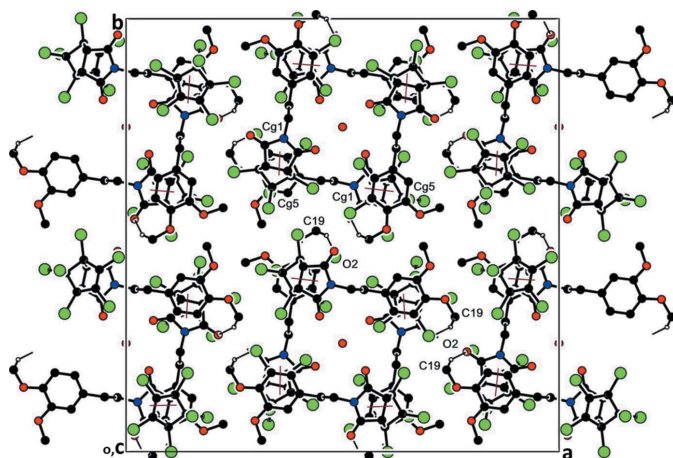


Figure 2
A view along the *c* axis of the crystal packing of the title compound. The C–H...O hydrogen bonds (thin black lines; Table 1) generate an $R_4^4(48)$ ring motif. The offset π - π interaction is shown as a thin red line. For clarity, H atoms not involved in hydrogen bonding have been omitted.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

Cg5 is the centroid of the C12–C17 benzene ring.

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C19–H19A...O2 ⁱ	0.96	2.57	3.408 (4)	146
C6–Cl6...Cg5 ⁱⁱ	1.77 (1)	3.41 (1)	4.894 (2)	140 (1)

Symmetry codes: (i) $y + \frac{1}{4}, -x + \frac{3}{4}, -z + \frac{7}{4}$; (ii) $-y + \frac{3}{4}, x - \frac{1}{4}, -z + \frac{3}{4}$.

are close to those found in similar compounds; see §4 Database survey.

3. Supramolecular features

In the crystal, weak C19–H19A...O2ⁱ hydrogen bonds link the molecules to form a cyclic $R_4^4(48)$ ring motif (Table 1 and Fig. 2). The molecules are stacked in layers held together by offset π - π interactions (Fig. 2), with an intercentroid distance $Cg1...Cg5^{iii}$ of $3.564(1) \text{ \AA}$ [$Cg1$ and $Cg5$ are the centroids of the pyrrolidine (N1/C1–C4) and benzene (C12–C17) rings, respectively, $\alpha = 9.80(12)^\circ$, interplanar distances are $3.448(1)$ and $3.547(1) \text{ \AA}$, offset = 0.353 \AA ; symmetry code: (iii) $-y + \frac{3}{4}, x - \frac{1}{4}, -z + \frac{3}{4}$]. There is also an intermolecular C–Cl... π interaction present, involving atom Cl6 and the centroid of the benzene ring (C12–C17); see Table 1.

4. Database survey

A search of the Cambridge Structural Database (CSD, V 5.40, update February 2019; Groom *et al.*, 2016) for the 4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisindole-1,3(2*H*)-dione skeleton yielded 17 hits (see supporting information). The majority of these compounds have thiophene substituents. One compound, 1,7,8,9,10,10-hexachloro-4-(2-phenylethyl)-4-azatricyclo[5.2.1.0^{2,6}]dec-8-ene-3,5-dione (CSD refcode EVEDIT; Manohar *et al.*, 2011), closely resembles the title compound but has a 2-phenethyl substituent rather than the 2-(3,4-dimethylphenethyl) group in the title compound. Here, the aryl ring is inclined to the pyrrolidine ring by $7.43(16)^\circ$ compared to $14.83(12)^\circ$ in the title compound, and the N–C–C–C_{ar} torsion angle is $-169.3(3)^\circ$ compared to $175.8(3)^\circ$ in the title compound.

In all 17 structures, the five-membered ring has envelope conformations and the six-membered ring a boat conformation. The bond lengths and bond angles are very similar to those reported here for the title compound. For example, the Csp^2 –Cl bond lengths are shorter than the Csp^3 –Cl bond lengths; the former vary from *ca* 1.681 to 1.717 \AA , while the latter vary from *ca* 1.725 to 1.798 \AA . In the title compound these bond lengths are $1.691(2)$ – $1.692(2) \text{ \AA}$ and $1.744(2)$ – $1.768(2) \text{ \AA}$, respectively.

5. Synthesis and crystallization

2-(3,4-Dimethoxyphenyl) ethanamine (1 equiv.) and 1,4,5,6,7,7-hexachloro-5-norbornene-2,3-dicarboxylic anhy-

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₉ H ₁₅ Cl ₆ NO ₄ [+solvent]
<i>M</i> _r	534.02
Crystal system, space group	Tetragonal, <i>I</i> ₄ / <i>a</i>
Temperature (K)	293
<i>a</i> , <i>c</i> (Å)	29.6250 (9), 10.2427 (4)
<i>V</i> (Å ³)	8989.4 (6)
<i>Z</i>	16
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.79
Crystal size (mm)	0.26 × 0.21 × 0.15
Data collection	
Diffractionmeter	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2008)
<i>T</i> _{min} , <i>T</i> _{max}	0.752, 0.863
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	10728, 5181, 3330
<i>R</i> _{int}	0.021
(sin θ/λ) _{max} (Å ⁻¹)	0.687
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.041, 0.101, 1.04
No. of reflections	5181
No. of parameters	273
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.33, -0.21

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXL2018* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

dride (1 equiv.) were stirred at room temperature in dry ethyl acetate for 30 min. The ethyl acetate was removed under reduced pressure and the resulting residue was dissolved in toluene. To this reaction mixture was added acetyl chloride (5 equiv.) and refluxed for 1 h. The reaction mixture was brought to room temperature and washed with aqueous Na₂CO₃ and dried over anhydrous Na₂SO₄. It was then filtered and the filtrate was concentrated under reduced pressure followed by silica gel column purification to afford the title compound in 82% yield. Colourless block-shaped crystals were obtained by slow evaporation of a solution in ethanol.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen atoms were placed in calculated positions and refined using a riding model: C—H = 0.93–0.98 Å with *U*_{iso}(H) = 1.5*U*_{eq}(C-methyl) and 1.2*U*_{eq}(C) for other H atoms. The contribution of the disordered solvent

to the scattering was removed using the SQUEEZE routine of *PLATON* (Spek, 2015). The solvent contribution was not included in the reported molecular weight and density. Further details are given in the archived CIF.

Funding information

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supporting information

Acta Cryst. (2019). E75, 562-564 [https://doi.org/10.1107/S2056989019004109]

Crystal structure of 4,5,6,7,8,8-hexachloro-2-(3,4-dimethoxyphenethyl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisindole-1,3(2*H*)-dione [+solvent]

R. Manohar, M. Harikrishna, S. Harikrishna Etti, C. Ramanathan and K. Gunasekaran

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL2018* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

4,5,6,7,8,8-Hexachloro-2-(3,4-dimethoxyphenethyl)-3a,4,7,7a-tetrahydro-1*H*-4,7-methanoisindole-1,3(2*H*)-dione

Crystal data

C₁₉H₁₅Cl₆NO₄[+solvent]
M_r = 534.02
 Tetragonal, *I*₄/a
a = 29.6250 (9) Å
c = 10.2427 (4) Å
V = 8989.4 (6) Å³
Z = 16
F(000) = 4320

D_x = 1.578 Mg m⁻³
 Mo *K*α radiation, λ = 0.71073 Å
 Cell parameters from 5181 reflections
 θ = 2.8–29.2°
 μ = 0.79 mm⁻¹
T = 293 K
 Block, colourless
 0.26 × 0.21 × 0.15 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
 ω and φ scans
 Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.752, *T_{max}* = 0.863
 10728 measured reflections

5181 independent reflections
 3330 reflections with *I* > 2σ(*I*)
R_{int} = 0.021
 θ_{max} = 29.2°, θ_{min} = 2.8°
h = -32→24
k = -40→24
l = -12→12

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2σ(*F*²)] = 0.041
wR(*F*²) = 0.101
S = 1.04
 5181 reflections
 273 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

$$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 2.6033P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$$

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.64197 (3)	0.18131 (2)	0.50159 (7)	0.0609 (2)
C12	0.53878 (2)	0.16505 (2)	0.39238 (6)	0.05182 (19)
C13	0.51735 (2)	0.05095 (2)	0.39790 (6)	0.04926 (18)
C14	0.60427 (3)	-0.00099 (2)	0.52552 (7)	0.0560 (2)
C15	0.68772 (2)	0.07881 (3)	0.59849 (7)	0.0604 (2)
C16	0.65299 (2)	0.08158 (2)	0.33757 (6)	0.05024 (19)
O1	0.55317 (7)	0.18699 (7)	0.73520 (19)	0.0638 (6)
O2	0.51935 (7)	0.03730 (7)	0.74848 (17)	0.0583 (5)
O3	0.29789 (7)	0.07109 (6)	0.78565 (19)	0.0606 (5)
O4	0.26332 (6)	0.14834 (6)	0.75279 (18)	0.0512 (5)
N1	0.52660 (7)	0.11436 (8)	0.74800 (18)	0.0436 (5)
C1	0.55897 (9)	0.14695 (10)	0.7253 (2)	0.0452 (6)
C2	0.60172 (8)	0.12358 (8)	0.6826 (2)	0.0374 (6)
H2	0.627206	0.131273	0.739349	0.045*
C3	0.59071 (7)	0.07269 (8)	0.6881 (2)	0.0345 (5)
H3	0.610647	0.056594	0.748616	0.041*
C4	0.54179 (9)	0.07055 (10)	0.7313 (2)	0.0419 (6)
C5	0.59788 (8)	0.05717 (7)	0.5446 (2)	0.0321 (5)
C6	0.63858 (7)	0.08698 (9)	0.5043 (2)	0.0359 (6)
C7	0.61330 (8)	0.13120 (8)	0.5366 (2)	0.0353 (5)
C8	0.57030 (7)	0.12315 (8)	0.45795 (19)	0.0304 (5)
C9	0.56157 (7)	0.07940 (8)	0.46217 (19)	0.0291 (5)
C10	0.47983 (9)	0.12501 (11)	0.7835 (2)	0.0561 (8)
H10A	0.478774	0.154042	0.827179	0.067*
H10B	0.468475	0.102335	0.843401	0.067*
C11	0.45025 (10)	0.12635 (15)	0.6621 (3)	0.0885 (13)
H11A	0.460751	0.150372	0.605383	0.106*
H11B	0.453546	0.098090	0.615245	0.106*
C12	0.40091 (10)	0.13382 (14)	0.6918 (3)	0.0630 (9)
C13	0.37364 (10)	0.09809 (11)	0.7279 (2)	0.0580 (8)
H13	0.386380	0.069607	0.737894	0.070*
C14	0.32777 (9)	0.10361 (9)	0.7495 (2)	0.0439 (6)
C15	0.30858 (8)	0.14660 (9)	0.7326 (2)	0.0396 (6)
C16	0.33546 (9)	0.18220 (10)	0.6993 (2)	0.0519 (7)
H16	0.322956	0.210806	0.689646	0.062*
C17	0.38163 (10)	0.17583 (13)	0.6796 (3)	0.0641 (9)

H17	0.399661	0.200407	0.657959	0.077*
C18	0.31333 (14)	0.02580 (11)	0.7890 (4)	0.0954 (13)
H18A	0.323689	0.017167	0.703745	0.143*
H18B	0.289057	0.006337	0.815147	0.143*
H18C	0.337711	0.023232	0.850281	0.143*
C19	0.24021 (10)	0.18878 (10)	0.7231 (3)	0.0670 (9)
H19A	0.249922	0.212192	0.781535	0.101*
H19B	0.208313	0.184150	0.732920	0.101*
H19C	0.246680	0.197481	0.634816	0.101*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0617 (5)	0.0460 (4)	0.0751 (5)	-0.0269 (4)	0.0008 (4)	0.0089 (3)
C12	0.0569 (4)	0.0473 (4)	0.0512 (4)	0.0131 (3)	-0.0095 (3)	0.0098 (3)
C13	0.0436 (4)	0.0551 (4)	0.0491 (4)	-0.0167 (3)	-0.0143 (3)	-0.0023 (3)
C14	0.0691 (5)	0.0336 (3)	0.0652 (4)	0.0060 (3)	0.0037 (4)	0.0058 (3)
C15	0.0315 (3)	0.0879 (6)	0.0618 (4)	0.0052 (4)	-0.0120 (3)	0.0078 (4)
C16	0.0448 (4)	0.0656 (5)	0.0404 (3)	-0.0024 (3)	0.0122 (3)	0.0030 (3)
O1	0.0729 (15)	0.0533 (13)	0.0651 (13)	0.0064 (11)	-0.0032 (11)	-0.0172 (10)
O2	0.0576 (12)	0.0645 (13)	0.0527 (11)	-0.0226 (11)	0.0096 (9)	0.0062 (10)
O3	0.0659 (13)	0.0456 (11)	0.0703 (13)	0.0102 (11)	-0.0031 (11)	0.0087 (10)
O4	0.0419 (11)	0.0452 (10)	0.0664 (12)	0.0106 (9)	-0.0006 (9)	0.0052 (9)
N1	0.0363 (12)	0.0636 (15)	0.0310 (10)	-0.0031 (11)	0.0025 (9)	-0.0060 (10)
C1	0.0504 (17)	0.0571 (17)	0.0282 (12)	-0.0019 (15)	-0.0080 (11)	-0.0082 (12)
C2	0.0345 (13)	0.0465 (15)	0.0312 (12)	-0.0078 (11)	-0.0062 (10)	-0.0023 (11)
C3	0.0310 (12)	0.0449 (14)	0.0275 (11)	-0.0035 (11)	-0.0047 (10)	0.0076 (10)
C4	0.0439 (15)	0.0561 (17)	0.0258 (12)	-0.0064 (14)	-0.0029 (11)	0.0023 (12)
C5	0.0362 (13)	0.0293 (12)	0.0309 (11)	-0.0027 (10)	-0.0018 (10)	0.0053 (10)
C6	0.0280 (12)	0.0471 (15)	0.0326 (12)	-0.0034 (11)	-0.0031 (10)	0.0063 (11)
C7	0.0341 (13)	0.0352 (13)	0.0366 (12)	-0.0143 (11)	-0.0020 (10)	0.0025 (11)
C8	0.0272 (12)	0.0397 (13)	0.0245 (10)	-0.0003 (10)	-0.0018 (9)	0.0029 (10)
C9	0.0261 (11)	0.0379 (13)	0.0234 (10)	-0.0044 (10)	-0.0026 (9)	-0.0002 (10)
C10	0.0403 (15)	0.089 (2)	0.0392 (14)	0.0055 (15)	0.0103 (12)	-0.0088 (14)
C11	0.0425 (17)	0.181 (4)	0.0419 (17)	0.017 (2)	0.0052 (14)	-0.009 (2)
C12	0.0434 (17)	0.115 (3)	0.0300 (14)	0.006 (2)	0.0000 (12)	-0.0106 (16)
C13	0.0549 (18)	0.086 (2)	0.0331 (14)	0.0287 (18)	-0.0063 (13)	-0.0089 (14)
C14	0.0463 (16)	0.0576 (17)	0.0278 (12)	0.0119 (14)	-0.0041 (11)	-0.0027 (12)
C15	0.0411 (15)	0.0490 (15)	0.0288 (12)	0.0042 (13)	-0.0035 (11)	-0.0023 (11)
C16	0.0534 (18)	0.0598 (18)	0.0426 (14)	-0.0016 (15)	0.0002 (13)	-0.0013 (14)
C17	0.0541 (19)	0.094 (3)	0.0438 (16)	-0.0127 (19)	0.0066 (14)	-0.0035 (17)
C18	0.114 (3)	0.056 (2)	0.116 (3)	0.029 (2)	-0.003 (3)	0.021 (2)
C19	0.0515 (18)	0.0576 (19)	0.092 (2)	0.0157 (16)	-0.0160 (17)	0.0047 (17)

Geometric parameters (\AA , $^\circ$)

C11—C7	1.748 (2)	C6—C7	1.545 (3)
C12—C8	1.692 (2)	C7—C8	1.526 (3)

C13—C9	1.691 (2)	C8—C9	1.322 (3)
C14—C5	1.744 (2)	C10—C11	1.522 (4)
C15—C6	1.763 (2)	C10—H10A	0.9700
C16—C6	1.768 (2)	C10—H10B	0.9700
O1—C1	1.203 (3)	C11—C12	1.509 (4)
O2—C4	1.201 (3)	C11—H11A	0.9700
O3—C14	1.360 (3)	C11—H11B	0.9700
O3—C18	1.418 (3)	C12—C17	1.375 (4)
O4—C15	1.358 (3)	C12—C13	1.382 (4)
O4—C19	1.413 (3)	C13—C14	1.386 (4)
N1—C1	1.380 (3)	C13—H13	0.9300
N1—C4	1.384 (3)	C14—C15	1.405 (4)
N1—C10	1.467 (3)	C15—C16	1.365 (4)
C1—C2	1.508 (3)	C16—C17	1.395 (4)
C2—C3	1.543 (3)	C16—H16	0.9300
C2—C7	1.550 (3)	C17—H17	0.9300
C2—H2	0.9800	C18—H18A	0.9600
C3—C4	1.516 (3)	C18—H18B	0.9600
C3—C5	1.554 (3)	C18—H18C	0.9600
C3—H3	0.9800	C19—H19A	0.9600
C5—C9	1.518 (3)	C19—H19B	0.9600
C5—C6	1.551 (3)	C19—H19C	0.9600
C14—O3—C18	117.8 (2)	C8—C9—C13	128.85 (18)
C15—O4—C19	118.6 (2)	C5—C9—C13	123.33 (17)
C1—N1—C4	114.1 (2)	N1—C10—C11	110.3 (2)
C1—N1—C10	123.2 (2)	N1—C10—H10A	109.6
C4—N1—C10	122.6 (2)	C11—C10—H10A	109.6
O1—C1—N1	125.2 (3)	N1—C10—H10B	109.6
O1—C1—C2	126.7 (3)	C11—C10—H10B	109.6
N1—C1—C2	108.1 (2)	H10A—C10—H10B	108.1
C1—C2—C3	105.1 (2)	C12—C11—C10	113.4 (2)
C1—C2—C7	113.51 (19)	C12—C11—H11A	108.9
C3—C2—C7	102.98 (18)	C10—C11—H11A	108.9
C1—C2—H2	111.6	C12—C11—H11B	108.9
C3—C2—H2	111.6	C10—C11—H11B	108.9
C7—C2—H2	111.6	H11A—C11—H11B	107.7
C4—C3—C2	104.7 (2)	C17—C12—C13	118.3 (3)
C4—C3—C5	113.19 (18)	C17—C12—C11	121.1 (4)
C2—C3—C5	103.01 (17)	C13—C12—C11	120.5 (3)
C4—C3—H3	111.8	C12—C13—C14	121.7 (3)
C2—C3—H3	111.8	C12—C13—H13	119.2
C5—C3—H3	111.8	C14—C13—H13	119.2
O2—C4—N1	124.8 (2)	O3—C14—C13	126.7 (3)
O2—C4—C3	127.3 (3)	O3—C14—C15	114.3 (2)
N1—C4—C3	107.9 (2)	C13—C14—C15	118.9 (3)
C9—C5—C6	98.95 (17)	O4—C15—C16	125.8 (2)
C9—C5—C3	107.51 (18)	O4—C15—C14	114.5 (2)

C6—C5—C3	100.94 (17)	C16—C15—C14	119.7 (3)
C9—C5—C14	116.28 (16)	C15—C16—C17	120.2 (3)
C6—C5—C14	116.64 (17)	C15—C16—H16	119.9
C3—C5—C14	114.41 (15)	C17—C16—H16	119.9
C7—C6—C5	92.81 (17)	C12—C17—C16	121.1 (3)
C7—C6—C15	113.55 (16)	C12—C17—H17	119.4
C5—C6—C15	114.70 (15)	C16—C17—H17	119.4
C7—C6—C16	113.64 (16)	O3—C18—H18A	109.5
C5—C6—C16	113.18 (16)	O3—C18—H18B	109.5
C15—C6—C16	108.47 (12)	H18A—C18—H18B	109.5
C8—C7—C6	99.14 (18)	O3—C18—H18C	109.5
C8—C7—C2	107.55 (17)	H18A—C18—H18C	109.5
C6—C7—C2	100.98 (18)	H18B—C18—H18C	109.5
C8—C7—C11	115.47 (16)	O4—C19—H19A	109.5
C6—C7—C11	116.16 (16)	O4—C19—H19B	109.5
C2—C7—C11	115.42 (16)	H19A—C19—H19B	109.5
C9—C8—C7	107.41 (19)	O4—C19—H19C	109.5
C9—C8—C12	128.61 (18)	H19A—C19—H19C	109.5
C7—C8—C12	123.74 (17)	H19B—C19—H19C	109.5
C8—C9—C5	107.74 (19)		
C4—N1—C1—O1	-179.4 (2)	C1—C2—C7—C8	-47.0 (3)
C10—N1—C1—O1	2.1 (4)	C3—C2—C7—C8	66.0 (2)
C4—N1—C1—C2	2.3 (3)	C1—C2—C7—C6	-150.4 (2)
C10—N1—C1—C2	-176.2 (2)	C3—C2—C7—C6	-37.3 (2)
O1—C1—C2—C3	179.7 (2)	C1—C2—C7—C11	83.5 (2)
N1—C1—C2—C3	-2.1 (2)	C3—C2—C7—C11	-163.44 (16)
O1—C1—C2—C7	-68.6 (3)	C6—C7—C8—C9	34.4 (2)
N1—C1—C2—C7	109.7 (2)	C2—C7—C8—C9	-70.2 (2)
C1—C2—C3—C4	1.1 (2)	C11—C7—C8—C9	159.29 (17)
C7—C2—C3—C4	-117.95 (19)	C6—C7—C8—C12	-150.73 (16)
C1—C2—C3—C5	119.72 (18)	C2—C7—C8—C12	104.6 (2)
C7—C2—C3—C5	0.6 (2)	C11—C7—C8—C12	-25.9 (3)
C1—N1—C4—O2	178.5 (2)	C7—C8—C9—C5	0.7 (2)
C10—N1—C4—O2	-3.0 (4)	C12—C8—C9—C5	-173.78 (16)
C1—N1—C4—C3	-1.6 (3)	C7—C8—C9—C13	177.45 (17)
C10—N1—C4—C3	176.95 (19)	C12—C8—C9—C13	3.0 (3)
C2—C3—C4—O2	-180.0 (2)	C6—C5—C9—C8	-35.4 (2)
C5—C3—C4—O2	68.6 (3)	C3—C5—C9—C8	69.1 (2)
C2—C3—C4—N1	0.1 (2)	C14—C5—C9—C8	-161.17 (16)
C5—C3—C4—N1	-111.3 (2)	C6—C5—C9—C13	147.60 (17)
C4—C3—C5—C9	45.4 (3)	C3—C5—C9—C13	-107.85 (19)
C2—C3—C5—C9	-67.1 (2)	C14—C5—C9—C13	21.9 (2)
C4—C3—C5—C6	148.5 (2)	C1—N1—C10—C11	94.0 (3)
C2—C3—C5—C6	36.1 (2)	C4—N1—C10—C11	-84.4 (3)
C4—C3—C5—C14	-85.4 (2)	N1—C10—C11—C12	175.8 (3)
C2—C3—C5—C14	162.17 (16)	C10—C11—C12—C17	99.6 (4)
C9—C5—C6—C7	52.57 (18)	C10—C11—C12—C13	-82.5 (4)

C3—C5—C6—C7	-57.35 (18)	C17—C12—C13—C14	1.1 (4)
C14—C5—C6—C7	178.05 (15)	C11—C12—C13—C14	-176.8 (2)
C9—C5—C6—C15	170.14 (16)	C18—O3—C14—C13	-7.2 (4)
C3—C5—C6—C15	60.2 (2)	C18—O3—C14—C15	172.3 (3)
C14—C5—C6—C15	-64.4 (2)	C12—C13—C14—O3	-179.7 (2)
C9—C5—C6—C16	-64.7 (2)	C12—C13—C14—C15	0.8 (4)
C3—C5—C6—C16	-174.59 (15)	C19—O4—C15—C16	7.7 (4)
C14—C5—C6—C16	60.8 (2)	C19—O4—C15—C14	-172.6 (2)
C5—C6—C7—C8	-52.15 (18)	O3—C14—C15—O4	-1.2 (3)
C15—C6—C7—C8	-170.68 (14)	C13—C14—C15—O4	178.4 (2)
C16—C6—C7—C8	64.71 (19)	O3—C14—C15—C16	178.5 (2)
C5—C6—C7—C2	57.87 (18)	C13—C14—C15—C16	-1.9 (3)
C15—C6—C7—C2	-60.66 (19)	O4—C15—C16—C17	-179.2 (2)
C16—C6—C7—C2	174.73 (15)	C14—C15—C16—C17	1.2 (4)
C5—C6—C7—C11	-176.50 (15)	C13—C12—C17—C16	-1.9 (4)
C15—C6—C7—C11	65.0 (2)	C11—C12—C17—C16	176.0 (2)
C16—C6—C7—C11	-59.6 (2)	C15—C16—C17—C12	0.8 (4)

Hydrogen-bond geometry (\AA , $^\circ$)

Cg5 is the centroid of the C12–C17 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C19—H19A \cdots O2 ⁱ	0.96	2.57	3.408 (4)	146
C6—C16 \cdots Cg5 ⁱⁱ	1.77 (1)	3.41 (1)	4.894 (2)	140 (1)

Symmetry codes: (i) $y+1/4, -x+3/4, -z+7/4$; (ii) $-y+3/4, x-1/4, -z+3/4$.