Crystal structure, DFT and MEP study of (*E*)-2-{[(3-chlorophenyl)imino]methyl}-6-methylphenol
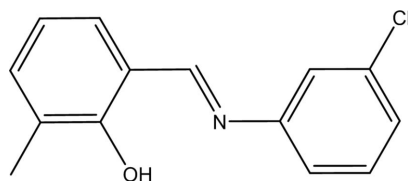
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In the crystal structure of the title compound, $C_{14}H_{12}ClNO$, the molecules are linked through C—H···O hydrogen bonds and C—H···π interactions, forming chains parallel to the [010] direction. π–π interactions and intramolecular hydrogen bonds are also observed. The molecular geometry of the title compound in the ground state has been calculated using density functional theory at the B3LYP level with the 6–311++G(2d,2p) basis set. Additionally, frontier molecular orbital and molecular electrostatic potential map analyses were performed.

1. Chemical context

Schiff bases, known as anils, imines or azomethines, have recently received considerable attention because of their good performance in coordination chemistry and anti-bacterial, anti-cancer and herbicidal applications (Piotr *et al.*, 2009; Schiff, 1864). The presence of a lone pair of electrons in an sp^2-hybridized orbital on the nitrogen atom of the azomethine group is of considerable chemical and biological importance (Sinha *et al.*, 2008). In a continuation of our interest in the chemical, herbicidal and biological properties of Schiff bases we synthesized the title compound, (I), as a potential anti-bacterial agent (Yılmaz *et al.*, 2012).

We report herein the synthesis, crystal structure and quantum chemical computational studies of the Schiff base compound, (I).

2. Structural commentary

The structure of the title compound (I) is shown in Fig. 1. It crystallizes in the orthorhombic space group *Pbca* with eight molecules in the unit cell. The molecular structure has two planar rings. The whole molecule is approximately planar, with a maximum deviation of −0.0236 (12) Å from planarity for the
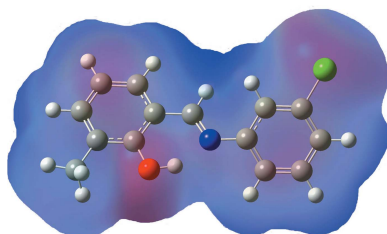
Table 1
Hydrogen-bond geometry (Å, °).

$Cg1$ and Cg are the centroids of the C1–C6 and C9–C14 rings, respectively.

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O1—H1$\cdots$N1	0.82	1.88	2.605 (2)	148
C10—H10$\cdots$O1^{i}	0.93	2.56	3.402 (2)	151
C2—H2$\cdots$Cg1^{ii}	0.93	2.75	3.561 (2)	147
C12—H12$\cdots$Cg2^{iii}	0.93	2.78	3.589 (2)	147

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, z$.

C8 atom of Schiff base. The title compound displays an E configuration with respect to the C8=N double bond. The dihedral angle between the two phenyl ring planes is 0.34 (9)° and the C5—C8—N1—C9 torsion angle is −179.81 (15)°. The planar molecular conformation is stabilized by the intramolecular O1—H1$\cdots$N1 hydrogen bond, which forms an $S(6)$ motif.

3. Supramolecular features

In the crystal, the molecules are linked by C10—H10$\cdots$O1 hydrogen bonds (Table 1), generating a $C_4^4(16)$ chain running parallel to the [010] direction (Fig. 2). C—H$\cdots\pi$ interactions occur between the two phenyl rings (Fig. 3, Table 1). π–π stacking interactions [centroid–centroid distance = 3.6389 (11) Å] between the chlorophenyl and methylphenol rings are also observed.

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40; update Nov. 2018; Groom *et al.*, 2016) gave eighteen hits for the (E)-2-{[(3-chlorophenyl)imino]methyl}-6-methylphenol structure. With a value of 1.271 (2) Å, the N1—C8 bond in the title compound (I) is the same length within standard uncertainties as those in the structures of 2-[(E)-(5-chloro-2-methylphenyl)iminomethyl]-4-methylphenol (AFILAE; Zheng, 2013*b*), 2,4-dibromo-6-{[(5-chloro-2-methylphenyl)-imino]methyl}phenol (AGEGUQ; Zheng, 2013*a*), 2-[(E)-
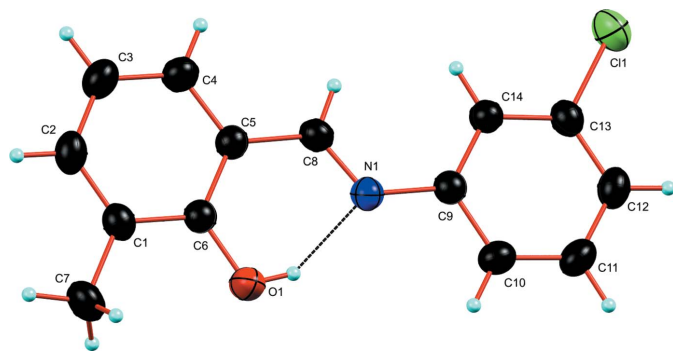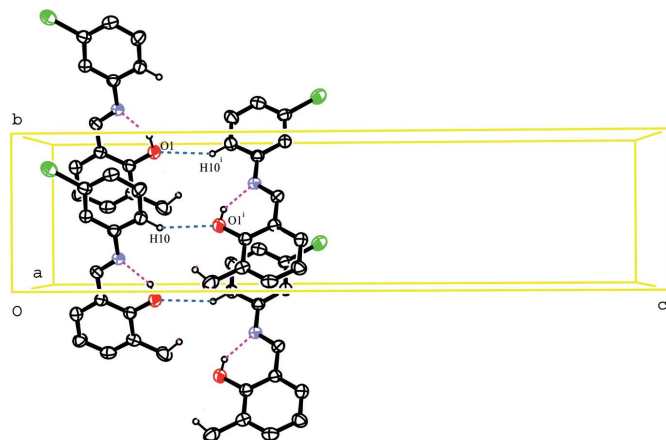

Figure 2
Diagram showing the hydrogen-bonding interactions in (I). Displacement ellipsoids are drawn at the 40% probability level. Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$.

(2,4,6-trichlorophenyl)iminomethyl]phenol (AWUSIV; Fun *et al.*, 2011), N-(2-methyl-5-chlorophenyl)salicylaldimine (BEYQEB; Elmalı & Elerman, 1998), (E)-2-[(3-chlorophenylimino)methyl]-4-methoxyphenol (DUBNAQ; Özek *et al.*, 2009), 3-{(E)-[(3,4-dichlorophenyl)imino]methyl}benzene-1,2-diol (MOYHAL; Tahir *et al.*, 2015) and N-(3-chlorophenyl)salicylaldimine (NADZUO; Karakaş *et al.*, 2004) where the C=N bond length varies from 1.266 (4) to 1.290 (3) Å. These structures also have an intramolecular O1—H1$\cdots$N1 hydrogen bond resulting in the formation of a six-membered ring and exhibit an E configuration.

5. Frontier molecular orbital analysis

The frontier molecular orbitals are important in the determination of the optical, electronic and anti-corrosion proper-

Figure 1
A view of the molecular structure of (I) with the atom labelling. The dotted line indicates the intramolecular O—H$\cdots$N hydrogen bond. Displacement ellipsoids are shown at the 40% probability level.
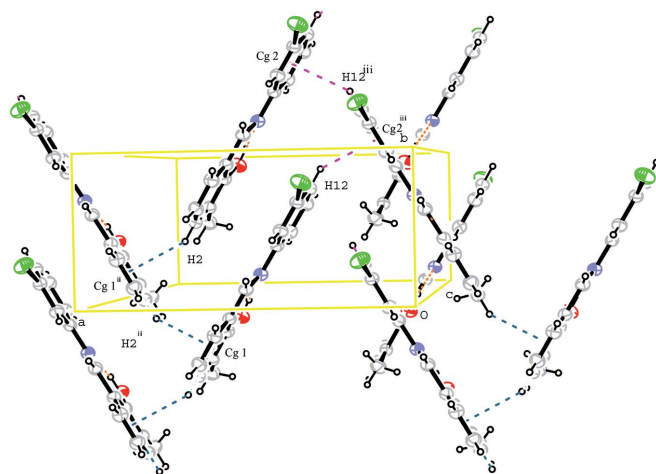

Figure 3
A partial packing diagram for (I) showing the C—H$\cdots\pi$ interactions as dashed lines. Symmetry codes: (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, z$.. $Cg1$ and $Cg2$ are the centroids of the methylphenol and chlorophenyl rings, respectively.

ties of a molecular system (Koepnick *et al.*, 2010; Solomon *et al.*, 2012; Jafari *et al.*, 2013). A molecule with a small frontier orbital gap is more polarizable than one with a large gap and is considered a soft molecule because of its high chemical reactivity and low kinetic stability (Prabavathi *et al.*, 2015). The energy levels of the HOMO (highest occupied molecular orbital), HOMO-1, LUMO (lowest occupied molecular orbital) and LUMO+1 orbitals calculated at the B3LYP/6-311++G(2*d*,2*p*) level (Frisch *et al.*, 2009; Dennington *et al.*, 2007) for (I) are shown in Fig. 4. The HOMO, HOMO-1 and LUMO orbitals are delocalized over the two phenyl rings connected by a Schiff base bridge and HOMO and HOMO-1 can be said to be π-bonding orbitals. The LUMO+1 orbitals are delocalized on the chlorophenyl ring and the C atom of the Schiff base. LUMO and LUMO+1 orbitals exhibit π^* anti-bonding character. The energy gap of (I) is 4.069 eV. The other molecular orbital energies are shown in Fig. 4. Electron
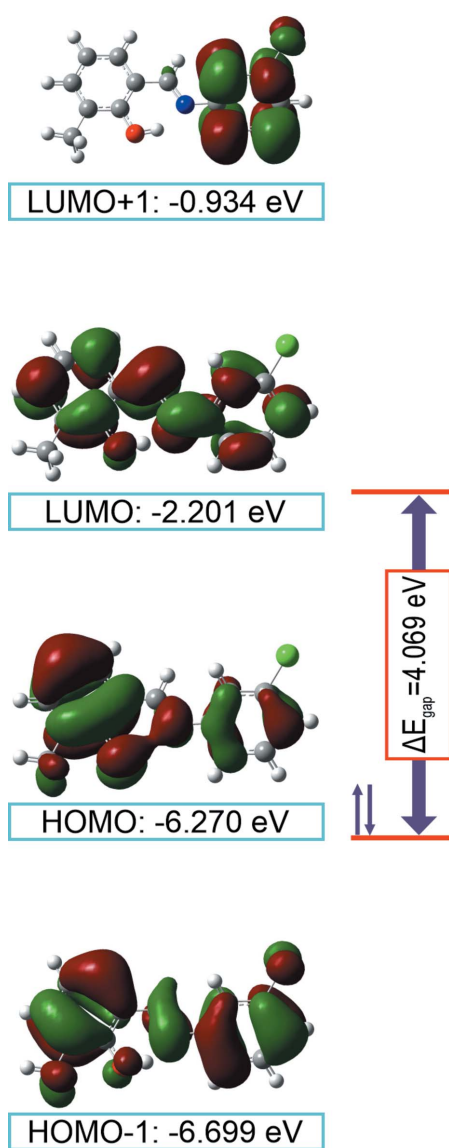
affinity (*A*) and ionization potential (*IP*) can be defined as $A = -E_{\mathrm{LUMO}}$ and $IP = -E_{\mathrm{HOMO}}$. Additionally, these values can also be used calculate the electronegativity (χ), chemical hardness (η) and chemical softness (S) (Prabavathi *et al.*, 2015; Karunakaran & Balachandran, 2014). For the title compound (I), $A = 2.201$ eV, $IP = 6.270$ eV, $\chi = 4.236$ eV, $\eta = 2.035$ eV, and $S = 0.246$ eV.

6. Molecular electrostatic potential surface analysis

The analysis of a three-dimensional plot of the molecular electrostatic potential (MEP) surface is a technique for mapping the electrostatic potential onto the isoelectronic density surface, providing information about the reactive sites. The surface simultaneously displays molecular size and shape and the electrostatic potential value. In the colour scheme adopted, red indicates an electron-rich region with a partial negative charge and blue an electron-deficient region with partial positive charge, light blue indicates a slightly electron-deficient region, yellow a slightly electron-rich region and green a neutral region (Politzer *et al.*, 2002). The MEP map of (I) was obtained by the B3LYP/6-311++G(2*d*,2*p*) method. In Fig. 5, it is shown that (I) has two possible sites of electrophilic attack. The negative region is localized on the protonated oxygen atom of methylphenol ring, O1, with a minimum value of −0.031 a.u. Positive potential sites of the compound are around hydrogen atoms. However, the maximum positive region is localized on the hydrogen atom bonded to the C atom forming the Schiff base, which can be considered as one possible site for nucleophilic attack, with a maximum value of 0.027 a.u.

7. Synthesis and crystallization

A mixture of 2-hydroxy-3-methylbenzaldehyde (34.0 mg, 0.25 mmol) and 4-chloroaniline (31.9 mg, 0.25 mmol) was stirred with ethanol (30 mL) at 377 K for 4 h, affording the title compound (43.0 mg, yield 70%, m.p. 362–364 K). Single

Figure 4
Plots of the frontier orbitals and the energy gap for (I).

LUMO+1: -0.934 eV

LUMO: -2.201 eV

$\Delta E_{\mathrm{gap}} = 4.069$ eV

HOMO: -6.270 eV

HOMO-1: -6.699 eV

Figure 5
Molecular electrostatic potential (MEP) map calculated at the B3LYP/6–311++G(2*d*,2*p*) level.

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crystals suitable for X-ray measurements were obtained by recrystallization from methanol at room temperature.

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed in calculated positions and refined using a riding model with C—H = 0.93–0.96 Å, $U_{iso}(H) = 1.2-1.5U_{eq}(C)$.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{12}ClNO$
M_r	245.70
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	296
a, b, c (Å)	14.0717 (8), 6.4811 (4), 26.767 (2)
V (Å³)	2441.1 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.29
Crystal size (mm)	$0.45 \times 0.43 \times 0.38$
Data collection	
Diffractometer	Stoe *IPDS* 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.820, 0.907
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10011, 2052, 1669
R_{int}	0.033
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.586
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.117, 1.05
No. of reflections	2052
No. of parameters	155
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.16, −0.24

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2002), *SHELXT2018* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2006) and *PLATON* (Spek, 2009).

Crystal structure, DFT and MEP study of (*E*)-2-{[(3-chlorophenyl)imino]-methyl}-6-methylphenol

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *Mercury* (Macrae *et al.*, 2006), *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

(*E*)-2-{[(3-Chlorophenyl)imino]methyl}-6-methylphenol

Crystal data

$C_{14}H_{12}ClNO$	$D_x = 1.337$ Mg m^{-3}
$M_r = 245.70$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pbca*	Cell parameters from 15471 reflections
$a = 14.0717$ (8) Å	$\theta = 1.5$–25.2°
$b = 6.4811$ (4) Å	$\mu = 0.29$ mm^{-1}
$c = 26.767$ (2) Å	$T = 296$ K
$V = 2441.1$ (3) Å^3	Prism, orange
$Z = 8$	$0.45 \times 0.43 \times 0.38$ mm
$F(000) = 1024$	

Data collection

Stoe IPDS 2 diffractometer	$T_{min} = 0.820$, $T_{max} = 0.907$
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	10011 measured reflections
	2052 independent reflections
Plane graphite monochromator	1669 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.033$
rotation method scans	$\theta_{max} = 24.6°$, $\theta_{min} = 1.5°$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -16 \rightarrow 16$
	$k = -6 \rightarrow 7$
	$l = -30 \rightarrow 31$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2 + 0.3364P]$
$wR(F^2) = 0.117$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
2052 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
155 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
0 restraints	
Primary atom site location: other	

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 (Å²)

	x	y	z	$U_{iso}*/U_{eq}$
Cl1	0.33517 (5)	0.79127 (10)	0.03649 (2)	0.0888 (3)
C12	0.32979 (13)	0.7525 (3)	0.13616 (8)	0.0632 (5)
H12	0.296569	0.876559	0.136229	0.076*
C13	0.35979 (13)	0.6646 (3)	0.09213 (7)	0.0565 (5)
C11	0.35033 (14)	0.6518 (3)	0.18009 (8)	0.0655 (5)
H11	0.330163	0.707801	0.210266	0.079*
C14	0.40948 (13)	0.4816 (3)	0.09088 (7)	0.0554 (5)
H14	0.428370	0.425004	0.060536	0.067*
C9	0.43105 (12)	0.3826 (3)	0.13554 (6)	0.0501 (4)
C10	0.40037 (13)	0.4690 (3)	0.18002 (7)	0.0581 (5)
H10	0.413635	0.403110	0.210087	0.070*
C8	0.51952 (12)	0.1055 (3)	0.10169 (7)	0.0533 (4)
H8	0.511386	0.163728	0.070226	0.064*
N1	0.48348 (10)	0.1964 (2)	0.13929 (5)	0.0524 (4)
C4	0.60571 (14)	−0.1837 (3)	0.06298 (7)	0.0617 (5)
H4	0.594284	−0.124767	0.031869	0.074*
C5	0.57270 (12)	−0.0849 (3)	0.10589 (6)	0.0507 (4)
C3	0.65470 (14)	−0.3660 (3)	0.06587 (8)	0.0658 (5)
H3	0.676683	−0.430204	0.037024	0.079*
C6	0.59085 (12)	−0.1759 (3)	0.15252 (6)	0.0511 (4)
O1	0.56117 (10)	−0.0861 (2)	0.19521 (4)	0.0668 (4)
H1	0.533250	0.021525	0.188623	0.100*
C2	0.67106 (13)	−0.4535 (3)	0.11231 (8)	0.0631 (5)
H2	0.703893	−0.577825	0.114078	0.076*
C1	0.64031 (13)	−0.3625 (3)	0.15602 (7)	0.0563 (5)
C7	0.65775 (16)	−0.4616 (4)	0.20614 (9)	0.0763 (6)
H7A	0.694377	−0.585261	0.201724	0.114*
H7B	0.598004	−0.495240	0.221426	0.114*
H7C	0.691973	−0.367515	0.227197	0.114*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1145 (5)	0.0730 (4)	0.0790 (4)	0.0241 (3)	−0.0112 (3)	0.0176 (3)
C12	0.0587 (11)	0.0503 (11)	0.0807 (15)	0.0027 (9)	0.0037 (9)	−0.0065 (10)
C13	0.0583 (10)	0.0475 (11)	0.0637 (11)	0.0008 (8)	−0.0049 (8)	0.0044 (9)
C11	0.0684 (12)	0.0645 (13)	0.0635 (12)	0.0014 (10)	0.0096 (9)	−0.0150 (10)
C14	0.0651 (11)	0.0511 (11)	0.0502 (10)	0.0032 (9)	−0.0001 (8)	0.0002 (8)
C9	0.0527 (9)	0.0450 (10)	0.0526 (9)	−0.0037 (8)	−0.0025 (7)	0.0014 (8)

C10	0.0644 (11)	0.0594 (12)	0.0506 (10)	−0.0040 (9)	0.0028 (8)	−0.0030 (9)
C8	0.0620 (11)	0.0483 (10)	0.0498 (9)	−0.0007 (8)	−0.0023 (8)	0.0062 (8)
N1	0.0595 (9)	0.0461 (9)	0.0517 (8)	0.0007 (7)	−0.0021 (6)	0.0006 (7)
C4	0.0693 (11)	0.0610 (13)	0.0546 (11)	0.0007 (10)	0.0075 (9)	0.0022 (9)
C5	0.0545 (9)	0.0454 (10)	0.0520 (10)	−0.0020 (8)	0.0018 (7)	0.0011 (8)
C3	0.0676 (12)	0.0597 (12)	0.0702 (13)	0.0030 (10)	0.0129 (9)	−0.0078 (10)
C6	0.0532 (9)	0.0483 (11)	0.0518 (10)	−0.0016 (8)	−0.0018 (7)	0.0006 (8)
O1	0.0889 (10)	0.0615 (9)	0.0500 (7)	0.0148 (7)	−0.0033 (6)	0.0003 (6)
C2	0.0545 (10)	0.0492 (11)	0.0854 (14)	0.0022 (8)	0.0064 (9)	0.0017 (10)
C1	0.0521 (9)	0.0512 (11)	0.0655 (11)	−0.0010 (8)	−0.0028 (8)	0.0064 (9)
C7	0.0836 (15)	0.0674 (14)	0.0779 (14)	0.0115 (11)	−0.0107 (11)	0.0173 (11)

Geometric parameters (Å, º)

Cl1—C13	1.7357 (19)	C4—C3	1.370 (3)
C12—C13	1.375 (3)	C4—C5	1.395 (2)
C12—C11	1.376 (3)	C4—H4	0.9300
C12—H12	0.9300	C5—C6	1.404 (2)
C13—C14	1.377 (3)	C3—C2	1.386 (3)
C11—C10	1.378 (3)	C3—H3	0.9300
C11—H11	0.9300	C6—O1	1.348 (2)
C14—C9	1.390 (2)	C6—C1	1.399 (3)
C14—H14	0.9300	O1—H1	0.8200
C9—C10	1.385 (2)	C2—C1	1.380 (3)
C9—N1	1.418 (2)	C2—H2	0.9300
C10—H10	0.9300	C1—C7	1.507 (3)
C8—N1	1.271 (2)	C7—H7A	0.9600
C8—C5	1.448 (2)	C7—H7B	0.9600
C8—H8	0.9300	C7—H7C	0.9600
C13—C12—C11	118.11 (18)	C5—C4—H4	119.4
C13—C12—H12	120.9	C4—C5—C6	118.61 (16)
C11—C12—H12	120.9	C4—C5—C8	119.96 (16)
C12—C13—C14	122.25 (18)	C6—C5—C8	121.42 (16)
C12—C13—Cl1	118.56 (15)	C4—C3—C2	119.16 (19)
C14—C13—Cl1	119.19 (15)	C4—C3—H3	120.4
C12—C11—C10	120.94 (18)	C2—C3—H3	120.4
C12—C11—H11	119.5	O1—C6—C1	118.05 (15)
C10—C11—H11	119.5	O1—C6—C5	121.05 (16)
C13—C14—C9	119.17 (17)	C1—C6—C5	120.90 (16)
C13—C14—H14	120.4	C6—O1—H1	109.5
C9—C14—H14	120.4	C1—C2—C3	122.26 (18)
C10—C9—C14	118.98 (17)	C1—C2—H2	118.9
C10—C9—N1	116.45 (16)	C3—C2—H2	118.9
C14—C9—N1	124.57 (16)	C2—C1—C6	117.95 (17)
C11—C10—C9	120.54 (18)	C2—C1—C7	121.44 (18)
C11—C10—H10	119.7	C6—C1—C7	120.61 (17)
C9—C10—H10	119.7	C1—C7—H7A	109.5

N1—C8—C5	122.65 (16)	C1—C7—H7B	109.5
N1—C8—H8	118.7	H7A—C7—H7B	109.5
C5—C8—H8	118.7	C1—C7—H7C	109.5
C8—N1—C9	123.07 (15)	H7A—C7—H7C	109.5
C3—C4—C5	121.12 (18)	H7B—C7—H7C	109.5
C3—C4—H4	119.4		
C11—C12—C13—C14	−0.3 (3)	N1—C8—C5—C4	176.22 (18)
C11—C12—C13—Cl1	−179.48 (15)	N1—C8—C5—C6	−2.7 (3)
C13—C12—C11—C10	0.6 (3)	C5—C4—C3—C2	0.3 (3)
C12—C13—C14—C9	−0.6 (3)	C4—C5—C6—O1	179.49 (16)
Cl1—C13—C14—C9	178.56 (14)	C8—C5—C6—O1	−1.6 (3)
C13—C14—C9—C10	1.2 (3)	C4—C5—C6—C1	−0.5 (3)
C13—C14—C9—N1	−178.54 (16)	C8—C5—C6—C1	178.43 (16)
C12—C11—C10—C9	−0.1 (3)	C4—C3—C2—C1	−0.5 (3)
C14—C9—C10—C11	−0.9 (3)	C3—C2—C1—C6	0.2 (3)
N1—C9—C10—C11	178.88 (16)	C3—C2—C1—C7	179.21 (19)
C5—C8—N1—C9	−179.81 (15)	O1—C6—C1—C2	−179.65 (16)
C10—C9—N1—C8	−176.76 (17)	C5—C6—C1—C2	0.3 (3)
C14—C9—N1—C8	3.0 (3)	O1—C6—C1—C7	1.3 (3)
C3—C4—C5—C6	0.2 (3)	C5—C6—C1—C7	−178.70 (17)
C3—C4—C5—C8	−178.79 (17)		

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg* are the centroids of the C1–C6 and C9–C14 rings, respectively.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1—H1⋯N1	0.82	1.88	2.605 (2)	148
C10—H10⋯O1[i]	0.93	2.56	3.402 (2)	151
C2—H2⋯*Cg*1[ii]	0.93	2.75	3.561 (2)	147
C12—H12⋯*Cg*2[iii]	0.93	2.78	3.589 (2)	147

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+3/2, *y*−1/2, *z*; (iii) −*x*+1/2, *y*+1/2, *z*.