

Crystal structure and Hirshfeld surface analysis of (*E*)-2-[[*(*2-iodophenyl)imino]methyl]-6-methylphenol

Sevgi Kansiz,^{a*} Tuggan Agar,^b Necmi Dege,^c Onur Erman Dogan,^d Ruby Ahmed^e and Eiad Saif^{f*}

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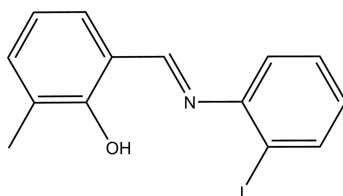
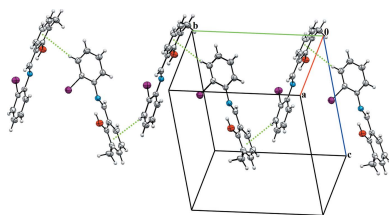
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^aSamsun University, Faculty of Engineering, Department of Fundamental Sciences, 55420, Samsun, Turkey, ^bYeditepe University, Department of Chemical Engineering, 34755, İstanbul, Turkey, ^cOndokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, 55139, Samsun, Turkey, ^dOndokuz Mayıs University, Faculty of Arts and Sciences, Department of Chemistry, 55139, Samsun, Turkey, ^eDepartment of Applied Chemistry, ZHCET, Aligarh Muslim University, Aligarh, 202002, UP, India, and ^fDepartment of Computer and Electronic Engineering Technology, Sana'a Community, College, Sana'a, Yemen. *Correspondence e-mail: sevgi.kansiz@samsun.edu.tr, eiad.saif@scc.edu.ye

The title compound, C₁₄H₁₂INO, was synthesized by condensation of 2-hydroxy-3-methylbenzaldehyde and 2-iodoaniline, and crystallizes in the orthorhombic space group *P*2₁2₁2₁. The 2-iodophenyl and benzene rings are twisted with respect to each other, making a dihedral angle of 31.38 (2)°. The molecular structure is stabilized by an O—H···N hydrogen bond, forming an *S*(6) ring motif. In the crystal, molecules are linked by C—H··· π interactions, resulting in the formation of sheets along the *a*-axis direction. Within the sheets, very weak π – π stacking interactions lead to additional stabilization. The Hirshfeld surface analysis and fingerprint plots reveal that the crystal structure is dominated by H···H (37.1%) and C···H (30.1%) contacts. Hydrogen bonding and van der Waals interactions are the dominant interactions in the crystal packing. The crystal studied was refined as a two-component inversion twin.

1. Chemical context

Imines derived from *o*-hydroxy aromatic carbonyls are of interest because of their ability to form an asymmetric intramolecular hydrogen bond between the oxygen atom of the hydroxyl group and the nitrogen atom of the imine moiety (Dominiak *et al.*, 2003). This ability has a decisive impact on the biological and thermo- or photochromic properties of *o*-hydroxy aromatic Schiff bases and makes them very useful compounds in chemistry, biochemistry, medicine, and technology (Vlad *et al.*, 2018; Bouhidel *et al.*, 2018; Faizi *et al.*, 2020*a,b*). A very important issue is determining the positions of tautomeric equilibria in these compounds and various instrumental research techniques are used to provide insight into the structure of molecules of studied *o*-hydroxy Schiff bases (Wojciechowski *et al.*, 2003; Faizi *et al.*, 2020*c,d*).



In the present study, a new Schiff base, (*E*)-2-[[*(*2-iodophenyl)imino]methyl]-6-methylphenol, was obtained in crystalline form from the reaction of 2-hydroxy-3-methylbenzaldehyde with 2-iodoaniline. We report here the synthesis and

Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the C8–C13 ring.

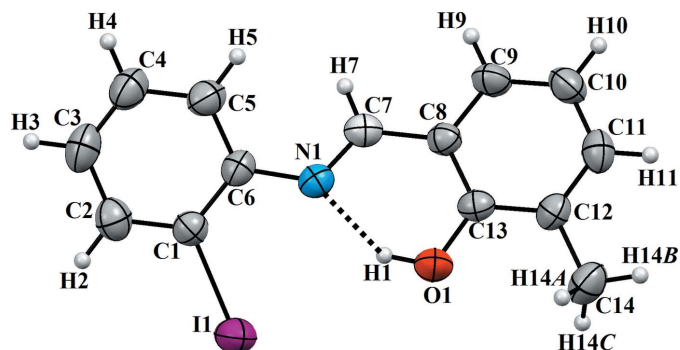
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H1 \cdots N1	0.93 (7)	1.82 (7)	2.634 (6)	144 (6)
C2–H2 \cdots Cg2 ⁱ	0.93	2.97 (6)	3.7445 (4)	142 (4)

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

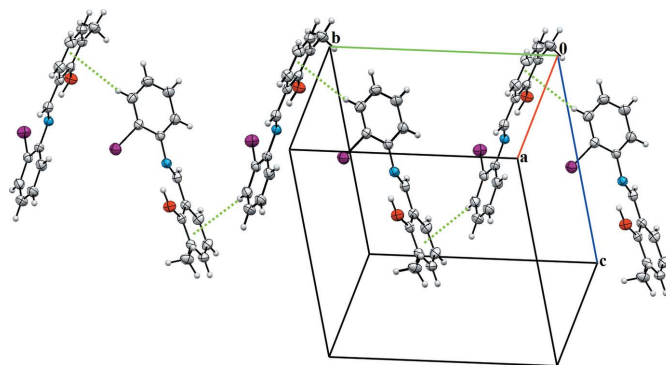
the crystal and molecular structures of the title compound, along with the results of a Hirshfeld surface analysis.

2. Structural commentary

Depending on the tautomers, two types of intramolecular hydrogen bonds are observed in Schiff bases: O–H \cdots N in enol–imine and N–H \cdots O in keto–amine tautomers. Most of these compounds are non-planar. The title compound, (I), is a Schiff base derivative from 2-hydroxy-3-methylbenzaldehyde, which crystallizes in the phenol–imine tautomeric form with an *E* configuration for the imine functionality. The asymmetric unit of (I) contains one molecule (Fig. 1). The molecule is non-planar with the 2-iodophenyl and benzene rings twisted with respect to each other at a dihedral angle of 31.38 (2)°. The hydroxyl H atom is involved in a strong intramolecular O–H \cdots N hydrogen bond, forming an *S*(6) ring motif, which stabilizes the molecular structure and induces the Schiff base atoms (N1, C7) to be coplanar with the methylphenol moiety. Of this planar unit (r.m.s deviation = 0.0274 Å), atoms O1 and N1 show the largest deviations from planarity in positive and negative directions [O1 = 0.035 (4) Å and N1 = –0.060 (4) Å]. The C7–N1 and C13–O1 bonds of the title compound are the most important indicators of the tautomeric type. The C13–O1 bond is of double-bond character for the keto–amine tautomer, whereas this bond displays single-bond character in the enol–imine tautomer. In addition, the C7–N1 bond is also a double bond in the enol–imine tautomer and a single bond length in the keto–amine tautomer. In the title compound, the enol–imine form is favored over the keto–amine form, as indicated by the C13–O1 [1.352 (6) Å] and C7–N1 [1.286 (8) Å] bonds, whose lengths indicate a high


Figure 1

The molecular structure of the title compound, with atom labelling. The intramolecular N–H \cdots O hydrogen bond (Table 1) is indicated by a dashed line. Displacement ellipsoids are drawn at the 40% probability level.


Figure 2

A view of the crystal packing of the title compound in a view parallel to the *bc* plane. C–H \cdots π (ring) interactions are indicated by dashed lines.

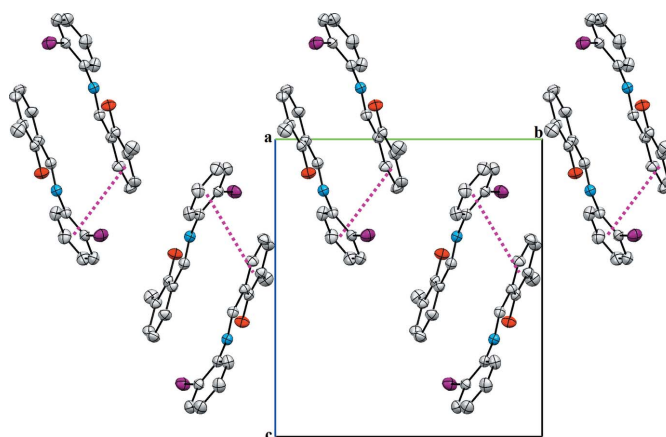
degree of single-bond and double-bond character, respectively. The shortest C–C distance (C3–C4) is 1.344 (11) Å in the C1–C6 ring with the weighted average ring bond distance being 1.376 (11) Å for this ring.

3. Supramolecular features

In the crystal structure, the molecules are connected into sheets extending along the *a*-axis direction by C2–H2 \cdots Cg2ⁱ interactions (Table 1; Fig. 2). Within the sheets, very weak π – π stacking interactions are observed with a centroid-to-centroid distance Cg1 \cdots Cg2ⁱⁱ of 4.093 (2) Å (Fig. 3), where Cg1 and Cg2 are the centroids of the C1–C6 and C8–C13 rings, respectively.

4. Hirshfeld surface analysis

A Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) was carried out using *CrystalExplorer17.5* (Turner *et al.*, 2017). The Hirshfeld surfaces and the associated two-dimensional fingerprint plots were used to quantify the various intermolecular interactions in the structure. The Hirshfeld surfaces (d_{norm} and shape-index) of the title compound are illustrated in Fig. 4. There are no prominent red spots on the surface,


Figure 3

A view of the crystal packing of the title compound along the *a* axis. π (Cg1) \cdots π (Cg2) interactions are indicated by dashed lines.

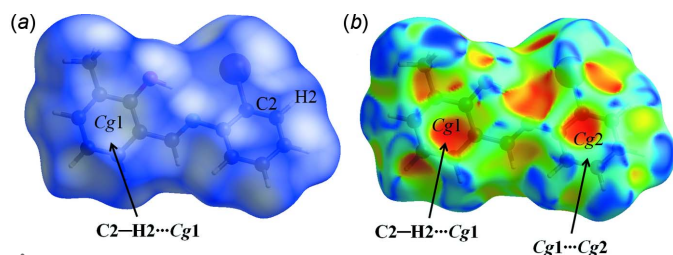


Figure 4
The Hirshfeld surfaces of the title compound mapped over (a) d_{norm} and (b) shape-index.

hence most of the interactions are weak non-covalent interactions. The diffuse white areas identified in Fig. 4a and red areas on phenyl rings mapped with shape-index (Fig. 4b) correspond to the $H \cdots \pi$ contacts resulting from hydrogen bond $C-H \cdots \pi(\text{ring})$ (Table 1) and $\pi-\pi$ stacking interactions. The major intermolecular interactions in the crystal structure are $H \cdots H$, $H \cdots C$ and $H \cdots I$ interactions, which make individual contributions of 37.1%, 30.1% and 18%, respectively. The fingerprint plots are shown in Fig. 5. There are also $O \cdots H$ (6.4%), $N \cdots H$ (3.6%) and $C \cdots C$ (23.3%) contacts. The Hirshfeld surface analysis confirms the importance of H-atom contacts in establishing the packing. The large number of $H \cdots H$ and $C \cdots H$ interactions suggest that van der Waals interactions play the major role in the crystal packing.

5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.41, update of November 2019; Groom *et al.*, 2016) for the

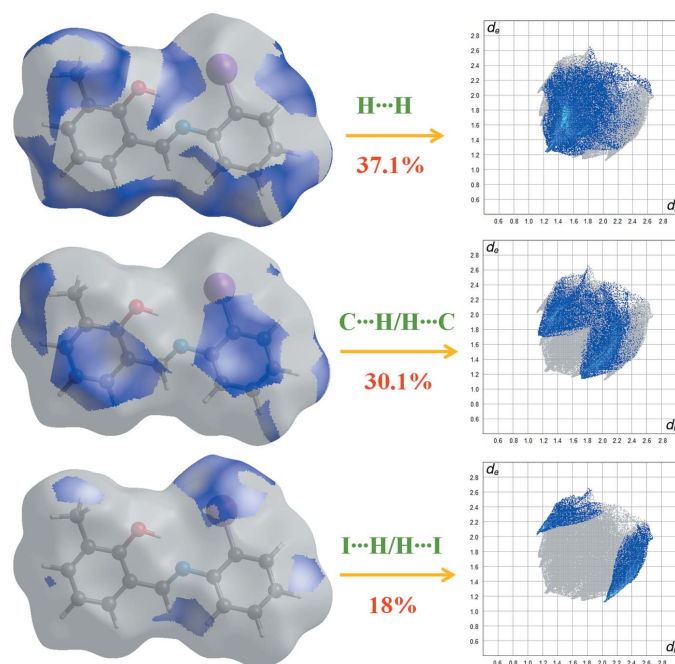


Figure 5
Two-dimensional fingerprint plots for the title compound, with a d_{norm} view and the relative contribution of the atom pairs to the Hirshfeld surface.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{12}INO$
M_r	337.15
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	296
a, b, c (Å)	8.1730 (4), 11.8143 (9), 13.1721 (8)
V (Å ³)	1271.88 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	2.50
Crystal size (mm)	0.66 × 0.34 × 0.13
Data collection	
Diffractometer	Stoe <i>IPDS 2</i>
Absorption correction	Integration (<i>X-RED32</i> ; Stoe & Cie, 2002)
T_{min}, T_{max}	0.365, 0.784
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5163, 2482, 1949
R_{int}	0.033
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.031, 0.063, 0.92
No. of reflections	2482
No. of parameters	160
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.46, -0.21

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2002), *SHELXT2017/1* (Sheldrick, 2015a), *SHELXL2017/1* (Sheldrick, 2015b), *PLATON* (Spek, 2020) and *WinGX* (Farrugia, 2012).

(*E*)-2-[(2-iodophenylimino)methyl]phenol gave six hits: bis[*N*-(2-iodophenyl)-2-oxynaphthaldimino-*N,O*]copper(II) (HABFIA; Unver, 2002), bis(*m*-methanolato)bis(2-[(5,7-diiodoquinolin-8-yl)imino]methyl)phenolato)bis(isothiocyanato)diiron(III) methanol solvate (HIDJOW; Sahadevan *et al.*, 2018), bis(*m*-oxo)bis(*m*-methanolato)tetrakis(2-[(5,7-diiodoquinolin-8-yl)imino]methyl)phenolato)bis(isothiocyanato)-tetrairon(III) dichloromethane solvate (HIDJUC; Sahadevan *et al.*, 2018), 2-[(5,7-diiodoquinolin-8-yl)imino]methyl)phenol (HIDKAJ; Sahadevan *et al.*, 2018), 2-iodo-salicylideneaniline (QQQANJ; Bernstein, 1967) and 2-[(2-iodophenyl)imino-methyl]phenol (RAVTIR; Elmali & Elerman, 1997). In HABFIA, the C—O bond length is 1.293 (3) Å, compared to 1.339 (5) Å for this bond in RAVTIR. Similar values are observed in the crystal of the title compound. The C—N bond lengths are 1.306 (3) and 1.267 (5) Å in HABFIA and RAVTIR, respectively. The molecules of HABFIA and RAVTIR have the same configuration as the title compound, while the other compounds listed above have different configurations.

6. Synthesis and crystallization

The title compound was prepared by refluxing mixed solutions of 2-hydroxy-3-methylbenzaldehyde (34.0 mg, 0.25 mmol) in ethanol (20 ml) and 2-iodoaniline (54.7 mg, 0.25 mmol) in ethanol (20 ml). The reaction mixture was stirred for 4 h under reflux. Single crystals of the title compound for X-ray analysis

were obtained by slow evaporation of an ethanol solution (yield 72%, m.p. 410–412 K).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were placed according to the difference-Fourier map and refined using a riding model: C–H = 0.93–0.96 Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C-methyl})$ and $1.2U_{\text{eq}}(\text{C})$ for other H atoms. Hydroxyl H atoms were placed according to a difference-Fourier map and were freely refined. The crystal studied was refined as a two-component inversion twin. This reflection file contains the non-overlapping reflections of the two twin components as well as the overlapping reflections. The BASF parameter for this two-component twin refined to -0.03242 (8).

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXT2017/1* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2020); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

(*E*)-2-[(2-Iodophenyl)imino]methyl}-6-methylphenol

Crystal data

C₁₄H₁₂INO

M_r = 337.15

Orthorhombic, *P*2₁2₁2₁

a = 8.1730 (4) Å

b = 11.8143 (9) Å

c = 13.1721 (8) Å

V = 1271.88 (14) Å³

Z = 4

F(000) = 656

D_x = 1.761 Mg m⁻³

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 6431 reflections

θ = 2.5–32.6°

μ = 2.50 mm⁻¹

T = 296 K

Rod, orange

0.66 × 0.34 × 0.13 mm

Data collection

Stoe IPDS 2

diffractometer

Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus

Plane graphite monochromator

Detector resolution: 6.67 pixels mm⁻¹

rotation method scans

Absorption correction: integration (X-RED32; Stoe & Cie, 2002)

T_{min} = 0.365, *T_{max}* = 0.784

5163 measured reflections

2482 independent reflections

1949 reflections with *I* > 2σ(*I*)

R_{int} = 0.033

θ_{max} = 26.0°, θ_{min} = 2.9°

h = -8→10

k = -14→14

l = -12→16

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.031

wR(*F*²) = 0.063

S = 0.92

2482 reflections

160 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

w = 1/[σ²(*F_o*²) + (0.0304*P*)²]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.001

Δρ_{max} = 0.46 e Å⁻³

Δρ_{min} = -0.21 e Å⁻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.

Refinement. Refined as a two-component inversion twin.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.5327 (7)	0.7863 (4)	0.8238 (6)	0.0512 (13)
C2	0.6359 (10)	0.8192 (5)	0.9003 (6)	0.0664 (19)
H2	0.598522	0.866780	0.951494	0.080*
C3	0.7966 (11)	0.7810 (6)	0.9008 (6)	0.076 (2)
H3	0.867715	0.803861	0.951899	0.092*
C4	0.8492 (8)	0.7109 (5)	0.8273 (7)	0.0720 (18)
H4	0.956517	0.684703	0.828468	0.086*
C5	0.7452 (7)	0.6773 (5)	0.7497 (6)	0.0632 (17)
H5	0.783507	0.629118	0.699235	0.076*
C6	0.5849 (7)	0.7150 (5)	0.7469 (5)	0.0508 (14)
C7	0.5196 (7)	0.6589 (5)	0.5815 (5)	0.0523 (13)
H7	0.628176	0.672300	0.564200	0.063*
C8	0.4100 (7)	0.6148 (4)	0.5043 (5)	0.0475 (14)
C9	0.4719 (8)	0.5869 (5)	0.4092 (5)	0.0599 (17)
H9	0.582202	0.598902	0.395435	0.072*
C10	0.3738 (9)	0.5425 (5)	0.3361 (6)	0.0661 (17)
H10	0.416758	0.523217	0.273023	0.079*
C11	0.2093 (10)	0.5262 (5)	0.3564 (5)	0.0624 (17)
H11	0.142297	0.496373	0.305986	0.075*
C12	0.1420 (8)	0.5532 (5)	0.4495 (5)	0.0535 (15)
C13	0.2432 (7)	0.5988 (4)	0.5232 (5)	0.0486 (15)
C14	-0.0374 (8)	0.5358 (6)	0.4703 (7)	0.075 (2)
H14A	-0.050482	0.493780	0.532175	0.113*
H14B	-0.085832	0.494527	0.415201	0.113*
H14C	-0.090242	0.607994	0.476842	0.113*
I1	0.29233 (6)	0.84637 (4)	0.82323 (4)	0.07511 (17)
O1	0.1754 (5)	0.6247 (4)	0.6139 (4)	0.0648 (12)
N1	0.4728 (6)	0.6802 (3)	0.6727 (5)	0.0507 (11)
H1	0.254 (8)	0.660 (5)	0.654 (6)	0.08 (2)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.050 (3)	0.050 (3)	0.053 (3)	-0.005 (2)	0.002 (4)	0.002 (3)
C2	0.074 (5)	0.058 (4)	0.067 (5)	-0.010 (3)	-0.003 (4)	-0.005 (3)
C3	0.073 (5)	0.075 (4)	0.081 (5)	-0.014 (4)	-0.025 (5)	-0.001 (4)
C4	0.058 (4)	0.068 (3)	0.090 (5)	-0.005 (3)	-0.015 (5)	-0.004 (5)
C5	0.050 (4)	0.057 (4)	0.083 (5)	0.002 (3)	-0.002 (3)	-0.007 (3)

C6	0.049 (4)	0.047 (3)	0.057 (4)	-0.002 (3)	-0.007 (3)	0.001 (3)
C7	0.049 (3)	0.050 (3)	0.058 (4)	0.002 (3)	0.008 (3)	0.001 (3)
C8	0.046 (3)	0.050 (3)	0.046 (3)	0.003 (2)	0.002 (3)	0.003 (2)
C9	0.054 (4)	0.070 (4)	0.056 (4)	-0.001 (3)	0.015 (3)	-0.003 (3)
C10	0.074 (5)	0.073 (4)	0.051 (4)	0.006 (4)	0.008 (4)	-0.012 (4)
C11	0.072 (4)	0.061 (3)	0.054 (4)	-0.001 (4)	-0.018 (4)	0.000 (3)
C12	0.049 (3)	0.057 (3)	0.055 (4)	-0.001 (3)	-0.006 (3)	0.005 (3)
C13	0.045 (4)	0.048 (3)	0.053 (3)	0.004 (2)	0.004 (3)	0.004 (3)
C14	0.053 (4)	0.089 (4)	0.084 (5)	-0.008 (4)	-0.009 (4)	0.006 (4)
I1	0.0656 (3)	0.0895 (3)	0.0703 (3)	0.0186 (2)	0.0053 (3)	-0.0094 (3)
O1	0.049 (3)	0.088 (3)	0.057 (3)	-0.002 (2)	0.009 (2)	-0.007 (2)
N1	0.047 (2)	0.050 (2)	0.055 (3)	-0.0006 (18)	-0.001 (3)	0.002 (3)

Geometric parameters (Å, °)

C1—C2	1.370 (10)	C8—C9	1.390 (9)
C1—C6	1.385 (9)	C8—C13	1.399 (8)
C1—I1	2.089 (6)	C9—C10	1.359 (10)
C2—C3	1.389 (11)	C9—H9	0.9300
C2—H2	0.9300	C10—C11	1.384 (10)
C3—C4	1.344 (11)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.382 (9)
C4—C5	1.387 (10)	C11—H11	0.9300
C4—H4	0.9300	C12—C13	1.384 (8)
C5—C6	1.384 (8)	C12—C14	1.505 (9)
C5—H5	0.9300	C13—O1	1.352 (7)
C6—N1	1.401 (8)	C14—H14A	0.9600
C7—N1	1.286 (8)	C14—H14B	0.9600
C7—C8	1.451 (9)	C14—H14C	0.9600
C7—H7	0.9300	O1—H1	0.93 (7)
C2—C1—C6	121.4 (6)	C10—C9—C8	121.0 (6)
C2—C1—I1	119.0 (5)	C10—C9—H9	119.5
C6—C1—I1	119.6 (5)	C8—C9—H9	119.5
C1—C2—C3	119.6 (7)	C9—C10—C11	119.3 (7)
C1—C2—H2	120.2	C9—C10—H10	120.3
C3—C2—H2	120.2	C11—C10—H10	120.3
C4—C3—C2	120.0 (7)	C12—C11—C10	121.8 (7)
C4—C3—H3	120.0	C12—C11—H11	119.1
C2—C3—H3	120.0	C10—C11—H11	119.1
C3—C4—C5	120.7 (7)	C11—C12—C13	118.3 (6)
C3—C4—H4	119.7	C11—C12—C14	121.2 (6)
C5—C4—H4	119.7	C13—C12—C14	120.5 (6)
C6—C5—C4	120.5 (6)	O1—C13—C12	117.6 (5)
C6—C5—H5	119.7	O1—C13—C8	121.7 (6)
C4—C5—H5	119.7	C12—C13—C8	120.7 (6)
C5—C6—C1	117.8 (6)	C12—C14—H14A	109.5
C5—C6—N1	122.9 (6)	C12—C14—H14B	109.5

C1—C6—N1	119.2 (5)	H14A—C14—H14B	109.5
N1—C7—C8	122.8 (6)	C12—C14—H14C	109.5
N1—C7—H7	118.6	H14A—C14—H14C	109.5
C8—C7—H7	118.6	H14B—C14—H14C	109.5
C9—C8—C13	118.9 (6)	C13—O1—H1	109 (4)
C9—C8—C7	119.4 (6)	C7—N1—C6	121.0 (5)
C13—C8—C7	121.7 (6)		
C6—C1—C2—C3	0.4 (10)	C8—C9—C10—C11	0.9 (10)
I1—C1—C2—C3	-179.2 (5)	C9—C10—C11—C12	-0.5 (10)
C1—C2—C3—C4	-0.9 (11)	C10—C11—C12—C13	0.8 (9)
C2—C3—C4—C5	0.9 (11)	C10—C11—C12—C14	179.6 (6)
C3—C4—C5—C6	-0.3 (11)	C11—C12—C13—O1	180.0 (5)
C4—C5—C6—C1	-0.3 (9)	C14—C12—C13—O1	1.2 (8)
C4—C5—C6—N1	-177.3 (6)	C11—C12—C13—C8	-1.4 (8)
C2—C1—C6—C5	0.2 (9)	C14—C12—C13—C8	179.8 (5)
I1—C1—C6—C5	179.8 (5)	C9—C8—C13—O1	-179.7 (5)
C2—C1—C6—N1	177.4 (5)	C7—C8—C13—O1	0.7 (8)
I1—C1—C6—N1	-3.1 (8)	C9—C8—C13—C12	1.7 (8)
N1—C7—C8—C9	-175.8 (6)	C7—C8—C13—C12	-177.9 (5)
N1—C7—C8—C13	3.8 (9)	C8—C7—N1—C6	175.4 (5)
C13—C8—C9—C10	-1.5 (9)	C5—C6—N1—C7	-33.7 (9)
C7—C8—C9—C10	178.2 (6)	C1—C6—N1—C7	149.2 (5)

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

$Cg2$ is the centroid of the C8—C13 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots N1	0.93 (7)	1.82 (7)	2.634 (6)	144 (6)
C2—H2 \cdots $Cg2^i$	0.93	2.97 (6)	3.7445 (4)	142 (4)

Symmetry code: (i) $-x+1, y+1/2, -z+1/2$.