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## 2-((*E*)-{3-[(*E*)-2-Hydroxy-3,5-diiodo-benzylideneamino]-2,2-dimethylpropyl}-iminomethyl)-4,6-diiodophenol

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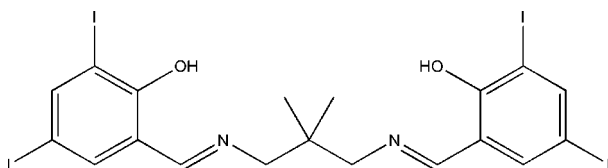
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Key indicators: single-crystal X-ray study;  $T = 291$  K; mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.079; data-to-parameter ratio = 22.1.

The asymmetric unit of the title compound,  $\text{C}_{19}\text{H}_{18}\text{I}_4\text{N}_2\text{O}_2$ , comprises a potentially tetradentate Schiff base ligand. The disordered H atoms on the N and O atoms were refined with site occupancies of 0.54 (8)/0.46 (8) and 0.59 (7)/0.41 (7), respectively. The dihedral angle between the benzene rings is  $73.3(3)^\circ$ . Intramolecular  $\text{O}-\text{H}\cdots\text{N}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds make  $S(6)$  ring motifs. Short  $\text{I}\cdots\text{I}$  [ $3.8919(7)$  Å] and  $\text{I}\cdots\text{Cg}$  [ $\text{Cg}$  is a ring centroid;  $3.911(2)$  Å] contacts are present in the crystal structure. The crystal structure is further stabilized by intermolecular  $\pi-\pi$  interactions [centroid-to-centroid distance =  $3.827(3)$  Å].

### Related literature

For related structures, see for example: Kargar *et al.* (2011, 2012); Kia *et al.* (2010). For standard values of bond lengths, see: Allen *et al.* (1987). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For van der Waals radii, see: Bondi (1964).



### Experimental

#### Crystal data

$\text{C}_{19}\text{H}_{18}\text{I}_4\text{N}_2\text{O}_2$   
 $M_r = 813.95$   
 Orthorhombic,  $Pbca$   
 $a = 12.2057(5)$  Å  
 $b = 11.8169(5)$  Å  
 $c = 31.8157(15)$  Å  
 $V = 4588.9(3)$  Å<sup>3</sup>  
 $Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 5.45$  mm<sup>-1</sup>  
 $T = 291$  K  
 $0.18 \times 0.12 \times 0.08$  mm

#### Data collection

Bruker SMART APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2005)  
 $T_{\min} = 0.441$ ,  $T_{\max} = 0.670$   
 39183 measured reflections  
 5472 independent reflections  
 2871 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.099$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.079$   
 $S = 1.00$   
 5471 reflections  
 248 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 1.11$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.94$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O1}$	0.72	1.90	2.526 (6)	145
$\text{O2}-\text{H2}\cdots\text{N2}$	0.82	1.82	2.548 (6)	148

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2150).

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## supporting information

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## 2-((*E*)-{3-[(*E*)-2-Hydroxy-3,5-diiodobenzylideneamino]-2,2-dimethylpropyl}-iminomethyl)-4,6-diiodophenol

Hadi Kargar, Reza Kia, Tayebeh Shakarami and Muhammad Nawaz Tahir

### S1. Comment

In continuation of our work on the crystal structure of Schiff base ligands (Kargar *et al.*, 2011, 2012; Kia *et al.*, 2010), we determined the X-ray structure of the title compound.

The asymmetric unit of the title compound, Fig. 1, comprises a potentially tetradentate Schiff base ligand. In the crystal structure the phenolic H atoms are disordered over a second position on the Schiff base N atoms. The bond lengths and angles are within the normal ranges (Allen *et al.*, 1987) and are comparable to related structures (Kargar *et al.*, 2011, 2012; Kia *et al.*, 2010).

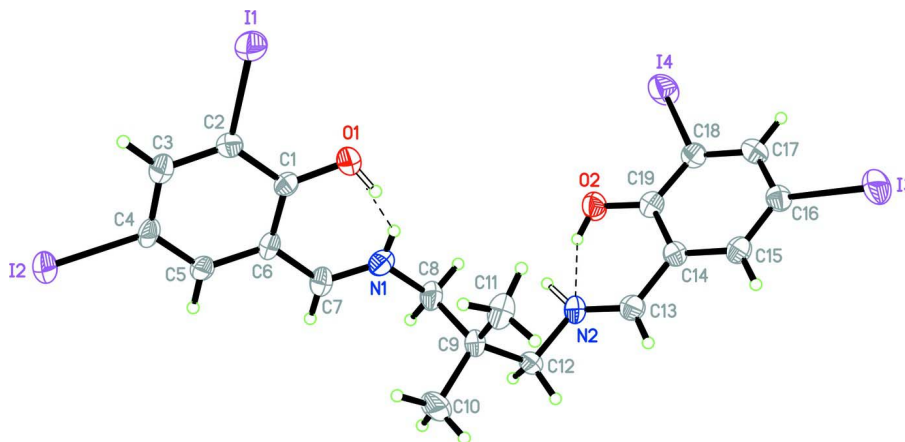
The intramolecular N—H $\cdots$ O and O—H $\cdots$ N hydrogen bonds (Table 1) make S(6) ring motifs (Bernstein *et al.*, 1995). The dihedral angle between the benzene rings is 73.3 (3)°. Short I(1) $\cdots$ I(2)<sup>i</sup> [3.8919 (7) Å; (i) 1/2 + x, 1/2 - y, 1 - z] and I4 $\cdots$ Cg2<sup>ii</sup> [3.911 (2) Å; (ii) 3/2 - x, -1/2 + y, z; Cg2 is the centroid of the C14–C19 ring] contacts are present in the crystal structure (Fig. 2). The crystal structure is further stabilized by the intermolecular  $\pi$ – $\pi$  interaction [Cg1 $\cdots$ Cg2<sup>i</sup> = 3.827 (3) Å; (i) 2 - x, 1/2 + y, 1/2 - z; Cg1 and Cg2 are the centroids of the C1–C6 and C14–C19 benzene rings].

### S2. Experimental

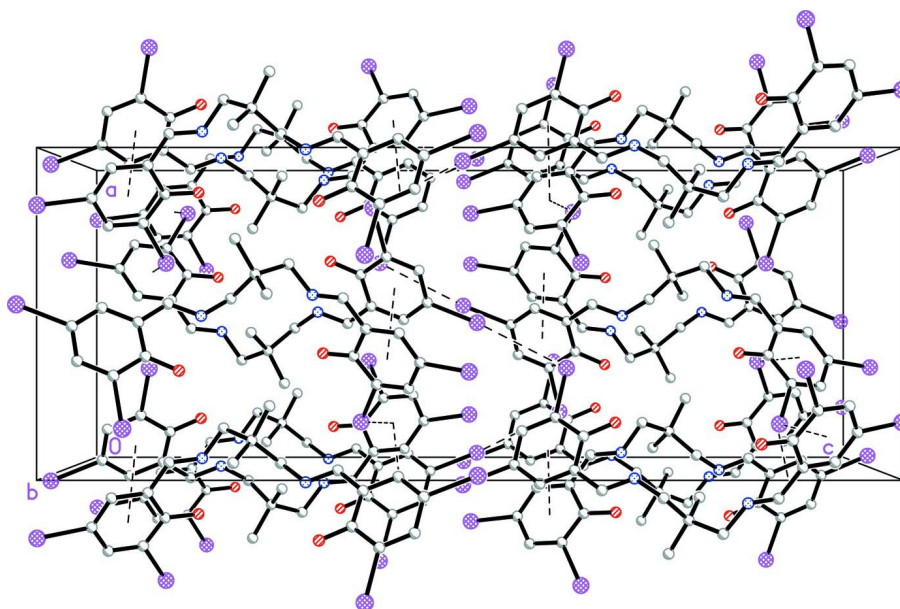
The title compound was synthesized by adding 3,5-diiodo-salicylaldehyde (2 mmol) to a solution of 2,2-dimethyl-1,3-propanediamine (1 mmol) in ethanol (30 ml). The mixture was refluxed with stirring for half an hour. The resultant solution was filtered. Yellow single crystals of the title compound suitable for X-ray structure determination were recrystallized from ethanol by slow evaporation of the solvents at room temperature over several days.

### S3. Refinement

The O- and N-bound H atoms were located in difference Fourier map and then constrained to refine to the parent atoms with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ , respectively. The C-bound H-atoms were included in calculated positions and treated as riding atoms: C—H = 0.93, 0.96 and 0.97 Å for CH, CH<sub>3</sub> and CH<sub>2</sub> H-atoms, respectively, with  $U_{\text{iso}}(\text{H}) = k \times U_{\text{eq}}(\text{C})$ , where  $k = 1.5$  for CH<sub>3</sub> H-atoms, and  $k = 1.2$  for all other H-atoms.

**Figure 1**

ORTEP plot of the title compound, showing 40% probability displacement ellipsoids and atomic numbering. The dashed lines show the intramolecular hydrogen bonds. The open bonds show the minor disordered components.

**Figure 2**

Packing diagram of the title compound viewed down the *b*-axis showing the short intermolecular I...I, I...Cg [C14–C19], and Cg [C1–C6]...Cg [C14–C19] contacts (dashed lines). All H atoms were omitted for clarity.

### 2-((*E*)-{3-[(*E*)-2-Hydroxy-3,5-diiodobenzylideneamino]-2,2-dimethylpropyl}iminomethyl)-4,6-diiodophenol

#### Crystal data

$C_{19}H_{18}I_4N_2O_2$

$M_r = 813.95$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 12.2057(5) \text{ \AA}$

$b = 11.8169(5) \text{ \AA}$

$c = 31.8157(15) \text{ \AA}$

$V = 4588.9(3) \text{ \AA}^3$

$Z = 8$

$F(000) = 2992$

$D_x = 2.356 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3211 reflections

$\theta = 2.5\text{--}27.5^\circ$

$\mu = 5.45 \text{ mm}^{-1}$   
 $T = 291 \text{ K}$

Block, yellow  
 $0.18 \times 0.12 \times 0.08 \text{ mm}$

*Data collection*

Bruker SMART APEXII CCD area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2005)  
 $T_{\min} = 0.441$ ,  $T_{\max} = 0.670$

39183 measured reflections  
 5472 independent reflections  
 2871 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.099$   
 $\theta_{\max} = 27.9^\circ$ ,  $\theta_{\min} = 1.3^\circ$   
 $h = -15 \rightarrow 16$   
 $k = -15 \rightarrow 14$   
 $l = -41 \rightarrow 39$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.079$   
 $S = 1.00$   
 5471 reflections  
 248 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0213P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.11 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.94 \text{ e } \text{Å}^{-3}$

*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.** 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{Å}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
I1	0.67018 (4)	0.26848 (5)	0.383838 (17)	0.06718 (18)	
I2	1.02767 (3)	0.17675 (4)	0.508635 (14)	0.04527 (13)	
I3	0.82622 (4)	0.00536 (4)	0.001078 (17)	0.06243 (17)	
I4	0.65930 (4)	-0.30987 (4)	0.131933 (17)	0.06028 (17)	
O1	0.8328 (3)	0.1220 (4)	0.32918 (15)	0.0501 (12)	
H1	0.8784	0.0964	0.3128	0.075*	0.46 (8)
O2	0.8775 (3)	-0.2231 (3)	0.17564 (15)	0.0475 (12)	
H2	0.9371	-0.2077	0.1860	0.071*	0.59 (7)
N1	0.9942 (4)	-0.0017 (4)	0.31029 (17)	0.0421 (14)	
H1A	0.9424	0.0253	0.3063	0.051*	0.54 (8)
N2	1.0582 (4)	-0.1182 (4)	0.18514 (18)	0.0421 (14)	
H1B	1.0104	-0.1580	0.2007	0.051*	0.41 (7)
C1	0.8751 (5)	0.1317 (5)	0.3665 (2)	0.0337 (15)	
C2	0.8201 (4)	0.1925 (5)	0.3985 (2)	0.0379 (16)	

C3	0.8633 (5)	0.2052 (5)	0.4382 (2)	0.0365 (16)
H3	0.8259	0.2468	0.4584	0.044*
C4	0.9642 (5)	0.1548 (5)	0.44789 (19)	0.0333 (15)
C5	1.0178 (5)	0.0919 (5)	0.41839 (19)	0.0331 (15)
H5	1.0838	0.0574	0.4254	0.040*
C6	0.9755 (5)	0.0782 (5)	0.37794 (19)	0.0313 (14)
C7	1.0307 (5)	0.0096 (5)	0.3477 (2)	0.0370 (16)
H7	1.0947	-0.0278	0.3554	0.044*
C8	1.0466 (5)	-0.0734 (5)	0.2792 (2)	0.0436 (17)
H8A	0.9906	-0.1139	0.2637	0.052*
H8B	1.0916	-0.1290	0.2935	0.052*
C9	1.1191 (5)	-0.0066 (5)	0.2478 (2)	0.0381 (16)
C10	1.2243 (5)	0.0305 (6)	0.2697 (2)	0.067 (2)
H10A	1.2693	0.0719	0.2503	0.100*
H10B	1.2634	-0.0350	0.2794	0.100*
H10C	1.2065	0.0780	0.2932	0.100*
C11	1.0597 (5)	0.0973 (5)	0.2311 (2)	0.054 (2)
H11A	1.1027	0.1317	0.2093	0.081*
H11B	1.0490	0.1505	0.2535	0.081*
H11C	0.9898	0.0752	0.2198	0.081*
C12	1.1517 (4)	-0.0858 (5)	0.2119 (2)	0.0426 (17)
H12A	1.2066	-0.0488	0.1947	0.051*
H12B	1.1844	-0.1537	0.2236	0.051*
C13	1.0478 (5)	-0.0796 (5)	0.1485 (2)	0.0392 (17)
H13	1.1029	-0.0336	0.1377	0.047*
C14	0.9534 (5)	-0.1038 (5)	0.1222 (2)	0.0340 (15)
C15	0.9413 (5)	-0.0561 (5)	0.0826 (2)	0.0359 (16)
H15	0.9962	-0.0092	0.0723	0.043*
C16	0.8510 (5)	-0.0761 (5)	0.0583 (2)	0.0361 (16)
C17	0.7708 (5)	-0.1491 (5)	0.0727 (2)	0.0406 (17)
H17	0.7100	-0.1646	0.0560	0.049*
C18	0.7804 (5)	-0.1982 (5)	0.1111 (2)	0.0352 (16)
C19	0.8699 (5)	-0.1780 (5)	0.1381 (2)	0.0329 (15)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
I1	0.0476 (3)	0.1081 (5)	0.0458 (3)	0.0294 (3)	0.0003 (3)	-0.0007 (3)
I2	0.0508 (3)	0.0558 (3)	0.0292 (2)	0.0012 (2)	-0.0041 (2)	-0.0020 (2)
I3	0.0643 (3)	0.0714 (4)	0.0516 (4)	0.0043 (2)	-0.0106 (3)	0.0231 (3)
I4	0.0551 (3)	0.0626 (3)	0.0631 (4)	-0.0240 (2)	-0.0120 (3)	0.0108 (3)
O1	0.041 (3)	0.078 (3)	0.031 (3)	0.007 (2)	-0.005 (2)	-0.010 (3)
O2	0.049 (3)	0.056 (3)	0.037 (3)	-0.012 (2)	-0.002 (2)	0.005 (2)
N1	0.038 (3)	0.053 (4)	0.035 (4)	-0.002 (3)	0.009 (3)	-0.007 (3)
N2	0.044 (3)	0.055 (4)	0.027 (4)	0.000 (3)	-0.002 (3)	-0.008 (3)
C1	0.030 (4)	0.043 (4)	0.028 (4)	-0.009 (3)	0.005 (3)	0.003 (3)
C2	0.029 (4)	0.052 (4)	0.033 (4)	-0.001 (3)	0.002 (3)	0.002 (3)
C3	0.044 (4)	0.034 (4)	0.032 (4)	-0.004 (3)	0.006 (3)	-0.004 (3)

C4	0.042 (4)	0.037 (4)	0.022 (4)	-0.006 (3)	0.006 (3)	0.005 (3)
C5	0.030 (3)	0.043 (4)	0.027 (4)	-0.002 (3)	0.004 (3)	0.007 (3)
C6	0.039 (4)	0.032 (4)	0.023 (4)	-0.001 (3)	0.006 (3)	0.000 (3)
C7	0.047 (4)	0.034 (4)	0.030 (4)	-0.002 (3)	0.004 (3)	-0.005 (3)
C8	0.047 (4)	0.053 (4)	0.031 (4)	-0.001 (3)	0.002 (3)	-0.009 (4)
C9	0.038 (4)	0.050 (4)	0.027 (4)	-0.002 (3)	-0.002 (3)	-0.009 (3)
C10	0.046 (5)	0.103 (7)	0.051 (6)	-0.016 (4)	-0.008 (4)	-0.033 (5)
C11	0.069 (5)	0.054 (5)	0.038 (5)	0.002 (4)	0.008 (4)	0.001 (4)
C12	0.030 (4)	0.066 (5)	0.032 (4)	-0.003 (3)	-0.002 (3)	-0.011 (4)
C13	0.036 (4)	0.043 (4)	0.038 (5)	0.003 (3)	0.003 (3)	-0.016 (4)
C14	0.034 (4)	0.038 (4)	0.030 (4)	-0.002 (3)	-0.002 (3)	-0.003 (3)
C15	0.040 (4)	0.032 (4)	0.036 (4)	0.001 (3)	0.005 (3)	-0.001 (3)
C16	0.039 (4)	0.034 (4)	0.035 (4)	0.010 (3)	-0.002 (3)	0.000 (3)
C17	0.035 (4)	0.044 (4)	0.043 (5)	0.000 (3)	-0.009 (3)	-0.002 (4)
C18	0.037 (4)	0.031 (4)	0.038 (4)	-0.007 (3)	0.000 (3)	-0.005 (3)
C19	0.040 (4)	0.024 (4)	0.034 (4)	0.002 (3)	0.005 (3)	-0.004 (3)

*Geometric parameters (Å, °)*

I1—C2	2.091 (6)	C8—C9	1.550 (8)
I2—C4	2.098 (6)	C8—H8A	0.9700
I3—C16	2.081 (6)	C8—H8B	0.9700
I4—C18	2.090 (6)	C9—C11	1.522 (8)
O1—C1	1.301 (7)	C9—C10	1.526 (8)
O1—H1	0.8203	C9—C12	1.530 (8)
O2—C19	1.312 (7)	C10—H10A	0.9600
O2—H2	0.8201	C10—H10B	0.9600
N1—C7	1.278 (8)	C10—H10C	0.9600
N1—C8	1.452 (7)	C11—H11A	0.9600
N1—H1A	0.7184	C11—H11B	0.9600
N2—C13	1.259 (8)	C11—H11C	0.9600
N2—C12	1.474 (7)	C12—H12A	0.9700
N2—H1B	0.8984	C12—H12B	0.9700
C1—C2	1.416 (8)	C13—C14	1.452 (8)
C1—C6	1.426 (8)	C13—H13	0.9300
C2—C3	1.376 (8)	C14—C15	1.388 (8)
C3—C4	1.403 (8)	C14—C19	1.436 (8)
C3—H3	0.9300	C15—C16	1.367 (8)
C4—C5	1.364 (8)	C15—H15	0.9300
C5—C6	1.396 (8)	C16—C17	1.383 (8)
C5—H5	0.9300	C17—C18	1.359 (8)
C6—C7	1.427 (8)	C17—H17	0.9300
C7—H7	0.9300	C18—C19	1.408 (8)
C1—O1—H1	110.0	C12—C9—C8	108.6 (5)
C19—O2—H2	109.8	C9—C10—H10A	109.5
C7—N1—C8	122.8 (6)	C9—C10—H10B	109.5
C7—N1—H1A	115.1	H10A—C10—H10B	109.5

C8—N1—H1A	121.8	C9—C10—H10C	109.5
C13—N2—C12	121.2 (6)	H10A—C10—H10C	109.5
C13—N2—H1B	129.4	H10B—C10—H10C	109.5
C12—N2—H1B	108.7	C9—C11—H11A	109.5
O1—C1—C2	120.8 (6)	C9—C11—H11B	109.5
O1—C1—C6	122.4 (6)	H11A—C11—H11B	109.5
C2—C1—C6	116.7 (6)	C9—C11—H11C	109.5
C3—C2—C1	122.2 (6)	H11A—C11—H11C	109.5
C3—C2—I1	119.6 (5)	H11B—C11—H11C	109.5
C1—C2—I1	118.2 (5)	N2—C12—C9	112.8 (5)
C2—C3—C4	119.5 (6)	N2—C12—H12A	109.0
C2—C3—H3	120.2	C9—C12—H12A	109.0
C4—C3—H3	120.2	N2—C12—H12B	109.0
C5—C4—C3	120.0 (6)	C9—C12—H12B	109.0
C5—C4—I2	121.6 (5)	H12A—C12—H12B	107.8
C3—C4—I2	118.4 (4)	N2—C13—C14	122.8 (6)
C4—C5—C6	121.3 (6)	N2—C13—H13	118.6
C4—C5—H5	119.3	C14—C13—H13	118.6
C6—C5—H5	119.3	C15—C14—C19	119.4 (6)
C5—C6—C1	120.1 (5)	C15—C14—C13	121.8 (6)
C5—C6—C7	120.9 (6)	C19—C14—C13	118.8 (6)
C1—C6—C7	119.0 (6)	C16—C15—C14	122.0 (6)
N1—C7—C6	121.5 (6)	C16—C15—H15	119.0
N1—C7—H7	119.2	C14—C15—H15	119.0
C6—C7—H7	119.2	C15—C16—C17	119.4 (6)
N1—C8—C9	113.2 (5)	C15—C16—I3	122.2 (5)
N1—C8—H8A	108.9	C17—C16—I3	118.4 (5)
C9—C8—H8A	108.9	C18—C17—C16	120.2 (6)
N1—C8—H8B	108.9	C18—C17—H17	119.9
C9—C8—H8B	108.9	C16—C17—H17	119.9
H8A—C8—H8B	107.8	C17—C18—C19	122.9 (6)
C11—C9—C10	109.2 (5)	C17—C18—I4	119.6 (5)
C11—C9—C12	110.9 (5)	C19—C18—I4	117.6 (5)
C10—C9—C12	107.3 (5)	O2—C19—C18	122.7 (6)
C11—C9—C8	111.4 (5)	O2—C19—C14	121.2 (6)
C10—C9—C8	109.4 (6)	C18—C19—C14	116.1 (6)

Hydrogen-bond geometry (Å, °)

<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>
N1—H1A...O1	0.72	1.90	2.526 (6)	145
O2—H2...N2	0.82	1.82	2.548 (6)	148