



# Crystal structure and Hirshfeld surface analysis of *N*-[(*Z*)-(2-hydroxyphenyl)methylidene]aniline *N*-oxide

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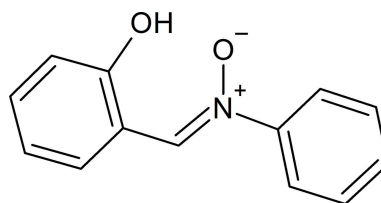
**Supporting information:** this article has supporting information at journals.iucr.org/e

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The conformation of the title compound, C<sub>13</sub>H<sub>11</sub>NO<sub>2</sub>, is partially determined by a strong, intramolecular O—H...O hydrogen bond. The crystal packing consists of strongly corrugated layers parallel to the *ac* plane and associated through C—H... $\pi$ (ring) interactions. A Hirshfeld surface analysis of the crystal structure indicates that the most significant contributions to the crystal packing are from H...H (44.1%), C...H/H...C (29.4%) and O...H/H...O (17.3%) contacts.

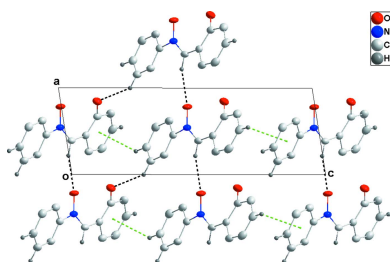
## 1. Chemical context

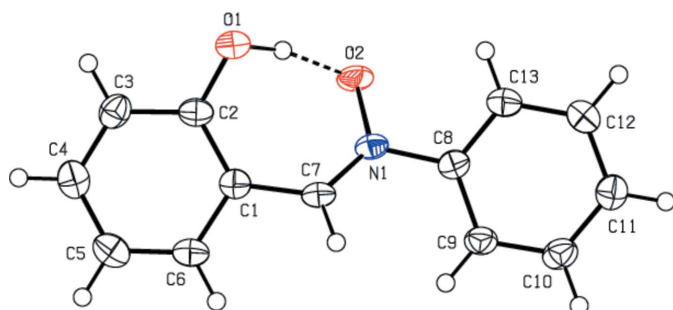
Nitrones are a very important class of organic compounds as a result of their medicinal and pharmaceutical applications. They show antifungal (Salman *et al.*, 2013), antibacterial (Chakraborty *et al.*, 2010), neuroprotective (Chioua *et al.*, 2012) and anticancer (Floyd *et al.*, 2011) activities. In addition, nitrone compounds are widely used as antioxidant agents (Al-Mowali *et al.*, 2014) because of their ability to scavenge free radicals. Based on these findings and following our interest in this area, we report herein the crystal structure of the title compound.



## 2. Structural commentary

The molecular structure of the title compound (Fig. 1) is almost planar, with maximum deviations of 0.398 (2) Å for O1 and -0.756 (2) Å for O2. The N1—O2 distance of 1.331 (2) Å is normal for a single bond and agrees well with those observed in other amine *N*-oxides. The dihedral angle between the aromatic rings (C1—C6 and C8—C13) is 1.94 (12)°. The torsion angles C2—C1—C7—N1, C1—C7—N1—C8, C1—C7—N1—O2, C7—N1—C8—C9 and O2—N1—C8—C9 are -30.2 (3), -179.7 (2), -0.4 (3), 27.3 (3) and -152.0 (2)°, respectively. The conformation of the title compound is partially determined by a strong, intramolecular O1—H1...O2 hydrogen bond (Table 1).





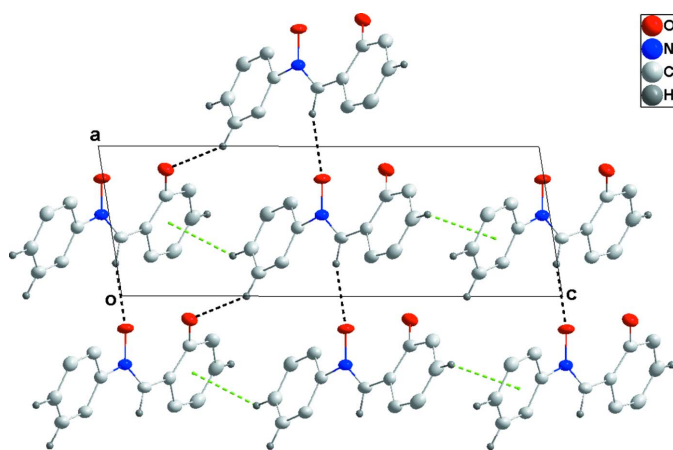
**Figure 1**  
The title molecule with labelling scheme and 50% probability ellipsoids. The intramolecular hydrogen bond is shown by a dashed line.

### 3. Supramolecular features

In the crystal,  $C7-H7 \cdots O2^i$  hydrogen bonds (Table 1) link the molecules, forming chains along the  $a$ -axis direction. The chains are linked into strongly corrugated sheets parallel to the  $ac$  plane by  $C10-H10 \cdots O2^{ii}$  hydrogen bonds and  $C11-H11 \cdots Cg1^{iii}$  interactions ( $Cg1$  is the centroid of the  $C1-C6$  hydroxyphenyl ring; Table 1 and Fig. 2). The sheets are stacked along the  $b$ -axis direction by  $C4-H4 \cdots Cg2^{iv}$  interactions ( $Cg2$  is the centroid of the  $C8-C13$  phenyl ring; Table 1 and Figs. 2 and 3).

### 4. Hirshfeld surface analysis

A Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) was carried out using *CrystalExplorer17.5* (Turner *et al.*, 2017) to visualize the intermolecular interactions in the title compound. The Hirshfeld surface mapped over  $d_{\text{norm}}$  (Fig. 4) shows the expected bright-red spots near atoms O1, O2, H7 and H10, which are involved in the  $C-H \cdots O$  hydrogen-bonding interactions. The bright-red spot near O1 indicates its role as a hydrogen-bond acceptor to  $(C10)H10$  (Fig. 4) and



**Figure 2**  
Detail of the intermolecular  $C-H \cdots O$  hydrogen bonds and the  $C-H \cdots \pi(\text{ring})$  interactions (black and green dashed lines, respectively) viewed along the  $b$ -axis direction.

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$Cg1$  and  $Cg2$  are the centroids of the  $C1-C6$  and  $C8-C13$  aromatic rings, respectively.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1-H1 \cdots O2$	0.97	1.53	2.479 (2)	167
$C7-H7 \cdots O2^i$	0.95	2.43	3.368 (3)	167
$C10-H10 \cdots O1^{ii}$	0.95	2.53	3.227 (3)	131
$C11-H11 \cdots Cg1^{iii}$	0.95	2.94	3.662 (3)	136
$C4-H4 \cdots Cg2^{iv}$	0.95	2.77	3.545 (3)	140

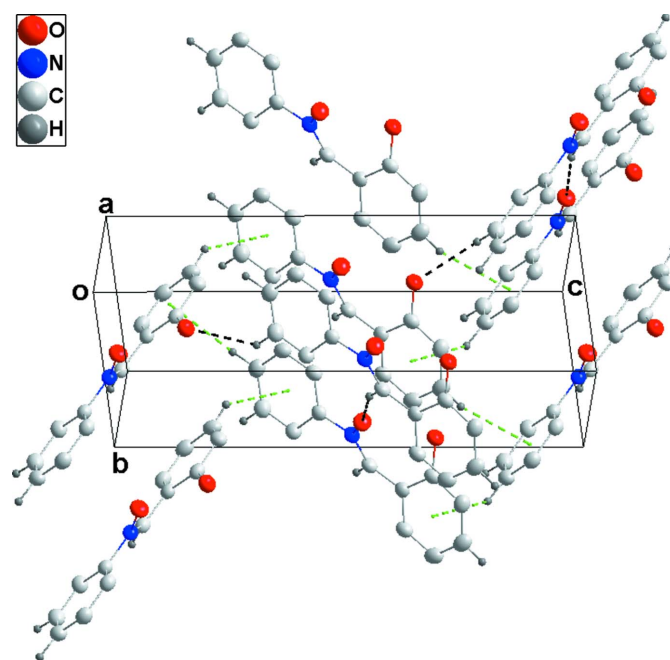
Symmetry codes: (i)  $x-1, y, z$ ; (ii)  $x-1, -y, z-\frac{1}{2}$ ; (iii)  $x, -y, z-\frac{1}{2}$ ; (iv)  $x, -y+1, z+\frac{1}{2}$ .

**Table 2**  
Summary of short interatomic contacts ( $\text{\AA}$ ) in the title compound.

Contact	Distance	Symmetry operation
$O2 \cdots H7$	2.43	$1+x, y, z$
$O1 \cdots H10$	2.53	$1+x, -y, \frac{1}{2}+z$
$O2 \cdots H12$	2.87	$x, 1+y, z$
$C3 \cdots H12$	3.02	$x, -y, \frac{1}{2}+z$
$H4 \cdots C11$	2.86	$x, 1-y, \frac{1}{2}+z$
$H6 \cdots H13$	2.46	$-1+x, 1+y, z$

another red region near O2 correlates with the  $C7-H7 \cdots O2$  interaction.

The two-dimensional fingerprint plots show the relative contributions of the various types of contacts to the Hirshfeld surface for the title compound (McKinnon *et al.*, 2007). The plots (Fig. 5) reveal that  $H \cdots H$  and  $C \cdots H/H \cdots C$  interactions make the greatest contributions to the surface contacts, while  $O \cdots H/H \cdots O$ ,  $C \cdots C$ ,  $N \cdots H/H \cdots N$ ,  $N \cdots C/C \cdots N$  and  $O \cdots C/C \cdots O$  contacts are less significant (Tables 2 and 3).



**Figure 3**  
Packing viewed along the  $(120)$  direction with intermolecular interactions shown as in Fig. 2.

Table 3

Percentage contributions of interatomic contacts to the Hirshfeld surface for the title compound.

Contact	Percentage contribution
H...H	44.1
C...H/H...C	29.4
O...H/H...O	17.3
C...C	5.3
N...C/C...N	1.7
N...H/H...N	1.5
O...C/C...O	0.7

### 5. Database survey

The four most closely related structures are (*Z*)-*N*-[(1,3-diphenyl-1*H*-pyrazol-4-yl)methanimine]-*N*-oxido (DEPVOM; Mohamed *et al.*, 2018), (*Z*)-1,2-bis(3-bromophenyl)diazene 1-oxide (SIYHAK01; Goswami *et al.*, 2018), (*Z*)-*N*-benzyl-

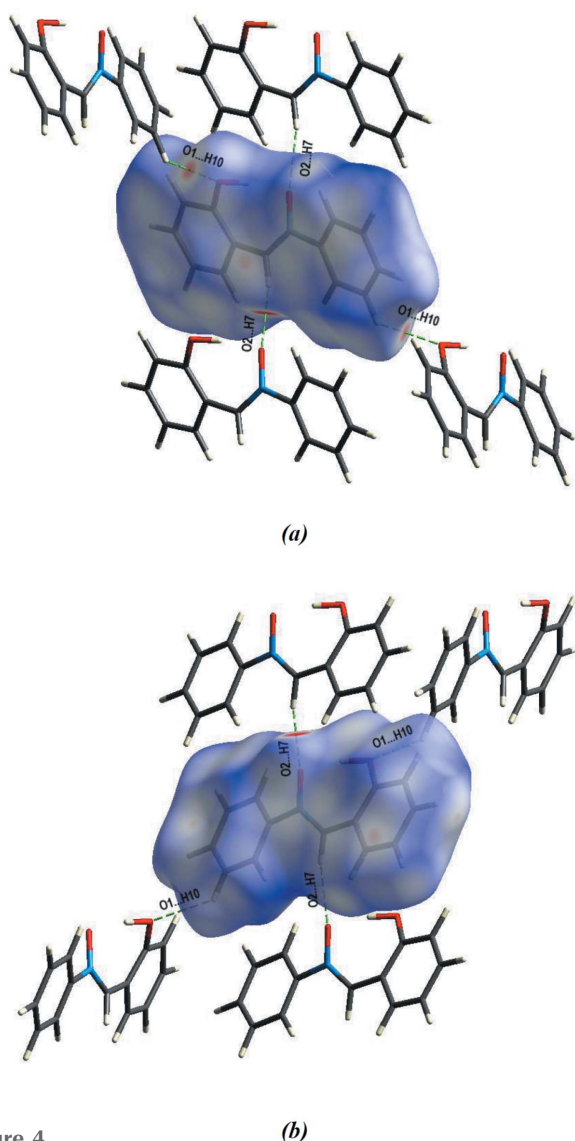


Figure 4 A view of the three-dimensional Hirshfeld surface with the C—H...O interactions for the title compound, plotted over  $d_{norm}$  in the range  $-0.2242$  to  $1.2146$  a.u. (a) front view, (b) back view.

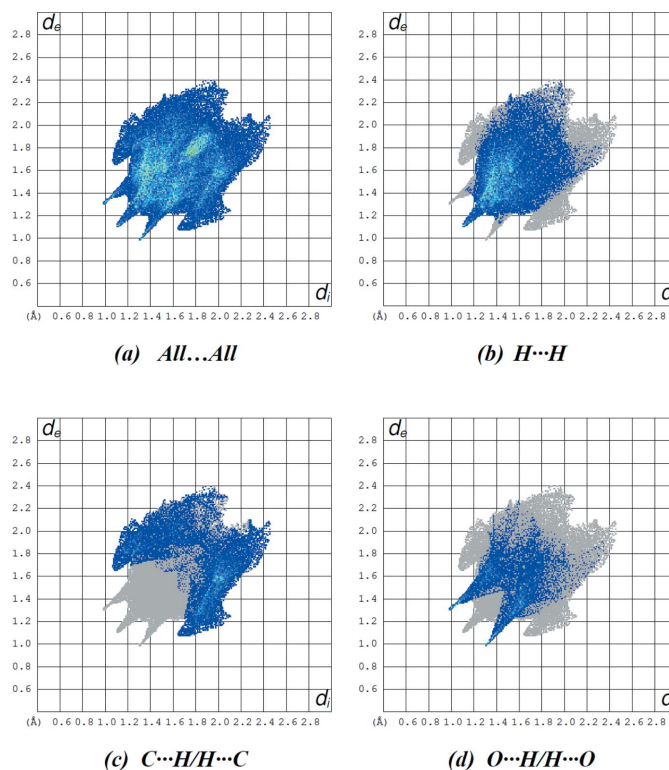


Figure 5 A view of the two-dimensional fingerprint plots for the title compound, showing (a) all interactions, and delineated into (b) H...H, (c) C...H/H...C and (d) O...H/H...O interactions. The  $d_i$  and  $d_e$  values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

idene-1-phenylmethanamine oxide hydrogen peroxide solvate (JELQOJ; Churakov *et al.*, 2017) and (*Z*)-*N*-(2-chlorobenzylidene)aniline *N*-oxide (ERIXEJ; Fu *et al.*, 2011).

In the crystal of DEPVOM, (101) layers are generated by C—H...O hydrogen bonds coupled with C—H... $\pi$ (ring) and offset  $\pi$ - $\pi$  stacking interactions. In the crystal of SIYHAK01, C—H...O and C—H...Br hydrogen bonds together with offset  $\pi$ - $\pi$  interactions stack the molecules along the *a*-axis direction. In the crystal of JELQOJ, the organic and peroxide molecules are linked through both peroxide O—H donor groups to oxide O-atom acceptors, giving one-dimensional chains extending along the *b*-axis direction. Weak intermolecular C—H...O hydrogen-bonding interactions are also present. In the crystal of ERIXEJ, the molecule is stabilized by an intramolecular C—H...O hydrogen bond. The geometry about the C=N bond is *Z* [C—C—N—O torsion angle =  $-4.2(3)^\circ$ ] and the phenyl and benzene rings are *trans*-oriented around the C=N bond. The phenyl and benzene rings make a dihedral angle of  $56.99(2)^\circ$ .

### 6. Synthesis and crystallization

(*Z*)-(2-Hydroxyphenyl)methylidene]benzenimine *N*-oxide (nitron) was prepared according to the reported procedures (Mobinikhaledi *et al.*, 2005). 0.7 ml (6 mmol) of salicylaldehyde were added to a warmed solution of 0.8 g (6 mmol)

Table 4

Experimental details.

Crystal data	
Chemical formula	C <sub>13</sub> H <sub>11</sub> NO <sub>2</sub>
<i>M<sub>r</sub></i>	213.23
Crystal system, space group	Monoclinic, <i>Pc</i>
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.5391 (1), 5.7873 (2), 16.0859 (4)
$\beta$ (°)	99.067 (1)
<i>V</i> (Å <sup>3</sup> )	509.21 (2)
<i>Z</i>	2
Radiation type	Cu <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.77
Crystal size (mm)	0.19 × 0.17 × 0.15
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.77, 0.89
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	3578, 1654, 1607
<i>R<sub>int</sub></i>	0.023
( $\sin \theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	0.033, 0.084, 1.06
No. of reflections	1654
No. of parameters	145
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.18, -0.18
Absolute structure	Flack <i>x</i> determined using 611 quotients [( <i>I</i> <sup>+</sup> ) - ( <i>I</i> <sup>-</sup> )] / [( <i>I</i> <sup>+</sup> ) + ( <i>I</i> <sup>-</sup> )] (Parsons <i>et al.</i> , 2013).
Absolute structure parameter	0.30 (13)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg & Putz, 2012) and *PLATON* (Spek, 2020).

*N*-phenylhydroxyamine in ethanol followed by stirring for 5 minutes, then standing at room temperature in the dark overnight gave the nitron, which was recrystallized from ethanol in 53% yield; m.p. 387–388 K.

## 7. Refinement

Crystal and refinement details are presented in Table 4. The H atom of the OH group was found in difference-Fourier maps, and its positional parameters were fixed using the AFIX 3 instruction in *SHELXL* and were refined with the isotropic displacement parameter  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . The C-bound H atoms were positioned geometrically, with C–H = 0.95 Å, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) =$

$1.2U_{\text{eq}}(\text{C})$ . Attempts to determine the absolute structure did not produce a definitive result, *viz.*: Flack *x* = 0.2 (3) by classical fit to all intensities 0.30 (14) from 611 selected quotients (Parsons' method). A round of TWIN/BASF refinement gave  $\text{BASF} = 0.2$  (4) with no improvement in the model.

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## supporting information

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## Crystal structure and Hirshfeld surface analysis of *N*-[(*Z*)-(2-hydroxyphenyl)-methylidene]aniline *N*-oxide

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### Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015*b*); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg & Putz, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

### *N*-[(*Z*)-(2-Hydroxyphenyl)methylidene]aniline *N*-oxide

#### Crystal data

$C_{13}H_{11}NO_2$	$F(000) = 224$
$M_r = 213.23$	$D_x = 1.391 \text{ Mg m}^{-3}$
Monoclinic, <i>Pc</i>	Cu <i>K</i> $\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
$a = 5.5391 (1) \text{ \AA}$	Cell parameters from 3430 reflections
$b = 5.7873 (2) \text{ \AA}$	$\theta = 5.6\text{--}72.4^\circ$
$c = 16.0859 (4) \text{ \AA}$	$\mu = 0.77 \text{ mm}^{-1}$
$\beta = 99.067 (1)^\circ$	$T = 150 \text{ K}$
$V = 509.21 (2) \text{ \AA}^3$	Block, yellow
$Z = 2$	$0.19 \times 0.17 \times 0.15 \text{ mm}$

#### Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer	$T_{\min} = 0.77, T_{\max} = 0.89$
Radiation source: INCOATEC $I\mu$ S micro-focus source	3578 measured reflections
Mirror monochromator	1654 independent reflections
Detector resolution: $10.4167 \text{ pixels mm}^{-1}$	1607 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.023$
Absorption correction: multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)	$\theta_{\max} = 72.4^\circ, \theta_{\min} = 5.6^\circ$
	$h = -6 \rightarrow 6$
	$k = -7 \rightarrow 7$
	$l = -19 \rightarrow 19$

#### Refinement

Refinement on $F^2$	Hydrogen site location: mixed
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 0.084P]$
$wR(F^2) = 0.084$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\max} < 0.001$
1654 reflections	$\Delta\rho_{\max} = 0.18 \text{ e \AA}^{-3}$
145 parameters	$\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$
2 restraints	

Absolute structure: Flack  $x$  determined using  
611 quotients  $[(F^-)-(F)]/[(F^+)+(F)]$  (Parsons *et al.*,  
2013).  
Absolute structure parameter: 0.30 (13)

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.8449 (3)	0.3532 (3)	0.64513 (12)	0.0342 (4)
H1	0.841875	0.289527	0.589214	0.051*
O2	0.7828 (3)	0.2215 (3)	0.49662 (12)	0.0338 (4)
N1	0.5424 (3)	0.1864 (3)	0.48272 (13)	0.0267 (4)
C1	0.4520 (4)	0.4953 (4)	0.57874 (14)	0.0260 (5)
C2	0.6705 (4)	0.5169 (4)	0.63617 (15)	0.0280 (5)
C3	0.7030 (4)	0.7093 (4)	0.68930 (16)	0.0328 (5)
H3	0.852651	0.728354	0.726592	0.039*
C4	0.5207 (5)	0.8717 (4)	0.68821 (18)	0.0348 (5)
H4	0.545906	1.001606	0.724635	0.042*
C5	0.3009 (4)	0.8470 (4)	0.63443 (17)	0.0349 (6)
H5	0.174797	0.958261	0.634589	0.042*
C6	0.2662 (4)	0.6611 (4)	0.58092 (16)	0.0304 (5)
H6	0.114410	0.643651	0.544695	0.036*
C7	0.3908 (4)	0.3082 (4)	0.51888 (15)	0.0270 (5)
H7	0.222390	0.270734	0.504648	0.032*
C8	0.4586 (4)	0.0034 (4)	0.42327 (14)	0.0263 (5)
C9	0.2257 (4)	0.0070 (4)	0.37527 (15)	0.0304 (5)
H9	0.116018	0.130115	0.380872	0.036*
C10	0.1571 (4)	-0.1720 (4)	0.31930 (17)	0.0340 (5)
H10	-0.001169	-0.171673	0.286384	0.041*
C11	0.3176 (5)	-0.3521 (4)	0.31083 (16)	0.0327 (5)
H11	0.269918	-0.473587	0.271973	0.039*
C12	0.5480 (5)	-0.3533 (4)	0.35956 (18)	0.0324 (5)
H12	0.657396	-0.477040	0.354374	0.039*
C13	0.6199 (4)	-0.1748 (4)	0.41587 (16)	0.0301 (5)
H13	0.778043	-0.175337	0.448865	0.036*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0260 (9)	0.0382 (9)	0.0363 (9)	0.0038 (6)	-0.0010 (7)	0.0001 (7)
O2	0.0137 (7)	0.0461 (9)	0.0418 (9)	-0.0015 (7)	0.0047 (7)	-0.0028 (8)
N1	0.0170 (9)	0.0340 (9)	0.0290 (10)	-0.0013 (7)	0.0031 (7)	0.0025 (8)
C1	0.0253 (12)	0.0287 (11)	0.0250 (12)	-0.0010 (8)	0.0073 (10)	0.0032 (8)

C2	0.0232 (12)	0.0314 (11)	0.0301 (12)	0.0004 (8)	0.0057 (10)	0.0066 (9)
C3	0.0308 (13)	0.0359 (12)	0.0320 (12)	-0.0082 (10)	0.0059 (10)	-0.0024 (10)
C4	0.0380 (14)	0.0300 (11)	0.0397 (13)	-0.0066 (9)	0.0166 (11)	-0.0022 (10)
C5	0.0346 (14)	0.0328 (12)	0.0403 (15)	0.0032 (9)	0.0150 (11)	0.0065 (10)
C6	0.0232 (11)	0.0362 (12)	0.0321 (12)	0.0026 (9)	0.0054 (9)	0.0071 (10)
C7	0.0185 (10)	0.0327 (11)	0.0293 (11)	0.0009 (8)	0.0028 (9)	0.0049 (9)
C8	0.0241 (11)	0.0292 (11)	0.0258 (13)	-0.0022 (8)	0.0044 (10)	0.0029 (8)
C9	0.0218 (11)	0.0379 (12)	0.0316 (13)	0.0017 (9)	0.0053 (10)	-0.0012 (9)
C10	0.0246 (11)	0.0448 (13)	0.0329 (12)	-0.0037 (9)	0.0052 (10)	-0.0013 (11)
C11	0.0328 (12)	0.0340 (12)	0.0328 (13)	-0.0066 (9)	0.0096 (10)	-0.0021 (10)
C12	0.0336 (12)	0.0307 (11)	0.0341 (12)	0.0044 (9)	0.0096 (10)	0.0023 (10)
C13	0.0249 (11)	0.0350 (12)	0.0307 (13)	0.0025 (8)	0.0056 (9)	0.0053 (9)

*Geometric parameters (Å, °)*

O1—C2	1.345 (3)	C5—H5	0.9500
O1—H1	0.9697	C6—H6	0.9500
O2—N1	1.331 (2)	C7—H7	0.9500
N1—C7	1.302 (3)	C8—C13	1.382 (3)
N1—C8	1.454 (3)	C8—C9	1.395 (3)
C1—C2	1.407 (3)	C9—C10	1.386 (4)
C1—C6	1.411 (3)	C9—H9	0.9500
C1—C7	1.453 (3)	C10—C11	1.391 (4)
C2—C3	1.398 (4)	C10—H10	0.9500
C3—C4	1.377 (4)	C11—C12	1.389 (4)
C3—H3	0.9500	C11—H11	0.9500
C4—C5	1.385 (4)	C12—C13	1.390 (4)
C4—H4	0.9500	C12—H12	0.9500
C5—C6	1.372 (4)	C13—H13	0.9500
C2—O1—H1	105.1	N1—C7—C1	126.9 (2)
C7—N1—O2	122.78 (18)	N1—C7—H7	116.6
C7—N1—C8	121.79 (18)	C1—C7—H7	116.6
O2—N1—C8	115.43 (17)	C13—C8—C9	121.2 (2)
C2—C1—C6	118.6 (2)	C13—C8—N1	117.2 (2)
C2—C1—C7	125.97 (19)	C9—C8—N1	121.66 (19)
C6—C1—C7	115.4 (2)	C10—C9—C8	118.9 (2)
O1—C2—C3	118.3 (2)	C10—C9—H9	120.5
O1—C2—C1	122.5 (2)	C8—C9—H9	120.5
C3—C2—C1	119.1 (2)	C9—C10—C11	120.6 (2)
C4—C3—C2	120.8 (2)	C9—C10—H10	119.7
C4—C3—H3	119.6	C11—C10—H10	119.7
C2—C3—H3	119.6	C12—C11—C10	119.6 (2)
C3—C4—C5	120.5 (2)	C12—C11—H11	120.2
C3—C4—H4	119.7	C10—C11—H11	120.2
C5—C4—H4	119.7	C11—C12—C13	120.5 (2)
C6—C5—C4	119.6 (2)	C11—C12—H12	119.8
C6—C5—H5	120.2	C13—C12—H12	119.8

C4—C5—H5	120.2	C8—C13—C12	119.2 (2)
C5—C6—C1	121.2 (2)	C8—C13—H13	120.4
C5—C6—H6	119.4	C12—C13—H13	120.4
C1—C6—H6	119.4		
C6—C1—C2—O1	172.1 (2)	C6—C1—C7—N1	153.4 (2)
C7—C1—C2—O1	-4.2 (3)	C7—N1—C8—C13	-153.0 (2)
C6—C1—C2—C3	-4.4 (3)	O2—N1—C8—C13	27.7 (3)
C7—C1—C2—C3	179.3 (2)	C7—N1—C8—C9	27.3 (3)
O1—C2—C3—C4	-174.0 (2)	O2—N1—C8—C9	-152.0 (2)
C1—C2—C3—C4	2.6 (3)	C13—C8—C9—C10	-0.1 (3)
C2—C3—C4—C5	0.1 (4)	N1—C8—C9—C10	179.6 (2)
C3—C4—C5—C6	-1.0 (4)	C8—C9—C10—C11	-0.2 (4)
C4—C5—C6—C1	-0.9 (4)	C9—C10—C11—C12	0.6 (4)
C2—C1—C6—C5	3.6 (3)	C10—C11—C12—C13	-0.7 (4)
C7—C1—C6—C5	-179.7 (2)	C9—C8—C13—C12	0.0 (3)
O2—N1—C7—C1	-0.4 (3)	N1—C8—C13—C12	-179.8 (2)
C8—N1—C7—C1	-179.7 (2)	C11—C12—C13—C8	0.4 (4)
C2—C1—C7—N1	-30.2 (3)		

#### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

*Cg*1 and *Cg*2 are the centroids of the C1—C6 and C8—C13 aromatic rings, respectively.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1—H1 $\cdots$ O2	0.97	1.53	2.479 (2)	167
C7—H7 $\cdots$ O2 <sup>i</sup>	0.95	2.43	3.368 (3)	167
C10—H10 $\cdots$ O1 <sup>ii</sup>	0.95	2.53	3.227 (3)	131
C11—H11 $\cdots$ <i>Cg</i> 1 <sup>iii</sup>	0.95	2.94	3.662 (3)	136
C4—H4 $\cdots$ <i>Cg</i> 2 <sup>iv</sup>	0.95	2.77	3.545 (3)	140

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