

## 3-Hydroxy-*N'*-[phenyl(2-pyridyl)methylene]-2-naphthohydrazide

Wen-Jun Kang, Jian-Min Dou,\* Da-Cheng Li and Da-Qi Wang

School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, People's Republic of China

Correspondence e-mail: jmdou@lcu.edu.cn

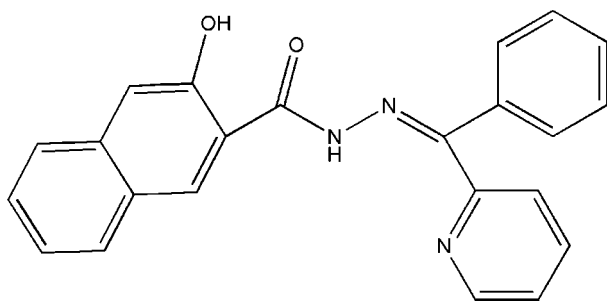
Received 14 June 2007; accepted 21 June 2007

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.045;  $wR$  factor = 0.152; data-to-parameter ratio = 12.5.

In the title molecule,  $\text{C}_{23}\text{H}_{17}\text{N}_3\text{O}_2$ , intramolecular  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds influence the molecular conformation. In the crystal structure,  $\pi-\pi$  interactions, with a distance of 3.611 (5) Å between the centroids of rings in neighbouring naphthalene rings, link the molecules into centrosymmetric dimers, and  $\text{C}-\text{H}\cdots\pi$  interactions link the dimers into chains running in the [101] direction.

### Related literature

For the crystal structure of an Ni complex with a related aroylhydrazone derivative, see: Liu *et al.* (2005). For general background, see Bai *et al.* (2005); for the specific biological activities of aroylhydrazones, see Mostafa & Haifaa (2007).



### Experimental

#### Crystal data

$\text{C}_{23}\text{H}_{17}\text{N}_3\text{O}_2$   
 $M_r = 367.40$

Monoclinic,  $P2_1/c$   
 $a = 13.9214$  (18) Å

$b = 17.238$  (2) Å  
 $c = 7.7751$  (16) Å  
 $\beta = 104.294$  (2)°  
 $V = 1808.0$  (5) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.38 \times 0.30 \times 0.28$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.967$ ,  $T_{\max} = 0.976$

9307 measured reflections  
3185 independent reflections  
1695 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.040$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.152$   
 $S = 1.01$   
3185 reflections  
254 parameters

1 restraint  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.20$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond and stacking geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O2}-\text{H2}\cdots\text{O1}$	0.82	1.86	2.571 (3)	145
$\text{N1}-\text{H1}\cdots\text{N3}$	0.86	2.01	2.648 (3)	130
$\text{C23}-\text{H23}\cdots\text{Cg}^i$	0.93	2.63	3.460 (7)	147

Symmetry code: (i)  $-x, 1-y, 1-z$ . Note:  $\text{Cg}$  is the centroid of the  $\text{N3/C13}-\text{C17}$  ring.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

The authors acknowledge the support of the National Natural Science Foundation of China (grant No. 20671048).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2265).

### References

- Bai, Y., Dang, D. B., Duan, C. Y., Song, Y. & Meng, Q. J. (2005). *Inorg. Chem.* **44**, 5972–5974.  
Liu, M.-L., Dou, J.-M., Wang, D.-Q. & Li, D.-C. (2005). *Acta Cryst.* **E61**, m1366–m1367.  
Mostafa, E. B. & Haifaa, E. T. (2007). *Spectrochim. Acta Part A*, **66**, 28–36.  
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
Sheldrick, G. M. (1997a). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.  
Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.  
Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

**supplementary materials**

*Acta Cryst.* (2007). E63, o3328 [ doi:10.1107/S160053680703036X ]

### 3-Hydroxy-*N'*-[phenyl(2-pyridyl)methylene]-2-naphthohydrazide

W.-J. Kang, J.-M. Dou, D.-C. Li and D.-Q. Wang

#### Comment

The chemistry of aroylhydrazones has gained a special attraction due to their coordination abilities to metal ions (Bai *et al.*, 2005) and their biological activities (Mostafa & Haifaa, 2007). As an extension of our work on the structural characterization of aroylhydrazone derivatives (Liu *et al.*, 2005), the title compound, (I), was synthesized and characterized.

In the title compound, the C1—O1 bond length is 1.228 (3) Å, indicating that the molecule is in the keto form. The bond distances and angles in (I) are normal. The three mean planes - naphthalene bicycle (A), benzene ring (B) and pyridine ring (C), make the following dihedral angles - A/B 75.7 (1)°, B/C 57.5 (1)° and A/C 25.1 (1)°. There are two intramolecular O2—H···O1 and N1—H···N3 hydrogen bonds (Table 1 and Fig. 1).

The  $\pi\cdots\pi$  interactions - proved by short distance Cg1···Cg2<sup>i</sup> of 3.611 (5) Å - link the molecules into centrosymmetric dimers [Cg1 and Cg2 are centroids of C2—C7 and C6—C11, respectively; symmetry code: (i) 1 - x, 1 - y, 2 - z]. The C—H··· $\pi$  interactions - C23—H23···Cg3<sup>ii</sup> 2.63 Å, 149°; Cg3 is a centroid of N3/C13—C17 [symmetry code: (ii) -x, 1 - y, 1 - z] - link dimers into chains running in direction [101] (Fig. 2).

#### Experimental

A solution of 2-benzoylpyridine (2.56 g, 14 mmol) in ethanol (10 ml) was added to a solution of 2-hydroxy-3-naphthoylhydrazine (2.02 g, 10 mmol) in ethanol (10 ml). The mixture was refluxed for 3 h, and then the precipitate was collected, washed several times with ethanol and dried *in vacuo* (yield 80%). A dichloromethane solution of the title compound was slowly evaporated and yellow crystal for X-ray diffraction was obtained after two weeks (m.p. 475–476 K). Analysis calculated for C<sub>23</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub>: C 75.19, H 4.67, N 11.44%; found: C 75.01, H 4.49, N 11.31%.

#### Refinement

All H atoms were placed in geometrically idealized positions (N—H 0.86 Å, O—H 0.82 Å and C—H 0.93 Å) and treated as riding on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

#### Figures

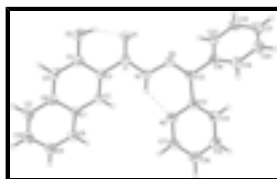


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

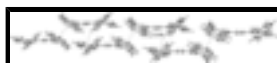


Fig. 2. Crystal packing of the title compound.

## 3-Hydroxy-*N*<sup>1</sup>-[phenyl(2-pyridyl)methylene]-2-naphthohydrazide

### Crystal data

$C_{23}H_{17}N_3O_2$	$F_{000} = 768$
$M_r = 367.40$	$D_x = 1.350 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 13.9214 (18) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 17.238 (2) \text{ \AA}$	Cell parameters from 1775 reflections
$c = 7.7751 (16) \text{ \AA}$	$\theta = 2.4\text{--}22.8^\circ$
$\beta = 104.294 (2)^\circ$	$\mu = 0.09 \text{ mm}^{-1}$
$V = 1808.0 (5) \text{ \AA}^3$	$T = 293 (2) \text{ K}$
$Z = 4$	Block, yellow
	$0.38 \times 0.30 \times 0.28 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer	3185 independent reflections
Radiation source: fine-focus sealed tube	1695 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.040$
$T = 293(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 1.5^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -16 \rightarrow 13$
$T_{\text{min}} = 0.967$ , $T_{\text{max}} = 0.976$	$k = -20 \rightarrow 19$
9307 measured reflections	$l = -8 \rightarrow 9$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.152$	$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.3761P]$
$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
3185 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
254 parameters	$\Delta\rho_{\text{max}} = 0.22 \text{ e \AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97, $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0079 (14)

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.12667 (15)	0.45180 (13)	0.8333 (3)	0.0502 (7)
H1	0.1275	0.5007	0.8551	0.060*
N2	0.04182 (16)	0.41633 (12)	0.7402 (3)	0.0475 (6)
N3	0.01643 (16)	0.57354 (13)	0.8659 (3)	0.0506 (6)
O1	0.21182 (14)	0.33844 (12)	0.8614 (3)	0.0826 (8)
O2	0.35617 (16)	0.32793 (12)	1.1398 (4)	0.0933 (9)
H2	0.3047	0.3140	1.0702	0.140*
C1	0.2092 (2)	0.40821 (17)	0.8904 (4)	0.0546 (8)
C2	0.3136 (2)	0.52678 (16)	0.9791 (4)	0.0520 (8)
H2A	0.2677	0.5553	0.8956	0.062*
C3	0.29691 (18)	0.44932 (16)	0.9980 (4)	0.0494 (8)
C4	0.3682 (2)	0.40554 (17)	1.1233 (5)	0.0624 (9)
C5	0.4488 (2)	0.44150 (19)	1.2260 (5)	0.0668 (10)
H5	0.4941	0.4125	1.3092	0.080*
C6	0.4661 (2)	0.52093 (18)	1.2106 (4)	0.0554 (8)
C7	0.39797 (19)	0.56455 (16)	1.0821 (4)	0.0505 (8)
C8	0.4168 (2)	0.64417 (17)	1.0631 (5)	0.0625 (9)
H8	0.3729	0.6732	0.9778	0.075*
C9	0.4980 (2)	0.6791 (2)	1.1672 (5)	0.0734 (11)
H9	0.5092	0.7317	1.1530	0.088*
C10	0.5644 (2)	0.6364 (2)	1.2949 (5)	0.0806 (12)
H10	0.6196	0.6608	1.3664	0.097*
C11	0.5499 (2)	0.5599 (2)	1.3165 (5)	0.0748 (11)
H11	0.5955	0.5323	1.4023	0.090*
C12	-0.0393 (2)	0.45569 (15)	0.6996 (4)	0.0440 (7)
C13	-0.05324 (19)	0.53912 (15)	0.7360 (4)	0.0449 (7)
C14	-0.1321 (2)	0.58120 (17)	0.6364 (4)	0.0568 (8)
H14	-0.1795	0.5569	0.5474	0.068*
C15	-0.1403 (2)	0.65894 (18)	0.6692 (5)	0.0677 (10)
H15	-0.1927	0.6877	0.6018	0.081*
C16	-0.0705 (2)	0.69346 (17)	0.8019 (5)	0.0641 (9)
H16	-0.0748	0.7459	0.8270	0.077*
C17	0.0057 (2)	0.64892 (16)	0.8969 (4)	0.0571 (8)

## supplementary materials

---

H17	0.0526	0.6724	0.9881	0.069*
C18	-0.1255 (2)	0.40909 (15)	0.6010 (4)	0.0463 (7)
C19	-0.2175 (2)	0.41381 (17)	0.6401 (4)	0.0575 (8)
H19	-0.2266	0.4482	0.7269	0.069*
C20	-0.2955 (2)	0.3681 (2)	0.5517 (5)	0.0666 (10)
H20	-0.3564	0.3710	0.5805	0.080*
C21	-0.2828 (3)	0.31836 (19)	0.4211 (5)	0.0687 (10)
H21	-0.3359	0.2888	0.3588	0.082*
C22	-0.1918 (2)	0.31210 (17)	0.3818 (4)	0.0632 (9)
H22	-0.1831	0.2777	0.2948	0.076*
C23	-0.1137 (2)	0.35729 (16)	0.4726 (4)	0.0519 (8)
H23	-0.0522	0.3527	0.4467	0.062*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0443 (14)	0.0329 (13)	0.0666 (17)	-0.0022 (11)	0.0006 (12)	-0.0055 (11)
N2	0.0420 (13)	0.0396 (13)	0.0570 (16)	-0.0049 (11)	0.0047 (12)	-0.0039 (11)
N3	0.0577 (15)	0.0356 (14)	0.0547 (16)	-0.0026 (11)	0.0069 (12)	-0.0014 (11)
O1	0.0583 (14)	0.0381 (13)	0.139 (2)	0.0034 (10)	0.0011 (14)	-0.0161 (13)
O2	0.0683 (15)	0.0448 (14)	0.148 (3)	0.0037 (11)	-0.0087 (16)	0.0215 (14)
C1	0.0452 (17)	0.0375 (17)	0.077 (2)	0.0031 (14)	0.0072 (16)	-0.0013 (15)
C2	0.0454 (17)	0.0410 (17)	0.064 (2)	0.0032 (13)	0.0027 (15)	-0.0027 (14)
C3	0.0398 (16)	0.0376 (16)	0.066 (2)	0.0041 (13)	0.0041 (15)	-0.0038 (14)
C4	0.0448 (17)	0.0416 (18)	0.094 (3)	0.0037 (14)	0.0048 (17)	0.0046 (17)
C5	0.0468 (18)	0.058 (2)	0.085 (3)	0.0122 (16)	-0.0047 (17)	0.0078 (18)
C6	0.0415 (17)	0.0525 (19)	0.068 (2)	0.0050 (14)	0.0054 (16)	-0.0070 (16)
C7	0.0421 (16)	0.0421 (17)	0.065 (2)	0.0011 (14)	0.0092 (15)	-0.0101 (15)
C8	0.057 (2)	0.0463 (19)	0.079 (2)	-0.0025 (15)	0.0065 (18)	-0.0070 (17)
C9	0.058 (2)	0.053 (2)	0.107 (3)	-0.0092 (17)	0.016 (2)	-0.022 (2)
C10	0.048 (2)	0.073 (3)	0.110 (3)	-0.0059 (19)	0.000 (2)	-0.033 (2)
C11	0.0466 (19)	0.076 (3)	0.091 (3)	0.0047 (17)	-0.0037 (18)	-0.017 (2)
C12	0.0446 (16)	0.0376 (16)	0.0476 (18)	-0.0017 (13)	0.0075 (14)	0.0010 (13)
C13	0.0437 (16)	0.0380 (16)	0.0522 (19)	0.0011 (13)	0.0102 (14)	0.0019 (13)
C14	0.0504 (17)	0.0480 (19)	0.068 (2)	0.0001 (15)	0.0065 (16)	0.0015 (15)
C15	0.058 (2)	0.051 (2)	0.087 (3)	0.0103 (16)	0.0052 (19)	0.0064 (18)
C16	0.071 (2)	0.0383 (17)	0.085 (3)	0.0091 (16)	0.023 (2)	-0.0006 (17)
C17	0.068 (2)	0.0374 (17)	0.062 (2)	-0.0037 (15)	0.0086 (17)	-0.0045 (15)
C18	0.0444 (17)	0.0389 (16)	0.0519 (19)	-0.0017 (13)	0.0049 (14)	0.0041 (14)
C19	0.0470 (18)	0.058 (2)	0.065 (2)	-0.0032 (15)	0.0102 (16)	-0.0014 (16)
C20	0.0471 (19)	0.072 (2)	0.078 (3)	-0.0076 (17)	0.0105 (18)	0.010 (2)
C21	0.061 (2)	0.060 (2)	0.072 (3)	-0.0209 (17)	-0.0093 (19)	0.0147 (19)
C22	0.075 (2)	0.0451 (19)	0.060 (2)	-0.0087 (16)	-0.0004 (18)	-0.0025 (15)
C23	0.0524 (18)	0.0420 (17)	0.058 (2)	-0.0021 (14)	0.0076 (15)	-0.0015 (15)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

N1—C1	1.352 (3)	C10—C11	1.351 (5)
N1—N2	1.368 (3)	C10—H10	0.9300

N1—H1	0.8600	C11—H11	0.9300
N2—C12	1.288 (3)	C12—C13	1.488 (4)
N3—C17	1.337 (3)	C12—C18	1.489 (4)
N3—C13	1.353 (3)	C13—C14	1.382 (4)
O1—C1	1.226 (3)	C14—C15	1.374 (4)
O2—C4	1.358 (3)	C14—H14	0.9300
O2—H2	0.8200	C15—C16	1.366 (4)
C1—C3	1.480 (4)	C15—H15	0.9300
C2—C3	1.369 (4)	C16—C17	1.369 (4)
C2—C7	1.408 (4)	C16—H16	0.9300
C2—H2A	0.9300	C17—H17	0.9300
C3—C4	1.423 (4)	C18—C23	1.379 (4)
C4—C5	1.356 (4)	C18—C19	1.389 (4)
C5—C6	1.400 (4)	C19—C20	1.380 (4)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.412 (4)	C20—C21	1.374 (5)
C6—C11	1.420 (4)	C20—H20	0.9300
C7—C8	1.412 (4)	C21—C22	1.378 (4)
C8—C9	1.358 (4)	C21—H21	0.9300
C8—H8	0.9300	C22—C23	1.382 (4)
C9—C10	1.389 (5)	C22—H22	0.9300
C9—H9	0.9300	C23—H23	0.9300
C1—N1—N2	118.5 (2)	C6—C11—H11	119.5
C1—N1—H1	120.7	N2—C12—C13	127.6 (2)
N2—N1—H1	120.7	N2—C12—C18	112.9 (2)
C12—N2—N1	119.0 (2)	C13—C12—C18	119.5 (2)
C17—N3—C13	118.0 (2)	N3—C13—C14	120.8 (3)
C4—O2—H2	109.5	N3—C13—C12	117.6 (2)
O1—C1—N1	123.1 (3)	C14—C13—C12	121.6 (3)
O1—C1—C3	121.0 (2)	C15—C14—C13	119.9 (3)
N1—C1—C3	115.8 (2)	C15—C14—H14	120.0
C3—C2—C7	122.0 (3)	C13—C14—H14	120.0
C3—C2—H2A	119.0	C16—C15—C14	119.3 (3)
C7—C2—H2A	119.0	C16—C15—H15	120.4
C2—C3—C4	118.9 (3)	C14—C15—H15	120.4
C2—C3—C1	123.0 (2)	C15—C16—C17	118.4 (3)
C4—C3—C1	118.1 (3)	C15—C16—H16	120.8
C5—C4—O2	119.9 (3)	C17—C16—H16	120.8
C5—C4—C3	119.8 (3)	N3—C17—C16	123.6 (3)
O2—C4—C3	120.4 (3)	N3—C17—H17	118.2
C4—C5—C6	122.1 (3)	C16—C17—H17	118.2
C4—C5—H5	119.0	C23—C18—C19	118.5 (3)
C6—C5—H5	119.0	C23—C18—C12	119.8 (3)
C5—C6—C7	118.8 (3)	C19—C18—C12	121.7 (3)
C5—C6—C11	123.1 (3)	C20—C19—C18	120.8 (3)
C7—C6—C11	118.1 (3)	C20—C19—H19	119.6
C2—C7—C8	122.7 (3)	C18—C19—H19	119.6
C2—C7—C6	118.5 (3)	C21—C20—C19	119.7 (3)
C8—C7—C6	118.8 (3)	C21—C20—H20	120.1

## supplementary materials

C9—C8—C7	121.2 (3)	C19—C20—H20	120.1
C9—C8—H8	119.4	C20—C21—C22	120.3 (3)
C7—C8—H8	119.4	C20—C21—H21	119.8
C8—C9—C10	120.0 (3)	C22—C21—H21	119.8
C8—C9—H9	120.0	C21—C22—C23	119.6 (3)
C10—C9—H9	120.0	C21—C22—H22	120.2
C11—C10—C9	120.9 (3)	C23—C22—H22	120.2
C11—C10—H10	119.6	C18—C23—C22	121.0 (3)
C9—C10—H10	119.6	C18—C23—H23	119.5
C10—C11—C6	121.1 (3)	C22—C23—H23	119.5
C10—C11—H11	119.5		
C1—N1—N2—C12	173.6 (3)	C5—C6—C11—C10	178.8 (3)
N2—N1—C1—O1	0.6 (5)	C7—C6—C11—C10	-0.3 (5)
N2—N1—C1—C3	-177.0 (2)	N1—N2—C12—C13	2.5 (4)
C7—C2—C3—C4	-1.2 (5)	N1—N2—C12—C18	-179.1 (2)
C7—C2—C3—C1	-179.5 (3)	C17—N3—C13—C14	1.2 (4)
O1—C1—C3—C2	153.4 (3)	C17—N3—C13—C12	178.5 (3)
N1—C1—C3—C2	-28.9 (4)	N2—C12—C13—N3	-20.4 (4)
O1—C1—C3—C4	-24.9 (5)	C18—C12—C13—N3	161.4 (3)
N1—C1—C3—C4	152.8 (3)	N2—C12—C13—C14	157.0 (3)
C2—C3—C4—C5	2.5 (5)	C18—C12—C13—C14	-21.3 (4)
C1—C3—C4—C5	-179.1 (3)	N3—C13—C14—C15	-0.1 (4)
C2—C3—C4—O2	-177.0 (3)	C12—C13—C14—C15	-177.3 (3)
C1—C3—C4—O2	1.3 (5)	C13—C14—C15—C16	-0.7 (5)
O2—C4—C5—C6	178.1 (3)	C14—C15—C16—C17	0.4 (5)
C3—C4—C5—C6	-1.4 (5)	C13—N3—C17—C16	-1.6 (5)
C4—C5—C6—C7	-1.0 (5)	C15—C16—C17—N3	0.8 (5)
C4—C5—C6—C11	179.9 (3)	N2—C12—C18—C23	-40.3 (4)
C3—C2—C7—C8	179.3 (3)	C13—C12—C18—C23	138.2 (3)
C3—C2—C7—C6	-1.1 (4)	N2—C12—C18—C19	136.9 (3)
C5—C6—C7—C2	2.2 (4)	C13—C12—C18—C19	-44.6 (4)
C11—C6—C7—C2	-178.6 (3)	C23—C18—C19—C20	-0.4 (4)
C5—C6—C7—C8	-178.2 (3)	C12—C18—C19—C20	-177.6 (3)
C11—C6—C7—C8	0.9 (4)	C18—C19—C20—C21	-1.3 (5)
C2—C7—C8—C9	178.7 (3)	C19—C20—C21—C22	2.1 (5)
C6—C7—C8—C9	-0.9 (5)	C20—C21—C22—C23	-1.2 (5)
C7—C8—C9—C10	0.2 (5)	C19—C18—C23—C22	1.3 (4)
C8—C9—C10—C11	0.5 (6)	C12—C18—C23—C22	178.6 (3)
C9—C10—C11—C6	-0.4 (6)	C21—C22—C23—C18	-0.5 (4)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2 $\cdots$ O1	0.82	1.86	2.571 (3)	145
N1—H1 $\cdots$ N3	0.86	2.01	2.648 (3)	130
C23—H23 $\cdots$ Cg <sup>i</sup>	0.93	2.63	3.460 (7)	147

Symmetry codes: (i)  $-x, -y+1, -z+1$ .



Fig. 1

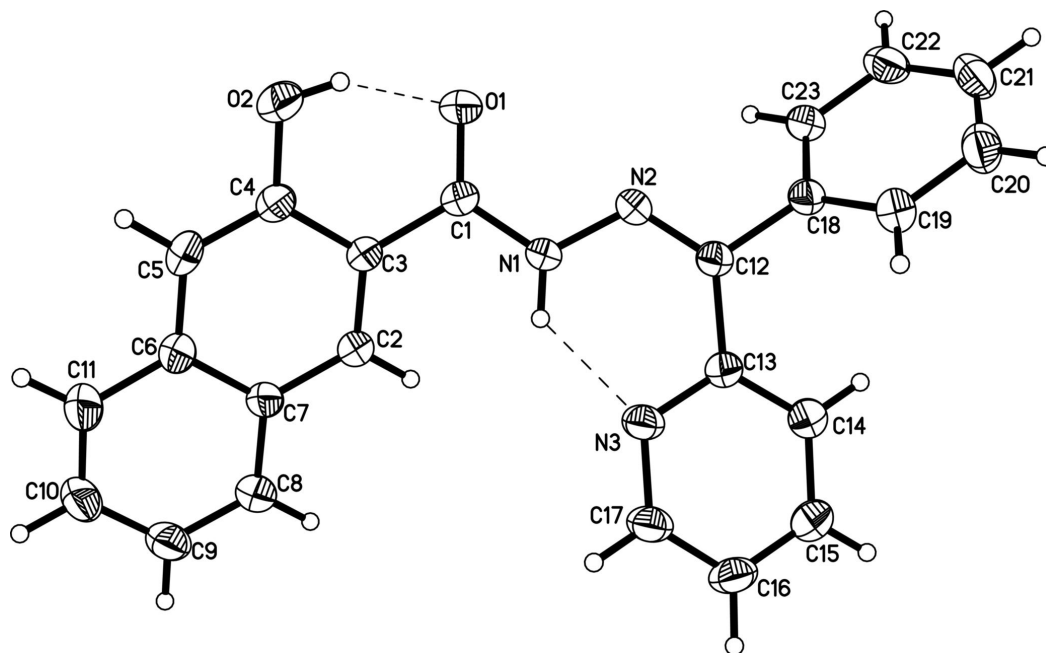


Fig. 2

