Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 3-Hydroxy-*N*′-[(*E*)-3-pyridylmethylidene]-2-naphthohydrazide

**Chuan Li, Xiuyun Zhang, Qingkun Wu and Handong Yin***

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: handongyin@163.com

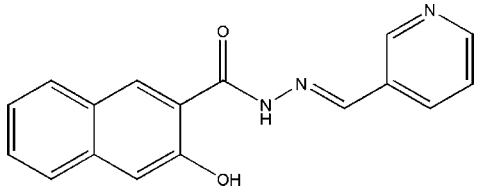
Received 17 June 2011; accepted 29 June 2011

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.039; $wR$ factor = 0.109; data-to-parameter ratio = 12.3.

The title compound, $C_{17}H_{13}N_3O_2$, displays an *E* configuration about the C=N bond. The mean planes of the pyridine and benzene rings make a dihedral angle of 31.2 (2)°. An intramolecular O—H···O hydrogen bond is observed. In the crystal, intermolecular N—H···N hydrogen bonding links the molecules into a chain along [101].

## Related literature

For related structures, see: Lv *et al.* (2006); Tarafder *et al.* (2002); Zhou *et al.* (2009); Huang (2009); Shafiq *et al.* (2009); Liang *et al.* (2008).




## Experimental

### *Crystal data*

$C_{17}H_{13}N_3O_2$
$M_r$ = 291.30
Orthorhombic, *Pbca*
$a$ = 11.0976 (11) Å
$b$ = 10.4422 (9) Å
$c$ = 23.9903 (17) Å
$V$ = 2780.1 (4) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 298 K
0.39 × 0.38 × 0.32 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.964, $T_{max}$ = 0.971
10663 measured reflections
2451 independent reflections
1486 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.043

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109
$S$ = 1.07
2451 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2···O1 | 0.82 | 1.87 | 2.6015 (18) | 147 |
| N1—H1···N3$^{i}$ | 0.86 | 2.12 | 2.956 (2) | 165 |

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We acknowledge the National Natural Science Foundation of China (20771053), the National Basic Research Program (No. 2010CB234601) and the Natural Science Foundation of Shandong Province (Y2008B48) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2338).

## References

Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Huang, H.-T. (2009). *Acta Cryst.* E**65**, o892.
Liang, Q.-F., Feng, H.-M. & Li, F.-Q. (2008). *Acta Cryst.* E**64**, o1008.
Lv, J., Liu, T., Cai, S., Wang, X., Liu, L. & Wang, Y. (2006). *J. Inorg. Biochem.* **100**, 1888–1896.
Shafiq, Z., Yaqub, M., Tahir, M. N., Nawaz, M. H. & Iqbal, M. S. (2009). *Acta Cryst.* E**65**, o2845–o2846.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tarafder, M. T. H., Jin, K. T., Crouse, K. A., Ali, A. M. & Yamin, B. M. (2002). *Polyhedron*, **21**, 2547–2554.
Zhou, J.-C., Li, N.-X., Zhang, C.-M. & Zhang, Z.-Y. (2009). *Acta Cryst.* E**65**, o1949.

# supplementary materials

*Acta Cryst.* (2011). E**67**, o1912 [ **doi:10.1107/S1600536811025591** ]

# 3-Hydroxy-*N*'-[(*E*)-3-pyridylmethylidene]-2-naphthohydrazide

**C. Li, X. Zhang, Q. Wu and H. Yin**

## Comment

Schiff bases have been extensively investigated because of their important applications in coordination chemistry, catalysis and biological processes. (Lv *et al.*, 2006; Tarafder *et al.*, 2002; Zhou *et al.*, 2009). In continuation of our research of organotin derivatives, the title compound, a novel Schiff base, was prepared and its crystal structure presented (Fig. 1). The structure of the molecule shows an *E* configuration about the C=N bond. The mean planes of the pyridine and benzene rings make the dihedral angle of 31.20 (15)°. Intramolecular O—H···O hydrogen bond was observed (Fig. 1 and Table 1). All bond lengths and angles are normal and correspond to those observed in the related componds (Huang (2009); Shafiq *et al.*, 2009; Liang *et al.*, 2008). In the crystal structure, intermolecular N—H···N hydrogen bonds link the molecules into a chain (Fig.2 and Table 1).

## Experimental

The methanol solution of 3-pyridinecarboxaldehyde(0.2 mol) was added dropwise to a solution of 3-hydroxy-2-naphtho-hydrazide(0.2 mol) in mehtanol. Then the mixture was stirred at room temperature for 6 h, during which time a brown precipitate was observed. The precipitate was filtrated off and the obtained solid was recrystallised from methanol. Anal. Calc (%) for $C_{17}H_{13}N_3O_2$ (291.30): C, 70.11; H, 4.45; N, 14.48. Found (%): C, 70.09; H, 4.50; N, 14.43.

## Refinement

All data were corrected using *SADABS* method and the final refinement was performed by mull-matrix least-square method with anisotropic parameters for non-hydrogen atoms on F2 using *SHELX97* program. The hydrogen atoms were added theoretically, riding on the concerned atoms and refined with fixed thermal factors ($U_{iso}$(H) = 1.2 $U_{eq}$(C, N); $U_{iso}$(H) = 1.5 $U_{eq}$(O)).

## Figures

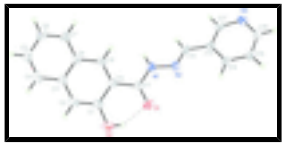


Fig. 1. The molecular structure of the title compound with 50% probability displacement ellipsoids. An O—H···O intramolecular hydrogen bond is shown as a dashed line.

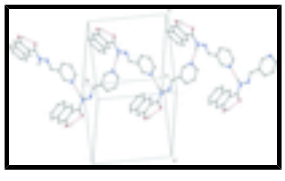


Fig. 2. View of the chain formed by N—H···N hydrogen bond.

### 3-Hydroxy-*N*'-[(*E*)-3-pyridylmethylidene]-2-naphthohydrazide

*Crystal data*

| | |
|---|---|
| $C_{17}H_{13}N_3O_2$ | $F(000) = 1216$ |
| $M_r = 291.30$ | $D_x = 1.392$ Mg m$^{-3}$ |
| Orthorhombic, *Pbca* | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 2315 reflections |
| $a = 11.0976$ (11) Å | $\theta = 2.5$–$24.7°$ |
| $b = 10.4422$ (9) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 23.9903$ (17) Å | $T = 298$ K |
| $V = 2780.1$ (4) Å$^3$ | Block, brown |
| $Z = 8$ | 0.39 × 0.38 × 0.32 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2451 independent reflections |
| Radiation source: fine-focus sealed tube | 1486 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.043$ |
| phi and ω scans | $\theta_{max} = 25.0°$, $\theta_{min} = 2.5°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -13 \rightarrow 13$ |
| $T_{min} = 0.964$, $T_{max} = 0.971$ | $k = -12 \rightarrow 12$ |
| 10663 measured reflections | $l = -16 \rightarrow 28$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.109$ | H-atom parameters constrained |
| $S = 1.07$ | $w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 1.2301P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2451 reflections | $(\Delta/\sigma)_{max} = 0.018$ |
| 200 parameters | $\Delta\rho_{max} = 0.16$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.18$ e Å$^{-3}$ |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.72696 (12) | 0.13202 (13) | 0.68223 (5) | 0.0454 (4) |
| H1 | 0.6567 | 0.1573 | 0.6719 | 0.055* |
| N2 | 0.73782 (12) | 0.03490 (13) | 0.72100 (5) | 0.0441 (4) |

| | | | | |
|---|---|---|---|---|
| N3 | 0.51884 (13) | −0.26353 (14) | 0.83141 (6) | 0.0517 (4) |
| O1 | 0.92858 (10) | 0.16623 (12) | 0.67932 (5) | 0.0587 (4) |
| O2 | 0.99947 (10) | 0.37468 (13) | 0.62980 (5) | 0.0631 (4) |
| H2 | 1.0011 | 0.3162 | 0.6526 | 0.095* |
| C1 | 0.89726 (14) | 0.36595 (16) | 0.59886 (7) | 0.0436 (5) |
| C2 | 0.88220 (15) | 0.44499 (16) | 0.55447 (7) | 0.0478 (5) |
| H2A | 0.9415 | 0.5053 | 0.5466 | 0.057* |
| C3 | 0.77958 (15) | 0.43855 (15) | 0.51990 (6) | 0.0425 (5) |
| C4 | 0.76205 (18) | 0.51752 (17) | 0.47290 (7) | 0.0559 (5) |
| H4 | 0.8195 | 0.5790 | 0.4640 | 0.067* |
| C5 | 0.66274 (19) | 0.50506 (18) | 0.44061 (7) | 0.0611 (6) |
| H5 | 0.6528 | 0.5587 | 0.4100 | 0.073* |
| C6 | 0.57495 (18) | 0.41305 (17) | 0.45245 (7) | 0.0594 (6) |
| H6 | 0.5079 | 0.4048 | 0.4295 | 0.071* |
| C7 | 0.58781 (16) | 0.33592 (16) | 0.49747 (7) | 0.0513 (5) |
| H7 | 0.5288 | 0.2754 | 0.5054 | 0.062* |
| C8 | 0.68986 (15) | 0.34632 (15) | 0.53254 (6) | 0.0409 (4) |
| C9 | 0.70638 (15) | 0.26731 (15) | 0.57943 (6) | 0.0415 (5) |
| H9 | 0.6471 | 0.2076 | 0.5881 | 0.050* |
| C10 | 0.80619 (14) | 0.27488 (15) | 0.61284 (6) | 0.0378 (4) |
| C11 | 0.82639 (15) | 0.18724 (16) | 0.66058 (6) | 0.0420 (5) |
| C12 | 0.64006 (16) | −0.00150 (16) | 0.74330 (6) | 0.0447 (5) |
| H12 | 0.5686 | 0.0406 | 0.7347 | 0.054* |
| C13 | 0.63850 (14) | −0.10870 (15) | 0.78229 (6) | 0.0388 (4) |
| C14 | 0.74226 (16) | −0.16753 (17) | 0.80160 (7) | 0.0478 (5) |
| H14 | 0.8176 | −0.1357 | 0.7918 | 0.057* |
| C16 | 0.62105 (17) | −0.31857 (17) | 0.84855 (7) | 0.0539 (5) |
| H15 | 0.6158 | −0.3916 | 0.8706 | 0.065* |
| C17 | 0.53001 (16) | −0.15897 (18) | 0.79985 (7) | 0.0486 (5) |
| H17 | 0.4599 | −0.1172 | 0.7890 | 0.058* |
| C15 | 0.73317 (16) | −0.27280 (17) | 0.83522 (7) | 0.0525 (5) |
| H18 | 0.8020 | −0.3128 | 0.8489 | 0.063* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0402 (8) | 0.0517 (8) | 0.0444 (7) | 0.0054 (7) | 0.0001 (6) | 0.0108 (7) |
| N2 | 0.0446 (8) | 0.0480 (8) | 0.0397 (7) | 0.0038 (7) | 0.0002 (7) | 0.0052 (7) |
| N3 | 0.0461 (8) | 0.0557 (9) | 0.0533 (8) | −0.0090 (8) | 0.0024 (7) | 0.0052 (8) |
| O1 | 0.0406 (7) | 0.0751 (8) | 0.0603 (7) | 0.0044 (7) | −0.0062 (6) | 0.0105 (7) |
| O2 | 0.0445 (7) | 0.0711 (8) | 0.0737 (8) | −0.0115 (7) | −0.0106 (6) | 0.0042 (7) |
| C1 | 0.0365 (9) | 0.0458 (9) | 0.0486 (10) | 0.0007 (8) | 0.0019 (8) | −0.0083 (8) |
| C2 | 0.0469 (10) | 0.0396 (9) | 0.0569 (10) | −0.0067 (9) | 0.0099 (9) | −0.0016 (9) |
| C3 | 0.0494 (10) | 0.0368 (9) | 0.0414 (9) | 0.0028 (8) | 0.0086 (8) | −0.0026 (8) |
| C4 | 0.0716 (13) | 0.0470 (10) | 0.0490 (10) | 0.0013 (10) | 0.0134 (10) | 0.0065 (9) |
| C5 | 0.0886 (14) | 0.0533 (11) | 0.0415 (10) | 0.0139 (11) | 0.0013 (10) | 0.0065 (9) |
| C6 | 0.0766 (13) | 0.0561 (11) | 0.0455 (10) | 0.0086 (11) | −0.0126 (10) | −0.0063 (9) |
| C7 | 0.0564 (11) | 0.0456 (10) | 0.0518 (10) | 0.0003 (9) | −0.0067 (9) | −0.0038 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0472 (10) | 0.0384 (9) | 0.0372 (8) | 0.0035 (8) | 0.0021 (8) | −0.0045 (8) |
| C9 | 0.0426 (10) | 0.0385 (9) | 0.0434 (9) | −0.0058 (8) | 0.0038 (8) | −0.0025 (8) |
| C10 | 0.0366 (9) | 0.0372 (9) | 0.0394 (8) | 0.0006 (8) | 0.0036 (7) | −0.0029 (7) |
| C11 | 0.0389 (9) | 0.0458 (10) | 0.0412 (9) | 0.0008 (8) | 0.0014 (8) | −0.0041 (8) |
| C12 | 0.0416 (10) | 0.0499 (10) | 0.0427 (9) | 0.0049 (9) | −0.0043 (8) | 0.0042 (8) |
| C13 | 0.0376 (9) | 0.0444 (9) | 0.0344 (8) | 0.0011 (8) | −0.0011 (7) | −0.0007 (8) |
| C14 | 0.0373 (9) | 0.0569 (11) | 0.0491 (9) | −0.0016 (9) | 0.0003 (8) | 0.0072 (9) |
| C16 | 0.0593 (12) | 0.0473 (10) | 0.0552 (11) | −0.0049 (10) | −0.0015 (9) | 0.0075 (9) |
| C17 | 0.0395 (10) | 0.0602 (11) | 0.0462 (9) | 0.0004 (9) | −0.0042 (8) | −0.0008 (9) |
| C15 | 0.0427 (10) | 0.0543 (11) | 0.0606 (11) | 0.0043 (9) | −0.0052 (9) | 0.0130 (9) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C11 | 1.349 (2) | C6—C7 | 1.355 (2) |
| N1—N2 | 1.3814 (17) | C6—H6 | 0.9300 |
| N1—H1 | 0.8600 | C7—C8 | 1.415 (2) |
| N2—C12 | 1.268 (2) | C7—H7 | 0.9300 |
| N3—C17 | 1.334 (2) | C8—C9 | 1.407 (2) |
| N3—C16 | 1.336 (2) | C9—C10 | 1.370 (2) |
| O1—C11 | 1.2395 (19) | C9—H9 | 0.9300 |
| O2—C1 | 1.3586 (19) | C10—C11 | 1.483 (2) |
| O2—H2 | 0.8200 | C12—C13 | 1.459 (2) |
| C1—C2 | 1.358 (2) | C12—H12 | 0.9300 |
| C1—C10 | 1.428 (2) | C13—C17 | 1.379 (2) |
| C2—C3 | 1.411 (2) | C13—C14 | 1.385 (2) |
| C2—H2A | 0.9300 | C14—C15 | 1.367 (2) |
| C3—C4 | 1.410 (2) | C14—H14 | 0.9300 |
| C3—C8 | 1.418 (2) | C16—C15 | 1.371 (2) |
| C4—C5 | 1.353 (3) | C16—H15 | 0.9300 |
| C4—H4 | 0.9300 | C17—H17 | 0.9300 |
| C5—C6 | 1.397 (3) | C15—H18 | 0.9300 |
| C5—H5 | 0.9300 | | |
| C11—N1—N2 | 120.11 (13) | C7—C8—C3 | 119.14 (15) |
| C11—N1—H1 | 119.9 | C10—C9—C8 | 122.64 (15) |
| N2—N1—H1 | 119.9 | C10—C9—H9 | 118.7 |
| C12—N2—N1 | 115.43 (14) | C8—C9—H9 | 118.7 |
| C17—N3—C16 | 116.59 (15) | C9—C10—C1 | 118.26 (14) |
| C1—O2—H2 | 109.5 | C9—C10—C11 | 122.59 (14) |
| C2—C1—O2 | 119.38 (15) | C1—C10—C11 | 119.04 (14) |
| C2—C1—C10 | 120.14 (15) | O1—C11—N1 | 122.22 (15) |
| O2—C1—C10 | 120.48 (15) | O1—C11—C10 | 121.84 (15) |
| C1—C2—C3 | 122.12 (15) | N1—C11—C10 | 115.94 (14) |
| C1—C2—H2A | 118.9 | N2—C12—C13 | 120.71 (15) |
| C3—C2—H2A | 118.9 | N2—C12—H12 | 119.6 |
| C4—C3—C2 | 123.62 (16) | C13—C12—H12 | 119.6 |
| C4—C3—C8 | 118.11 (15) | C17—C13—C14 | 117.05 (15) |
| C2—C3—C8 | 118.26 (14) | C17—C13—C12 | 119.88 (15) |
| C5—C4—C3 | 120.91 (17) | C14—C13—C12 | 123.02 (15) |
| C5—C4—H4 | 119.5 | C15—C14—C13 | 119.52 (16) |

| | | | |
|---|---|---|---|
| C3—C4—H4 | 119.5 | C15—C14—H14 | 120.2 |
| C4—C5—C6 | 121.16 (17) | C13—C14—H14 | 120.2 |
| C4—C5—H5 | 119.4 | N3—C16—C15 | 123.29 (17) |
| C6—C5—H5 | 119.4 | N3—C16—H15 | 118.4 |
| C7—C6—C5 | 119.82 (18) | C15—C16—H15 | 118.4 |
| C7—C6—H6 | 120.1 | N3—C17—C13 | 124.45 (16) |
| C5—C6—H6 | 120.1 | N3—C17—H17 | 117.8 |
| C6—C7—C8 | 120.84 (17) | C13—C17—H17 | 117.8 |
| C6—C7—H7 | 119.6 | C14—C15—C16 | 119.00 (17) |
| C8—C7—H7 | 119.6 | C14—C15—H18 | 120.5 |
| C9—C8—C7 | 122.31 (15) | C16—C15—H18 | 120.5 |
| C9—C8—C3 | 118.54 (15) | | |
| C11—N1—N2—C12 | 172.76 (15) | O2—C1—C10—C9 | −178.18 (15) |
| O2—C1—C2—C3 | 178.39 (15) | C2—C1—C10—C11 | 178.32 (15) |
| C10—C1—C2—C3 | −1.8 (2) | O2—C1—C10—C11 | −1.9 (2) |
| C1—C2—C3—C4 | −178.81 (16) | N2—N1—C11—O1 | −9.7 (2) |
| C1—C2—C3—C8 | 0.2 (2) | N2—N1—C11—C10 | 170.29 (13) |
| C2—C3—C4—C5 | 178.62 (17) | C9—C10—C11—O1 | 156.80 (16) |
| C8—C3—C4—C5 | −0.4 (2) | C1—C10—C11—O1 | −19.4 (2) |
| C3—C4—C5—C6 | −0.5 (3) | C9—C10—C11—N1 | −23.2 (2) |
| C4—C5—C6—C7 | 1.1 (3) | C1—C10—C11—N1 | 160.67 (14) |
| C5—C6—C7—C8 | −0.6 (3) | N1—N2—C12—C13 | 176.15 (13) |
| C6—C7—C8—C9 | −179.64 (16) | N2—C12—C13—C17 | −170.56 (16) |
| C6—C7—C8—C3 | −0.3 (2) | N2—C12—C13—C14 | 6.9 (2) |
| C4—C3—C8—C9 | −179.83 (15) | C17—C13—C14—C15 | 1.8 (2) |
| C2—C3—C8—C9 | 1.1 (2) | C12—C13—C14—C15 | −175.73 (15) |
| C4—C3—C8—C7 | 0.8 (2) | C17—N3—C16—C15 | 0.0 (3) |
| C2—C3—C8—C7 | −178.27 (15) | C16—N3—C17—C13 | 2.9 (2) |
| C7—C8—C9—C10 | 178.50 (16) | C14—C13—C17—N3 | −3.8 (2) |
| C3—C8—C9—C10 | −0.9 (2) | C12—C13—C17—N3 | 173.85 (15) |
| C8—C9—C10—C1 | −0.7 (2) | C13—C14—C15—C16 | 0.7 (3) |
| C8—C9—C10—C11 | −176.86 (15) | N3—C16—C15—C14 | −1.7 (3) |
| C2—C1—C10—C9 | 2.0 (2) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···O1 | 0.82 | 1.87 | 2.6015 (18) | 147 |
| N1—H1···N3$^{i}$ | 0.86 | 2.12 | 2.956 (2) | 165 |

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

**Fig. 1**

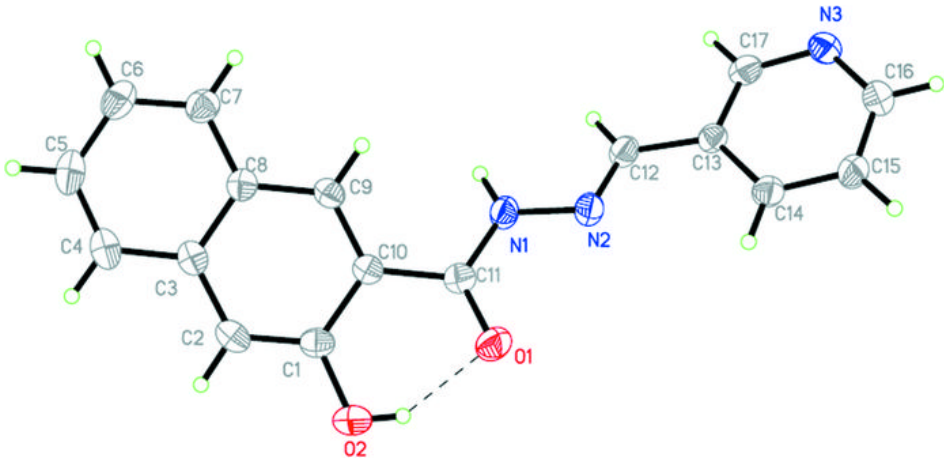

N3
C17
C16
C6
C7
C5
C8
C9
C12
C13
C15
C4
C10
N1
N2
C14
C3
C11
C2
C1
O1
O2

**Fig. 2**