Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

1-{2-[(2-Hydroxy-1-naphthyl)methyleneamino]phenyliminiomethyl}-2-naphtholate methanol hemisolvate

Naser Eltaher Eltayeb,[a]‡ Siang Guan Teoh,[a] Jeannie Bee-Jan Teh,[b] Hoong-Kun Fun[b]* and Kamarulazizi Ibrahim[c]

[a]School of Chemical Sciences, Universiti Sains Malaysia, Minden, Penang, Malaysia, [b]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [c]School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

‡ On study leave from International University of Africa, Sudan; e-mail: nasertaha90@hotmail.com

Correspondence e-mail: hkfun@usm.my

Received 15 November 2006
Accepted 24 November 2006

Key indicators

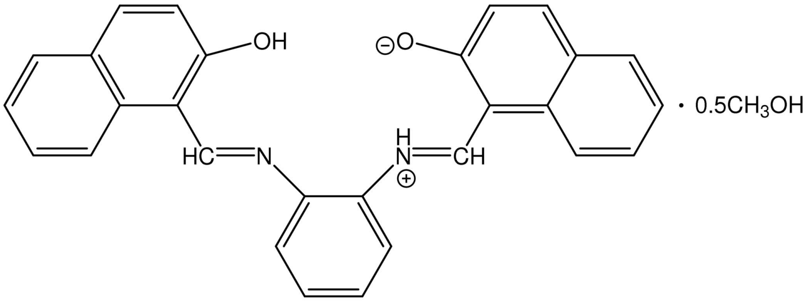
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.108
Data-to-parameter ratio = 10.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{28}H_{40}N_2O_2 \cdot 0.5CH_3OH$, crystallizes with two molecules of 1-{2-[(2-hydroxy-1-naphthyl)methyleneamino]phenyliminiomethyl}-2-naphtholate and one methanol solvent molecule in the asymmetric unit. All bond lengths and angles are normal. The crystal structure is stabilized by π–π, O—H···O and C—H···π interactions.

Comment

Considerable interest has been paid to Schiff base compounds in the past decades, owing to their easy preparation and modification of the steric and electronic properties using different substituents. In addition, some of these compounds exhibit various pharmacological activities, *viz*. anticancer (Dao *et al.*, 2000), anti-HIV (Sriram *et al.*, 2006), antibacterial and antifungal (Karthikeyan *et al.*, 2006). In addition, some of them may be used as analytical reagents for the determination of trace elements (Eltayeb & Ahmed, 2005*a*,*b*). In this paper, we report the crystal structure of the title compound, obtained by the reaction of *o*-phenylenediamine and 2-hydroxy-1-naphthaldehyde, which crystallized as the methanol solvate, (I). The molecule of 1-{2-[(2-hydroxy-1-naphthyl)methyleneamino]phenyliminiomethyl}-2-naphtholate, (II), in the title compound, (I), exists in the zwitterionic form, in which one of the two imine N atoms is protonated to counter-balance the proximal phenolate anion. Popovic *et al.* (2001) have previously reported the crystal structure of another solvate of (II).



(I)

The title compound crystallizes with two molecules of (II) (*A* and *B*) and one methanol solvent molecule in the asymmetric unit (Fig. 1). All bond lengths and angles in (I) have normal values (Allen *et al.*, 1987). In molecule *A*, the dihedral angles C12*A*–C17*A*^C1*A*–C10*A*, C12*A*–C17*A*^C19*A*–C28*A* and C1*A*–C10*A*^C19*A*–C28*A* are 56.39 (9), 5.84 (9) and

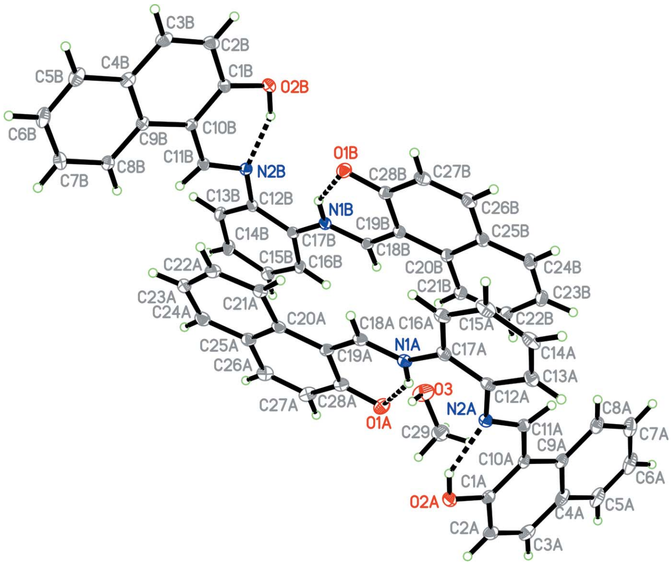


Figure 1
The asymmetric unit of the title compound, showing the atomic numbering and 30% probability displacement ellipsoids. Hydrogen bonds are shown as dashed lines.

54.47 (7)°, respectively. In molecule *B*, the dihedral angles C12*B*–C17*B*^C1*B*–C10*B*, C12*B*–C17*B*^C19*B*–C28*B* and C1*B*–C10*B*^C19*B*–C28*B* are 54.26 (9), 3.71 (9) and 50.74 (6)°, respectively. Intramolecular N—H···O and O—H···N hydrogen bonds (Table 2) generate *S*(6) ring motifs (Bernstein *et al.*, 1995) in the molecules of (II).

The crystal structure is stabilized by intermolecular *π*–*π*, C—H···*π* and O—H···O interactions (Tables 1 and 2).

Experimental

To a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol (30 ml) was added 2-hydroxy-1-naphthaldehyde (0.688 g, 4 mmol). The mixture was refluxed with stirring for 30 min. An orange precipitate was then obtained. Red crystals suitable for X-ray diffraction analysis formed after several weeks on slow evaporation of a ethanol–methanol–dichloromethane (4:1:4) solution at room temperature (m.p. 495–496 K).

Crystal data

$C_{28}H_{20}N_2O_2\cdot0.5CH_4O$
$M_r = 432.48$
Orthorhombic, $Pna2_1$
$a = 19.3610\ (3)$ Å
$b = 12.5103\ (2)$ Å
$c = 17.7128\ (2)$ Å
$V = 4290.25\ (11)$ Å^3
$Z = 8$
$D_x = 1.339$ Mg m^{-3}
Mo *Kα* radiation
$\mu = 0.09$ mm^{-1}
$T = 100.0\ (1)$ K
Block, red
0.31 × 0.30 × 0.18 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min} = 0.962$, $T_{\max} = 0.985$
52989 measured reflections
6547 independent reflections
5671 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.041$
$\theta_{\max} = 30.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.108$
$S = 1.03$
6547 reflections
616 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.8098P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.34$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

Table 1
π–*π*Interactions (Å).

*Cg*1, *Cg*2, *Cg*3, *Cg*4, *Cg*5 and *Cg*6 are the centroids of rings C1*A*–C4*A*/C9*A*–C10*A*, C19*B*–C20*B*/C25*B*–C28*B*, C1*B*–C4*B*/C9*B*–C10*B*, C19*A*–C20*A*/C25*A*–C28*A*, C12*A*–C17*A* and C20*B*–C25*B*, respectively.

*Cg*1···*Cg*2$^{\rm i}$	3.569 (1)	*Cg*5···*Cg*6	3.637 (1)
*Cg*3···*Cg*4$^{\rm ii}$	3.562 (1)		

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

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*7 are the centroids of rings C1*A*–C4*A*/C9*A*–C10*A* and C4*B*–C9*B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3*A*—H3*AA*···*Cg*7$^{\rm iii}$	0.93	2.67	3.575 (3)	163
C29—H29*C*···*Cg*1	0.96	2.78	3.668 (3)	154
N1*A*—H1*NA*···O1*A*	0.88 (4)	1.78 (4)	2.542 (2)	143 (3)
N1*B*—H1*NB*···O1*B*	0.91 (3)	1.78 (3)	2.560 (2)	143 (2)
O2*A*—H2*OA*···N2*A*	0.86 (3)	1.84 (4)	2.588 (2)	145 (3)
O2*B*—H2*OB*···N2*B*	0.95 (4)	1.72 (4)	2.600 (2)	153 (3)
O3—H*O*3···O1*A*	0.94 (5)	1.84 (5)	2.763 (3)	168 (3)

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

N- and O-bound H atoms were located in difference maps and refined isotropically. The remaining H atoms were positioned geometrically and treated as riding, with C—H = 0.93–0.96 Å and the $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}$(methyl C). In the absence of significant anomalous scattering effects, 6149 Friedel pairs were merged.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government, Academy of Sciences Malaysia and Universiti Sains Malaysia for the research grant and facilities. International University of Africa (Sudan) is acknowledged for providing study leave to NEE.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12A) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Dao, V.-T., Gaspard, C., Mayer, M., Werner, G. H., Nguyen, S. N. & Michelot, R. J. (2000). *Eur. J. Med. Chem.* **35**, 805–813.
Eltayeb, N. E. & Ahmed, T. A. (2005*a*). *J. Sci. Tech.* **6**, 51–59.

o118 Eltayeb *et al.* • $C_{28}H_{20}N_2O_2\cdot0.5CH_4O$ *Acta Cryst.* (2007). E**63**, o117–o119

Eltayeb, N. E. & Ahmed, T. A. (2005*b*). *Sudan J. Basic Sci.* **7**, 97–108.

Karthikeyan, M. S., Prasad, D. J., Poojary, B., Bhat, K. S., Holla, B. S. & Kumari, N. S. (2006). *Bioorg. Med. Chem.* **14**, 7482–7489.

Popovic, Z., Roje, V., Pavlovic, G., Matkovic-Calogovic, D. & Giester, G. (2001). *J. Mol. Struct.* **597**, 39–47.

Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Sriram, D., Yogeeswari, P., Myneedu, N. S. & Saraswat, V. (2006). *Bioorg. Med. Chem. Lett.* **16**, 2127–2129.

Acta Cryst. (2007). E**63**, o117–o119 Eltayeb *et al.* • $C_{28}H_{20}N_2O_2\cdot0.5CH_4O$ **o119**