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1-[(Z)-(5-Methyl-2-pyridyl)iminio-methyl]-2-naphtholate

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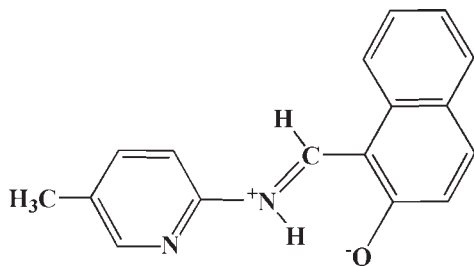
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.038; wR factor = 0.109; data-to-parameter ratio = 9.1.

In the zwitterionic title compound, $\text{C}_{17}\text{H}_{14}\text{N}_2\text{O}$, the dihedral angle between the naphthalene and pyridine ring systems is 3.56 (9°) and an intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond generates an $S(6)$ ring. In the crystal, molecules are linked by $\text{C}-\text{H}\cdots\text{O}$ interactions.

Related literature

For a related structure, see: Eltayeb *et al.* (2007).

Experimental

Crystal data

$\text{C}_{17}\text{H}_{14}\text{N}_2\text{O}$
 $M_r = 262.30$
 Monoclinic, $P2_1$

$a = 4.8703$ (2) Å
 $b = 9.5525$ (5) Å
 $c = 14.0804$ (6) Å

$\beta = 98.353$ (2) $^\circ$
 $V = 648.12$ (5) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 0.09$ mm⁻¹
 $T = 296$ K
 $0.47 \times 0.10 \times 0.09$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.961$, $T_{\max} = 0.992$

6930 measured reflections
 1660 independent reflections
 1321 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.109$
 $S = 0.98$
 1660 reflections
 182 parameters

1 restraint
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.15$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{O1}$	0.86	1.89	2.571 (3)	135
$\text{C3}-\text{H3}\cdots\text{O1}^1$	0.93	2.46	3.346 (3)	159

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

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); 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: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5298).

References

- Bruker (2005). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
 Eltayeb, N. E., Teoh, S. G., Teh, J. B.-J., Fun, H.-K. & Ibrahim, K. (2007). *Acta Cryst.* E63, o117–o119.
 Sheldrick, G. M. (2008). *Acta Cryst.* A64, 112–122.

supplementary materials

Acta Cryst. (2010). E66, o309 [doi:10.1107/S1600536810000346]

1-[(Z)-(5-Methyl-2-pyridyl)imino]methyl]-2-naphtholate

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Comment

One similar compound as 1-{2-[(2-hydroxy-1-naphthyl)methyleneamino] phenylimino]methyl}-2-naphtholate methanol hemisolvate has been synthesized and characterized by X-ray diffraction (Eltayeb *et al.*, 2007). We now report on the title compound, (I), whose structure was determined by X-ray diffraction (Fig. 1).

This compound, which has a non-planar molecular structure, contains two aromatic rings linked through a imine group. The dihedral angle between the two aromatic rings C2—C3—C4—C5—N1—C6 and C8—C9—C14—C15—C16—C17 is 3.46(0.16)°. Intramolecular N—H···O hydrogen bonds are observed in the molecular structure, similar to those reported structure (Eltayeb *et al.*, 2007). The molecules is formed a one-dimensional zigzag chain through intermolecular C—H···O hydrogen bonds, which make the molecule more stabile.

As seen in Fig. 2, the molecules are linked into a one-dimensional chain by intermolecular C—H···O hydrogen bonds (Table 2).

Experimental

2-Hydroxy-1-naphthaldehyde (1 mmol, 172.2 mg) were added with stirring to anhydrous ethanol (30 ml) to make a solution. It was slowly dropped into the anhydrous ethanol solution (15 ml) containing (1 mmol, 108.1 mg) 5-methylpyridin-2-amine at 339 K and mixture was stirred at 339 K for 4 h, a mass of deep yellow grain was separated out. The product was collected by filtration and washed several times with anhydrous ethanol and dried under vacuum. Yellow needles of (I) were obtained by slow evaporation at room temperature from anhydrous ethanol solution after 4 days.

Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement. All H-atoms were positioned geometrically (C—H = 0.93–0.96 Å, N—H = 0.86 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

Figures

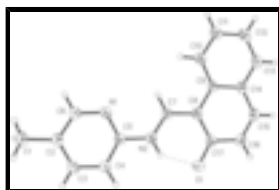


Fig. 1. The structure of (I) showing 30% probability displacement ellipsoids.

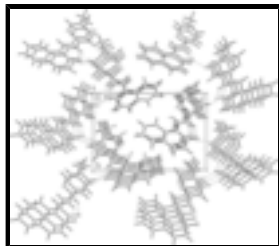


Fig. 2. The crystal packing of (I), viewed approximately along the *a* axis.

1-[(Z)-(5-Methyl-2-pyridyl)iminiomethyl]-2-naphtholate

Crystal data

$C_{17}H_{14}N_2O$

$M_r = 262.30$

Monoclinic, $P2_1$

Hall symbol: P 2yb

$a = 4.8703$ (2) Å

$b = 9.5525$ (5) Å

$c = 14.0804$ (6) Å

$\beta = 98.353$ (2)°

$V = 648.12$ (5) Å³

$Z = 2$

$F(000) = 276$

$D_x = 1.344$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1877 reflections

$\theta = 2.6$ – 25.6 °

$\mu = 0.09$ mm⁻¹

$T = 296$ K

Needle, yellow

$0.47 \times 0.10 \times 0.09$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2005)

$T_{\min} = 0.961$, $T_{\max} = 0.992$

6930 measured reflections

1660 independent reflections

1321 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 28.1$ °, $\theta_{\min} = 2.6$ °

$h = -6 \rightarrow 6$

$k = -12 \rightarrow 11$

$l = -18 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.109$

$S = 0.98$

1660 reflections

182 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.0757P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.18$ e Å⁻³

1 restraint

$$\Delta\rho_{\min} = -0.15 \text{ e } \text{\AA}^{-3}$$

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	-0.5458 (5)	-0.0508 (3)	0.8827 (2)	0.0561 (6)
H1A	-0.6558	-0.0735	0.8224	0.084*
H1B	-0.6646	-0.0178	0.9266	0.084*
H1C	-0.4484	-0.1328	0.9086	0.084*
C2	-0.3401 (5)	0.0616 (2)	0.86752 (16)	0.0431 (5)
C3	-0.2411 (5)	0.1558 (3)	0.93834 (17)	0.0518 (6)
H3	-0.3011	0.1508	0.9980	0.062*
C4	-0.0533 (5)	0.2576 (3)	0.92116 (16)	0.0492 (6)
H4	0.0127	0.3223	0.9683	0.059*
C5	0.0341 (4)	0.2610 (2)	0.83229 (15)	0.0382 (5)
C6	-0.2414 (5)	0.0762 (3)	0.78108 (16)	0.0478 (6)
H6	-0.3082	0.0143	0.7322	0.057*
C7	0.3255 (4)	0.3752 (2)	0.73144 (15)	0.0398 (5)
H7	0.2584	0.3151	0.6815	0.048*
C8	0.5254 (4)	0.4749 (2)	0.71574 (15)	0.0383 (5)
C9	0.6227 (4)	0.4846 (2)	0.62325 (15)	0.0371 (5)
C10	0.5226 (5)	0.3996 (3)	0.54463 (16)	0.0468 (6)
H10	0.3905	0.3315	0.5518	0.056*
C11	0.6141 (5)	0.4140 (3)	0.45734 (16)	0.0501 (6)
H11	0.5423	0.3566	0.4064	0.060*
C12	0.8133 (5)	0.5138 (3)	0.44477 (17)	0.0525 (6)
H12	0.8743	0.5238	0.3855	0.063*
C13	0.9182 (5)	0.5968 (3)	0.51987 (18)	0.0510 (6)
H13	1.0539	0.6623	0.5116	0.061*
C14	0.8257 (4)	0.5857 (2)	0.60997 (16)	0.0413 (5)
C15	0.9323 (5)	0.6740 (3)	0.68904 (18)	0.0499 (6)
H15	1.0677	0.7395	0.6804	0.060*
C16	0.8457 (5)	0.6663 (3)	0.77458 (18)	0.0484 (6)
H16	0.9224	0.7259	0.8236	0.058*
C17	0.6352 (5)	0.5673 (2)	0.79247 (16)	0.0430 (5)
N1	-0.0571 (4)	0.1724 (2)	0.76194 (13)	0.0462 (5)

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N2	0.2284 (4)	0.3625 (2)	0.81358 (13)	0.0424 (4)
H2	0.2877	0.4203	0.8588	0.051*
O1	0.5562 (4)	0.5643 (2)	0.87507 (11)	0.0567 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0517 (14)	0.0467 (15)	0.0725 (16)	-0.0048 (12)	0.0176 (12)	0.0080 (13)
C2	0.0391 (10)	0.0397 (12)	0.0520 (12)	0.0037 (10)	0.0115 (9)	0.0067 (11)
C3	0.0604 (14)	0.0536 (15)	0.0459 (12)	-0.0031 (13)	0.0230 (11)	0.0044 (12)
C4	0.0581 (14)	0.0484 (14)	0.0438 (12)	-0.0078 (12)	0.0163 (10)	-0.0060 (11)
C5	0.0403 (10)	0.0341 (11)	0.0416 (11)	0.0036 (9)	0.0108 (8)	0.0026 (9)
C6	0.0525 (13)	0.0435 (13)	0.0478 (12)	-0.0049 (11)	0.0081 (10)	-0.0027 (11)
C7	0.0436 (11)	0.0356 (11)	0.0418 (11)	0.0025 (9)	0.0116 (8)	0.0036 (9)
C8	0.0411 (10)	0.0322 (11)	0.0429 (11)	0.0033 (9)	0.0106 (8)	0.0024 (9)
C9	0.0370 (10)	0.0337 (11)	0.0421 (10)	0.0038 (9)	0.0103 (8)	0.0058 (9)
C10	0.0496 (13)	0.0447 (14)	0.0481 (12)	-0.0016 (11)	0.0136 (10)	0.0000 (11)
C11	0.0555 (14)	0.0529 (15)	0.0437 (12)	0.0054 (12)	0.0135 (10)	-0.0005 (11)
C12	0.0590 (14)	0.0553 (15)	0.0475 (13)	0.0092 (12)	0.0225 (10)	0.0091 (11)
C13	0.0504 (13)	0.0447 (14)	0.0615 (15)	0.0012 (11)	0.0203 (11)	0.0108 (12)
C14	0.0404 (11)	0.0356 (12)	0.0493 (12)	0.0033 (10)	0.0113 (9)	0.0055 (10)
C15	0.0486 (12)	0.0385 (13)	0.0645 (14)	-0.0057 (11)	0.0145 (10)	0.0025 (12)
C16	0.0508 (13)	0.0365 (12)	0.0582 (14)	-0.0035 (11)	0.0086 (10)	-0.0055 (11)
C17	0.0492 (12)	0.0356 (12)	0.0460 (12)	0.0033 (10)	0.0125 (9)	0.0016 (10)
N1	0.0536 (11)	0.0441 (11)	0.0430 (10)	-0.0029 (10)	0.0146 (8)	-0.0014 (9)
N2	0.0497 (11)	0.0370 (10)	0.0425 (9)	-0.0017 (9)	0.0134 (8)	-0.0010 (8)
O1	0.0721 (11)	0.0548 (11)	0.0463 (9)	-0.0073 (10)	0.0187 (8)	-0.0083 (8)

Geometric parameters (\AA , $^\circ$)

C1—C2	1.504 (3)	C8—C9	1.452 (3)
C1—H1A	0.9600	C9—C10	1.402 (3)
C1—H1B	0.9600	C9—C14	1.413 (3)
C1—H1C	0.9600	C10—C11	1.374 (3)
C2—C3	1.377 (4)	C10—H10	0.9300
C2—C6	1.379 (3)	C11—C12	1.390 (4)
C3—C4	1.380 (4)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.360 (4)
C4—C5	1.379 (3)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.410 (3)
C5—N1	1.329 (3)	C13—H13	0.9300
C5—N2	1.407 (3)	C14—C15	1.433 (3)
C6—N1	1.339 (3)	C15—C16	1.335 (3)
C6—H6	0.9300	C15—H15	0.9300
C7—N2	1.317 (3)	C16—C17	1.444 (3)
C7—C8	1.402 (3)	C16—H16	0.9300
C7—H7	0.9300	C17—O1	1.277 (3)
C8—C17	1.436 (3)	N2—H2	0.8600

C2—C1—H1A	109.5	C14—C9—C8	119.20 (19)
C2—C1—H1B	109.5	C11—C10—C9	121.8 (2)
H1A—C1—H1B	109.5	C11—C10—H10	119.1
C2—C1—H1C	109.5	C9—C10—H10	119.1
H1A—C1—H1C	109.5	C10—C11—C12	120.4 (2)
H1B—C1—H1C	109.5	C10—C11—H11	119.8
C3—C2—C6	116.3 (2)	C12—C11—H11	119.8
C3—C2—C1	122.3 (2)	C13—C12—C11	119.4 (2)
C6—C2—C1	121.5 (2)	C13—C12—H12	120.3
C2—C3—C4	120.3 (2)	C11—C12—H12	120.3
C2—C3—H3	119.8	C12—C13—C14	121.5 (2)
C4—C3—H3	119.8	C12—C13—H13	119.3
C5—C4—C3	118.4 (2)	C14—C13—H13	119.3
C5—C4—H4	120.8	C13—C14—C9	119.4 (2)
C3—C4—H4	120.8	C13—C14—C15	121.8 (2)
N1—C5—C4	123.2 (2)	C9—C14—C15	118.72 (19)
N1—C5—N2	117.42 (18)	C16—C15—C14	122.9 (2)
C4—C5—N2	119.4 (2)	C16—C15—H15	118.6
N1—C6—C2	125.2 (2)	C14—C15—H15	118.6
N1—C6—H6	117.4	C15—C16—C17	121.3 (2)
C2—C6—H6	117.4	C15—C16—H16	119.4
N2—C7—C8	123.2 (2)	C17—C16—H16	119.4
N2—C7—H7	118.4	O1—C17—C8	122.9 (2)
C8—C7—H7	118.4	O1—C17—C16	119.3 (2)
C7—C8—C17	119.32 (18)	C8—C17—C16	117.86 (19)
C7—C8—C9	120.61 (19)	C5—N1—C6	116.61 (19)
C17—C8—C9	120.07 (19)	C7—N2—C5	124.41 (19)
C10—C9—C14	117.45 (19)	C7—N2—H2	117.8
C10—C9—C8	123.34 (19)	C5—N2—H2	117.8
C6—C2—C3—C4	-0.1 (4)	C10—C9—C14—C13	0.0 (3)
C1—C2—C3—C4	-179.7 (2)	C8—C9—C14—C13	-179.1 (2)
C2—C3—C4—C5	-0.8 (4)	C10—C9—C14—C15	-179.9 (2)
C3—C4—C5—N1	1.1 (4)	C8—C9—C14—C15	1.0 (3)
C3—C4—C5—N2	-179.1 (2)	C13—C14—C15—C16	179.2 (2)
C3—C2—C6—N1	0.9 (4)	C9—C14—C15—C16	-0.9 (4)
C1—C2—C6—N1	-179.5 (2)	C14—C15—C16—C17	-0.3 (4)
N2—C7—C8—C17	1.0 (3)	C7—C8—C17—O1	-1.0 (3)
N2—C7—C8—C9	-179.45 (19)	C9—C8—C17—O1	179.5 (2)
C7—C8—C9—C10	1.4 (3)	C7—C8—C17—C16	178.5 (2)
C17—C8—C9—C10	-179.1 (2)	C9—C8—C17—C16	-1.1 (3)
C7—C8—C9—C14	-179.55 (19)	C15—C16—C17—O1	-179.3 (2)
C17—C8—C9—C14	0.0 (3)	C15—C16—C17—C8	1.2 (3)
C14—C9—C10—C11	-0.8 (3)	C4—C5—N1—C6	-0.3 (3)
C8—C9—C10—C11	178.3 (2)	N2—C5—N1—C6	179.8 (2)
C9—C10—C11—C12	0.6 (4)	C2—C6—N1—C5	-0.7 (3)
C10—C11—C12—C13	0.4 (4)	C8—C7—N2—C5	-178.1 (2)
C11—C12—C13—C14	-1.2 (4)	N1—C5—N2—C7	-0.1 (3)
C12—C13—C14—C9	1.0 (3)	C4—C5—N2—C7	-180.0 (2)
C12—C13—C14—C15	-179.1 (2)		

supplementary materials

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>
N2—H2···O1	0.86	1.89	2.571 (3)	135
C3—H3···O1 ⁱ	0.93	2.46	3.346 (3)	159

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

Fig. 1

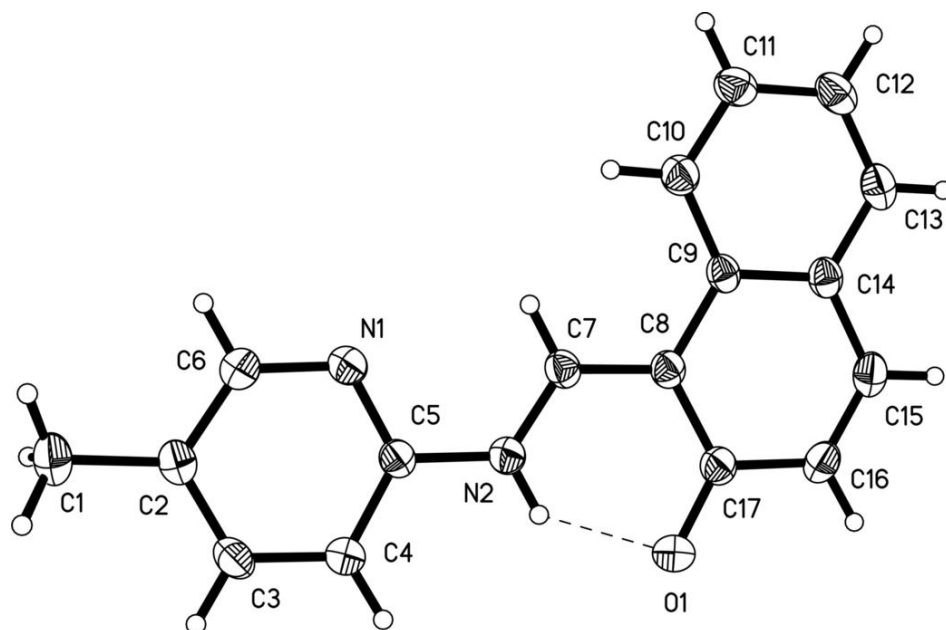


Fig. 2

