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N,*N*′-Bis(4-pyridylmethylene)naphthalene-1,5-diamine

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.108
Data-to-parameter ratio = 11.8

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

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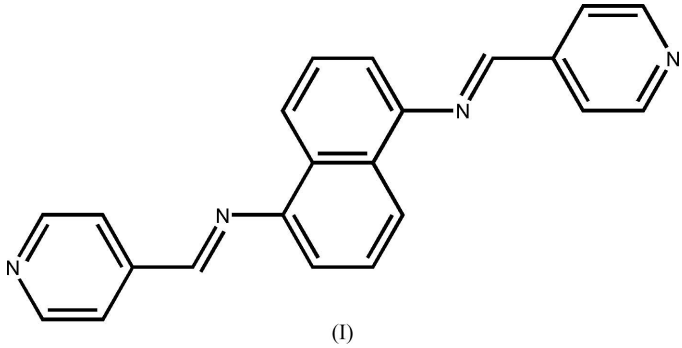
In the title compound, $C_{22}H_{16}N_4$, there are two crystallographically independent molecules, both of which are centrosymmetric and adopt a non-planar conformation.

Comment

Rigid bipyridyl-type bidentate Schiff base ligands have been utilized intensively to assemble various coordination polymers with diverse structures and interesting topology (Barnett & Champness, 2003). We have previously reported two interesting ladder structures assembled from the title compound with different metal ions (Su *et al.*, 2004); one has a non-interpenetrated one-dimensional ladder structure hosting solvent molecules, while the other has a rare fourfold interlocked three-dimensional structure of one-dimensional ladders. We report here the crystal structure of the title ligand, (I).



(I)

In the crystal structure, there are two crystallographically independent molecules. Both of them are centrosymmetric with an inversion center located at the center of the naphthalene ring system, as shown in Figs. 1 and 2. In both cases,

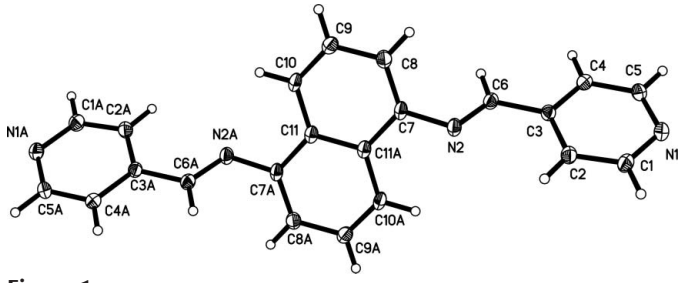


Figure 1
View of one independent molecule of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size. Atoms labeled with the suffix A are generated by the symmetry operation $(1 - x, -y, 2 - z)$.

the pyridyl and naphthalene rings are not coplanar; the dihedral angles between the planes of the rings are 53.97 (5) and 57.69 (7)°. Such a non-planar conformation of a rigid conjugated Schiff base compound has been observed in a related system (Wang *et al.*, 2005). The crystal packing indicates that these two molecules exhibit alternate layer stacking, as shown in Fig. 3.

Experimental

The title compound was prepared from the condensation reaction between pyridine-4-carboxaldehyde (100 mmol) and 1,5-naphthalenediamine (50 mmol) in tetrahydrofuran; yield 86%. Single crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution at room temperature.

Crystal data

$C_{22}H_{16}N_4$
M_r = 336.39
Triclinic, $P\overline{1}$
a = 7.6684 (7) Å
b = 10.2831 (9) Å
c = 11.6172 (10) Å
α = 102.895 (2)°
β = 102.286 (2)°
γ = 102.822 (2)°
V = 836.89 (13) Å^3
Z = 2
D_x = 1.335 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2932 reflections
θ = 2.8–25.0°
μ = 0.08 mm^{-1}
T = 150 (2) K
Block, green–brown
0.22 × 0.18 × 0.12 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.972, T_{max} = 0.990
6742 measured reflections
2957 independent reflections
2357 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.0°
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 1.01
2957 reflections
251 parameters
Only H-atom displacement parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.1827P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

H atoms were idealized and included as riding atoms with refined isotropic displacement parameters (C—H = 0.95 Å).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

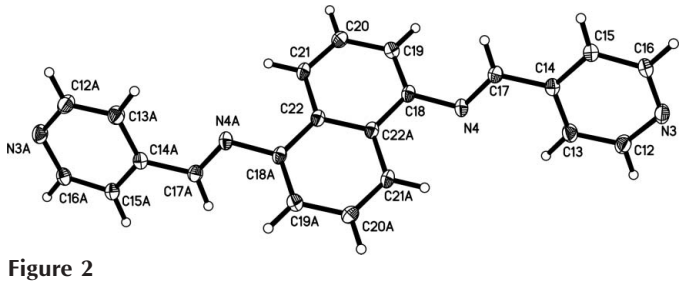


Figure 2
View of the other independent molecule of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size. Atoms labeled with the suffix A are generated by the symmetry operation $(-x, 1-y, 1-z)$.

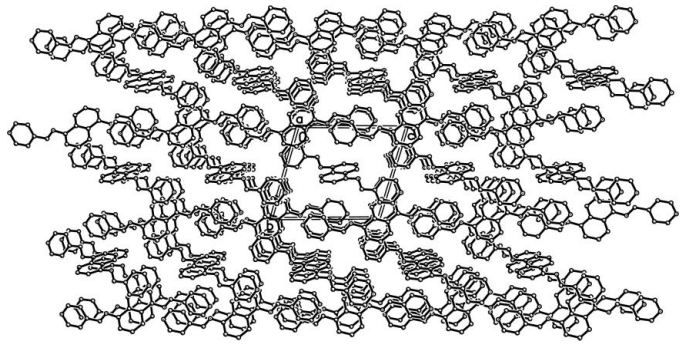


Figure 3
The molecular packing, viewed along the *a* axis. H atoms have been omitted for clarity.

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