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

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.139
Data-to-parameter ratio = 16.5

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

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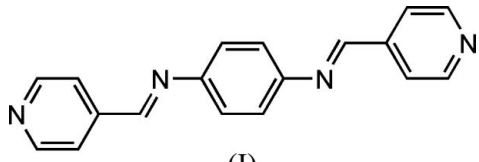
In the crystal structure of the title compound, $C_{18}H_{14}N_4$, there are two independent centrosymmetric molecules with different conformations. The two molecules are linked to each other *via* weak C—H···N hydrogen bonds and C—H···π interactions.

Comment

The title compound, (I), was synthesized by Grasso *et al.* (1981) and has been used as a bridging ligand to construct supramolecular systems (Moriuchi *et al.*, 2000; Diskin-Posner *et al.*, 2001). We present here its crystal structure.



(I)

The molecular structure of (I) is shown in Fig. 1. In the unit cell, there are two independent centrosymmetric molecules with different conformations. For the molecules containing atoms N1 and N3, the dihedral angles between the pyridine and benzene rings are 58.23 (14) and 53.29 (8)°, respectively.

The two molecules of (I) are linked to each other *via* weak C—H···N hydrogen bonds (Table 1). A C—H···π interaction is observed between molecules, with H3···Cg^{iv} = 2.65 Å and C—H···Cg^{iv} = 159° [symmetry code: (iv) *x*, *y*, −1 + *z*], where *Cg* is the centroid of the benzene ring containing atom C16.

Experimental

The title compound was prepared according to the procedure reported by Grasso *et al.* (1981). Single crystals of (I) were obtained by slow diffusion of petroleum ether into an ethanol solution of (I).

Crystal data

$C_{18}H_{14}N_4$
M_r = 286.33
Triclinic, $P\overline{1}$
a = 7.5282 (15) Å
b = 9.6334 (19) Å
c = 10.975 (2) Å
α = 79.66 (3)°
β = 81.89 (3)°
γ = 71.31 (3)°
V = 738.7 (3) Å^3
Z = 2
D_x = 1.287 Mg m^{-3}
Mo *Kα* radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
Block, yellow
0.56 × 0.23 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
6161 measured reflections
3278 independent reflections
2067 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.5^{\circ}$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.139$
$S = 1.08$
3278 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0662P)^2 + 0.0465P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···N3^{i}	0.93	2.56	3.443 (3)	158

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

H atoms were placed in geometrically idealized positions, with C—H = 0.93 Å, and were constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

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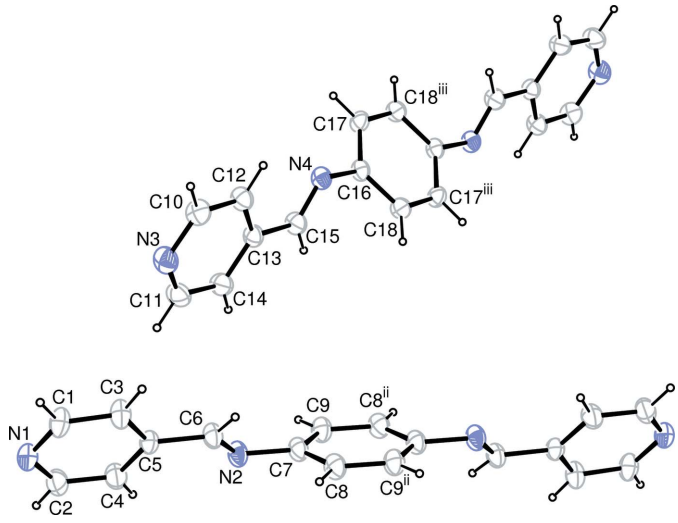

Figure 1
The structure of the two independent molecules of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). [Symmetry codes: (ii) $-x, -y, 1-z$; (iii) $-x, 1-y, 2-z$.]

References

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Diskin-Posner, Y., Patra, G. K. & Goldberg, I. (2001). *J. Chem. Soc. Dalton Trans.* pp. 2775–2782.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Grasso, D., Buemi, G., Fasone, S. & Gandolfo, C. (1981). *Croat. Chem. Acta*, **54**, 85–90.
Moriuchi, T., Bandoh, S., Kamikawa, M. & Hirao, T. (2000). *Chem. Lett.* pp. 148–149.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.