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Structure of *N*-[Di(2-pyridyl)methylene]aniline

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Abstract. $C_{17}H_{13}N_3$, $M_r = 259{\cdot}31$, triclinic, $P\bar{1}$, $a = 8{\cdot}217\ (4)$, $b = 8{\cdot}809\ (4)$, $c = 9{\cdot}847\ (4)$ Å, $\alpha = 81{\cdot}48\ (4)$, $\beta = 78{\cdot}86\ (4)$, $\gamma = 83{\cdot}71\ (4)°$, $V = 689\ (1)$ Å^3, $Z = 2$, $D_x = 1{\cdot}250$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0{\cdot}07$ mm^{-1}, $F(000) = 272$, $T = 291\ (1)$ K, final $R = 0{\cdot}070$ for 1879 unique observed $[F \geq 3{\cdot}0\sigma(F)]$ diffractometer data. The crystal structure of a condensation product of di-2-pyridyl ketone with aniline was determined by the X-ray diffraction method. There are no unusual bond distances and angles in the molecule and no short contacts between the molecules.

Experimental. The title compound was prepared by reaction of 1 g of di-2-pyridyl ketone and 1·2 ml aniline in 90 ml boiling toluene with 3 mg *p*-toluenesulfonic acid as a catalyst (yield: 83%). In order to keep the reaction water free a watertrap was used. Yellow-orange needle-shaped crystals (m.p. 314–315 K) were obtained by multifold recrystallization from ethanol. The IR spectrum shows a C=N band at 1635 cm^{-1}. Crystal size ~ 0·38 × 0·26 × 0·38 mm; $\omega/2\theta$ scan, scan speed 1·5–14·6° min^{-1} in θ; Nicolet *R*3*m*/V diffractometer, graphite-monochromated Mo $K\alpha$; lattice parameters from least-squares fit with 25 reflections up to $2\theta = 24{\cdot}5°$; six standard reflections recorded every 2·5 h, only random deviations; 4999 reflections measured, $1{\cdot}5 \leq \theta \leq 25{\cdot}0°$, $-10 \leq h \leq 10$, $-11 \leq k \leq 11$, $-12 \leq l \leq 12$; after averaging ($R_{int} = 0{\cdot}024$): 2446 unique reflections, 1879 with $F \geq 3{\cdot}0\sigma(F)$; Lorentz–polarization correction, no absorption correction; structure solution in space group $P\bar{1}$ *via* direct methods, ΔF syntheses and full-matrix least-squares refinement with anisotropic temperature factors for all non-H atoms and a common isotropic temperature factor for H atoms, which were placed in geometrically calculated positions (C–H 0·96 Å), the phenyl group was refined as a rigid body (C–C 1·935 Å, C–C–C and C–C–H 120°); refinement on *F* with 1879 reflections and 170 refined parameters; $w = 1{\cdot}0/[\sigma^2(F) + (0{\cdot}0005F^2)]$; $S = 1{\cdot}94$, $R = 0{\cdot}070$, $wR = 0{\cdot}069$, $(\Delta/\sigma)_{max} = 0{\cdot}04$, no extinction correction; largest peak in final ΔF map $\pm 0{\cdot}2\ (1)$ e Å^{-3},

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2 × 10^3)

$U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

	x	*y*	*z*	U_{eq}
N(1)	0·3540 (3)	0·4905 (3)	0·8320 (2)	54
N(2)	0·1826 (3)	0·1337 (2)	0·9727 (2)	52
N(3)	0·1550 (4)	0·3230 (3)	0·6545 (3)	86
C(1)	0·2557 (3)	0·3828 (3)	0·8551 (3)	41
C(2)	0·2816 (3)	0·2487 (3)	0·9634 (3)	42
C(3)	0·3977 (4)	0·2441 (3)	1·0490 (3)	55
C(4)	0·4130 (4)	0·1174 (4)	1·1477 (3)	63
C(5)	0·3127 (4)	−0·0012 (3)	1·1581 (3)	58
C(6)	0·2003 (4)	0·0118 (3)	1·0689 (3)	56
C(7)	0·1138 (3)	0·3789 (3)	0·7800 (3)	44
C(8)	−0·0415 (3)	0·4268 (3)	0·8416 (4)	61
C(9)	−0·1670 (5)	0·4177 (5)	0·7683 (7)	115
C(10)	−0·1347 (9)	0·3609 (6)	0·6435 (9)	163
C(11)	0·0208 (9)	0·3157 (5)	0·5918 (5)	135
C(13)	0·1952 (2)	0·7358 (2)	0·7716 (2)	58
C(14)	0·1790 (2)	0·8736 (2)	0·6832 (2)	64
C(15)	0·2947 (2)	0·9019 (2)	0·5604 (2)	60
C(16)	0·4267 (2)	0·7924 (2)	0·5261 (2)	57
C(17)	0·4429 (2)	0·6546 (2)	0·6146 (2)	52
C(12)	0·3271 (2)	0·6263 (2)	0·7374 (2)	48

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Table 2. *Bond distances* (Å), *angles* (°), *least-squares planes and dihedral angles* (°)

N(1)–C(1)	1·280 (3)	C(2)–C(3)	1·384 (4)
N(1)–C(12)	1·428 (3)	C(3)–C(4)	1·379 (4)
N(2)–C(2)	1·349 (4)	C(4)–C(5)	1·380 (5)
N(2)–C(6)	1·337 (3)	C(5)–C(6)	1·378 (5)
N(3)–C(7)	1·367 (4)	C(7)–C(8)	1·354 (4)
N(3)–C(11)	1·376 (8)	C(8)–C(9)	1·383 (7)
C(1)–C(2)	1·495 (3)	C(9)–C(10)	1·36 (1)
C(1)–C(7)	1·502 (4)	C(10)–C(11)	1·32 (1)

C(1)–N(1)–C(12)	121·1 (3)	C(4)–C(5)–C(6)	118·5 (3)
C(2)–N(2)–C(6)	117·5 (3)	N(2)–C(6)–C(5)	123·4 (3)
C(7)–N(3)–C(11)	113·8 (4)	N(3)–C(7)–C(1)	115·6 (3)
N(1)–C(1)–C(7)	124·8 (3)	C(1)–C(7)–C(8)	118·6 (3)
N(1)–C(1)–C(2)	119·0 (3)	N(3)–C(7)–C(8)	125·8 (3)
C(2)–C(1)–C(7)	116·2 (3)	C(7)–C(8)–C(9)	115·7 (4)
N(2)–C(2)–C(1)	115·3 (3)	C(8)–C(9)–C(10)	121·4 (5)
C(1)–C(2)–C(3)	122·2 (3)	C(9)–C(10)–C(11)	118·6 (7)
N(2)–C(2)–C(3)	122·5 (3)	N(3)–C(11)–C(10)	124·7 (5)
C(2)–C(3)–C(4)	118·9 (3)	N(1)–C(12)–C(17)	119·0 (2)
C(3)–C(4)–C(5)	119·2 (3)	N(1)–C(12)–C(13)	120·8 (2)

No.	Plane through atoms	Equation of the plane (x along **a**; y in the plane **ab**; z along **c***)	ψ^2
1	N(2),C(2),C(3),C(4),C(5), C(6)	$+0{\cdot}523x-0{\cdot}534y-0{\cdot}6644z=-5{\cdot}65$ Å	0·74
2	N(3),C(7),C(8),C(9),C(10), C(11)	$0{\cdot}141x+0{\cdot}8715y-0{\cdot}470z=0{\cdot}63$ Å	12·97
3	C(12),C(13),C(14),C(15), C(16),C(17)	$-0{\cdot}7173x-0{\cdot}4921y-0{\cdot}4933z=-10{\cdot}007$ Å	0·00
4	N(1),C(1),C(2),C(7)	$0{\cdot}434x-0{\cdot}575y-0{\cdot}693z-6{\cdot}45$ Å	1·27

Dihedral angles: 1,2 94·6 (1)°; 1,3 77·55 (8)°; 1,4 5·9 (1)°; 2,3 107·4 (1)°; 2,4 96·6 (1)°; 3,4 71·7 (1)°

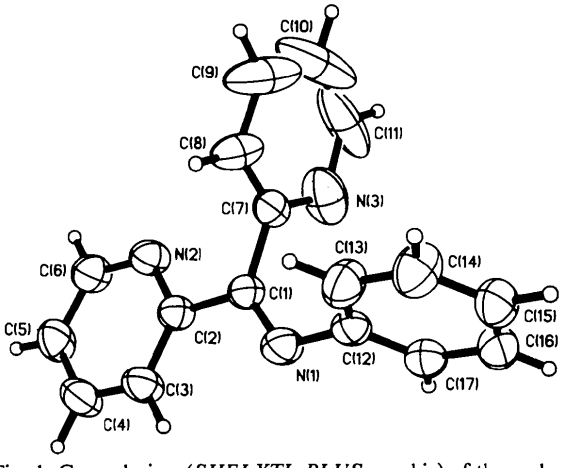

Fig. 1. General view (*SHELXTL PLUS* graphic) of the molecule, showing the atom-numbering scheme.

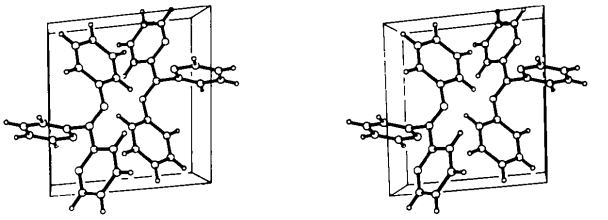

Fig. 2. Stereoscopic view (*SHELXTL PLUS* graphic) of the unit cell (**b** vertical, **a** nearly horizontal).

atomic scattering factors for neutral atoms and real and imaginary dispersion terms from *International Tables for X-ray Crystallography* (1974); programs: *SHELXTL PLUS* (Sheldrick, 1987), *PARST* (Nardelli, 1983), *PCK*83 (Williams, 1984). The molecule and the numbering scheme are shown in Fig. 1 and a stereoscopic view of the unit cell in Fig. 2. Positional parameters and the equivalent values of the anisotropic temperature factors for the non-H atoms are given in Table 1.* Bond lengths, bond angles, least-squares planes and dihedral angles are given in Table 2. There are no short contacts between the molecules.

Related literature. Martinez, Valcarcel & Pino (1976).

* Lists of H-atom coordinates, anisotropic thermal parameters and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51082 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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