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2,6-Diphenylpyridine

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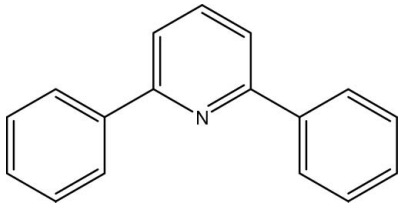
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.006 Å; R factor = 0.055; wR factor = 0.163; data-to-parameter ratio = 9.8.

In the title compound, $C_{17}H_{13}N$, the dihedral angles between the pyridine ring and the phenyl rings are 29.68 (18) and 26.58 (17)°. In the crystal structure, the molecules are linked by a weak C—H$\cdots\pi$ interaction, leading to [0$\bar{1}$1] chains. There are no further significant intermolecular interactions.

Related literature

For related literature, see: Crispini & Neve (2002); Silva *et al.* (1997). For a previous synthesis, see: Miyaura & Suzuki (1995).



Experimental

Crystal data

$C_{17}H_{13}N$
M_r = 231.28
Orthorhombic, $Pna2_1$
a = 16.1368 (16) Å
b = 12.5371 (14) Å
c = 6.2969 (4) Å
V = 1273.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 120 (2) K
0.70 × 0.32 × 0.14 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.953, T_{max} = 0.990
29987 measured reflections
1596 independent reflections
1147 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.163
S = 1.07
1596 reflections
163 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

*Cg*1 is the centroid of the pyridine ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C64—H64$\cdots$*Cg*1^{i}	0.95	2.74	3.534 (4)	142

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

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *FLIPPER* (Oszlányi & Süto, 2004, 2005; program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* (Sheldrick 1997) and *WORDPERFECT* macro *PRPKAPPA* (Ferguson, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2646).

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supplementary materials

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2,6-Diphenylpyridine

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Comment

The bonds and angles are in agreement with those found for related structures described by Crispini & Neve. (2002) and Silva *et al.*(1997). The angles between the mean planes of the pyridine rings and the phenyl rings are 29.68 (18)° (ring attached to C2), and 26.58 (17)° (ring attached to C6). The molecules are linked into chains along [0$\bar{1}$1] by a weak C—H..π interaction (Fig. 2 and Table 1); C64—H64.·*Cg*1(−*x* + 1/2, *y* + 1/2, *z* − 1/2), where *Cg*1 is the centroid of the pyridine ring. There are no further intermolecular interactions.

Experimental

The title compound was synthesized by adapting the procedure described by Miyaura & Suzuki (1995). A solution of 2,6-dibromopyridine (1.9 g), palladium(II) acetate (0.02 g) and phenylboronic acid (5.5 g) in *N*,*N*'-dimethylformamide was added to an aqueous solution of potassium carbonate (4.3 g). The mixture was refluxed for 5 h at 373 K. The cooled solution was extracted with 4 × 50 ml e thyl acetate/acetone (5:1 *v*/*v*) and the extract was filtered out. The solvent was evaporated under low pressure at 353 K. The resulting solid was recrystallized from ethanol to yield colourless blocks of (I). Found (%w) for $C_{17}H_{13}N$: C 88.97, H 5.32, N 5.71; calculated (%w): C 88.28, H 5.67, N 6.06. m.p. 351 K.

Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement. H atoms were treated as riding atoms with C—H = 0.95Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

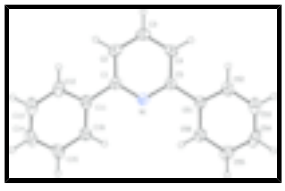

Fig. 1. A view of (I) with isplacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms).

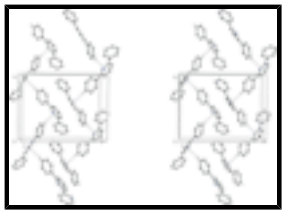

Fig. 2. A stereoscopic view of symmetry related chains of molecules linked by the C—H..π interaction. H atoms not involved in the interaction are omitted for clarity.

2,6-Diphenylpyridine

Crystal data

$C_{17}H_{13}N$	$D_x = 1.206$ Mg m^{-3}
$M_r = 231.28$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, $Pna2_1$	Cell parameters from 1596 reflections
$a = 16.1368$ (16) Å	$\theta = 3.5$–27.5º
$b = 12.5371$ (14) Å	$\mu = 0.07$ mm^{-1}
$c = 6.2969$ (4) Å	$T = 120$ (2) K
$V = 1273.9$ (2) Å^3	Block, colourless
$Z = 4$	0.70 × 0.32 × 0.14 mm
$F_{000} = 488$	

Data collection

Bruker–Nonius CCD diffractometer	1596 independent reflections
Radiation source: Bruker-Nonius FR591 rotating anode	1147 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.053$
Detector resolution: 9.091 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 120(2)$ K	$\theta_{min} = 3.5$º
π & ω scans	$h = -20 \rightarrow 20$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$k = -16 \rightarrow 16$
$T_{min} = 0.953$, $T_{max} = 0.990$	$l = -8 \rightarrow 8$
29987 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.055$	H-atom parameters constrained
$wR(F^2) = 0.163$	$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2 + 0.6523P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
1596 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
163 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. The scale factors in the experimental table are calculated from the 'size' command in the *SHELXL97* input file.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.40272 (15)	0.4122 (2)	0.3621 (5)	0.0353 (6)
C2	0.4510 (2)	0.3407 (3)	0.4621 (6)	0.0356 (8)
C3	0.4702 (2)	0.3502 (3)	0.6756 (6)	0.0412 (8)
C4	0.4376 (2)	0.4338 (3)	0.7908 (7)	0.0443 (9)
C5	0.3893 (2)	0.5073 (3)	0.6890 (6)	0.0406 (8)
C6	0.37309 (19)	0.4956 (2)	0.4725 (6)	0.0345 (7)
C21	0.4814 (2)	0.2503 (3)	0.3325 (6)	0.0407 (8)
C22	0.5556 (2)	0.1994 (3)	0.3788 (8)	0.0503 (10)
C23	0.5826 (3)	0.1144 (3)	0.2567 (9)	0.0624 (13)
C24	0.5356 (3)	0.0782 (3)	0.0889 (9)	0.0635 (12)
C25	0.4618 (3)	0.1281 (3)	0.0410 (8)	0.0594 (12)
C26	0.4351 (3)	0.2137 (3)	0.1592 (6)	0.0468 (9)
C61	0.32310 (19)	0.5744 (3)	0.3538 (6)	0.0386 (8)
C62	0.3186 (2)	0.6797 (3)	0.4181 (7)	0.0512 (10)
C63	0.2743 (3)	0.7541 (3)	0.3035 (9)	0.0613 (12)
C64	0.2330 (2)	0.7237 (4)	0.1205 (9)	0.0629 (13)
C65	0.2361 (2)	0.6181 (3)	0.0548 (8)	0.0556 (11)
C66	0.2814 (2)	0.5446 (3)	0.1690 (6)	0.0434 (9)
H3	0.5055	0.2996	0.7421	0.049*
H4	0.4486	0.4402	0.9385	0.053*
H5	0.3668	0.5659	0.7652	0.049*
H22	0.5881	0.2231	0.4953	0.060*
H23	0.6338	0.0808	0.2888	0.075*
H24	0.5539	0.0192	0.0067	0.076*
H25	0.4292	0.1032	−0.0744	0.071*
H26	0.3846	0.2483	0.1229	0.056*
H62	0.3466	0.7013	0.5437	0.061*
H63	0.2721	0.8261	0.3500	0.074*
H64	0.2028	0.7748	0.0405	0.076*
H65	0.2069	0.5965	−0.0691	0.067*
H66	0.2842	0.4728	0.1214	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0342 (13)	0.0336 (14)	0.0381 (15)	−0.0040 (11)	0.0018 (14)	0.0020 (13)
C2	0.0335 (16)	0.0326 (16)	0.0408 (19)	−0.0040 (13)	0.0022 (15)	0.0032 (16)
C3	0.0344 (16)	0.049 (2)	0.041 (2)	−0.0077 (15)	−0.0038 (16)	0.0062 (18)
C4	0.0417 (18)	0.052 (2)	0.039 (2)	−0.0110 (16)	−0.0035 (17)	0.0011 (18)
C5	0.0391 (17)	0.0454 (19)	0.0371 (19)	−0.0072 (15)	0.0058 (16)	−0.0080 (17)

C6	0.0311 (15)	0.0338 (17)	0.0384 (19)	−0.0021 (13)	0.0009 (15)	−0.0015 (16)
C21	0.0453 (18)	0.0320 (15)	0.045 (2)	0.0002 (14)	0.0075 (18)	0.0058 (16)
C22	0.049 (2)	0.0365 (18)	0.066 (3)	0.0026 (15)	0.006 (2)	0.012 (2)
C23	0.063 (2)	0.039 (2)	0.085 (3)	0.0123 (18)	0.019 (3)	0.013 (2)
C24	0.090 (3)	0.0358 (18)	0.065 (3)	0.011 (2)	0.024 (3)	0.003 (2)
C25	0.088 (3)	0.0359 (19)	0.054 (3)	0.005 (2)	0.006 (3)	0.0004 (19)
C26	0.061 (2)	0.0344 (18)	0.045 (2)	0.0022 (16)	0.000 (2)	0.0007 (17)
C61	0.0307 (14)	0.0407 (17)	0.0444 (19)	0.0019 (13)	0.0034 (17)	−0.0021 (16)
C62	0.050 (2)	0.045 (2)	0.059 (3)	0.0085 (17)	0.0038 (19)	−0.005 (2)
C63	0.056 (2)	0.048 (2)	0.079 (4)	0.0154 (18)	0.011 (2)	0.000 (2)
C64	0.0384 (19)	0.068 (3)	0.083 (4)	0.0231 (19)	0.003 (2)	0.017 (3)
C65	0.0374 (19)	0.073 (3)	0.057 (3)	0.0057 (19)	−0.0049 (19)	0.005 (2)
C66	0.0331 (16)	0.0495 (19)	0.048 (2)	0.0032 (15)	0.0001 (18)	0.0013 (19)

Geometric parameters (Å, °)

N1—C6	1.344 (4)	C24—C25	1.378 (7)
N1—C2	1.344 (4)	C24—H24	0.95
C2—C3	1.385 (5)	C25—C26	1.376 (5)
C2—C21	1.481 (5)	C25—H25	0.95
C3—C4	1.378 (5)	C26—H26	0.95
C3—H3	0.95	C61—C62	1.383 (5)
C4—C5	1.368 (5)	C61—C66	1.395 (5)
C4—H4	0.95	C62—C63	1.379 (6)
C5—C6	1.395 (5)	C62—H62	0.95
C5—H5	0.95	C63—C64	1.384 (7)
C6—C61	1.478 (5)	C63—H63	0.95
C21—C22	1.387 (5)	C64—C65	1.388 (6)
C21—C26	1.400 (5)	C64—H64	0.95
C22—C23	1.384 (6)	C65—C66	1.380 (5)
C22—H22	0.95	C65—H65	0.95
C23—C24	1.378 (8)	C66—H66	0.95
C23—H23	0.95		
C6—N1—C2	118.9 (3)	C25—C24—H24	120.2
N1—C2—C3	121.8 (3)	C23—C24—H24	120.2
N1—C2—C21	116.4 (3)	C26—C25—C24	120.5 (5)
C3—C2—C21	121.8 (3)	C26—C25—H25	119.8
C4—C3—C2	119.4 (4)	C24—C25—H25	119.8
C4—C3—H3	120.3	C25—C26—C21	120.6 (4)
C2—C3—H3	120.3	C25—C26—H26	119.7
C5—C4—C3	118.9 (4)	C21—C26—H26	119.7
C5—C4—H4	120.6	C62—C61—C66	118.3 (3)
C3—C4—H4	120.6	C62—C61—C6	121.2 (3)
C4—C5—C6	119.6 (3)	C66—C61—C6	120.4 (3)
C4—C5—H5	120.2	C63—C62—C61	121.3 (4)
C6—C5—H5	120.2	C63—C62—H62	119.3
N1—C6—C5	121.3 (3)	C61—C62—H62	119.3
N1—C6—C61	116.9 (3)	C62—C63—C64	119.9 (4)
C5—C6—C61	121.7 (3)	C62—C63—H63	120.0

C22—C21—C26	118.3 (4)	C64—C63—H63	120.0
C22—C21—C2	121.5 (4)	C63—C64—C65	119.6 (4)
C26—C21—C2	120.2 (3)	C63—C64—H64	120.2
C23—C22—C21	120.6 (4)	C65—C64—H64	120.2
C23—C22—H22	119.7	C66—C65—C64	120.0 (4)
C21—C22—H22	119.7	C66—C65—H65	120.0
C24—C23—C22	120.4 (4)	C64—C65—H65	120.0
C24—C23—H23	119.8	C65—C66—C61	120.8 (4)
C22—C23—H23	119.8	C65—C66—H66	119.6
C25—C24—C23	119.6 (4)	C61—C66—H66	119.6
C6—N1—C2—C3	0.7 (5)	C22—C23—C24—C25	0.9 (7)
C6—N1—C2—C21	179.7 (3)	C23—C24—C25—C26	0.1 (7)
N1—C2—C3—C4	1.4 (5)	C24—C25—C26—C21	−1.2 (6)
C21—C2—C3—C4	−177.5 (3)	C22—C21—C26—C25	1.3 (5)
C2—C3—C4—C5	−2.1 (5)	C2—C21—C26—C25	−178.4 (4)
C3—C4—C5—C6	0.8 (5)	N1—C6—C61—C62	−152.9 (3)
C2—N1—C6—C5	−2.1 (4)	C5—C6—C61—C62	26.8 (5)
C2—N1—C6—C61	177.6 (3)	N1—C6—C61—C66	25.0 (4)
C4—C5—C6—N1	1.4 (5)	C5—C6—C61—C66	−155.3 (3)
C4—C5—C6—C61	−178.3 (3)	C66—C61—C62—C63	−0.1 (6)
N1—C2—C21—C22	151.8 (3)	C6—C61—C62—C63	177.7 (4)
C3—C2—C21—C22	−29.2 (5)	C61—C62—C63—C64	0.2 (6)
N1—C2—C21—C26	−28.5 (5)	C62—C63—C64—C65	0.5 (6)
C3—C2—C21—C26	150.5 (3)	C63—C64—C65—C66	−1.3 (6)
C26—C21—C22—C23	−0.2 (5)	C64—C65—C66—C61	1.4 (6)
C2—C21—C22—C23	179.4 (4)	C62—C61—C66—C65	−0.7 (5)
C21—C22—C23—C24	−0.8 (6)	C6—C61—C66—C65	−178.6 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C64—H64···Cg1^{i}	0.95	2.74	3.534 (4)	142

Symmetry codes: (i) −*x*+1/2, *y*+1/2, *z*−1/2.

Fig. 1

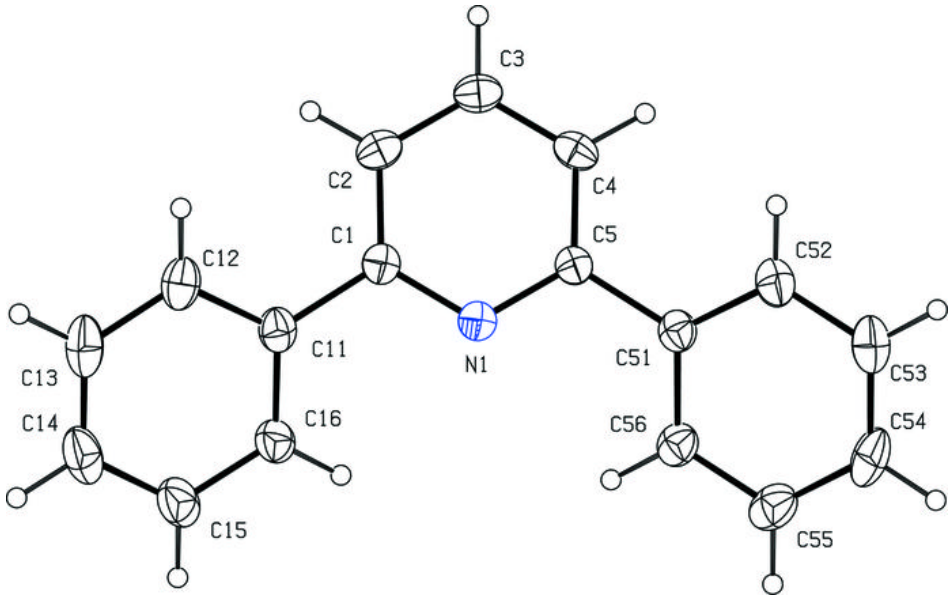

Fig. 2