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2,6-Bis[1-(2-isopropylphenylimino)ethyl]-pyridine

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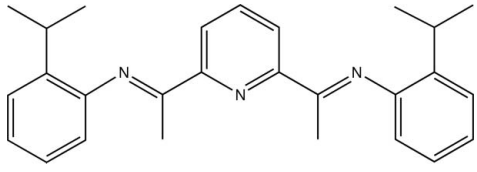
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.061; wR factor = 0.188; data-to-parameter ratio = 15.6.

The title compound, $C_{27}H_{31}N_3$, has E substitution at each imine double bond where the two N atoms adopt a *trans–trans* relationship. The benzene rings are twisted out of the mean plane of the pyridine ring; the mean planes of the aromatic groups are rotated by 63.0 (1) and 72.58 (8)°. The crystal structure is sustained mainly by C—H$\cdots\pi$ and hydrophobic methyl–methyl interactions.

Related literature

For related literature, see: Alyea & Merrel (1974); Bernstein *et al.* (1995); Bianchini & Hon Man (2000); Britovsek *et al.* (1999); Huang *et al.* (2006); Mentes *et al.* (2001); Orrell *et al.* (1997); Small & Brookhart (1998); Togni & Venanzi (1994); Çetinkaya *et al.* (1999).



Experimental

Crystal data

$C_{27}H_{31}N_3$
M_r = 397.55
Monoclinic, $P2_1/c$
a = 16.9462 (18) Å
b = 6.791 (4) Å
c = 21.801 (4) Å
β = 104.551 (13)°
V = 2428.3 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.06 mm^{-1}
T = 295 (2) K
0.48 × 0.40 × 0.20 mm

Data collection

Rigaku AFC-7*S* diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.963, T_{max} = 0.987
4402 measured reflections
4248 independent reflections
2520 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
3 standard reflections
every 150 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.188
S = 1.02
4248 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the rings N1/C1–C5, C8–C13 and C19–C24, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C7—H7$A\cdots$N1	0.96	2.46	2.799 (3)	100
C14—H14$\cdots$N2	0.98	2.46	2.830 (4)	101
C18—H18$A\cdots$N1	0.96	2.47	2.819 (3)	101
C25—H25$\cdots$N3	0.98	2.39	2.892 (4)	111
C3—H3$\cdots Cg1^{i}$	0.93	2.75	3.450 (3)	133
C23—H23$\cdots Cg2^{ii}$	0.93	2.97	3.801 (4)	149
C12—H12$\cdots Cg3^{ii}$	0.93	3.16	3.961 (10)	146
C15—H15$B\cdots Cg1^{iii}$	0.96	3.17	3.757 (13)	121
C15—H15$C\cdots Cg1^{iii}$	0.96	3.44	3.757 (13)	102

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x, -y, -z+1$.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXTL-NT* (Bruker, 1998); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT* and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL-NT* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2609).

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supplementary materials

Acta Cryst. (2008). E**64**, o28-o29 [**doi:10.1107/S1600536807060254**]

2,6-Bis[1-(2-isopropylphenylimino)ethyl]pyridine

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Comment

The development of new ligand politopics bearing nitrogen heterocyclic units has been receiving increasing interest in the coordination chemistry of transition-metal based homogeneous catalysis (Togni & Venanzi, 1994). In this context, the planar tridentate–or potentially bidentate–ligand 2,6-bis(imino)pyridine and its derivatives (Orrell *et al.*, 1997) have attracted great attention and the bis(arylimino)pyridine ligand [2,6-(ArN═CR)$_2$C$_5$H$_3$N] by (Alyea & Merrel, 1974). There are several recent examples of reactions catalyzed by complexes bearing the ligand 2,6-bis(arylimino)pyridine ligands such as epoxidation of olefins (Çetinkaya *et al.*, 1999), cyclopropanation of styrene (Bianchini *et al.*, 2000). Specially, it has been nearly a decade since sterically demanding bis(arylimino)pyridine ligands were found to impart transitions metals, iron and cobalt, catalytic activities for olefin polymerization (Small & Brookhart, 1998; Britovsek *et al.*, 1999). Many reports have appared in the literature concerning the effects (sterically and/or electronic) of ligand modifications, to find a structure–activity relationships. The crystal structure of different 2,6-bis(arylimino)pyridine ligands and their transition metal complexes offer the possibilty to compare directly structural parameters. Here we report the synthesis and crystal structure of the title compound, (I), (Fig. 1).

The molecule adopts a nonplanar conformation in which an E configuration around each C═N imine group is observed, likewise the two N atoms display a *trans-trans* relationship. The conformation of the system N–N–N system is of course different in each case. In general, X-ray structures of bis(arylimino)pyridines reveal that in the solid state the imino nitrogen atoms prefer to be disposed *trans* with respect to the central pyridine nitrogen (Mentes, *et al.* 2001; Huang *et al.*, 2006) in order to minimize the interaction between the nitrogen lone pairs. The phenyl rings in (I) are twisted out of the mean plane of the pyridine ring, the mean planes of C8–C13 and C19–C24 being rotated by 63.0 (1)° and 72.58 (8)°, respectively. This molecular conformation is determined by the formation of pairs of intramolecular C—H···N hydrogen bonds, involving methyl groups with the N of the pyridine ring and isopropyl groups with imine groups with a range of distances C···N = 2.799 (3)–2.892 (4) Å (Fig. 2). These interactions lead to the formation of five-membered rings described by graph-set simbol S(5) (Bernstein *et al.*, 1995).

The crystal structure of (I) consists of dimers linked by self-complementary C—H···π interactions related by an inversion centre C15···*Cg*1 = 3.757 Å; were *Cg*1 is the centroid of the N1,C1–C5 ring (Fig. 2). Neighbouring dimers are connected through additional C—H···π between phenyl rings (Fig. 3), generating supramolecular sheets parallel to the *c* axis. Details of geometrical parameters of these hydrogen bonding interactions are summarized in Table 2. Finally, the stacking of adjacent sheets is sustained by hydrophobic methyl-methyl interactions along the *a* axis (Fig. 4).

Experimental

The tile compound was synthetized by condensation of 2,6-diacetylpiridine (1.63 g, 10 mmol) with 2-iso-propylaniline (2.74 g, 20.3 mmol) in 25 ml dry methanol and five drops of formic acid. The solution was refluxed for 18 h. Upon slow cooling to room temperature and overnight to 273 K. Yellow prisms of (I) were obtained and filtered with a yield 75%.

^{1}H-NMR (300 MHz, $CDCl_3$); (δ, p.p.m.) 1.16 (d, 12 H), 2.23(s, 6H), 2.75(sept,2 H), 6. 54(tt, 2H), 7.08(tt, 2 H), 7.20(tt, 2 H), 7.44(dd, 2 H), 7.95(t, 1 H), 8.43(d, 2 H). Elemental analysis calcd. for $C_{27}H_{31}N_3$ (%): C 81.57; H 7.85; N 10.57%. Found: C 81.33; H 7.69; N 10.41%.

Refinement

All H atoms bound to carbon were included in calculated positions (C—H = 0.93–096 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

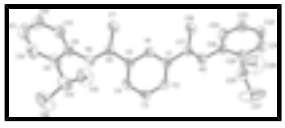


Fig. 1. Molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level (H atoms omitted for clarity).

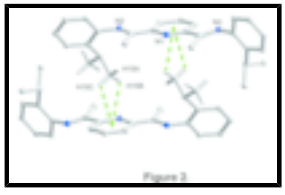


Fig. 2. Ball and stick representation, showing the centrosymmetric dimer generated by C—H···π interactions (dashed lines). Most H atoms have been omitted for clarity.

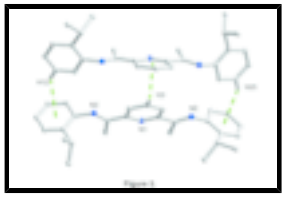


Fig. 3. Ball and stick representation, showing side C—H···π interactions between adjacent molecules (dashed lines). Most H atoms have been omitted for clarity.

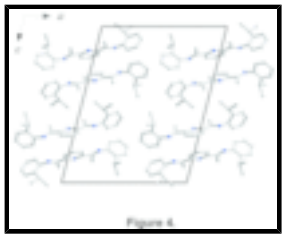


Fig. 4. View of the packing of (I) along the *b* axis

2,6-Bis[1-(2-isopropylphenylimino)ethyl]pyridine

Crystal data

$C_{27}H_{31}N_3$	F_{000} = 856
M_r = 397.55	D_x = 1.087 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
a = 16.9462 (18) Å	θ = 32.2–38.4°
b = 6.791 (4) Å	μ = 0.06 mm^{-1}
c = 21.801 (4) Å	T = 295 (2) K

β = 104.551 (13)º	Prism, yellow
V = 2428.3 (16) Å^3	0.48 × 0.40 × 0.20 mm
Z = 4	

Data collection

Rigaku AFC-7S diffractometer	R_{int} = 0.016
Radiation source: normal-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 1.9º
T = 295(2) K	h = 0→20
ω/2θ scans	k = 0→8
Absorption correction: ψ scan (North *et al.*, 1968)	l = −25→25
T_{min} = 0.963, T_{max} = 0.987	3 standard reflections
4402 measured reflections	every 150 reflections
4248 independent reflections	intensity decay: none
2520 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.061	H-atom parameters constrained
$wR(F^2)$ = 0.188	$w = 1/[\sigma^2(F_o^2) + (0.0887P)^2 + 0.6215P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
4248 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
272 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}

N1	0.05494 (11)	0.3071 (3)	0.34591 (9)	0.0579 (5)
C1	0.11172 (13)	0.2115 (4)	0.32418 (11)	0.0557 (6)
N2	−0.14528 (12)	0.2343 (3)	0.36370 (10)	0.0626 (6)
C2	0.10199 (15)	0.0180 (4)	0.30294 (12)	0.0628 (7)
H2	0.1427	−0.0446	0.2885	0.075*
N3	0.23456 (12)	0.2431 (3)	0.29399 (10)	0.0677 (6)
C3	0.03083 (15)	−0.0796 (4)	0.30372 (12)	0.0638 (7)
H3	0.0233	−0.2102	0.2907	0.077*
C4	−0.02878 (14)	0.0191 (4)	0.32408 (12)	0.0610 (7)
H4	−0.0778	−0.0428	0.3238	0.073*
C5	−0.01505 (14)	0.2114 (4)	0.34492 (11)	0.0550 (6)
C6	−0.07766 (14)	0.3213 (4)	0.36847 (12)	0.0588 (6)
C7	−0.05481 (19)	0.5194 (4)	0.39720 (18)	0.0984 (11)
H7A	−0.0209	0.5859	0.3745	0.148*
H7B	−0.0256	0.5043	0.4408	0.148*
H7C	−0.1033	0.5955	0.3948	0.148*
C8	−0.20994 (14)	0.3228 (4)	0.38484 (13)	0.0656 (7)
C9	−0.23417 (16)	0.2357 (5)	0.43497 (13)	0.0732 (8)
C10	−0.3013 (2)	0.3205 (6)	0.45150 (17)	0.0961 (11)
H10	−0.3181	0.2696	0.4858	0.115*
C11	−0.3430 (2)	0.4763 (7)	0.4187 (2)	0.1101 (13)
H11	−0.3876	0.5285	0.4307	0.132*
C12	−0.3195 (2)	0.5553 (6)	0.3686 (2)	0.1071 (12)
H12	−0.3483	0.6601	0.3461	0.129*
C13	−0.25291 (17)	0.4787 (5)	0.35161 (16)	0.0873 (9)
H13	−0.2366	0.5323	0.3175	0.105*
C14	−0.1887 (2)	0.0594 (5)	0.46845 (15)	0.0950 (10)
H14	−0.1738	−0.0204	0.4356	0.114*
C15	−0.1087 (2)	0.1186 (7)	0.51467 (17)	0.1210 (13)
H15A	−0.0777	0.1996	0.4932	0.181*
H15B	−0.0780	0.0025	0.5306	0.181*
H15C	−0.1201	0.1909	0.5493	0.181*
C16	−0.2374 (3)	−0.0741 (8)	0.5009 (2)	0.173 (2)
H16A	−0.2872	−0.1117	0.4712	0.260*
H16B	−0.2498	−0.0055	0.5358	0.260*
H16C	−0.2060	−0.1898	0.5162	0.260*
C17	0.18765 (14)	0.3230 (4)	0.32340 (12)	0.0599 (6)
C18	0.20231 (18)	0.5140 (4)	0.35833 (19)	0.0993 (11)
H18A	0.1516	0.5832	0.3529	0.149*
H18B	0.2395	0.5925	0.3420	0.149*
H18C	0.2252	0.4892	0.4026	0.149*
C19	0.30842 (15)	0.3356 (4)	0.28902 (13)	0.0647 (7)
C20	0.38249 (15)	0.2764 (4)	0.32815 (13)	0.0679 (7)
C21	0.45263 (16)	0.3592 (5)	0.31692 (15)	0.0803 (8)
H21	0.5030	0.3230	0.3427	0.096*
C22	0.45021 (17)	0.4919 (5)	0.26932 (16)	0.0860 (9)
H22	0.4983	0.5439	0.2630	0.103*
C23	0.37679 (18)	0.5477 (5)	0.23106 (16)	0.0920 (10)
H23	0.3745	0.6379	0.1986	0.110*

C24	0.30616 (17)	0.4692 (5)	0.24102 (15)	0.0856 (9)
H24	0.2561	0.5070	0.2150	0.103*
C25	0.38646 (18)	0.1294 (6)	0.38095 (15)	0.0966 (11)
H25	0.3302	0.1035	0.3828	0.116*
C26	0.4307 (3)	0.2107 (8)	0.4446 (2)	0.168 (2)
H26A	0.4317	0.1134	0.4767	0.252*
H26B	0.4030	0.3264	0.4536	0.252*
H26C	0.4855	0.2443	0.4439	0.252*
C27	0.4219 (5)	−0.0611 (8)	0.3690 (3)	0.236 (4)
H27A	0.4222	−0.1495	0.4035	0.354*
H27B	0.4767	−0.0410	0.3656	0.354*
H27C	0.3898	−0.1166	0.3303	0.354*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0471 (11)	0.0610 (13)	0.0652 (12)	−0.0048 (10)	0.0137 (9)	0.0046 (10)
C1	0.0489 (13)	0.0587 (15)	0.0586 (14)	0.0008 (11)	0.0121 (11)	0.0055 (12)
N2	0.0496 (11)	0.0725 (14)	0.0655 (13)	−0.0081 (10)	0.0142 (9)	−0.0009 (11)
C2	0.0577 (14)	0.0622 (17)	0.0693 (16)	0.0020 (13)	0.0173 (12)	−0.0003 (13)
N3	0.0527 (12)	0.0752 (15)	0.0763 (14)	−0.0045 (11)	0.0183 (11)	−0.0030 (12)
C3	0.0672 (16)	0.0561 (15)	0.0671 (16)	−0.0067 (13)	0.0149 (13)	−0.0039 (13)
C4	0.0566 (14)	0.0612 (16)	0.0639 (15)	−0.0085 (13)	0.0127 (12)	0.0029 (13)
C5	0.0528 (14)	0.0574 (15)	0.0537 (14)	−0.0035 (11)	0.0115 (11)	0.0052 (11)
C6	0.0554 (14)	0.0571 (15)	0.0656 (15)	−0.0063 (12)	0.0185 (12)	0.0044 (12)
C7	0.084 (2)	0.074 (2)	0.155 (3)	−0.0210 (17)	0.062 (2)	−0.032 (2)
C8	0.0478 (14)	0.0778 (18)	0.0709 (17)	−0.0125 (13)	0.0142 (12)	−0.0101 (15)
C9	0.0609 (16)	0.092 (2)	0.0688 (17)	−0.0269 (15)	0.0208 (13)	−0.0149 (16)
C10	0.076 (2)	0.131 (3)	0.090 (2)	−0.035 (2)	0.0366 (18)	−0.029 (2)
C11	0.067 (2)	0.135 (3)	0.135 (3)	−0.006 (2)	0.038 (2)	−0.036 (3)
C12	0.071 (2)	0.117 (3)	0.135 (3)	0.016 (2)	0.027 (2)	−0.005 (3)
C13	0.0643 (17)	0.098 (2)	0.101 (2)	0.0080 (18)	0.0230 (16)	0.0075 (19)
C14	0.103 (2)	0.105 (3)	0.080 (2)	−0.026 (2)	0.0289 (18)	0.008 (2)
C15	0.115 (3)	0.144 (4)	0.092 (2)	−0.015 (3)	0.005 (2)	0.014 (3)
C16	0.193 (5)	0.163 (4)	0.175 (5)	−0.063 (4)	0.069 (4)	0.040 (4)
C17	0.0464 (13)	0.0598 (15)	0.0724 (16)	0.0031 (12)	0.0132 (12)	0.0073 (13)
C18	0.0725 (18)	0.0693 (19)	0.168 (3)	−0.0142 (16)	0.052 (2)	−0.027 (2)
C19	0.0505 (14)	0.0728 (17)	0.0737 (17)	−0.0027 (13)	0.0213 (12)	−0.0031 (15)
C20	0.0533 (15)	0.0814 (19)	0.0700 (17)	0.0003 (14)	0.0174 (12)	0.0014 (15)
C21	0.0514 (15)	0.095 (2)	0.094 (2)	0.0048 (15)	0.0187 (14)	0.0033 (19)
C22	0.0593 (17)	0.095 (2)	0.111 (2)	−0.0059 (16)	0.0351 (17)	0.006 (2)
C23	0.0702 (19)	0.097 (2)	0.112 (3)	0.0009 (17)	0.0287 (17)	0.030 (2)
C24	0.0594 (16)	0.098 (2)	0.099 (2)	0.0039 (16)	0.0182 (15)	0.0255 (19)
C25	0.0681 (18)	0.131 (3)	0.089 (2)	0.0062 (19)	0.0168 (16)	0.030 (2)
C26	0.213 (5)	0.196 (5)	0.084 (3)	0.006 (4)	0.016 (3)	0.025 (3)
C27	0.437 (11)	0.107 (4)	0.206 (6)	0.065 (6)	0.157 (7)	0.059 (4)

Geometric parameters (Å, °)

N1—C1	1.342 (3)	C14—H14	0.9800
N1—C5	1.348 (3)	C15—H15A	0.9600
C1—C2	1.389 (4)	C15—H15B	0.9600
C1—C17	1.496 (3)	C15—H15C	0.9600
N2—C6	1.270 (3)	C16—H16A	0.9600
N2—C8	1.424 (3)	C16—H16B	0.9600
C2—C3	1.380 (3)	C16—H16C	0.9600
C2—H2	0.9300	C17—C18	1.493 (4)
N3—C17	1.263 (3)	C18—H18A	0.9600
N3—C19	1.429 (3)	C18—H18B	0.9600
C3—C4	1.376 (3)	C18—H18C	0.9600
C3—H3	0.9300	C19—C24	1.378 (4)
C4—C5	1.382 (3)	C19—C20	1.388 (4)
C4—H4	0.9300	C20—C21	1.391 (4)
C5—C6	1.490 (3)	C20—C25	1.512 (4)
C6—C7	1.494 (4)	C21—C22	1.367 (4)
C7—H7A	0.9600	C21—H21	0.9300
C7—H7B	0.9600	C22—C23	1.366 (4)
C7—H7C	0.9600	C22—H22	0.9300
C8—C13	1.383 (4)	C23—C24	1.376 (4)
C8—C9	1.392 (4)	C23—H23	0.9300
C9—C10	1.401 (4)	C24—H24	0.9300
C9—C14	1.509 (4)	C25—C27	1.476 (6)
C10—C11	1.369 (5)	C25—C26	1.506 (6)
C10—H10	0.9300	C25—H25	0.9800
C11—C12	1.363 (5)	C26—H26A	0.9600
C11—H11	0.9300	C26—H26B	0.9600
C12—C13	1.375 (4)	C26—H26C	0.9600
C12—H12	0.9300	C27—H27A	0.9600
C13—H13	0.9300	C27—H27B	0.9600
C14—C16	1.516 (5)	C27—H27C	0.9600
C14—C15	1.526 (4)		
C1—N1—C5	117.9 (2)	C14—C15—H15C	109.5
N1—C1—C2	122.6 (2)	H15A—C15—H15C	109.5
N1—C1—C17	117.0 (2)	H15B—C15—H15C	109.5
C2—C1—C17	120.3 (2)	C14—C16—H16A	109.5
C6—N2—C8	121.9 (2)	C14—C16—H16B	109.5
C3—C2—C1	118.8 (2)	H16A—C16—H16B	109.5
C3—C2—H2	120.6	C14—C16—H16C	109.5
C1—C2—H2	120.6	H16A—C16—H16C	109.5
C17—N3—C19	121.6 (2)	H16B—C16—H16C	109.5
C4—C3—C2	119.0 (2)	N3—C17—C18	126.0 (2)
C4—C3—H3	120.5	N3—C17—C1	116.2 (2)
C2—C3—H3	120.5	C18—C17—C1	117.9 (2)
C3—C4—C5	119.3 (2)	C17—C18—H18A	109.5
C3—C4—H4	120.3	C17—C18—H18B	109.5

C5—C4—H4	120.3	H18A—C18—H18B	109.5
N1—C5—C4	122.4 (2)	C17—C18—H18C	109.5
N1—C5—C6	116.9 (2)	H18A—C18—H18C	109.5
C4—C5—C6	120.7 (2)	H18B—C18—H18C	109.5
N2—C6—C5	116.4 (2)	C24—C19—C20	120.4 (2)
N2—C6—C7	125.9 (2)	C24—C19—N3	119.3 (2)
C5—C6—C7	117.6 (2)	C20—C19—N3	120.0 (2)
C6—C7—H7A	109.5	C19—C20—C21	117.1 (3)
C6—C7—H7B	109.5	C19—C20—C25	121.3 (2)
H7A—C7—H7B	109.5	C21—C20—C25	121.6 (3)
C6—C7—H7C	109.5	C22—C21—C20	122.4 (3)
H7A—C7—H7C	109.5	C22—C21—H21	118.8
H7B—C7—H7C	109.5	C20—C21—H21	118.8
C13—C8—C9	121.1 (3)	C23—C22—C21	119.7 (3)
C13—C8—N2	120.0 (2)	C23—C22—H22	120.2
C9—C8—N2	118.5 (3)	C21—C22—H22	120.2
C8—C9—C10	116.5 (3)	C22—C23—C24	119.4 (3)
C8—C9—C14	120.1 (3)	C22—C23—H23	120.3
C10—C9—C14	123.4 (3)	C24—C23—H23	120.3
C11—C10—C9	121.9 (3)	C23—C24—C19	121.0 (3)
C11—C10—H10	119.0	C23—C24—H24	119.5
C9—C10—H10	119.0	C19—C24—H24	119.5
C12—C11—C10	120.4 (3)	C27—C25—C26	110.7 (4)
C12—C11—H11	119.8	C27—C25—C20	112.8 (3)
C10—C11—H11	119.8	C26—C25—C20	112.1 (3)
C11—C12—C13	119.4 (4)	C27—C25—H25	107.0
C11—C12—H12	120.3	C26—C25—H25	107.0
C13—C12—H12	120.3	C20—C25—H25	107.0
C12—C13—C8	120.6 (3)	C25—C26—H26A	109.5
C12—C13—H13	119.7	C25—C26—H26B	109.5
C8—C13—H13	119.7	H26A—C26—H26B	109.5
C9—C14—C16	115.4 (3)	C25—C26—H26C	109.5
C9—C14—C15	111.8 (3)	H26A—C26—H26C	109.5
C16—C14—C15	110.3 (3)	H26B—C26—H26C	109.5
C9—C14—H14	106.2	C25—C27—H27A	109.5
C16—C14—H14	106.2	C25—C27—H27B	109.5
C15—C14—H14	106.2	H27A—C27—H27B	109.5
C14—C15—H15A	109.5	C25—C27—H27C	109.5
C14—C15—H15B	109.5	H27A—C27—H27C	109.5
H15A—C15—H15B	109.5	H27B—C27—H27C	109.5

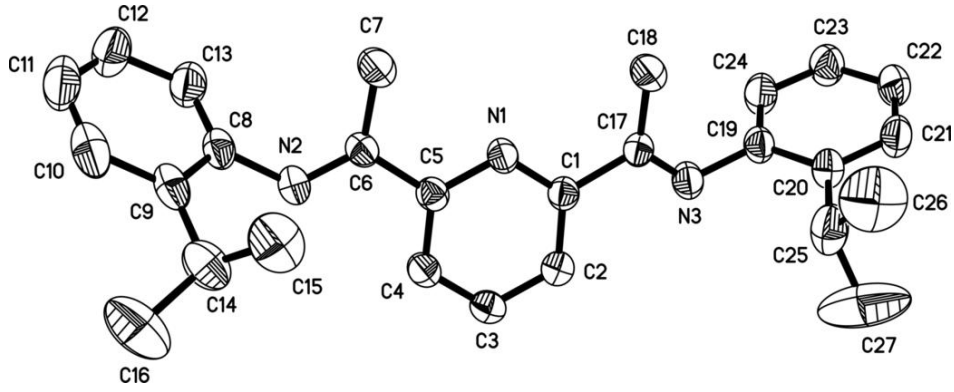
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7A···N1	0.96	2.46	2.799 (3)	100
C14—H14···N2	0.98	2.46	2.830 (4)	101
C18—H18A···N1	0.96	2.47	2.819 (3)	101
C25—H25···N3	0.98	2.39	2.892 (4)	111
C3—H3···Cg1^{i}	0.93	2.75	3.450 (3)	133

C23—H23···Cg2^{ii}	0.93	2.97	3.801 (4)	149
C12—H12···Cg3^{ii}	0.93	3.16	3.961 (10)	146
C15—H15B···Cg1^{iii}	0.96	3.17	3.757 (13)	121
C15—H15C···Cg1^{iii}	0.96	3.44	3.757 (13)	102

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

Fig. 1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C7
C18
C23
C11
C13
C24
C22
C8
N1
C17
C19
C21
N2
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C1
C10
C6
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C9
N3
C25
C15
C2
C14
C4
C3
C27
C16

Fig. 2

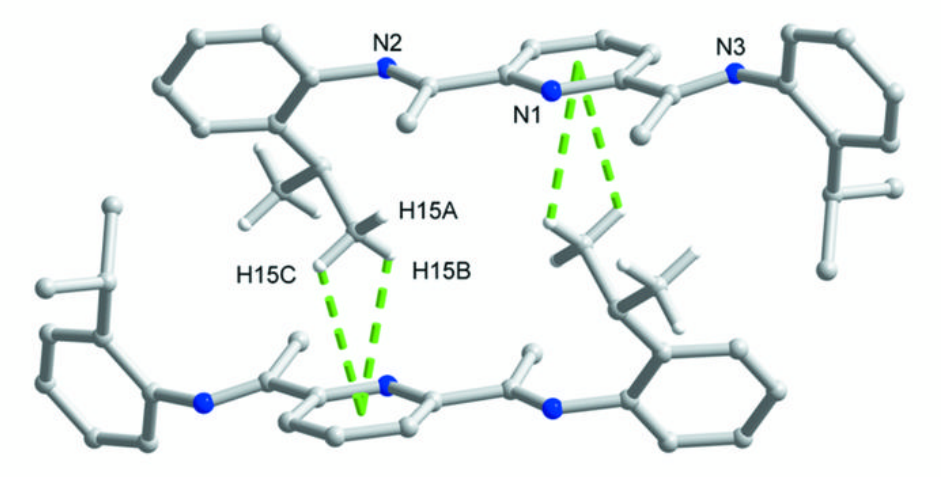

Figure 2.

Fig. 3

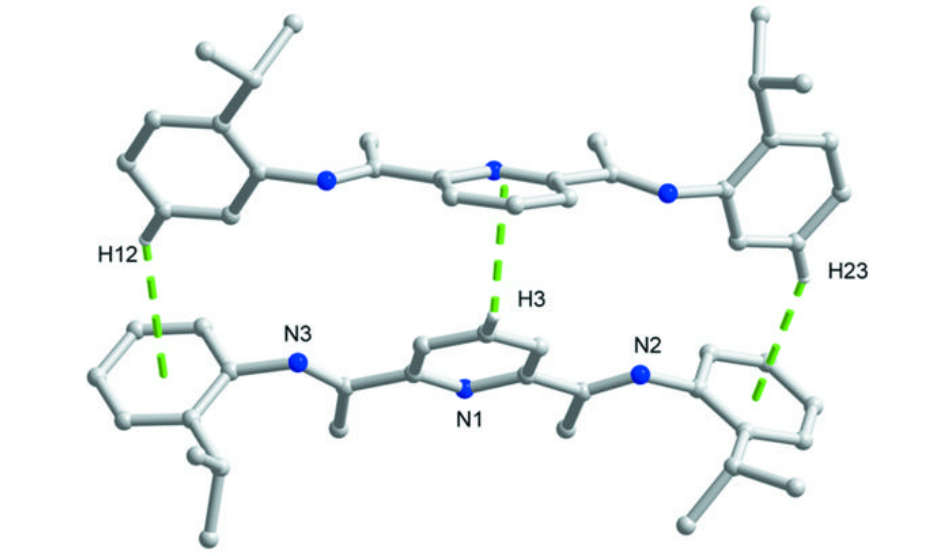

Figure 3.

Fig. 4

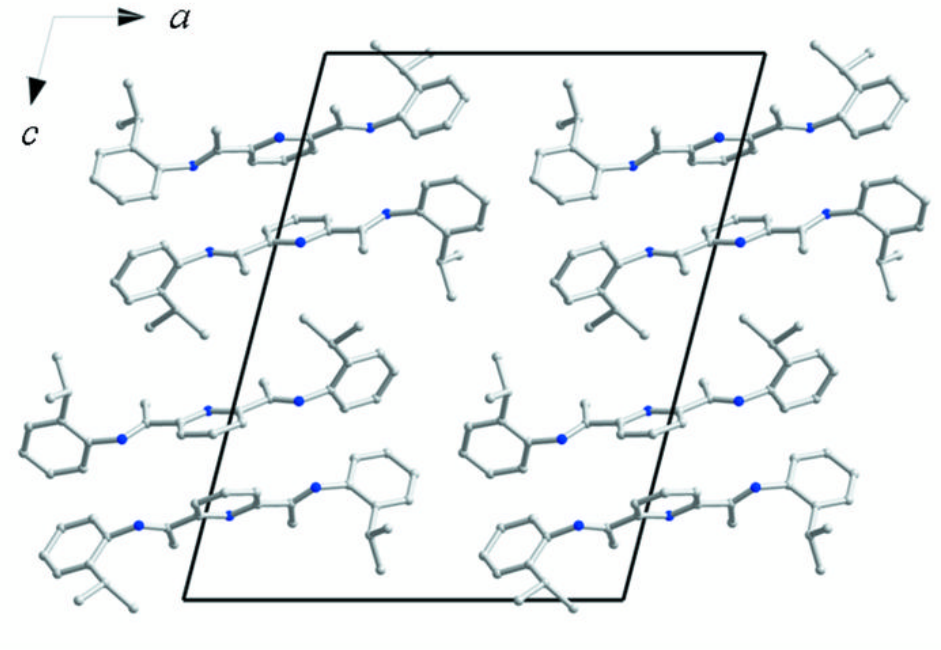

Figure 4.