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

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Key indicators

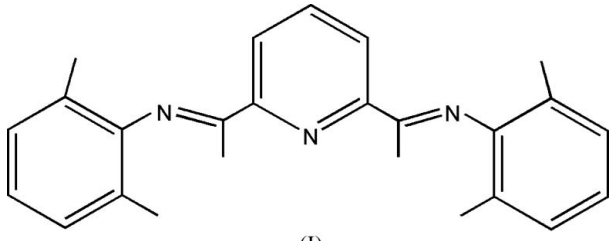
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.053
wR factor = 0.180
Data-to-parameter ratio = 19.6

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

In the molecule of the title compound, $C_{25}H_{27}N_3$, the two 2,6-dimethyl-substituted phenyl rings are connected to the pyridine ring *via* the C=N imine bonds. Although the compound includes three N atoms, there are no obvious hydrogen-bond or π–π interactions in the crystal structure.

Comment

Recently, much attention has been focused on multidentate complexes of late transition metals which show high catalytic activity for olefin polymerization (Ittel *et al.*, 2000). One of the most effective ethylene polymerization catalysts is an Fe^{II} or Co^{II} *N*,*N*,*N*-diiminopyridyl-type complex (Small & Brookhart, 1998; Small *et al.*, 1998; Britovsek *et al.*, 1999; Kooistra *et al.*, 2003). It is well known that the steric bulk of the *ortho* substituents on the imino nitrogen donors of the diimino-pyridyl catalysts plays a pivotal role in determining the selectivity of the catalyst. Here, we present the crystal structure of the title compound, (I).



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The two imino C=N bonds have distinctive double-bond character. Rings 1 (atoms N1/C1–C5), 2 (atoms C10–C15) and 3 (atoms C18–C23) make the following dihedral angles: 1/2 = 86.71 (3)°, 1/3 = 66.70 (4)° and 2/3 = 51.31 (5)°.

As can be seen from the packing diagram (Fig. 2), the molecules are extended along the *c* axis and stacked along the *b* axis. Dipole–dipole and van der Waals interactions are also effective in the molecular packing in the crystal structure.

Experimental

The title compound was synthesized according to the literature method of Britovsek *et al.* (1999). 2,6-Dimethylaniline (0.177 ml, 1.426 mmol) was added to a solution of 2,6-diacetylpyridine (120 mg, 0.713 mmol) in absolute ethanol (10 ml). After the addition of a few drops of glacial acetic acid, the solution was refluxed overnight. Upon cooling to room temperature, single crystals were obtained by slow evaporation of a solution in ethanol/methanol (1:1).

Crystal data

$C_{25}H_{27}N_3$
M_r = 369.51
Monoclinic, $P2_1/n$
a = 10.340 (6) Å
b = 14.433 (5) Å
c = 15.185 (7) Å
β = 105.92 (2)°
V = 2179.2 (17) Å^3
Z = 4
D_x = 1.126 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 296 (2) K
Block, yellow
0.65 × 0.58 × 0.55 mm

Data collection

Rigaku Weissenberg IP diffractometer
ω scans
Absorption correction: multi-scan (*TEXSAN*; Molecular Structure Corporation, 1998)
T_{min} = 0.861, T_{max} = 0.994
20802 measured reflections
4978 independent reflections
3655 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.180
S = 1.08
4978 reflections
254 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0998P)^2 + 0.19P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.025 (3)

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.3364 (18)	N2—C10	1.4247 (18)
N1—C5	1.3406 (17)	N3—C8	1.2705 (18)
N2—C6	1.2651 (19)	N3—C18	1.423 (2)
C1—N1—C5	118.24 (12)	N1—C5—C8	116.21 (12)
C6—N2—C10	121.59 (13)	N2—C6—C1	116.74 (13)
C8—N3—C18	121.45 (13)	N2—C6—C7	125.68 (13)
N1—C1—C2	122.72 (13)	N3—C8—C9	125.63 (14)
N1—C1—C6	116.72 (12)	N3—C8—C5	117.37 (13)
N1—C5—C4	122.38 (13)		

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.2 for aromatic and x = 1.5 for methyl H atoms.

Data collection: *TEXSAN* (Molecular Structure Corporation, 1998); cell refinement: *TEXSAN*; data reduction: *TEXSAN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL97*.

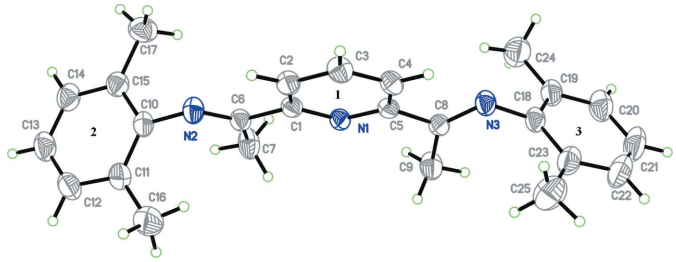


Figure 1
The molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

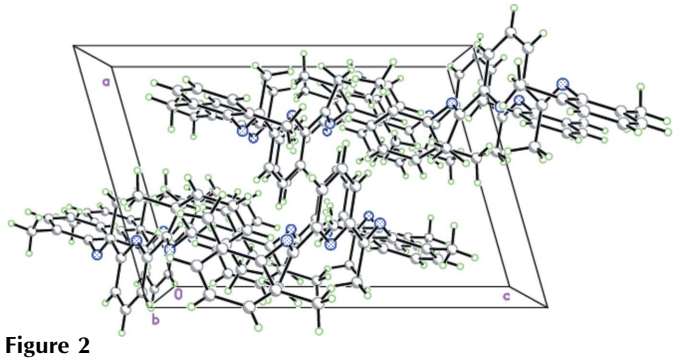


Figure 2
A packing diagram of (I), viewed along the *b* axis.

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