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6-Methyl-2-[2,2,6,6-tetramethyl-5-(2-pyridyl)-hepta-3,4-dien-3-yl]pyridine

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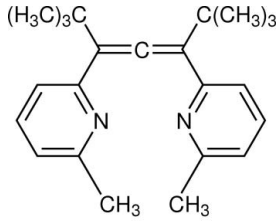
The title compound, $C_{21}H_{26}N_2$, a potential chiral ligand for transition metal-catalysed reactions, crystallizes with one molecule in the asymmetric unit; the molecule has a pseudo-twofold axis perpendicular to the central C=C=C fragment.



(I)

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.110
Data-to-parameter ratio = 20.1

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

Experimental

The title compound, (I), was synthesized in racemic form by S_N2' substitution of a propargyl acetate with a cyanocuprate (Krause & Hoffmann-Röder, 2004). It was dissolved in a small amount of tetrahydrofuran and hexane, and crystals were obtained by evaporation.

Crystal data

$C_{23}H_{30}N_2$
M_r = 334.49
Triclinic, $P\overline{1}$
a = 9.6201 (8) Å
b = 10.4931 (12) Å
c = 11.1713 (11) Å
α = 90.172 (6)°
β = 110.536 (6)°
γ = 97.963 (6)°
V = 1044.22 (18) Å^3
Z = 2
D_x = 1.064 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 16854 reflections
θ = 3.0–27.5°
μ = 0.06 mm^{-1}
T = 291 (1) K
Block, colourless
0.30 × 0.30 × 0.25 mm

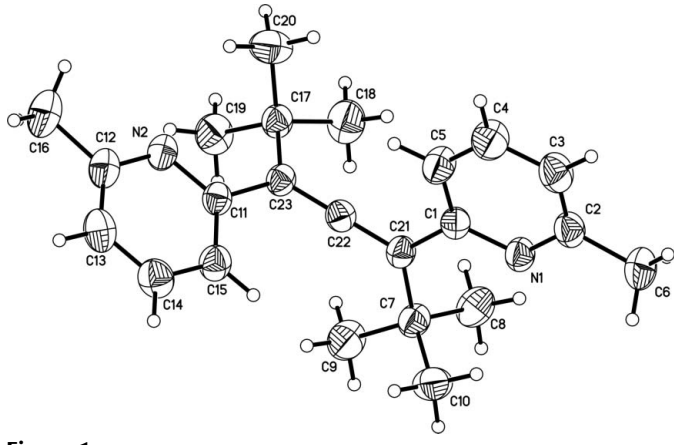


Figure 1
The molecular structure of the title compound, showing the labellng of all non-H atoms. Displacement ellipsoids are shown at the 30% probability level.

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.032$
ω scans	$\theta_{max} = 27.5^\circ$
Absorption correction: none	$h = -12 \rightarrow 12$
16854 measured reflections	$k = -13 \rightarrow 13$
4706 independent reflections	$l = -14 \rightarrow 13$
1974 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.110$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.12$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
4706 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
234 parameters	

H atoms were placed in calculated positions, with C—H = 0.93–0.96 Å, and were refined as riding, with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl or $1.2U_{eq}(C)$ for others; the methyl groups were allowed to rotate but not to tip.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*, *PARST95* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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