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2,6-Dimethylquinoline

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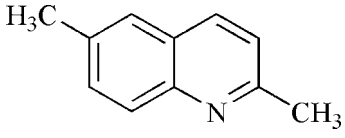
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.101; data-to-parameter ratio = 10.8.

The title compound, $C_{11}H_{11}N$, excluding the methyl H atoms, is planar. The H atoms of the methyl groups are disordered over two sites of equal occupancy.

Related literature

For related literature, see: Beadle *et al.* (2005); Geneste *et al.* (2006); Schäfer *et al.* (2003).



Experimental

Crystal data

$C_{11}H_{11}N$
M_r = 157.21
Orthorhombic, $P2_12_12_1$
a = 5.9497 (3) Å
b = 10.6987 (8) Å
c = 13.4021 (12) Å
V = 853.10 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 113 (2) K
0.20 × 0.16 × 0.14 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Molecular Structure Corporation & Rigaku, 1999)
T_{min} = 0.986, T_{max} = 0.990
10784 measured reflections
1202 independent reflections
1098 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.102
S = 1.15
1202 reflections
111 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2096).

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supplementary materials

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Comment

The derivatives of quinoline are of great significance as a result of their various bioactivities. For example, they can be used as antagonists, matrix metalloproteinase inhibitors and glucocorticoid mimetics (Geneste, *et al.* 2006; Beadle, *et al.*, 2005; Schäfer, *et al.*, 2003). In this paper we present the crystal structure of the title compound, 2,6-dimethylquinoline, (I).

The two methyl groups are coplanar with the quinoline ring, which is almost planar, with an r. m. s. derivation of 0.0111 (2) Å. The H atoms of the methyl groups are disordered 50:50 over two sites.

Experimental

The title compound was bought from Shanghai Kuilin Chemical Co., Ltd. as the synthetic raw material. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a CH_2Cl_2 solution.

Refinement

All H atoms were positioned geometrically and refined as riding with C—H = 0.95 and 0.98 Å. For the CH groups, U_{iso}(H) values are set equal to 1.2U_{eq}(carrier atom) and for the methyl groups they are set equal to 1.5U_{eq}(carrier atom). The H atoms of the methyl groups are disordered over two sites [both occupancies 0.50:0.50].

Figures

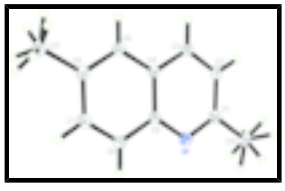

Fig. 1. View of a molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

2,6-dimethylquinoline

Crystal data

$C_{11}H_{11}N$	D_x = 1.224 Mg m^{-3}
M_r = 157.21	Melting point: 328 K
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71070 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2085 reflections
a = 5.9497 (3) Å	θ = 3.0–25.0°
b = 10.6987 (8) Å	μ = 0.07 mm^{-1}

c = 13.4021 (12) Å	T = 113 (2) K
V = 853.10 (11) Å^3	Plate, colourless
Z = 4	0.20 × 0.16 × 0.14 mm
F_{000} = 336	

Data collection

Rigaku Saturn diffractometer	R_{int} = 0.048
Radiation source: rotating anode	θ_{max} = 27.9º
Monochromator: confocal	θ_{min} = 2.4º
T = 113(2) K	h = −7→7
ω scans	k = −14→14
Absorption correction: multi-scan (Crystalclear; Molecular Structure Corporation & Rigaku, 1999)	l = −17→17
T_{min} = 0.986, T_{max} = 0.990	Standard reflections: .;
10784 measured reflections	every . reflections
1202 independent reflections	intensity decay: .
1098 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.041	$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 0.0963P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.102	$(\Delta/\sigma)_{max} < 0.001$
S = 1.15	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
1202 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
111 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.046 (7)
Secondary atom site location: difference Fourier map	

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}	Occ. (<1)
N1	1.0066 (2)	0.52180 (13)	0.07529 (10)	0.0232 (4)	
C1	0.9191 (3)	0.46134 (15)	−0.00134 (13)	0.0226 (4)	
C2	0.7025 (3)	0.48864 (16)	−0.04071 (13)	0.0228 (4)	
H2	0.6453	0.4420	−0.0954	0.027*	
C3	0.5771 (3)	0.58242 (15)	0.00067 (12)	0.0216 (4)	
H3	0.4325	0.6019	−0.0251	0.026*	
C4	0.6660 (3)	0.65016 (15)	0.08253 (12)	0.0192 (4)	
C5	0.8820 (3)	0.61591 (15)	0.11774 (12)	0.0201 (4)	
C6	0.9720 (3)	0.68026 (16)	0.20107 (13)	0.0240 (4)	
H6	1.1162	0.6582	0.2259	0.029*	
C7	0.8528 (3)	0.77392 (17)	0.24591 (13)	0.0258 (4)	
H7	0.9168	0.8167	0.3011	0.031*	
C8	0.6361 (3)	0.80873 (15)	0.21201 (13)	0.0231 (4)	
C9	0.5470 (3)	0.74754 (15)	0.13096 (12)	0.0211 (4)	
H9	0.4028	0.7710	0.1070	0.025*	
C10	1.0594 (4)	0.35966 (16)	−0.04720 (15)	0.0314 (5)	
H10A	1.2025	0.3532	−0.0113	0.047*	0.50
H10B	1.0884	0.3796	−0.1174	0.047*	0.50
H10C	0.9789	0.2800	−0.0428	0.047*	0.50
H10D	0.9774	0.3220	−0.1030	0.047*	0.50
H10E	1.0914	0.2956	0.0031	0.047*	0.50
H10F	1.2010	0.3952	−0.0716	0.047*	0.50
C11	0.5081 (4)	0.90984 (16)	0.26553 (14)	0.0306 (5)	
H11A	0.5989	0.9418	0.3209	0.046*	0.50
H11B	0.3671	0.8755	0.2915	0.046*	0.50
H11C	0.4749	0.9780	0.2190	0.046*	0.50
H11D	0.3617	0.9217	0.2334	0.046*	0.50
H11E	0.5935	0.9881	0.2627	0.046*	0.50
H11F	0.4857	0.8856	0.3353	0.046*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0235 (7)	0.0234 (7)	0.0227 (7)	0.0014 (7)	0.0019 (6)	0.0027 (6)
C1	0.0255 (9)	0.0203 (8)	0.0220 (8)	−0.0001 (7)	0.0037 (7)	0.0034 (7)
C2	0.0262 (9)	0.0208 (8)	0.0213 (9)	−0.0043 (8)	0.0002 (7)	0.0000 (7)
C3	0.0189 (8)	0.0243 (8)	0.0218 (8)	−0.0024 (7)	0.0001 (7)	0.0023 (7)
C4	0.0199 (8)	0.0193 (8)	0.0185 (8)	−0.0021 (7)	0.0019 (7)	0.0029 (7)
C5	0.0198 (8)	0.0204 (8)	0.0200 (8)	−0.0005 (7)	0.0023 (7)	0.0039 (7)
C6	0.0211 (9)	0.0305 (9)	0.0205 (9)	−0.0022 (8)	−0.0020 (7)	0.0027 (7)
C7	0.0285 (10)	0.0270 (9)	0.0219 (9)	−0.0045 (8)	−0.0014 (8)	−0.0006 (7)
C8	0.0278 (9)	0.0202 (8)	0.0213 (9)	−0.0017 (7)	0.0048 (8)	0.0014 (7)
C9	0.0196 (8)	0.0213 (8)	0.0225 (8)	0.0002 (7)	0.0028 (7)	0.0035 (7)
C10	0.0348 (11)	0.0266 (9)	0.0327 (10)	0.0047 (9)	0.0031 (9)	−0.0022 (8)

C11	0.0381 (10)	0.0259 (9)	0.0279 (10)	0.0033 (9)	0.0055 (8)	−0.0024 (7)

Geometric parameters (Å, °)

N1—C1	1.321 (2)	C8—C9	1.375 (2)
N1—C5	1.374 (2)	C8—C11	1.505 (2)
C1—C2	1.423 (2)	C9—H9	0.9500
C1—C10	1.503 (2)	C10—H10A	0.9800
C2—C3	1.368 (2)	C10—H10B	0.9800
C2—H2	0.9500	C10—H10C	0.9800
C3—C4	1.417 (2)	C10—H10D	0.9800
C3—H3	0.9500	C10—H10E	0.9800
C4—C9	1.417 (2)	C10—H10F	0.9800
C4—C5	1.418 (2)	C11—H11A	0.9800
C5—C6	1.417 (2)	C11—H11B	0.9800
C6—C7	1.367 (2)	C11—H11C	0.9800
C6—H6	0.9500	C11—H11D	0.9800
C7—C8	1.417 (3)	C11—H11E	0.9800
C7—H7	0.9500	C11—H11F	0.9800
C1—N1—C5	117.92 (15)	H10A—C10—H10D	141.1
N1—C1—C2	123.02 (16)	H10B—C10—H10D	56.3
N1—C1—C10	116.98 (16)	H10C—C10—H10D	56.3
C2—C1—C10	120.00 (17)	C1—C10—H10E	109.5
C3—C2—C1	119.62 (17)	H10A—C10—H10E	56.3
C3—C2—H2	120.2	H10B—C10—H10E	141.1
C1—C2—H2	120.2	H10C—C10—H10E	56.3
C2—C3—C4	119.05 (17)	H10D—C10—H10E	109.5
C2—C3—H3	120.5	C1—C10—H10F	109.5
C4—C3—H3	120.5	H10A—C10—H10F	56.3
C9—C4—C3	122.98 (15)	H10B—C10—H10F	56.3
C9—C4—C5	119.38 (15)	H10C—C10—H10F	141.1
C3—C4—C5	117.63 (15)	H10D—C10—H10F	109.5
N1—C5—C6	118.59 (16)	H10E—C10—H10F	109.5
N1—C5—C4	122.76 (16)	C8—C11—H11A	109.5
C6—C5—C4	118.65 (15)	C8—C11—H11B	109.5
C7—C6—C5	120.43 (17)	H11A—C11—H11B	109.5
C7—C6—H6	119.8	C8—C11—H11C	109.5
C5—C6—H6	119.8	H11A—C11—H11C	109.5
C6—C7—C8	121.59 (17)	H11B—C11—H11C	109.5
C6—C7—H7	119.2	C8—C11—H11D	109.5
C8—C7—H7	119.2	H11A—C11—H11D	141.1
C9—C8—C7	118.64 (16)	H11B—C11—H11D	56.3
C9—C8—C11	121.58 (17)	H11C—C11—H11D	56.3
C7—C8—C11	119.77 (17)	C8—C11—H11E	109.5
C8—C9—C4	121.29 (16)	H11A—C11—H11E	56.3
C8—C9—H9	119.4	H11B—C11—H11E	141.1
C4—C9—H9	119.4	H11C—C11—H11E	56.3
C1—C10—H10A	109.5	H11D—C11—H11E	109.5
C1—C10—H10B	109.5	C8—C11—H11F	109.5

H10A—C10—H10B	109.5	H11A—C11—H11F	56.3
C1—C10—H10C	109.5	H11B—C11—H11F	56.3
H10A—C10—H10C	109.5	H11C—C11—H11F	141.1
H10B—C10—H10C	109.5	H11D—C11—H11F	109.5
C1—C10—H10D	109.5	H11E—C11—H11F	109.5
C5—N1—C1—C2	−0.6 (2)	C9—C4—C5—C6	0.3 (2)
C5—N1—C1—C10	179.40 (14)	C3—C4—C5—C6	−178.47 (15)
N1—C1—C2—C3	0.8 (2)	N1—C5—C6—C7	−179.55 (15)
C10—C1—C2—C3	−179.16 (15)	C4—C5—C6—C7	−0.4 (2)
C1—C2—C3—C4	−0.3 (2)	C5—C6—C7—C8	0.8 (3)
C2—C3—C4—C9	−179.10 (15)	C6—C7—C8—C9	−1.1 (3)
C2—C3—C4—C5	−0.4 (2)	C6—C7—C8—C11	178.20 (16)
C1—N1—C5—C6	178.96 (15)	C7—C8—C9—C4	1.0 (2)
C1—N1—C5—C4	−0.2 (2)	C11—C8—C9—C4	−178.31 (15)
C9—C4—C5—N1	179.40 (14)	C3—C4—C9—C8	178.10 (15)
C3—C4—C5—N1	0.6 (2)	C5—C4—C9—C8	−0.6 (2)

Fig. 1