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Methyl 2-(2-pyridyl)quinoline-4-carboxylate

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.107
Data-to-parameter ratio = 8.5

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

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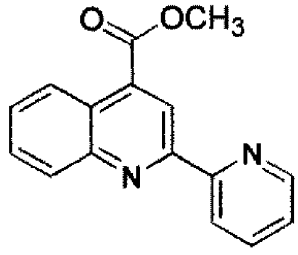
The synthesis and structure of the title compound, $C_{16}H_{12}N_2O_2$, are described. The observed conformation in the solid state is similar to that determined previously by ^{1}H NMR and two-dimensional COSY NMR analysis.

Comment

The photophysical properties and the excited-state chemistry of tris(bipyridyl)ruthenium(II) complexes have been investigated to a great extent because of their unique and interesting features such as chemical stability, reversible redox property, long excited-state life time and chelation properties (Juris *et al.*, 1988). 2,2′-Bipyridine is the prototype ligand of almost all reported Ru^{II} tris-chelate complexes (Kaes *et al.*, 2000). Synthetically, it lacks a suitable peripheral chemical functionality that allows it to be bound into a diverse array of substrates. To address this dilemma, a rigorous synthetic research effort towards the structural variation of the commonly used ligands, such as bipyridines, phenanthrolines and terpyridines, must be conducted in order to develop such analogues, where differences in electronic and steric properties may lead to modification of the resulting metal complexes. We have synthesized and characterized a novel diimine ligand, methyl 2-(2-pyridyl)quinoline-4-carboxylate, (I), and covalently bound it into a polymeric matrix (Farah *et al.*, 2000) and on to CdS nanoparticle (Veinot *et al.*, 2000). We report here the synthesis and crystal structure of (I).



(I)

The *ORTEP*II (Johnson, 1976) diagram of (I) (Fig. 1) reveals the expected conformation of the ligand in the solid state as the two N atoms are in the *trans* configuration to minimize electronic repulsion. The packing (Fig. 2) also precludes interaction between adjacent molecules and reveals an alternating flat/tilt array typical of molecular crystals (Gray & Goodby, 1984). All observed C—C, C—N and C—O bond lengths are in good agreement with those reported in the literature and do not merit any further discussion (*International Tables for Crystallography*, 1995, Vol. C).

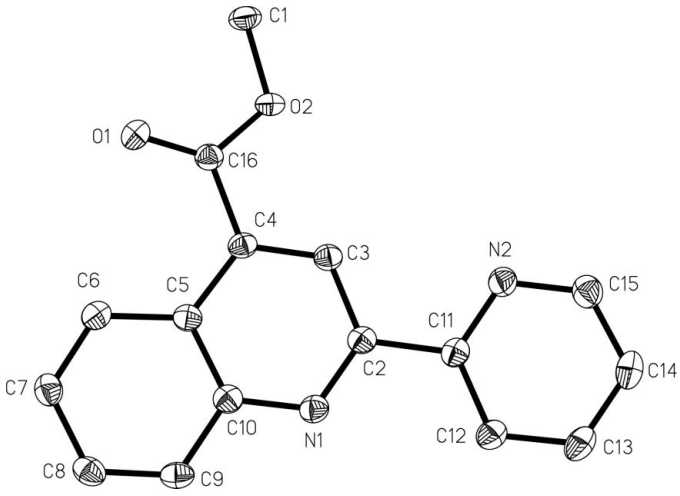


Figure 1
*ORTEP*II drawing with atomic numbering of the title compound. Displacement ellipsoids are plotted with 50% probability. H atoms have been omitted for clarity.

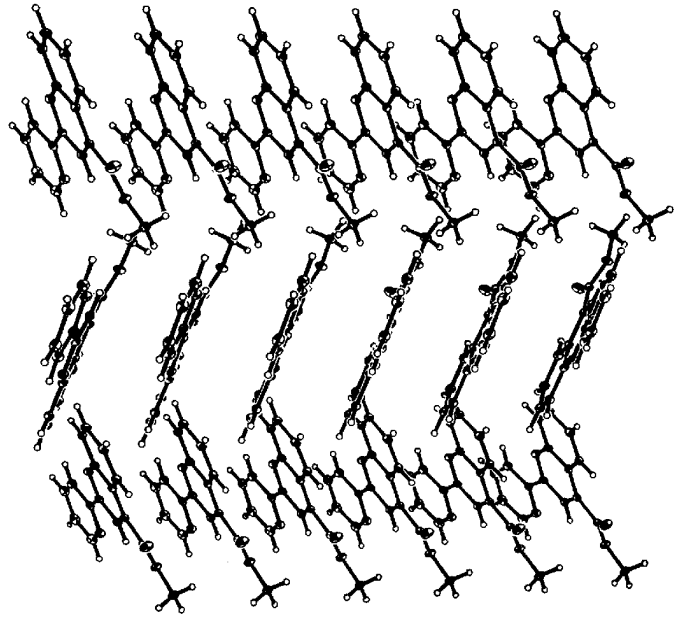


Figure 2
Packing diagram of the title compound viewed along the *b* axis.

Experimental

4.00 g (16 mmol) of 2-(2-pyridyl)-4-carboxyquinolic acid were dissolved in 70 ml of freshly distilled benzene. 4.10 g (128 mmol) of methanol and 5 ml of H_2SO_4 were added successively and the reaction mixture was refluxed overnight. The reaction product was then poured into 150 ml of water and extracted with (3 × 30 ml) of ether. The ethereal layer was washed with 5% $NaHCO_3$, then with water and was dried over $MgSO_4$. After removal of the solvent the resultant product was recrystallized from ethanol; yield: 3.47 g (81%).

Crystal data

$C_{16}H_{12}N_2O_2$	D_x = 1.420 Mg m^{-3}
M_r = 264.28	Mo $K\alpha$ radiation
Monoclinic, *C*2	Cell parameters from 9674 reflections
a = 29.332 (3) Å	θ = 2.6–27.5°
b = 3.8551 (2) Å	μ = 0.10 mm^{-1}
c = 11.0753 (11) Å	*T* = 100 (2) K
β = 99.341 (3)°	Needle, light gold
V = 1235.76 (19) Å^3	0.20 × 0.10 × 0.05 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	1352 reflections with $I > 2\sigma(I)$
φ scans, and ω scans with κ offsets	R_{int} = 0.024
Absorption correction: multi-scan (*DENZO–SMN*; Otwinowski & Minor, 1997)	θ_{max} = 27.4°
T_{min} = 0.981, T_{max} = 0.995	*h* = 0 → 37
9674 measured reflections	*k* = 0 → 4
1538 independent reflections	*l* = −14 → 14
	Intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0647P)^2 + 0.8852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.041	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.107	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
S = 0.89	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
1538 reflections	
181 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.322 (3)	O2—C16	1.335 (3)
N1—C10	1.364 (3)	O2—C1	1.456 (3)
N2—C15	1.338 (3)	C2—C3	1.418 (3)
N2—C11	1.346 (3)	C3—C4	1.369 (3)
O1—C16	1.204 (3)		
C2—N1—C10	118.25 (19)	N1—C2—C3	122.7 (2)
C15—N2—C11	117.3 (2)	N1—C2—C11	117.32 (19)
C16—O2—C1	115.88 (17)	C4—C3—C2	120.2 (2)

Data collection: *COLLECT* (Nonius, 1997–2001); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *SHELXTL/PC* (Sheldrick 1999); program(s) used to refine structure: *SHELXTL/PC*; molecular graphics: *SHELXTL/PC*.

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