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1-(6-Methylpyridin-2-yl)-2-phenylethanedione

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.066
wR factor = 0.153
Data-to-parameter ratio = 12.9

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

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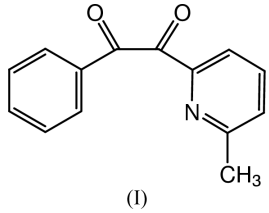
The phenyl and pyridyl rings of the title compound, $C_{14}H_{11}NO_2$, are nearly perpendicular to each other, with a dihedral angle of 86.1 (1)°. In the crystal, the molecules exist as centrosymmetrically hydrogen-bonded C—H···O dimers and the molecular packing is stabilized by C—H···π and π···π interactions.

Comment

Recently, we have investigated photo-induced oxygenation reactions of indolizine derivatives (Tian *et al.*, 2001). In a continuation of this work, we report here the crystal structure of the title compound, (I), which was obtained by photo-induced oxygenation of 1-benzoyl-5-methyl-2-phenyl-indolizine in acetonitrile.



(I)

The bond lengths in the title compound (Fig. 1) are comparable to the mean values reported by Allen *et al.* (1987). The C6—C7 distance of 1.536 (3) Å is significantly longer than the value of 1.48 Å expected for a Csp^2—Csp^2 bond. This lengthening may be due to the repulsion between the two O atoms. The two aromatic rings, phenyl and pyridyl rings, are mutually nearly orthogonal, with a dihedral angle of 86.1 (1)°. In the solid state, the molecules form centrosymmetrically C4—H4···O1^{i} [symmetry code: (i) = $-x, 2-y, -z$] hydrogen-bonded dimers (Table 1). Weak intermolecular C2—H2···π_{phenyl} interactions link the dimers to form infinite one-dimensional molecular chains parallel to [110] (Fig. 2). The crystal packing is further stabilized by π···π stacking interactions involving the pyridyl ring and its symmetry equivalent at $(-x, 1-y, -z)$ [centroid separation 3.659 (1) Å].

Experimental

The title compound was isolated from the reaction mixture, obtained by the photo-oxygenation of 1-benzoyl-5-methyl-2-phenylindolizine in acetonitrile, by column chromatography on silica gel. Single crystals suitable for X-ray crystallographic measurement were grown by slow evaporation of a petroleum ether-ethyl acetate solution (5:1 *v*/*v*) of the compound.

Crystal data

$C_{14}H_{11}NO_2$	$Z = 2$
$M_r = 225.24$	$D_x = 1.310$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.9526$ (9) Å	Cell parameters from 1413 reflections
$b = 8.0441$ (10) Å	$\theta = 2.5$–$28.3°$
$c = 9.1229$ (11) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 90.953$ (2)°	$T = 293$ (2) K
$\beta = 101.247$ (2)°	Slab, pale yellow
$\gamma = 93.647$ (2)°	0.50 × 0.42 × 0.10 mm
$V = 570.99$ (12) Å^3	

Data collection

Siemens SMART CCD area detector diffractometer	1820 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.011$
ω scans	$\theta_{max} = 27.0°$
Absorption correction: none	$h = -10 \rightarrow 9$
3296 measured reflections	$k = -10 \rightarrow 9$
2408 independent reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.2157P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.066$	
$wR(F^2) = 0.153$	
$S = 1.15$	$(\Delta/\sigma)_{max} < 0.001$
2408 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
187 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.92 (2)	2.54 (2)	3.442 (3)	169 (2)
C2—H2···Cg(phenyl)^{ii}	0.96 (3)	2.99 (4)	3.931 (4)	167 (2)

Symmetry codes: (i) $-x, 2-y, -z$; (ii) $1-x, 1-y, -z$.

The H atoms of the aromatic rings were located from a difference Fourier map and were refined isotropically; those attached to the methyl C14 were fixed geometrically and treated as riding atoms, with a C—H distance of 0.96 Å and U_{iso}(H) set equal to $1.5U_{eq}$(C). Owing to a large fraction of weak data at higher angles, the 2θ maximum was limited to 54° during the refinement.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* and *SADABS* (Sheldrick, 1996); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

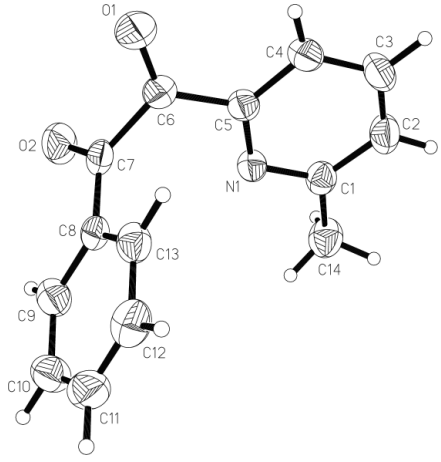


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

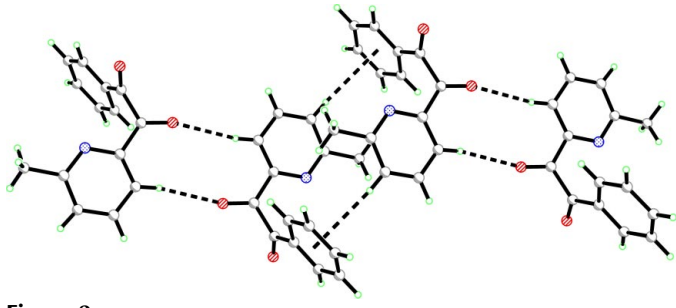


Figure 2
Arrangement of hydrogen-bonded dimers and π-stacking, viewed normal to (110).

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