Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

8-Quinolyl benzoate

Gang Lei

Department of Chemistry, China West Normal University, Nanchong 637002, People's Republic of China

Correspondence e-mail: leigang307@yahoo.com.cn

Received 18 September 2006
Accepted 20 September 2006

In the title compound, $C_{16}H_{11}NO_2$, the ester group is twisted away from the quinoline benzene ring by 77.32 (4)°. Molecules are linked into centrosymmetric $R_2^2(16)$ dimers by C—H···O hydrogen bonds.

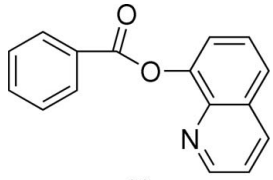
Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.124
Data-to-parameter ratio = 16.1

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

Comment

8-Hydroxyquinoline benzoates were developed as a new set of derivatives for highly sensitive fluorescent chemosensors for transition metal ions (Zhang *et al.*, 2005). We report here the crystal structure of the title compound, (I).



(I)

Bond lengths and angles in (I) are normal. The quinoline ring system is planar with a maximum deviation of 0.011 (1) Å for atom N1. As a result of steric effects, the substituent group at atom C8 is twisted away from the plane of the quinoline ring system (Fig. 1). The O1/O2/C8/C10 and C4–C9 planes form a dihedral angle of 77.32 (4)°. The O1/O2/C8/C10 and C11–C16 planes are inclined at an angle of 4.55 (9)°.

The molecules are linked into centrosymmetric $R_2^2(16)$ dimers by C—H···O hydrogen bonds (Table 1). The dimers are stacked along the a axis with weak π–π interactions between the quinoline ring systems, with $Cg1\cdots Cg2^{ii}$ = $Cg2\cdots Cg1^{ii}$ = 3.7020 (7) Å [symmetry code: (ii) $2-x, 1-y, 1-z$], where $Cg1$ and $Cg2$ are the centroids of rings N1/C1–C4/C9 and C4–C9, respectively.

Experimental

Compound (I) was prepared according to the reported precedure of Zhang *et al.* (2005). Yellow single crystals suitable for X-ray diffraction were obtained by recrystallization from ethyl acetate.

Crystal data

$C_{16}H_{11}NO_2$
M_r = 249.26
Monoclinic, $P2_1/c$
a = 6.6322 (3) Å
b = 8.5401 (4) Å
c = 21.5578 (10) Å
β = 92.798 (1)°
V = 1219.57 (10) Å^3
Z = 4
D_x = 1.358 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 (2) K
Block, yellow
0.45 × 0.17 × 0.16 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
11407 measured reflections
2784 independent reflections
2270 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5^{\circ}$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.125$
$S = 1.01$
2784 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2 + 0.1478P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.013 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.95	2.55	3.4128 (15)	151

Symmetry code: (i) $-x+1, -y+1, -z+1$.

All H atoms were placed in calculated positions and refined using a riding model, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

The author thanks the Centre for Testing and Analysis, Cheng Du Branch, Chinese Academy of Sciences, for analytical support.

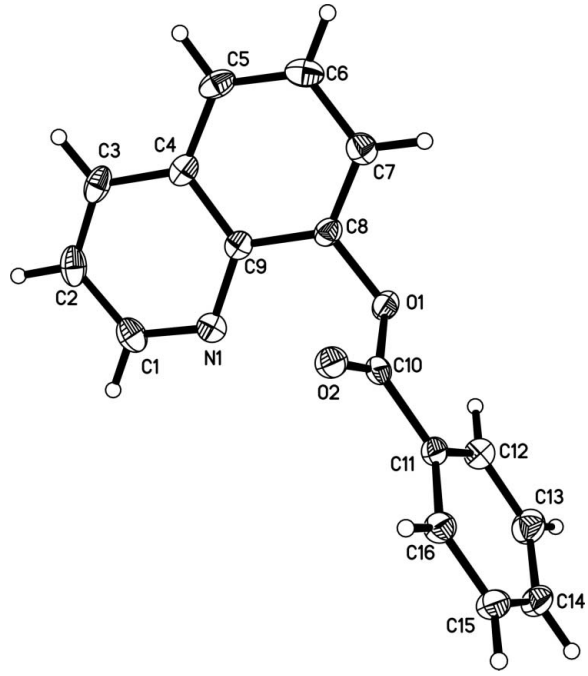


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

References

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Rigaku/MSC (2004). *RAPID-AUTO*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, H., Han, L. F., Zachariasse, K. A. & Jiang, Y. B. (2005). *Org. Lett.* **7**, 4217–4220.