Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*R*)-*N*-(1-Phenylethyl)quinoline-2-carboxamide

Qi-Yun Yang,[a] Zhong-Yuan Zhou[b] and Jian-Ying Qi[a]*

[a]Department of Chemistry, Yunnan Normal University, Kunming, Yunnan, People's Republic of China, and [b]Chengdu Institute of Organic Chemistry, Chinese Academy of Science, Chengdu, Sichuan, People's Republic of China

Correspondence e-mail: bcqijy@polyu.edu.hk

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.090
Data-to-parameter ratio = 12.5

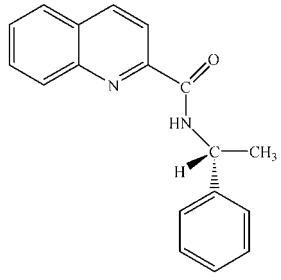
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 20 August 2001
Accepted 30 August 2001
Online 29 September 2001

The quinolyl and phenyl rings in the title compound, $C_{18}H_{16}N_2O$, form a dihedral angle of 89.07 (5)°. The amide group is rotated out of the quinoline ring plane, with a dihedral angle of 21.19 (1)°.

Comment

Recently, we have reported the structure of the tridentate ligand *N*,*N*′-di-2-naphthylpyridine-2,6-dicarboxamide (Qi *et al.*, 2001). Because of the steric effect, the bulky naphthyl ring will hinder coordination of the ligand to a metal ion, so a new chiral bidentate ligand, (I), containing the quinoline-2-carboxamide moiety was synthesized. It is expected that the N atom of the quinoline ring and the amide N atom will coordinate to a metal ion and form a complex with a five-membered ring structure. The quinolyl and phenyl rings in (I) (Fig. 1) are not coplanar, and form a dihedral angle of 89.07 (5)°. The amide group is rotated out of the quinoline ring plane, forming a dihedral angle of 21.19 (1)°. The title compound could have practical applications as a new chiral ligand (Noyori, 1989).



(I)

Experimental

The title compound was synthesized from 2-quinolinecarboxylic acid and (*D*)-α-methylbenzylamine according to the general procedure of Johnson *et al.* (1960). Therefore, the absolute configuration of the chiral centre was known in advance as *R*. The crystal used for the data collection was obtained by slow evaporation from a saturated DMF–water (10:1) solution at room temperature.

Crystal data

$C_{18}H_{16}N_2O$
M_r = 276.33
Monoclinic, $P2_1$
a = 5.5955 (11) Å
b = 10.684 (2) Å
c = 12.224 (2) Å
β = 98.687 (4)°
V = 722.4 (2) Å^3
Z = 2
D_x = 1.270 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2871 reflections
θ = 1–27.5°
μ = 0.08 mm^{-1}
T = 294 (2) K
Plate, colourless
0.28 × 0.20 × 0.10 mm

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.992
4900 measured reflections
2371 independent reflections
1768 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°
$h = -7 \rightarrow 7$
$k = -13 \rightarrow 9$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.090
S = 0.96
2371 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2	0.86	2.41	2.754 (2)	104

The C-bound H atoms were placed at geometrically calculated positions and included in the final refinement using the riding-model approximation.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SHELXTL-NT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

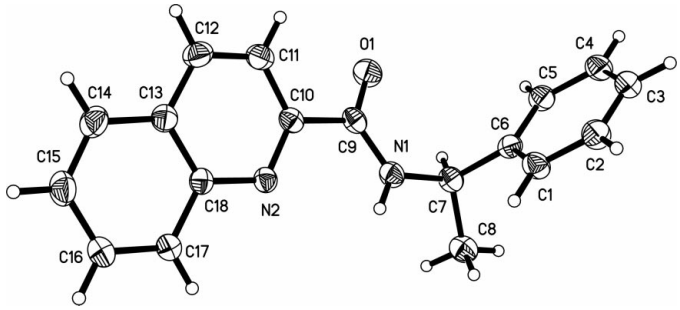


Figure 1
The molecular structure of (I) showing ellipsoids plotted at the 30% probability level (Siemens, 1995).

We acknowledge the financial support of the National Natural Science Foundation of China for this study and the help of the Hong Kong Polytechnic University with the X-ray analysis.

References

Johnson, W. A., King, T. J. & Turner, J. R. (1960). *J. Chem. Soc.* pp. 1509–1511.
Noyori, R. (1989). *Chem. Soc. Rev.* **18**, 187–208.
Qi, J.-Y., Zhou, Z.-Y., Chan, A. S. C. (2001). *Acta Cryst.* E**57**, o749–o750.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Siemens (1995). *SMART* (Version 5.0) and *SHELXTL-NT* (Version 5.10). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.