Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

4-(Quinolin-4-yloxy)phthalonitrile

Hai-Yan Yu, Jin-Ping Xue,* Nai-Sheng Chen and Jin-Ling Huang

Department of Chemistry, Fuzhou University, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: xuejinping66@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.125
Data-to-parameter ratio = 16.0

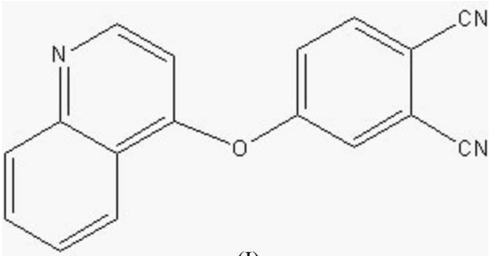
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 November 2005
Accepted 21 December 2005

In the title compound, $C_{17}H_9N_3O$, the dihedral angle between the quinoline group and the dicyanobenzene ring is 66.54 (5)°.

Comment

The title compound, (I), is a precursor in the synthesis of substituted phthalocyanines (Leznoff & Lever, 1996). Phthalocyanines are traditionally used as dyes and pigments (Moser & Thomas, 1983), and they also have other widespread applications, such as photosensitizers for the photodynamic therapy of cancer, semiconductive materials, liquid crystals and nonlinear optics (Leznoff & Lever, 1996).



(I)

The N2—C16 and N3—C17 bond distances (Table 1) agree with the literature values (Subbiah Pandi *et al.*, 2002). The C—C bond distances and C—C—C angles in (I) are in agreement with the expected values for aromatic rings (Allen *et al.*, 1987). The quinoline group is essentially planar and makes a dihedral angle of 66.54 (5)° with the dicyanobenzene ring (Fig. 1).

Experimental

4-Quinolinol (0.36 g, 2.5 mmol) and 4-nitrophthalonitrile (0.433 g, 2.5 mmol) were dissolved in dry dimethylformamide (8 ml). After stirring for about 15 min at room temperature, dry potassium carbonate (0.71 g, 5.1 mmol) was added portionwise over 3 h with stirring. The reaction was stirred for 24 h at room temperature and poured into ice–water (100 g). The reaction mixture was filtered off and washed with water until the filtrate was neutral. Recrystallization from ethanol gave a white product (yield 30%). Single crystals of (I) were obtained from ethanol at room temperature by slow evaporation (m.p. 448.2–449 K).

Crystal data

$C_{17}H_9N_3O$
M_r = 271.27
Orthorhombic, *Pbca*
a = 7.1044 (5) Å
b = 15.5318 (8) Å
c = 24.6393 (2) Å
V = 2718.8 (2) Å^3
Z = 8
D_x = 1.325 Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 11450 reflections
θ = 1.6–27.5°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.55 × 0.20 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.908$, $T_{\max} = 0.989$
15500 measured reflections
3047 independent reflections
1821 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.026$
$\theta_{\max} = 27.5^\circ$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 20$
$l = 0 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.125$
$S = 1.03$
3047 reflections
190 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.1058P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.12$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C10	1.3790 (18)	N1—C1	1.367 (2)
O1—C7	1.3852 (18)	N2—C16	1.142 (2)
N1—C9	1.313 (2)	N3—C17	1.135 (2)
C10—O1—C7	120.20 (12)	C8—C7—O1	124.38 (14)
C9—N1—C1	116.44 (15)	O1—C10—C14	121.96 (14)

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *SHELXL97*.

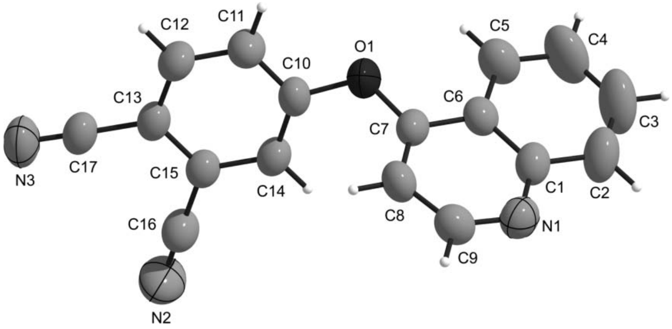


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

This work was supported by the Natural Science Research Foundation of Fujian Province, China (Project No. E0310013), and the Science Technology Research Foundation of Fujian Province, China (Project No. 2003I018).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Brandenburg, K. (2004). *DIAMOND*. Version 3.0. University of Bonn, Germany.

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

Leznoff, C. C. & Lever, A. B. P. (1996). *Phthalocyanines: Properties and Applications*, Vols. 1–4. Weinheim: VCH.

Molecular Structure Corporation (1999). *TEXRAY* (Version 1.10) and *TEXSAN* (Version 1.10). MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.

Moser, F. H. & Thomas, A. L. (1983). *The Phthalocyanines*, Vols. 1 and 2. Boca Raton: CRC Press.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Subbiah Pandi, A., Rajakannan, V., Velmurugan, D., Parvez, M., Kim, M. J., Senthilvelan, A. & Narasinga Rao, S. (2002). *Acta Cryst.* C**58**, o164–o167.

Acta Cryst. (2006). E**62**, o480–o481 Yu *et al.* • $C_{17}H_9N_3O$ **o481**