

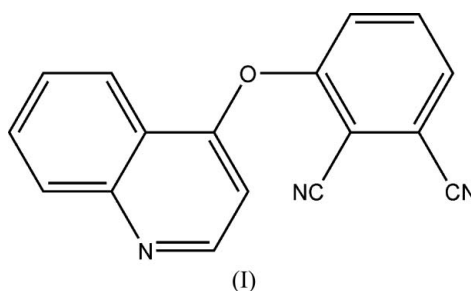
3-(Quinolin-4-yloxy)phthalonitrile

Jin-Ping Xue,* Li-Xuan Cai,
Hai-Yan Yu and Nai-Sheng ChenDepartment of Chemistry, Fuzhou University,
Fuzhou, Fujian 350002, People's Republic of
ChinaCorrespondence e-mail:
xuejinping66@yahoo.com.cn

Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.045
 wR factor = 0.122
Data-to-parameter ratio = 15.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The title compound, $\text{C}_{17}\text{H}_9\text{N}_3\text{O}$, is built up from two planar groups (quinoline and phthalonitrile), with a dihedral angle of $53.96(5)^\circ$ between them. The crystal structure is stabilized by weak $\text{C}-\text{H}\cdots\text{N}$ hydrogen-bond and $\text{C}-\text{N}\cdots\pi$ interactions.Received 11 July 2006
Accepted 15 September 2006

Comment

Substituted phthalonitriles have been used as starting materials for phthalocyanines. Phthalocyanines and metallophthalocyanines have been investigated for many years because of their wide applications, including use in chemical sensors, electrochromism, batteries, semiconducting materials, liquid crystals, Langmuir–Blodgett films and non-linear optics (Leznoff & Lever, 1989–1996). The title compound, (I) (Fig. 1), contains two ring systems, quinoline and phthalonitrile, linked by an O atom. The phthalonitrile ring exhibits normal geometry and is planar. The two cyano groups deviate from this plane by 0.011 (2) and 0.043 (3) Å at atoms N2 and N3, respectively. The quinoline system is also planar, with a maximum deviation of 0.021 (2) Å for atom C2. The phthalonitrile and quinoline groups make a dihedral angle of $53.96(5)^\circ$. The $\text{C}\equiv\text{N}$ bond lengths [$\text{N}2\equiv\text{C}16 = 1.135(2)\text{ \AA}$ and $\text{N}3\equiv\text{C}17 = 1.137(2)\text{ \AA}$] compare well with values reported in the literature (Subbiah Pandi *et al.*, 2002). As expected, the $\text{N}\equiv\text{C}-\text{C}$ angles [$\text{N}2\equiv\text{C}-\text{C} = 179.4(2)^\circ$ and $\text{N}3\equiv\text{C}-\text{C} = 178.6(2)^\circ$] are linear.The crystal structure is stabilized by weak $\text{C}-\text{H}\cdots\text{N}$ hydrogen-bond and $\text{C}-\text{N}\cdots\pi$ interactions (Table 1).

Experimental

3-Nitrophthalonitrile (0.86 g, 5 mmol) and 4-quinolinol (0.72 g, 5 mmol) were dissolved in dry dimethyl sulfoxide (15 ml) and heated at 333 K under an argon atmosphere. After stirring for about 20 min, dry fine-powdered potassium carbonate (1.4 g, 10 mmol) was added portionwise over 2 h with vigorous stirring. The reaction was stirred for 12 h at 333 K. After cooling, the product was poured into ice-water (200 g). The reaction mixture was then filtered and the solid

washed with water until the filtrate was neutral. Recrystallization from ethanol gave a light-yellow product (yield 30%). Single crystals were obtained by slow evaporation of an absolute ethanol solution at room temperature (m.p. 478–479 K).

Crystal data

$C_{17}H_9N_3O$
 $M_r = 271.27$
 Monoclinic, $P2_1/c$
 $a = 8.500$ (5) Å
 $b = 12.679$ (6) Å
 $c = 12.428$ (6) Å
 $\beta = 99.96$ (2)°
 $V = 1319.2$ (11) Å³

$Z = 4$
 $D_x = 1.366$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 293$ (2) K
 Needle, colourless
 $0.50 \times 0.10 \times 0.05$ mm

Data collection

Rigaku Weissenberg IP diffractometer
 ω scans
 Absorption correction: none
 12608 measured reflections

3003 independent reflections
 1707 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.046$
 $\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.122$
 $S = 1.01$
 3003 reflections
 199 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0581P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.14$ e Å⁻³
 $\Delta\rho_{min} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C14-H14\cdots N1^i$	0.93	2.46	3.330 (2)	156
$C1-H1\cdots N3^{ii}$	0.93	2.62	3.454 (3)	149
$C16-N2\cdots Cg^{iii}$	1.14 (1)	3.63 (1)	4.737 (3)	166 (1)

Symmetry codes: (i) $-x + 1, -y + 1, -z$; (ii) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$. Cg is the centroid of the C10–C15 ring.

H atoms were positioned geometrically and allowed to ride on their parent atoms, with $C-H = 0.93$ Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

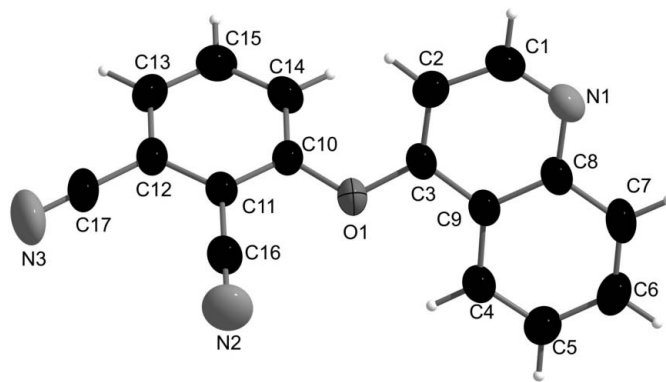


Figure 1

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

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*.

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. 20031018).

References

Brandenburg, K. (2004). *DIAMOND*. Version 3.0. University of Bonn, Germany.
 Leznoff, C. C. & Lever, A. B. P. (1989–1996). *Phthalocyanines: Properties and Applications*, Vols. 1–4. Weinheim, New York: VCH Publishers Inc.
 Molecular Structure Corporation (1999). *TEXRAY* (Version 1.10) and *TEXSAN* (Version 1.10). MSC, The Woodlands, Texas, USA.
 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.* **C58**, o164–o167.