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4-(8-Quinolinoxy)phthalonitrile

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The title compound, $C_{17}H_9N_3O$, cyrstallizes with two molecules in the asymmetric unit. Both independent molecules have essentially the same geometry. The angles between the planes of the quinoline group and the phenyl ring of the phthalonitrile group in the two molecules are 84.36 (4) and 83.69 (4)°.

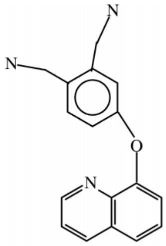
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.115
Data-to-parameter ratio = 13.8

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

Comment

Substituted phthalonitriles have been used as starting materials for phthalocyanines (McKeown, 1988). In addition to their extensive use as dyes and pigments, phthalocyanines have found widespread applications in catalysis, in optical recording, in photoconductive materials, in photodynamic therapy and as chemical sensors (Leznoff & Lever, 1993).



(I)

Fig. 1 shows a perspective view of the asymmetric unit of the title compound, (I), with the numbering scheme. The C10—O1 bond distance is 1.3779 (19) Å in molecule A and 1.3717 (19) Å in molecule B. The triple C≡N bond distances in molecules A and B are in good agreement with those in a related structure in the literature (Karadaı *et al.*, 2003). The

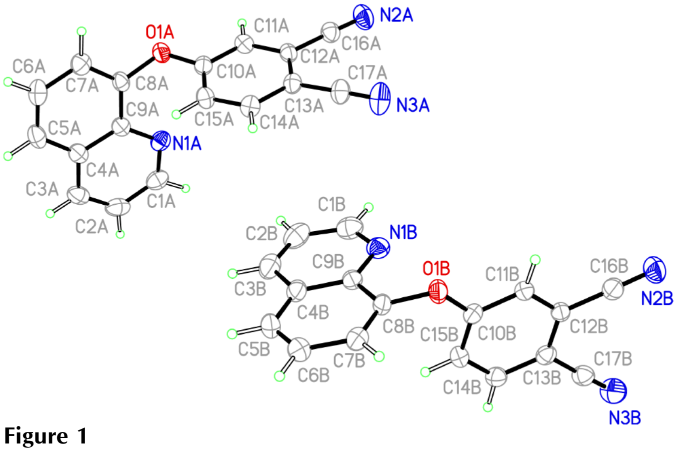


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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quinoline group is essentially planar. The angle between the least-squares planes C1–C9/N1 and C10–C15 is 84.36 (4)° in molecule *A* and 83.69 (4)° in molecule *B*; the maximum deviation from planarity is −0.041 (2) Å for atom C2*A* in the C1*A*–C9*A*/N1*A* ring.

Experimental

8-Quinolinol (1.31 g, 9.03 mmol) and 4-nitrophthalonitrile (1.36 g, 7.86 mmol) were dissolved in dry dimethylformamide (40 ml). After stirring for 30 min at room temperature, dry fine-powdered potassium carbonate (3.25 g, 23.55 mmol) was added portionwise over 2 h with vigorous stirring. The reaction was stirred for 24 h at room temperature and poured into ice-water (200 g). The product was filtered off and washed with (5% *w*/*w*) NaOH solution and water until the filtrate was neutral. Recrystallization from ethanol gave a white product; yield 1.30 g (6.03%). Single crystals were obtained in ethanol at room temperature *via* slow evaporation. Calculated: C 75.27, H3.34, N 15.49%; found: C 75.25, H 3.30, N 15.53%. IR data (Vmax/cm^{-1}): 3060–3020 (Ar—CH), 2210 (CN), 1668, 1596, 1560, 1480, 1464, 1416, 1384, 1364, 1312, 1276, 1236, 1188, 1160, 1128, 1090, 1070, 1050, 1024, 990, 944, 880, 825, 790, 772, 736, 725, 705, 660, 640, 625, 575, 525. ^{1}H NMR (acetone-d_6): 7.30–8.02 (*m*, 7H); 8.48 (*d*, 1H); 8.80 (*d*, 1H). ^{13}C NMR (acetone-d$_6$): 109.03, 116.11, 116.67, 117.92, 122.08, 122.29, 123.21, 127.51, 127.79, 131.39, 136.49, 137.24, 141.80, 150.28, 151.49, 164.03.

Crystal data

$C_{17}H_9N_3O$
M_r = 271.28
Monoclinic, $P2_1/c$
a = 12.7510 (11) Å
b = 14.7398 (12) Å
c = 15.0377 (13) Å
β = 110.3240 (10)°
V = 2650.3 (4) Å^3
Z = 8

D_x = 1.360 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 22448 reflections
θ =1.70–28.70°
μ = 0.09 mm^{-1}
T = 150 (1) K
Plate, colourless
0.36 × 0.27 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min}$ = 0.941, $T_{\rm max}$ = 10.996
21956 measured reflections

6214 independent reflections
4311 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.031
$\theta_{\rm max}$ = 28.7°
$h = -16 \rightarrow 16$
$k = -18 \rightarrow 19$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.115
S = 1.03
6214 reflections
451 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.6288P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.51 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1*B*—C10*B*	1.3717 (19)	C16*A*—N2*A*	1.148 (2)
O1*B*—C8*B*	1.3990 (18)	N1*B*—C1*B*	1.316 (2)
O1*A*—C10*A*	1.3779 (19)	N1*B*—C9*B*	1.368 (2)
O1*A*—C8*A*	1.4048 (18)	C17*B*—N3*B*	1.150 (2)
N1*A*—C1*A*	1.316 (2)	C16*B*—N2*B*	1.149 (2)
N1*A*—C9*A*	1.370 (2)	C17*A*—N3*A*	1.150 (2)
C10*B*—O1*B*—C8*B*	118.22 (12)	C10*A*—O1*A*—C8*A*	117.76 (12)

H atoms were located in a difference Fourier map and refined independently with isotropic displacement parameters. The final C—H distances ranged from 0.94 (2) to 1.01 (2) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

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