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4-(2-Naphthoxy)phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.112
Data-to-parameter ratio = 19.5

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

The title compound, $C_{18}H_{10}N_2O$, is built up from two planar groups (naphthoxy and phthalonitrile), with a dihedral angle of 66.14 (4)° between them. The crystal structure is stabilized by weak $C—H\cdots N$ and $C—H\cdots\pi$ hydrogen-bond interactions.

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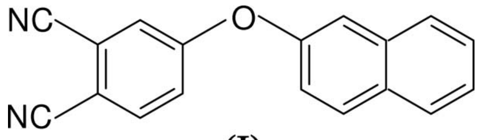
Comment

Tetrasubstituted phthalocyanines are generally obtained from monosubstituted phthalonitriles, *e.g.* 4-(2-naphthoxy)-phthalonitrile (McKeown, 1998). Phthalocyanines are of enormous technological importance for the manufacture of blue and green pigments. Other areas of current interest include applications in colours, catalysis, chemical sensors, electrochromism, batteries, photodynamic theraphy, semi-conductive materials, liquid crystals and modified supports for gas–solid chromatography, as a result of newly synthesized compounds (Leznoff & Lever, 1989–1996).



(I)

The title compound, (I), contains two cyclic groups, a naphthoxy and a phthalonitrile, bridged by an O atom. The phthalonitrile ring exhibits normal geometry and is planar, with a maximum deviation of 0.001 (1) Å for atom C4. The two cyano groups deviate from this plane by only 0.028 (3) and −0.053 (4) Å at atoms N1 and N2, respectively. The naphthoxy system is also planar, with a maximum deviation of 0.017 (2) Å for atom C9. The phthalonitrile and naphthyloxy groups make a dihedral angle of 66.14 (4)°. The $C\equiv N$ bond lengths [$N1\equiv C1$ = 1.141 (2) Å and $N2\equiv C2$ = 1.142 (2) Å] compare well with values reported in the literature [1.142 (5) Å in $C_{38}H_{36}N_8O_4S_2$ (Çoruh *et al.*, 2002), 1.141 (4) Å in $C_{17}H_{13}BrN_2O_3$ (Ocak Ískeleli *et al.*, 2005) and 1.148 (2) Å in $C_8H_4F_3N$ (Boitsov *et al.*, 2002)]. As expected, The $N\equiv C—C$ angles [$N1\equiv C1—C8$ = 178.8 (2)° and $N2\equiv C2—C3$ = 179.5 (3)°] are linear.

The crystal structure of (I) is stabilized by weak intermolecular $C—H\cdots N$ and $C—H\cdots\pi$ ring-centroid hydrogen-bond interactions (Table 1 and Fig. 2).

Experimental

2-Naphthol (1.34 g, 9.30 mmol) and 4-nitrophthalonitrile (1.43 g, 8.26 mmol) were dissolved in dry dimethylformamide (35 ml). After

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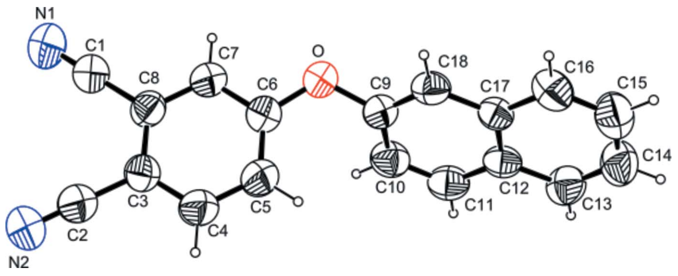

Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

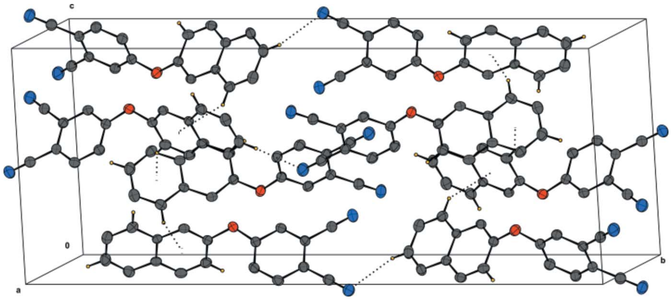

Figure 2
A view showing the weak C—H···N and C—H···π interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

stirring for 30 min at room temperature, dry fine-powdered potassium carbonate (3.00 g, 21.7 mmol) was added portionwise over 2 h with constant 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 NaOH solution (10% *w*/*w*) and water until the filtrate was neutral. Recrystallization from methanol gave a white product (yield 1.40 g, 62.8%). Single crystals of (I) were obtained from a solution in ethanol at room temperature by slow evaporation (m.p. 393–394 K). Elemental analysis calculated for $C_{18}H_{10}N_2O$: C 79.99, H 3.73, N 10.36%; found: C 79.90, H 3.70, N 10.40%.

Crystal data

$C_{18}H_{10}N_2O$
$M_r = 270.28$
Orthorhombic, *Pbca*
$a = 8.1630$ (7) Å
$b = 29.3272$ (9) Å
$c = 11.436$ (3) Å
$V = 2737.9$ (8) Å^3
$Z = 8$
$D_x = 1.311$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 1187 reflections
$\theta = 2.3$–29.2°
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Tablet, colourless
0.60 × 0.48 × 0.15 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.949$, $T_{\max} = 0.988$
8351 measured reflections
3710 independent reflections

1187 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.113$
$\theta_{\max} = 29.2°$
$h = -11 \rightarrow 11$
$k = - \rightarrow 40$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.112$
$S = 0.63$
3710 reflections
190 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.061P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.13$ e Å^{-3}

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

*Cg*1 is the centroid of the C3–C8 ring and *Cg*2 is the centroid of the C9–C12/C17/C18 ring

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···N2$^{\rm i}$	0.93	2.64	3.384 (3)	137
C10—H10···*Cg*1$^{\rm ii}$	0.93	2.60	3.4703 (19)	156
C16—H16···*Cg*2$^{\rm iii}$	0.93	2.86	3.633 (2)	141

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+2$; (iii) $x-\frac{1}{2}, y, -z+\frac{3}{2}$.

The H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H = 0.93 Å and $U_{\rm iso}$(H)= 1.2$U_{\rm eq}$(C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

References

Boitsov, S., Songstad, J. & Törnroos, K. W. (2002). *Acta Cryst.* C**58**, o66–o68.

Çoruh, U., Akdemir, N., Ağar, E., Vázquez-López, E. M. & Erdönmez, A. (2002). *Acta Cryst.* E**58**, o896–o897.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Leznoff, C. C. & Lever, A. B. P. (1989–1996). *Phthalocyanines: Properties and Applications*, Vols. 1, 2, 3 and 4. New York: Weinheim-VCH Publishers Inc.

McKeown, N. B. (1998). *Phthalocyanine Materials: Synthesis, Structure and Function*. Cambridge University Press.

Ocak Ískeleli, N., Atalay, Ş., Ağar, E. & Akdemir, N. (2005). *Acta Cryst.* E**61**, o2294–o2295.

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

Stoe & Cie (2002). *X-AREA* (Version 1.17) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.

Watkin, D. M., Pearce, L. & Prout, C. K. (1993). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.