organic papers

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.069
Data-to-parameter ratio = 10.2

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

4,5-Bis(1-naphthoxy)phthalonitrile

In the title molecule, $C_{28}H_{16}N_2O_2$, the dihedral angles between the planes of the two naphthalene moieties and the benzene ring are 84.78 (9) and 76.66 (9)°. The molecular structure is influenced by C—H···O and C—H···π interactions and the crystal structure is stabilized by π–π interactions.

Comment

4,5–Bis(1-naphthoxy)phthalonitrile, (I), is a starting material in the synthesis of peripherally tetrasubstituted phthalocyanines (Leznoff & Lever, 1996). Phthalocyanines have continuously been the subject of research due to their wide applications. The fundamental optical and electronic properties of these materials are explained and their potential in non-linear optics, optical data storage, electronic sensors, xerography, solar energy conversion, nuclear chemistry, molecular magnetism, electrochromic displays and heterogeneous catalysis are evaluated by McKeown (1998). In view of this importance, the crystal structure determination of (I) was carried out.

(I)
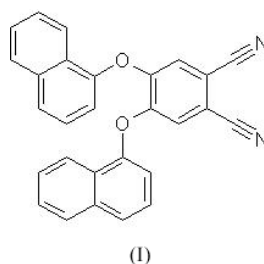
The structure of (I) is shown in Fig. 1. The molecule consists of three planar regions, a benzene ring and two naphthalene ring systems. The triple-bond distances, N1≡C6 [1.128 (3) Å] and N2≡C7 [1.130 (3) Å], agree with the mean values of 1.134 (2) Å reported by Allen et al. (1987). The C1—O1 [1.379 (2) Å] and C8—O2 [1.363 (2) Å] bond lengths show normal values (Gales et al., 2001). The dihedral angles between the least-squares planes through the naphthalene moieties and the plane of the benzene ring are 84.78 (9) and 76.66 (9)°.

The molecular structure is stabilized by C—H···O and C—H···π interactions (Table 2). In the crystal structure, the inversion-related naphthalene ring systems are stacked with $Cg2\cdots Cg3^i$, $Cg4\cdots Cg5^{ii}$ and $Cg5\cdots Cg5^{ii}$ distances of 3.626 (2), 3.775 (2) and 3.655 (2) Å, respectively, indicating π–π interactions [symmetry codes: (i) $1 - x, 2 - y, -z$; (ii) $2 - x, 2 - y, 1 - z$; in Table 2 and above, $Cg1$, $Cg2$, $Cg3$, $Cg4$ and $Cg5$ denote the centroids of aromatic rings C1–C5/C8, C9–C14,

C13–C18, C19–C24 and C23–C28, respectively]. The structure is further stabilized by C—H···π interactions (Table 2).

Experimental

4,5-Bis(1-naphthoxy)phthalonitrile was synthesized according to the procedures reported by Matlaba & Nyokong (2002). Single crystals were obtained from DMF at room temperature by slow evaporation.

Crystal data

$C_{28}H_{16}N_2O_2$	$Z = 2$
$M_r = 412.43$	$D_x = 1.338$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 9.9667$ (14) Å	Cell parameters from 5492
$b = 10.4946$ (15) Å	reflections
$c = 11.2637$ (16) Å	$\theta = 2.1$–$29.5°$
$\alpha = 116.931$ (11)°	$\mu = 0.09$ mm^{-1}
$\beta = 99.441$ (11)°	$T = 293$ (2) K
$\gamma = 93.570$ (12)°	Plate, brown
$V = 1023.6$ (3) Å^3	$0.80 \times 0.35 \times 0.03$ mm

Data collection

Stoe IPDS 2 diffractometer	$R_{int} = 0.090$
φ scans	$\theta_{max} = 25.0°$
Absorption correction: none	$h = -11 \rightarrow 11$
13294 measured reflections	$k = -12 \rightarrow 12$
3606 independent reflections	$l = -13 \rightarrow 13$
1694 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0125P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.069$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.80$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
3606 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
354 parameters	Extinction correction: SHELXL97
All H-atom parameters refined	Extinction coefficient: 0.0086 (10)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.379 (2)	O2—C19	1.409 (2)
O1—C9	1.415 (2)	N1—C6	1.128 (3)
O2—C8	1.363 (2)	N2—C7	1.130 (3)
C1—O1—C9	115.68 (15)	C10—C9—O1	122.4 (2)
C8—O2—C19	118.56 (15)	O1—C9—C14	114.9 (2)
C2—C1—O1	119.98 (18)	C20—C19—O2	119.2 (2)
O1—C1—C8	119.72 (18)	C24—C19—O2	117.4 (2)
C5—C4—C7	118.71 (19)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···O1	0.98 (2)	2.41 (2)	2.775 (3)	101 (1)
C25—H25···O2	0.88 (2)	2.48 (2)	2.815 (3)	103 (2)
C25—H25···Cg2	0.88 (2)	3.04 (2)	3.882 (3)	160 (2)
C26—H26···Cg1^{ii}	0.97 (3)	3.10 (3)	3.879 (3)	138 (2)
C28—H28···Cg3^{iii}	0.90 (2)	2.90 (2)	3.793 (3)	176 (2)

Symmetry codes: (ii) $2 - x, 2 - y, 1 - z$; (iii) $1 - x, 2 - y, 1 - z$.

H atoms were located in a difference Fourier map and their positional and isotropic displacement parameters were refined. The C—H distances lie in the range 0.88 (2)–1.03 (2) Å.

Data collection: X-AREA (Stoe & Cie, 2001); cell refinement: X-AREA; data reduction: X-RED (Stoe & Cie, 2001); 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 PLATON (Spek, 1990); software used to prepare material for publication: WinGX (Farrugia, 1999).
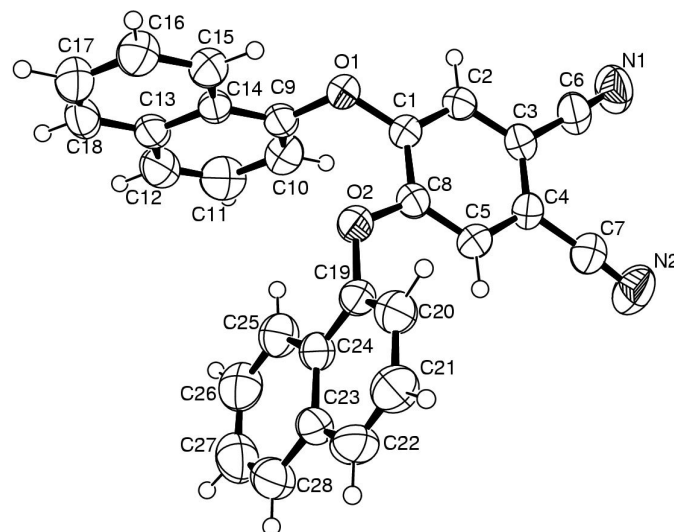

Figure 1
An ORTEP-3 (Farrugia, 1997) drawing of (I), showing the atom-numbering scheme. Displacement ellipsoids of non-H atoms are shown at the 50% probability level.
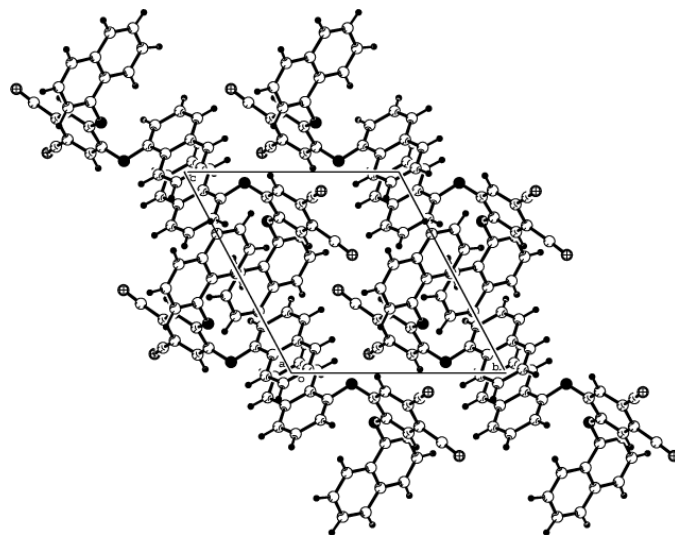

Figure 2
A view of the molecular packing down the a axis, showing part of the molecular stacking.

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