

## 2,7-Bis(3,4-dicyanophenoxy)naphthalene

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## Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$

$R$  factor = 0.036

$wR$  factor = 0.084

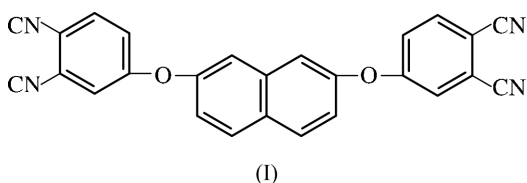
Data-to-parameter ratio = 13.3

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

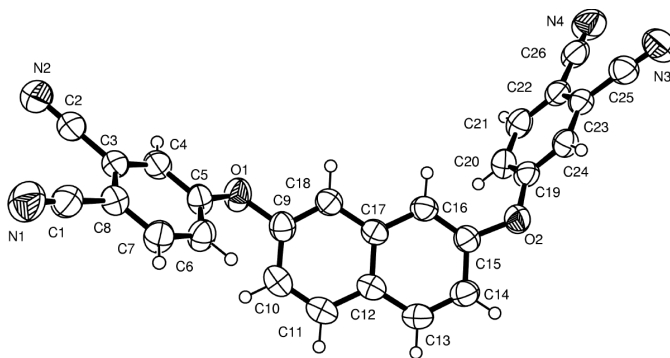
The molecule of the title compound, 4,4'-naphthalene-2,7-dioxydibenzene-1,2-dicarbonitrile,  $\text{C}_{26}\text{H}_{12}\text{N}_4\text{O}_2$ , has an asymmetric conformation, with the two benzene rings approximately orthogonal to each other [dihedral angle =  $77.18(5)^\circ$ ] and forming unequal dihedral angles of  $55.14(5)$  and  $67.62(5)^\circ$  with the naphthalene plane. The structure is stabilized by relatively weak  $\text{C}-\text{H}\cdots\text{N}$  interactions, linking the molecules into infinite chains running along the diagonal of the  $ac$  plane of the unit cell.

## Comment

The title compound, (I), belongs to the family of diphthalonitrile derivatives, which are used as starting materials for network polymeric phthalocyanines and high-performance aromatic polymers (McKeown, 1998; Takekoshi, 1987). Phthalocyanines represent an interesting class of compounds with increasingly diverse industrial and biomedical applications including photosensitization, linear optics, catalysis, liquid crystals and gas sensing (McKeown, 1998; Leznoff & Lever, 1989–1996). Polymeric phthalocyanines have been reported to be used as dyes and industrial high-technology materials and are also of interest because of their high thermostability (Leznoff & Lever, 1989–1996).



An *ORTEP*III (Burnett & Johnson, 1996) plot of the molecule of (I) is shown in Fig. 1. Considering its two-



**Figure 1**

An *ORTEP*III (Burnett & Johnson, 1996) drawing of the title compound, showing the atomic numbering. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

dimensional representation, the molecule could have had  $C_{2v}$  symmetry. This is certainly not the case in practice, as the naphthalene moiety is planar to within 0.03 Å and forms dihedral angles of 55.14 (5) and 67.62 (5)° with the planes of aromatic rings C3–C8 and C19–C24, respectively; the benzene rings form a dihedral angle of 77.18 (5)° with each other.

The crystal structure of (I) is stabilized by C–H···N intermolecular interactions, namely C16–H16···N4<sup>i</sup> and C7–H7···N3<sup>ii</sup> [symmetry codes: (i)  $1 - x, -y, -z$ ; (ii)  $x + \frac{1}{2}, -y - \frac{1}{2}, z + \frac{1}{2}$ ], which link the molecules into infinite chains stretching along the diagonal of the *ac* plane of the unit cell (Fig. 2 and Table 2).

## Experimental

2,7-Naphthalenediol (0.46 g, 2.88 mmol) and 4-nitrophthalodinitrile were dissolved in dry dimethylsulfoxide (40 ml) with stirring under N<sub>2</sub>. Dry fine-powdered potassium carbonate (1.0 g, 7.24 mmol) was added in portions (10 × 1 mmol) every 10 min. The reaction mixture was stirred for 48 h at room temperature and poured into ice-water (150 g). The product was filtered off and washed with NaOH solution (10% w/w) and water until the filtrate was neutral. The product was then refluxed in ethanol, filtered and dried (yield 1.08 g, 91.01%). Single crystals were obtained from dimethylformamide at room temperature by slow evaporation (m.p. 464 K). Elemental analysis calculated for C<sub>26</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>: C 75.72, H 2.93, N 13.56%; found: C 75.60, H 2.86, N 13.60%; IR (cm<sup>-1</sup>): 3093–3041 (Ar-CH<sub>2</sub>), 2229 (CN), 1631, 1595, 1562, 1483, 1458, 1435, 1415, 1369, 1277, 1244, 1203, 1165, 1138, 1086, 964, 903, 870, 839, 725.

## Crystal data

C <sub>26</sub> H <sub>12</sub> N <sub>4</sub> O <sub>2</sub>	$D_x = 1.399 \text{ Mg m}^{-3}$
$M_r = 412.40$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 8818 reflections
$a = 8.3592 (10) \text{ \AA}$	$\theta = 2.0\text{--}25.7^\circ$
$b = 7.5300 (5) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 31.368 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 97.400 (9)^\circ$	Prism, colourless
$V = 1958.0 (3) \text{ \AA}^3$	$0.50 \times 0.31 \times 0.07 \text{ mm}$
$Z = 4$	

## Data collection

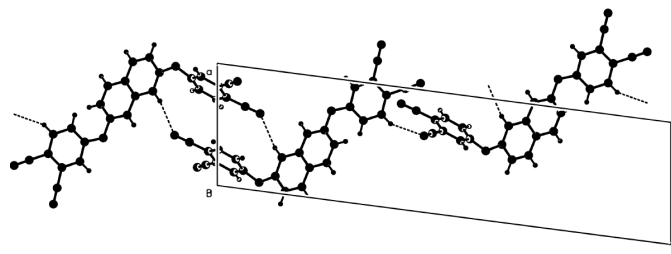
Stoe IPDS-2 diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 21357 measured reflections  
 3856 independent reflections  
 1929 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.064$   
 $\theta_{\text{max}} = 26.0^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -9 \rightarrow 9$   
 $l = -38 \rightarrow 38$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.084$   
 $S = 0.77$   
 3856 reflections  
 290 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.0097 (8)



**Figure 2**

The crystal packing of the title compound, with the C–H···N interactions shown as dashed lines.

**Table 1**

Selected bond lengths (Å).

O1–C5	1.376 (2)	N1–C1	1.142 (2)
O1–C9	1.405 (2)	N2–C2	1.139 (2)
O2–C15	1.3961 (19)	N3–C25	1.144 (2)
O2–C19	1.3730 (19)	N4–C26	1.136 (2)

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C16–H16···N4 <sup>i</sup>	0.93	2.56	3.397 (2)	151
C7–H7···N3 <sup>ii</sup>	0.93	2.62	3.486 (3)	155

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

The H atoms were positioned geometrically and included in the refinement in a riding-model approximation, with aromatic C–H distances fixed at 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

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: *ORTEP3* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

## References

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