4-(1-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 = 0.032

wR factor = 0.074

Data-to-parameter ratio = 12.6

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

The title compound, $C_{18}H_{10}N_2O$, crystallizes with two molecules in the asymmetric unit. The molecules are non-planar and the two independent molecules have different orientations. The dihedral angles between the least-squares planes of the naphthalene and the benzene ring in the independent molecules are 85.52 (3) and 73.40 (3)°.

Comment

4-(1-Naphthoxy)phthalonitrile is a starting material in the synthesis of peripherally tetra-substituted phthalocyanines (Leznoff & Lever, 1996). Since their discovery earlier this century, phthalocyanines have been of great interest to chemists, physicists and industrial scientists. Phthalocyanines have continuously been the subject of research due to their wide application fields. These include thin film fabrication, including molecular epitaxic deposition and composites, liquid crystals and self-assembled materials. 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 is evaluated by McKeown (1998).
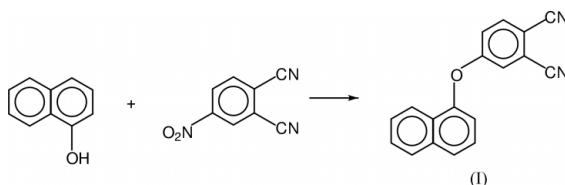
The title compound, (I), contains two molecules (denoted A and B, Fig. 1) in the asymmetric unit. The triple-bond distances C17A≡N1A and C18A≡N2A, 1.136 (2) and 1.134 (2) Å, respectively, agree with the literature values (Allen et al., 1986; Öztürk et al., 2000). The bond angles around C17A and C18A agree with the triple-bond character of C17A≡N1A and C18A≡N2A. The C11A—O1A bond length is 1.3657 (17) Å, similar to that in 2-(3,4-dimethoxyphenoxy)benzoic acid [1.376(2) Å; Gales et al., 2001]. Selected bond lengths and angles for compound (I) are listed in Table 1. The two independent molecules have different orientations. The dihedral angles between the naphthalene and the benzene ring are 85.52 (3)° for A and 73.40 (3)° for B.

Experimental

1-Naphthol (1.24 g, 7.6 mmol) was dissolved in dry DMF (40 ml) and 4-nitrophthalonitrile (1.32 g, 7.6 mmol) was added. After stirring for
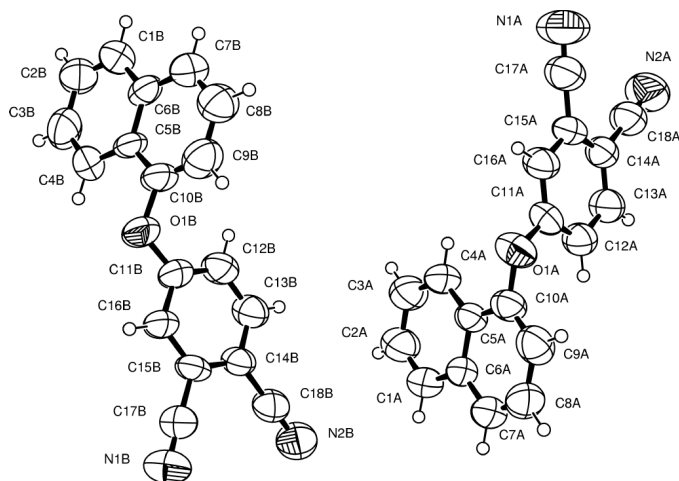
Figure 1
An *ORTEP*III (Burnett & Johnson, 1996) drawing of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.
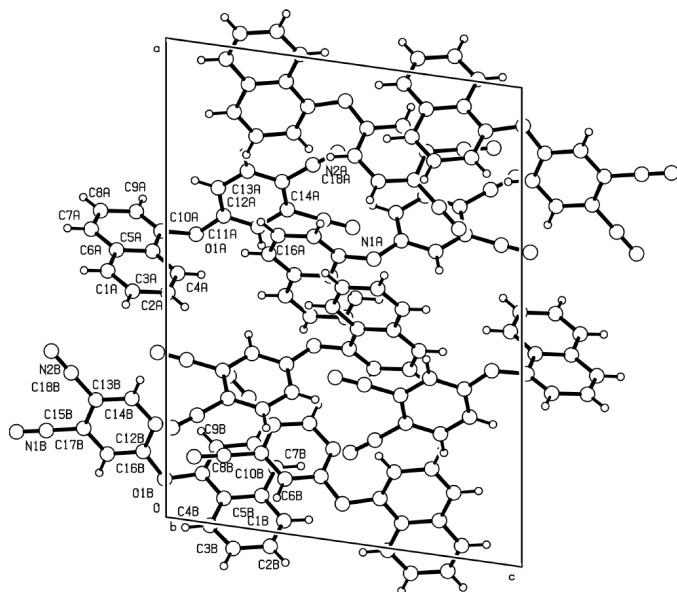

Figure 2
PLATON/PLUTON plot (Spek, 1997), viewed down the *b* axis, showing part of the stacking of molecules.

30 min at room temperature, dry fine-powdered potassium carbonate (3.00 g, 21.7 mmol) was added portionwise over 2 h with vigorous stirring. The reaction was stirred for 24 h at room temperature and then poured into ice-water (150 g). The product was filtered off and washed with (%10 w/w) NaOH solution and water until the filtrate was neutral. Recrystallization from ethanol gave a brown product. Yield 1.45 (70.4%). Single crystals were obtained from ethanol at room temperature *via* slow evaporation (m.p. 401–403 K); elemental analysis, calculated for $C_{18}H_{10}N_2O$: C 79.99, H 3.73, N 10.36%; found: C 79.97, H 3.76, N 10.40%. IR(ν_{max}, cm^{-1}): 3080–3025(Ar—CH), 2210(CN), 1622, 1590, 1555, 1500, 1472, 1452, 1416, 1380, 1276, 1208, 1190, 1052, 1084, 1064, 1032, 1008, 940, 880, 854, 828, 800, 780, 740, 716, 696, 656, 624, 612, 590, 568, 516. ^{1}H NMR (acetone–d_6): 7.22–8.14 (*m*, 10H). ^{13}C NMR (acetone–d_6): 109.71, 115.89, 116.31, 117.67, 118.93, 121.97, 122.38, 122.74, 126.91, 127.04, 127.39, 127.78, 127.93, 129.15, 136.26, 136.84, 150.57, 163.02.

Table 1
Selected geometric parameters (Å, °).

N2A—C18A	1.134 (2)	C17B—N1B	1.1385 (18)
N2B—C18B	1.136 (2)	C10B—O1B	1.4075 (18)
C11B—O1B	1.3675 (18)	C11A—O1A	1.3657 (17)
N1A—C17A	1.136 (2)	C10A—O1A	1.4078 (17)
C15A—C14A—C18A	119.45 (15)	C11B—O1B—C10B	119.61 (13)
C15B—C14B—C18B	120.16 (15)	O1A—C11A—C12A	123.64 (14)
O1B—C11B—C12B	123.31 (14)	O1A—C11A—C16A	115.76 (15)
O1B—C11B—C16B	115.41 (16)	C9A—C10A—O1A	119.30 (18)
C9B—C10B—O1B	121.23 (17)	C5A—C10A—O1A	117.96 (15)
C5B—C10B—O1B	116.44 (18)	C11A—O1A—C10A	118.66 (12)

The H atoms were refined using riding model, with C—H distances of 0.93 Å.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); structure solution: *SHELXS*97 (Sheldrick, 1997); structure refinement: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 1997).

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