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4-(2-Methoxy-1-naphthylmethoxy)-phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.087
Data-to-parameter ratio = 14.5

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

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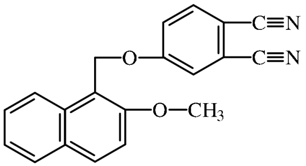
The title compound, $C_{20}H_{14}N_2O_2$, crystallizes in the centrosymmetric space group $P2_1/c$ with two molecules in the asymmetric unit. Both independent molecules have the same geometry.

Comment

Tetrasubstituted phthalocyanines are generally obtained from monosubstituted phthalonitriles [4-(2-methoxy-1-naphthalenemethanoxy)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 therapy, semiconductors, liquid crystals and modified supports for gas–solid chromatography as a result of newly synthesized compounds (Leznoff & Lever, 1989–1996). Fig. 1 shows a perspective view of the asymmetric unit of the title compound, (I), with the atom-numbering scheme.



(I)

The average triple C≡N bond distance in the cyano groups [1.143 (3) Å] is short enough to indicate their triple-bond character, and is in good agreement with those in a related structure (Ocak *et al.*, 2003).

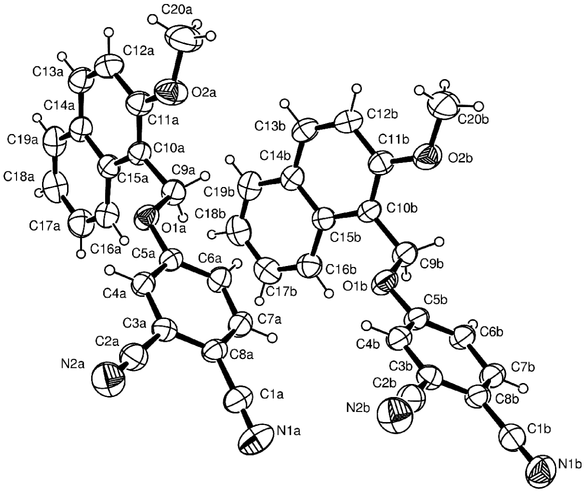


Figure 1
The structure of the asymmetric unit of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

The benzene ring of the phthalonitrile group and the naphthalene ring system are perpendicular to each other, with an angle of 84.21 (7)° in molecule *A* and 89.52 (6)° in *B*. The title compound has intramolecular C—H···O-type contacts, namely C9*A*—H9*A*2···O2*A* and C9*B*—H9*B*2···O2*B*.

Experimental

2-Methoxy-1-naphthalenemethanol (1.10 g, 5.85 mmol) and 4-nitrophthalonitrile (1.00 g, 5.78 mmol) were dissolved in dry DMSO (50 ml). After stirring for 30 min at room temperature dry fine-powdered potassium carbonate (1.40 g, 10.0 mmol) was added portionwise over 2 h with stirring. The reaction was stirred for 48 h at room temperature and poured into ice–water (200 g). The product was filtered off and washed with NaOH (10% *w*/*w*) solution and water until the filtrate was neutral. Recrystallization from methanol gave a white product (yield: 0.16 g, 8.80%). Single crystals were obtained from ethanol at room temperature *via* slow evaporation (m.p. = 393–394 K); elemental analysis, calculated for $C_{20}H_{14}N_2O_2$: C 76.42, H 4.49, N 8.91%; found: C 76.20, H 4.36, N 8.70%. IR data ($\nu_{\max}$/cm^{-1}): 3078, 3025 (Ar-CH), 2993, 2839 (C—H), 2210 (C—N), 1593, 1502, 1475, 1358, 1279, 1247, 1159, 1090, 989, 816, 748.

Crystal data

$C_{20}H_{14}N_2O_2$
$M_r = 314.34$
Monoclinic, $P2_1/c$
$a = 13.1166\ (9)$ Å
$b = 12.0736\ (12)$ Å
$c = 20.9806\ (15)$ Å
$\beta = 104.454\ (5)°$
$V = 3217.4\ (5)$ Å^3
$Z = 8$

$D_x = 1.298$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8964 reflections
$\theta = 1.6$–$22.9°$
$\mu = 0.09$ mm^{-1}
$T = 293\ (2)$ K
Plate, yellow
$0.30 \times 0.23 \times 0.12$ mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{\min} = 0.976$, $T_{\max} = 0.990$
37 155 measured reflections

6304 independent reflections
2114 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.101$
$\theta_{\max} = 26.0°$
$h = -15 \rightarrow 16$
$k = -14 \rightarrow 14$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.087$
$S = 0.68$
6304 reflections
436 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.11$ e Å^{-3}
$\Delta\rho_{\min} = -0.12$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0031 (2)

Table 1
Selected geometric parameters (Å, °).

O2*A*—C20*A*	1.408 (3)	C2*A*—N2*A*	1.143 (3)
O2*B*—C20*B*	1.420 (3)	O1*B*—C5*B*	1.355 (2)
O1*A*—C5*A*	1.360 (2)	O1*B*—C9*B*	1.452 (2)
O1*A*—C9*A*	1.442 (2)	C1*B*—N1*B*	1.146 (3)
C1*A*—N1*A*	1.141 (3)	C2*B*—N2*B*	1.141 (3)
C11*A*—O2*A*—C20*A*	118.7 (2)	C11*B*—O2B—C20*B*	119.1 (2)
C5*A*—O1*A*—C9*A*—C10*A*	173.32 (19)	C5*B*—O1*B*—C9*B*—C10*B*	−167.0 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9A—H9*A*2···O2*A*	0.97	2.38	2.716 (3)	100
C9*B*—H9*B*2···O2*B*	0.97	2.31	2.724 (3)	105

H atoms were positioned geometrically and refined using a riding model, with $C_{\rm aromatic}$—H = 0.93, $C_{\rm methylene}$—H = 0.97 and $C_{\rm methyl}$—H = 0.96 Å and $U_{\rm iso} = 1.2$ or $1.5U_{\rm eq}$ of the parent atom. The intensity data collected for the title structure are generally weak, so the least-squares goodness-of-fit parameter lies outside the normal range. In addition, some atoms show high displacement parameters and are possibly affected by unresolved disorder.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

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