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4-(1-Indanyloxy)phthalonitrile

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In the title compound, $C_{17}H_{12}N_2O$, the phthalonitrile group is coplanar with the three-atom bridge linking the phthalonitrile group with the indanyloxy group. The five-membered ring of the indanyloxy moiety adopts an envelope conformation. The crystal structure of the title compound is stabilized by two C—H$\cdots\pi$ interactions and van der Waals interactions.

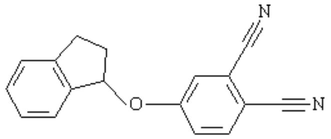
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.067
Data-to-parameter ratio = 14.7

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

Comment

Phthalonitriles are known precursors to phthalocyanines, an important class of molecules with wide applications (Leznoff & Lever, 1989–1996), ranging from catalysis to solid-state materials. Phthalocyanines are traditionally used as dyes and pigments (Moser & Thomas, 1983). 4-(1-Indanoxy)phthalonitrile is a precursor in the synthesis of phthalocyanines and subphthalocyanines (McKeown, 1998). Phthalocyanines and metallophthalocyanines have been investigated for many years because of their wide range of applications, including use in chemical sensors, liquid crystals, Langmuir–Blodgett films, non-linear optics and optical data storage, and as carrier generation materials in near-IR (Leznoff & Lever, 1989–1996). In view of these important properties of phthalocyanines, we have undertaken the X-ray diffraction study of the title compound, (I).



(I)

The molecule of (I) consists of two fragments, namely the phthalonitrile group (N1/N2/C1–C8) and the indanyloxy group (C9–C17). The phthalonitrile group is coplanar with the

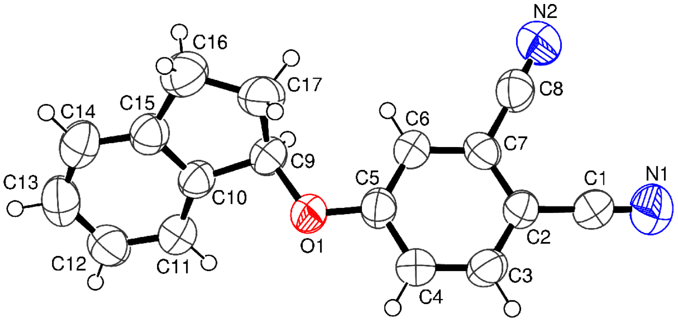


Figure 1
An *ORTEP*-3 (Farrugia, 1997) drawing of (I), showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

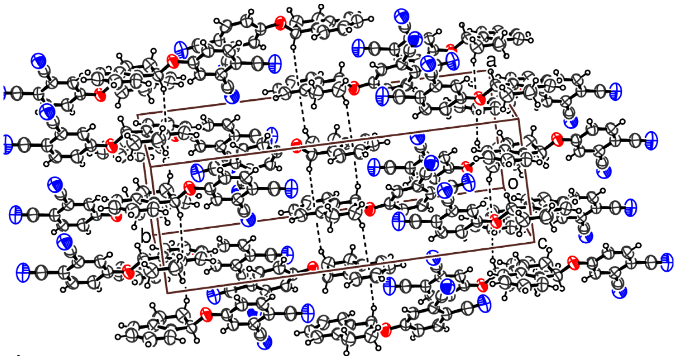


Figure 2
An *ORTEP*-3 (Farrugia, 1997) drawing of (I), illustrating the stacking of molecules and C—H···π interactions (dashed lines).

three-atom bridge (C5—O1—C9) to the indanyloxy group. The N1≡C1 and N2≡C8 triple-bond distances are 1.148 (3) and 1.135 (3) Å, respectively, in good agreement with values reported in the literature (Dinçer *et al.*, 2004; Nesi *et al.*, 1998).

Fig. 1 shows the molecular structure and conformation of (I), with the atomic numbering scheme. Selected bond lengths and angles are listed in Table 1. As expected, the C10–C15 ring is planar to within 0.012 (3) Å. However, the five-membered indanyloxy ring (C9/C10/C15–C17) is close to an envelope conformation, with atom C17 deviating by −0.108 (3) Å, and puckering parameters (Cremer & Pople, 1975) Q_2 = 0.1708 (33) Å and φ_2 = 328.5 (11)°.

In the crystal structure, inter- and intramolecular interactions are not observed. The crystal structure contains only two C—H···π interactions. In the first of these, atom C9 in the molecule at (*x*, *y*, *z*) forms a C—H···π contact (Table 2) with the centroid, *Cg*3, of the C10–C15 ring of the molecule at (1 − *x*, −*y*, 2 − *z*). In the second, atom C17 in the molecule at (*x*, *y*, *z*) forms a C—H···π contact with the centroid, *Cg*3, of the C10–C15 ring of the molecule at (−*x*, −*y*, 2 − *z*). The centroid of the C10–C15 ring acts as a single acceptor for both C—H···π interactions. Such an arrangement results in the formation of infinite chains extending parallel to the *a* axis of the crystal structure (Fig. 2). These interactions, as well as van der Waals interactions, stabilize the molecular structure and packing.

Experimental

1-Indanol (0.77 g, 5.74 mmol) and 4-nitrophthalonitrile (0.95 g, 5.49 mmol) were heated at 333 K in dry dimethylformamide (35 ml) with stirring under N_2. Dry fine-powdered potassium carbonate (0.96 g, 6.96 mmol) was added portionwise over a period of 2 h, with stirring. The reaction mixture was stirred for 48 h at 333 K and then poured into iced water (100 g). The product was filtered off and washed with NaOH (10%, *w*/*w*) solution and water until the filtrate was neutral. Recrystallization from ethanol gave a yellow product. Yield 0.40 g (28.2%). Single crystals were obtained from ethanol at room temperature *via* slow evaporation (m.p. 413 K). Analysis calculated for $C_{17}H_{12}N_2O$: C 78.44, H 4.64, N 10.76%; found: C 78.50, H 4.50, N 11.70%.

Crystal data

$C_{17}H_{12}N_2O$
M_r = 260.29
Monoclinic, $P2_1/c$
a = 8.0560 (16) Å
b = 23.950 (3) Å
c = 7.8057 (16) Å
β = 117.069 (14)°
V = 1341.1 (4) Å^3
Z = 4
D_x = 1.289 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 2365 reflections
θ = 1.7–22.9°
μ = 0.08 mm^{-1}
T = 293 (2) K
Plate, colourless
0.50 × 0.25 × 0.02 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{\min}$ = 0.979, $T_{\max}$ = 0.998
9063 measured reflections
2498 independent reflections
767 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.086
$\theta_{\max}$ = 25.5°
h = −9 → 9
k = −28 → 26
l = −9 → 9

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.067
S = 0.74
2498 reflections
170 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0101P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.12 e Å^{-3}
$\Delta\rho_{\min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0034 (3)

Table 1
Selected geometric parameters (Å, °).

O1—C5	1.362 (3)	C9—C17	1.529 (3)
O1—C9	1.448 (3)	C10—C15	1.367 (3)
C1—C2	1.430 (4)	C16—C17	1.525 (3)
C7—C8	1.452 (3)		
C5—O1—C9	117.8 (2)	C6—C7—C8	118.3 (3)
N1—C1—C2	179.0 (4)	C2—C7—C8	120.3 (3)
C3—C2—C1	120.8 (3)	N2—C8—C7	178.0 (3)
C7—C2—C1	120.6 (3)	O1—C9—C10	109.0 (2)
O1—C5—C4	115.5 (3)	O1—C9—C17	113.1 (2)
O1—C5—C6	124.2 (3)		

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

*Cg*3 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···*Cg*3$^{\rm i}$	0.98	2.689	3.625 (4)	160
C17—H17*A*···*Cg*3$^{\rm ii}$	0.97	2.993	3.917 (4)	160

Symmetry codes: (i) 1 − *x*, −*y*, 2 − *z*; (ii) −*x*, −*y*, 2 − *z*.

H atoms were positioned geometrically and treated using a riding model, with C—H distances of 0.98 Å for atom C9, 0.97 Å for atoms C16 and C17, and 0.93 Å for the aromatic atoms, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier atom).

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*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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