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4-(5-Indanyloxy)phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.088
Data-to-parameter ratio = 8.4

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

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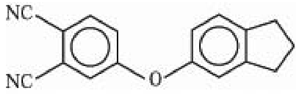
Im the title compound, $C_{17}H_{12}N_2O$, the aromatic rings are twisted by 62.84 (4)° with respect to each other. There are no unusually short contacts between the molecules and the crystal packing is controlled by weak van der Waals interactions.

Comment

4-Substituted phthalonitriles are generally used to prepare both symmetrically and unsymmetrically substituted phthalocyanines and subphthalocyanines (McKeown, 1998; Leznoff & Lever, 1989–1996). The annual worldwide production of phthalocyanines, used in the preparation of dyes and pigments, is around 80,000 tons (Wörhle, 2001). Phthalocyanines have been the subject of ongoing research due to their application in a variety of fields, such as organic pigments, chemical sensors, electrochromic display devices, photovoltaic cells, optical disks and photosensitizers for photodynamic therapy, and in xerography, catalysis, and nonlinear optics (Leznoff & Lever, 1989–1996). Against this background, we present here the crystal structure of the title compound, (I).



(I)

The five-membered ring of (I) (C11–C15) adopts an envelope conformation, with atom C13 at the flap position. The N1≡C7 and N2≡C8 triple-bond distances are both 1.138 (3) Å, in good agreement with values reported in the literature (Yazıcı *et al.*, 2004). The dihedral angle between the aromatic rings of the cyanophenoxy and indane moieties is 62.84 (4)°. Crystal packing is controlled by van der Waals forces.

Experimental

5-Indanol (1.00 g, 7.45 mmol) and 4-nitrophthalonitrile (1.00 g, 5.78 mmol) were dissolved in dry dimethylformamide (40 ml) with stirring under N_2. Dry fine-powdered potassium carbonate (1.5 g, 10.87 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 (200 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 white product, yield 1.06 g (70.67%). Single crystals of (I) were obtained from absolute ethanol at room temperature *via* slow evaporation (m.p. 360 K). Elemental analysis, calculated for $C_{17}H_{12}N_2O$: C 78.44, H 4.65, N 10.76%; found: C 78.46 H 4.70 N 10.74%.

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Crystal data

$C_{17}H_{12}N_2O$
$M_r = 260.29$
Orthorhombic, $P2_12_12_1$
$a = 7.7260$ (3) Å
$b = 11.7276$ (5) Å
$c = 14.6536$ (8) Å
$V = 1327.73$ (11) Å^3
$Z = 4$
$D_x = 1.302$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 28 036 reflections
$\theta = 2.2$–$29.9°$
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
$0.42 \times 0.32 \times 0.13$ mm

Data collection

Stoe IPDS 2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.969$, $T_{\max} = 0.989$
16 681 measured reflections
1515 independent reflections

1380 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.051$
$\theta_{\max} = 26.0°$
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 14$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.088$
$S = 1.07$
1515 reflections
181 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 0.3188P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

H atoms were included in calculated positions and refined using a riding model, with C—H distances of 0.97 Å for atoms C14, C13 and C12, and 0.93 Å for the aromatic H atoms, and with $U_{\rm iso}(H) = 1.5U_{\rm eq}(C)$. The absolute configuration could not be determined from the X-ray data, as no strong anomalous scatterers are present; 1515 Friedel pairs were therefore merged before refinement.

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

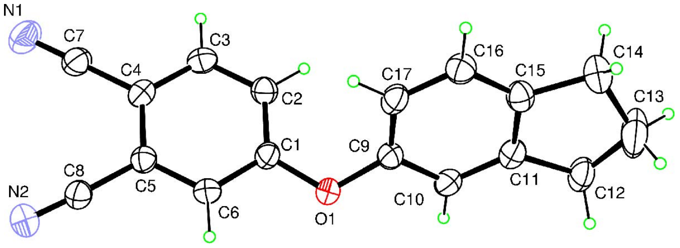

Figure 1
An *ORTEP* view of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

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