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4-(2-Allylphenoxy)phthalonitrile

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Key indicators

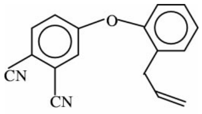
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.006 Å
R factor = 0.058
wR factor = 0.178
Data-to-parameter ratio = 9.8

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

In the title compound, $C_{17}H_{12}N_2O$, the mutual orientation of the two aromatic rings [dihedral angle 80.8 (1)°] is mainly determined by the presence of an intramolecular C—H···O hydrogen bond.

Comment

4-(2-Allylphenoxy)phthalonitrile, (I), is a starting material in the synthesis of peripherally tetra-substituted phthalocyanines (Leznoft & Lever, 1996). Phthalocyanines and metallophthalocyanines have been investigated in detail for many years because of their wide range of applications, including use in chemical sensors, liquid crystals, Langmuir–Blodgett films, non-linear optics, optical data storage and as carrier generation materials in the near IR (Leznoft & Lever, 1996).



(I)

In the molecule, the bond lengths and angles are consistent with the reported structures of similar compounds (Çoruh *et al.*, 2002). The dihedral angle between the C1–C6 and C7–C12 mean planes is 80.8 (1)°.

The displacement parameters of atoms C15, C16 and C17 of the allyl group are larger than those for other atoms. The high values of the anisotropic displacement parameters associated with the allyl group suggest this group could be affected by high thermal motion.

The compound has intramolecular C—H···O- and intermolecular C—H···N-type contacts, *viz.* C15—H15*A*···O1, C8—H8···N1^{i}, respectively (symmetry code in Table 2). The C15—H15*A*···O1 intramolecular hydrogen bond seems to drive the relative orientation of the two aromatic rings. As can be seen from the packing diagram (Fig. 2), the crystal structure of (I) involves intermolecular C8—H8···N1^{i} contacts, resulting in an infinite network structure. Details of these interactions are given in Table 2.

Experimental

2-Allylphenol (1.97 g, 14.68 mmol) was dissolved in dry DMF (60 ml) and 4-nitrophthalonitrile (2.28 g, 13.18 mmol) was added. After stirring for 20 min, finely ground anhydrous potassium carbonate (2.80 g, 20.29 mmol) was added in portions during 2 h with vigorous stirring. The reaction mixture was stirred for 24 h at room temperature and then poured into ice-water (250 g). The product was filtered and washed with (5% *w*/*w*) NaOH solution and water until the filtrate was neutral. Recrystallization from ethanol gave a green product (yield 1.94 g, 56.73%). Single crystals were obtained from ethanol at room temperature *via* slow evaporation. Calculated: C 78.44, H 4.65, N 19.64%; found: C 78.42, H 4.60, N 10.74%. IR data (ν_{max}/cm^{-1}): 3088, 3020 (Ar—CH), 2920, 2840 (C—H), 2220 (C≡N), 1684, 1632, 1580, 1476, 1448, 1428, 1405, 1352, 1300, 1272, 1240, 1204, 1168, 1152, 1112, 1076, 1036, 1004, 985, 960, 944, 912, 880, 864, 840, 784, 768, 732, 724, 703, 624, 564, 524 (aromatic). ^{1}H NMR (acetone–d_6): 3.36 (*d*, 2H), 4.95–5.04 (*m*, 2H), 5.83–5.96 (*m*, 1H), 7.14–8.03 (*m*, 7H). ^{13}C NMR (acetone–d_6): 34.67, 109.45, 115.93, 116.35, 116.69, 118.27, 122.03, 122.10, 122.34, 127.33, 129.35, 132.30, 133.36, 136.80, 152.61, 162.68.

Crystal data

$C_{17}H_{12}N_2O$
$M_r = 260.29$
Orthorhombic, $Pna2_1$
$a = 14.1639$ (14) Å
$b = 11.2630$ (11) Å
$c = 8.6098$ (8) Å
$V = 1373.5$ (2) Å^3
$Z = 4$
$D_x = 1.258$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 10384 reflections
$\theta = 2.3$–28.7°
$\mu = 0.08$ mm^{-1}
$T = 150$ (2) K
Block, green
0.31 × 0.25 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.975$, $T_{max} = 0.991$
9839 measured reflections

1777 independent reflections
1468 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 28.7°$
$h = -18 \rightarrow 15$
$k = -14 \rightarrow 14$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.178$
$S = 1.08$
1777 reflections
181 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1037P)^2 + 0.3289P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.72$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C10	1.355 (4)	N2—C14	1.141 (5)
O1—C1	1.399 (4)	C15—C16	1.498 (7)
N1—C13	1.144 (5)	C16—C17	1.238 (9)
C10—O1—C1	121.8 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···N1^{i}	0.93	2.53	3.325 (3)	144
C15—H15A···O1	0.97	2.49	2.884 (5)	104

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

The absolute polarity of the structure was not determined. Friedel pairs were merged before the final refinement. H atoms were positioned geometrically and refined using a riding model, fixing the aromatic C—H distance at 0.93 Å and the aliphatic C—H distance at 0.97 Å.

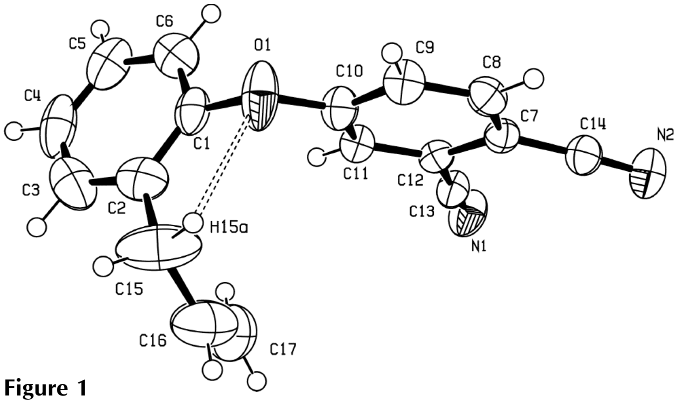


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

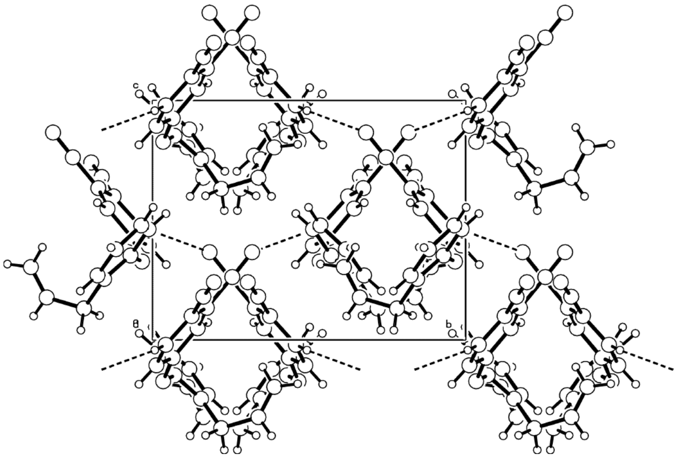


Figure 2
A packing diagram of (I), illustrating the hydrogen-bonding network.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); 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, 1997) and *PARST* (Nardelli, 1995).

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