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4-(2-Formylphenoxy)phthalonitrile

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The crystal structure of the title phthalonitrile derivative, $C_{15}H_8N_2O_2$, is stabilized by intermolecular C—H···O contacts.

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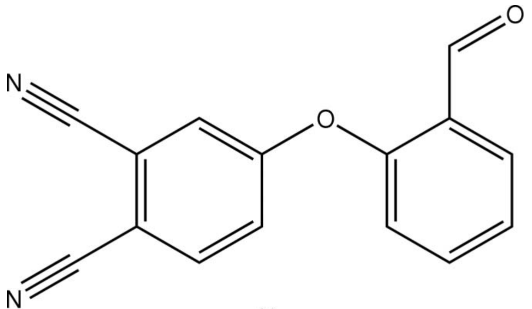
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.110
Data-to-parameter ratio = 17.2

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

Comment

Substituted phthalonitriles are generally used for preparing symmetrically and unsymmetrically peripherally and non-peripherally substituted phthalocyanines and subphthalocyanines (McKeown, 1998; Leznoff & Lever, 1989–1996). In addition to their extensive use as dyes and pigments, phthalocyanines have found widespread application in catalysis, optical recording, photoconductive materials and photodynamic therapy, and as chemical sensors (Leznoff & Lever, 1989–1996).



(I)

The molecule of the title compound, (I) is not planar: the dihedral angle between the phthalonitrile moiety and the 2-formylphenoxy group is 62.68 (4)°. The lengths of the two N≡C triple bonds [C1≡N1 = 1.3333 (17) Å and C2≡N2 = 1.1409 (17) Å] are consistent with those found in similar compounds (Ocak *et al.*, 2003, 2004; Atalay *et al.*, 2003; Erdem *et al.*, 2004).

The crystal structure of (I) is stabilized by C—H···O intermolecular contacts (Table 1, Fig. 2).

Experimental

To a solution of salicylaldehyde (1.4 g, 1,3 ml, 11.47 mmol) in dimethylformamide (DMF, 20 ml) was added potassium carbonate (3.16 g, 22.95 mmol). The mixture was stirred for 30 min under N_2. 4-Nitrophtalonitrile (1.98 g, 11.47 mmol) solution in DMF (30 ml) was added. The mixture was stirred for 48 h at 323 K under N_2 and poured into ice–water (150 g). The product was filtered off and washed with water and then recrystallized from ethanol to obtain 4-(2-formylphenoxy)phthalonitrile as a colourless solid. Crystals of (I) suitable for X-ray analysis were obtained from ethanol at room temparature *via* slow evaporation (yield 83%, m.p. 427 K).

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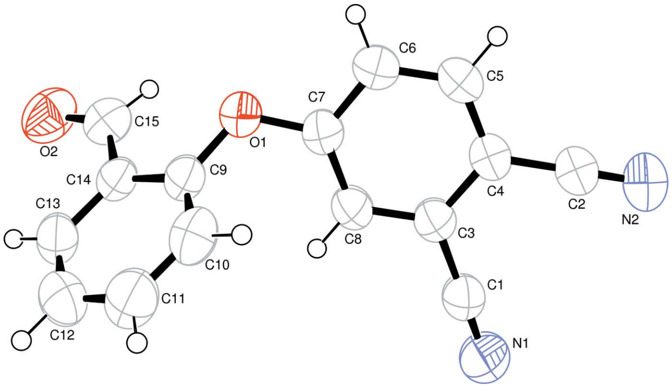

Figure 1
A drawing of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Crystal data

$C_{15}H_8N_2O_2$
$M_r = 248.23$
Monoclinic, $C2/c$
$a = 23.0524\ (16)$ Å
$b = 8.1639\ (8)$ Å
$c = 15.3994\ (11)$ Å
$\beta = 120.621\ (5)^\circ$
$V = 2494.0\ (4)$ Å^3
$Z = 8$

$D_x = 1.322$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13844 reflections
$\theta = 2.1$–28.0°
$\mu = 0.09$ mm^{-1}
$T = 293\ (2)$ K
Prism, colourless
$0.42 \times 0.34 \times 0.23$ mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.970$, $T_{\max} = 0.982$
16362 measured reflections
2982 independent reflections

1934 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 27.9^\circ$
$h = -30 \rightarrow 28$
$k = -10 \rightarrow 10$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.110$
$S = 1.04$
2982 reflections
173 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.0525P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.14$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0113 (15)

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C8—H8$\cdots$O2$^{\rm i}$	0.93	2.39	3.2722 (15)	159
C11—H11$\cdots$O2$^{\rm ii}$	0.93	2.42	3.3199 (17)	164

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

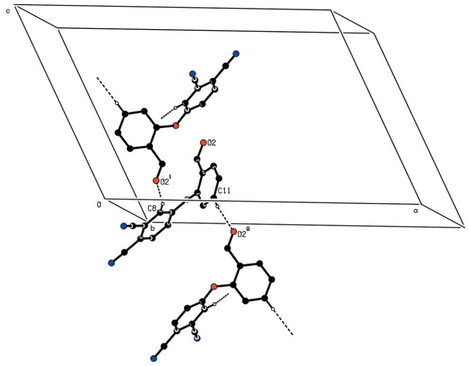

Figure 2
A partial packing diagram for (I), showing the C—H$\cdots$O hydrogen-bonding interactions as dashed lines. [Symmetry codes: (i) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $x, 1 - y, z - \frac{1}{2}$].

H atoms were included in calculated positions and treated using a riding model, with C—H(aromatic) = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

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: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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