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4-(Benzyloxy)phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.107
Data-to-parameter ratio = 11.0

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

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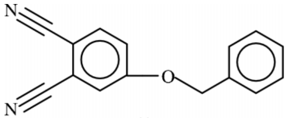
The molecule of the title compound, $C_{15}H_{10}N_2O$, has two planar fragments. The phthalonitrile group forms a dihedral angle of 84.15 (8)° with the plane of the phenyl ring. The crystal structure is stabilized by one intermolecular hydrogen bond, two π–π interactions and one C—H$\cdots\pi$ interaction.

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). Monosubstituted phthalonitriles [4-(benzyloxy)phthalonitrile] are generally used for synthesis of tetrasubstituted phthalocyanines and subphthalocyanines (McKeown, 1998). For many years, phthalocyanines have attracted continued interest in various research fields, such as chemical sensors, electrochromism, batteries, photosensitizers for the photodynamic therapy of cancer, semiconductive materials, liquid crystals and non-linear optics (Leznoff & Lever, 1989–1996). High-performance phthalonitrile-terminated polymers have also been developed and used for many applications (Keller, 1987, 1988). Phthalonitrile-based prepolymers with low molecular weight are stable at room temperature and the prepolymers can be processed to form void-free cross-linked polymers by heating in the presence of thermally stable aromatic amines (Keller, 1987, 1988). Taking into account the importance of phthalonitriles, we have undertaken an X-ray diffraction study of the title compound, (I).


(I)

The molecule of (I) contains two planar fragments. The phthalonitrile group (N1/N2/C1–C8) is coplanar with the four-atom bridge (C5—O1—C9—C10) to the phenyl ring, the torsion angle being −176.45 (14)°. The second plane is the phenyl ring (C10–C15). The phthalonitrile group is almost perpendicular with the plane of the phenyl ring, the dihedral angle being 84.15 (8)°. The N1≡C1 and N2≡C8 triple-bond distances are 1.142 (2) and 1.139 (2) Å, respectively, in good agreement with the values reported in the literature (Nesi *et al.*, 1998).

There is only one hydrogen bond in the structure. Atom H4 of the phthalonitrile group (C4) forms an intermolecular hydrogen bond with a phthalonitrile group N atom (N2) of a symmetry-related molecule [C4$\cdots$N2^{i} = 3.563 (2) Å;

symmetry code: (i) x, $1+y$, z]. The crystal structure also contains two π–π interactions and one C—H$\cdots\pi$ interaction per molecule. Equal distances of 3.8 Å are found for $Cg1\cdots Cg1^{\rm iii}$ and $Cg1\cdots Cg1^{\rm iv}$, involving centrosymmetrically related pairs of phthalonitrile rings in π–π interactions [symmetry codes: (iii) $-x$, $1-y$, $1-z$; (iv) $1-x$, $1-y$, $1-z$]. In the C—H$\cdots\pi$ interaction, C3$\cdots$*Cg*2 is 3.586 (2) Å. (*Cg*1 and *Cg*2 denote the centroids of rings C2–C7 and C10–C15, respectively.)

Experimental

Phenylcarbinol (1.56 g, 14.44 mmol) and 4-nitrophthalonitrile (1.60 g, 9.25 mmol) were dissolved in dry DMF (30 ml). After stirring for 30 min at room temperature, dry fine-powdered potassium carbonate (2.50 g, 18.12 mmol) was added portionwise over 2 h with efficient stirring. The reaction was stirred for 24 h at room temperature and poured into ice-water (200 g). The product was filtered off and washed with water until the filtrate was neutral. Recrystallization from methanol gave a green product (yield 1.12 g, 51.8%). Single crystals were obtained from absolute ethanol at room temperature *via* slow evaporation (m.p. 362–363 K).

Crystal data

$C_{15}H_{10}N_2O$
$M_r = 234.25$
Triclinic, $P\overline{1}$
$a = 6.8962$ (10) Å
$b = 8.8884$ (11) Å
$c = 9.8343$ (13) Å
$\alpha = 91.449$ (11)°
$\beta = 91.639$ (11)°
$\gamma = 92.858$ (11)°
$V = 601.59$ (14) Å^3

$Z = 2$
$D_x = 1.293$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6062 reflections
$\theta = 2.1$–28.2°
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Rectangular block, green
0.27 × 0.22 × 0.17 mm

Data collection

Stoe IPDS-2 diffractometer
φ scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{\rm min} = 0.981$, $T_{\rm max} = 0.988$
8792 measured reflections

2247 independent reflections
1487 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.070$
$\theta_{\rm max} = 25.5°$
$h = -8 \rightarrow 7$
$k = -10 \rightarrow 10$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.107$
$S = 0.96$
2247 reflections
204 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.19$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.041 (7)

Table 1
Selected geometric parameters (Å, °).

O1—C5	1.3490 (17)	N2—C8	1.139 (2)
O1—C9	1.4425 (19)	C1—C2	1.435 (2)
N1—C1	1.142 (2)	C7—C8	1.437 (2)
C5—O1—C9	118.97 (11)	O1—C5—C4	115.34 (12)
N1—C1—C2	177.62 (17)	C6—C7—C8	119.14 (14)
C3—C2—C1	119.35 (14)	C2—C7—C8	119.98 (13)
C7—C2—C1	122.04 (12)	N2—C8—C7	179.8 (2)
O1—C5—C6	124.86 (13)	O1—C9—C10	106.52 (12)

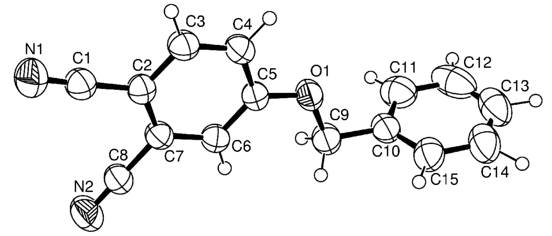


Figure 1
An *ORTEP*-3 (Farrugia, 1997) drawing of the title compound, (I), showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

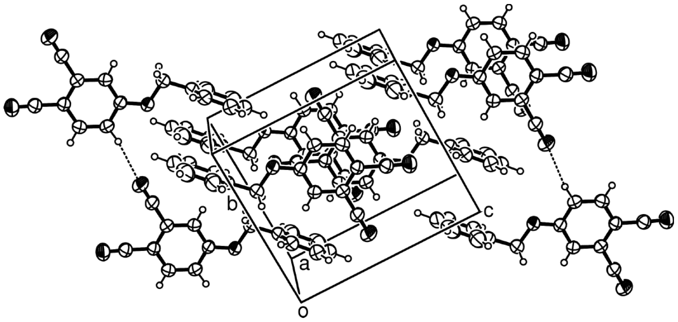


Figure 2
An *ORTEP*-3 (Farrugia, 1997) drawing of the title compound, (I), showing the hydrogen bonding and the stacking of molecules.

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
C4—H4$\cdots$N2$^{\rm i}$	0.975 (17)	2.597 (18)	3.563 (2)	170.4 (14)
C3—H3$\cdots$*Cg*2$^{\rm ii}$	0.946 (17)	2.641 (19)	3.586 (2)	171.7 (17)

Symmetry codes: (i) $x, 1+y, z$; (ii) $x, y, 1+z$. *Cg*2 denotes the centroid of ring C10–C15.

The H atoms were located in a difference Fourier map and their positional and isotropic displacement parameters were refined. The C—H distances lie in the range 0.88 (3)–1.10 (3) Å.

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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