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Key indicators

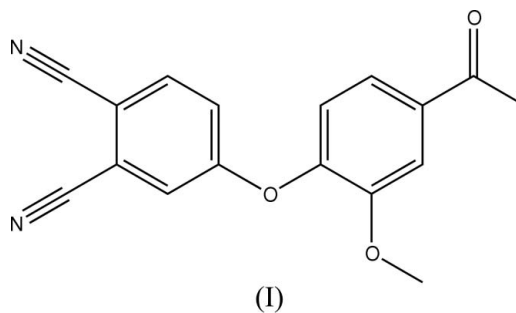
Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
R factor = 0.074
wR factor = 0.143
Data-to-parameter ratio = 16.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

4-(4-Acetyl-2-methoxyphenoxy)benzene-1,2-dicarbonitrile

The molecule of the title compound, $\text{C}_{17}\text{H}_{12}\text{N}_2\text{O}_3$, is not planar. The dihedral angle between the phthalonitrile unit and methoxyacetophenone group is $81.1 (1)^\circ$.Received 22 May 2006
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Comment

Substituted phthalonitriles have been used as starting materials for synthesizing peripherally substituted phthalocyanines and subphthalocyanines (McKeown, 1998). Phthalocyanines are among the most extensively investigated chemical species because of their uses in chemical sensors, low-dimensional conductors, nonlinear optics and liquid crystals, as well as their utility as catalysts and dyes (Leznoff & Lever, 1989–1996). The production of phthalocyanines for use in dyes and pigments is around 80 000 tonnes per year (Wöhrle, 2001). We present here the crystal structure of the title phthalonitrile derivative, (I).

The molecule of compound (I) is not planar (Fig. 1). The dihedral angle between the phthalonitrile unit and methoxyacetophenone group is $81.1 (1)^\circ$. The lengths of the two $\text{N}\equiv\text{C}$ triple bonds [$\text{C1}\equiv\text{N1} = 1.150 (5) \text{ \AA}$ and $\text{C2}\equiv\text{N2} = 1.145 (5) \text{ \AA}$] are consistent with the values found in similar compounds (Ocak *et al.*, 2003, 2004; Atalay *et al.*, 2003; Erdem *et al.*, 2004; Kartal *et al.*, 2006).

Experimental

4'-Hydroxy-3'-methoxyacetophenone (1.04 g, 6.26 mmol) and 4-nitrophthalonitrile (1.0 g, 5.78 mmol) were dissolved in dry dimethylformamide (50 ml). After stirring for 1 h at room temperature, dry fine-powdered potassium carbonate (1.40 g, 10.0 mmol) was added portionwise over a period of 2 h with thorough stirring. The reaction was stirred for 48 h at room temperature and then poured into ice-water (200 g). The product was filtered off and washed with NaOH solution (10% w/w) and water until the filtrate was neutral. Recrystallization from ethanol gave the title compound (yield 0.45 g, 24.68%). Single crystals of (I) were obtained from a solution in absolute ethanol at room temperature *via* slow evaporation.

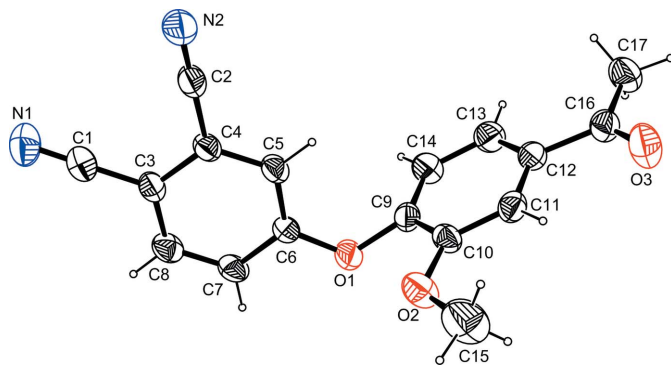


Figure 1

The molecular structure, showing the atomic numbering. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii.

Crystal data

$C_{17}H_{12}N_2O_3$

$M_r = 292.29$

Orthorhombic, *Pbca*

$a = 8.3942(7) \text{ \AA}$

$b = 22.426(2) \text{ \AA}$

$c = 15.855(2) \text{ \AA}$

$V = 2984.6(5) \text{ \AA}^3$

$Z = 8$

$D_x = 1.301 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\mu = 0.09 \text{ mm}^{-1}$

$T = 293(2) \text{ K}$

Prism, colourless

$0.64 \times 0.33 \times 0.02 \text{ mm}$

Data collection

Stoe IPDS II diffractometer

φ scans

Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)

$T_{\min} = 0.971$, $T_{\max} = 0.998$

17381 measured reflections

3260 independent reflections

1152 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.181$

$\theta_{\max} = 27.0^\circ$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.074$

$wR(F^2) = 0.143$

$S = 0.99$

3260 reflections

201 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.14 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.14 \text{ e \AA}^{-3}$

R_{int} is very high because of the poor data quality. H atoms were included in calculated positions and treated as riding on their parent C atoms, with C–H(aromatic) = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. Methyl H atoms were idealized by refining the torsion angle from the electron density map; C–H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$.

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

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