Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(2-Benzoyl-5-methoxyphenoxy)benzene-1,2-dicarbonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.085
Data-to-parameter ratio = 15.1

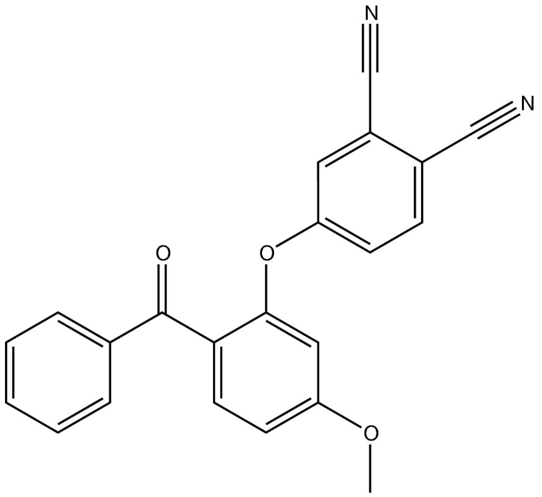
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 1 April 2005
Accepted 18 April 2005
Online 23 April 2005

The title compound, $C_{22}H_{14}N_2O_3$, contains three benzene rings, pairs of which form dihedral angles of 55.37 (5), 68.47 (4) and 82.82 (4)°. The average C—O—C angle is 119.0 (1)°.

Comment

The title compound, (I), is a precursor in the synthesis of peripherally tetrasubstituted phthalocyanines (Leznoff & Lever, 1989–1996). For many years, phthalocyanines have attracted continued interest in various research fields, such as chemical sensors, electrochromism, batteries, photodynamic therapy, semiconductor materials, liquid crystals and non-linear optics (Leznoff & Lever, 1989–1996; McKeown, 1998).


(I)

The molecular structure of (I) and a packing diagram are shown in Figs. 1 and 2, respectively. Some selected bond lengths and angles are listed in Table 1. The C≡N, C=O and C—O bond lengths agree with literature values (Ocak *et al.*, 2004; Iskeleli & Ağar, 2005; Erdem, Atalay, Akdemir, Ağar & Kantar, 2004; Erdem, Atalay, Akdemir, Ağar & Özil, 2004; Atalay *et al.*, 2003, 2004).

Compound (I) consists of one benzene rings, *A* (C1–C6), *B* (C8–C13) and *C* (C14–C19). The dihedral angles between the least-squares planes of the rings are *A*/*B* = 55.37 (5), *A*/*C* = 68.47 (4) and *B*/*C* = 82.82 (4)°.

Experimental

2-Hydroxy-4-methoxybenzophenone (1.58 g, 6.92 mmol) and 4-nitrophthalonitrile (1.00 g, 5.78 mmol) were dissolved in dry dimethylformamide (40 ml) with stirring under N_2 at 313 K. Dry fine-

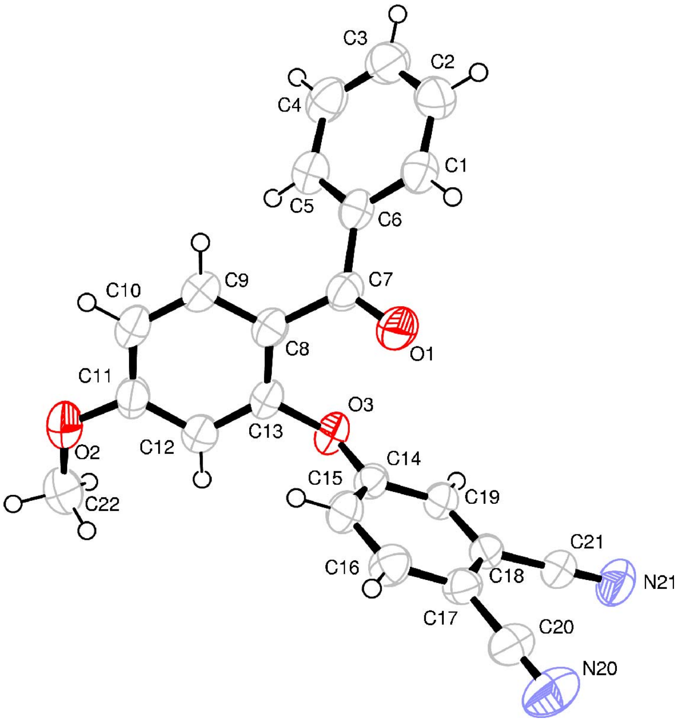


Figure 1
A view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids.

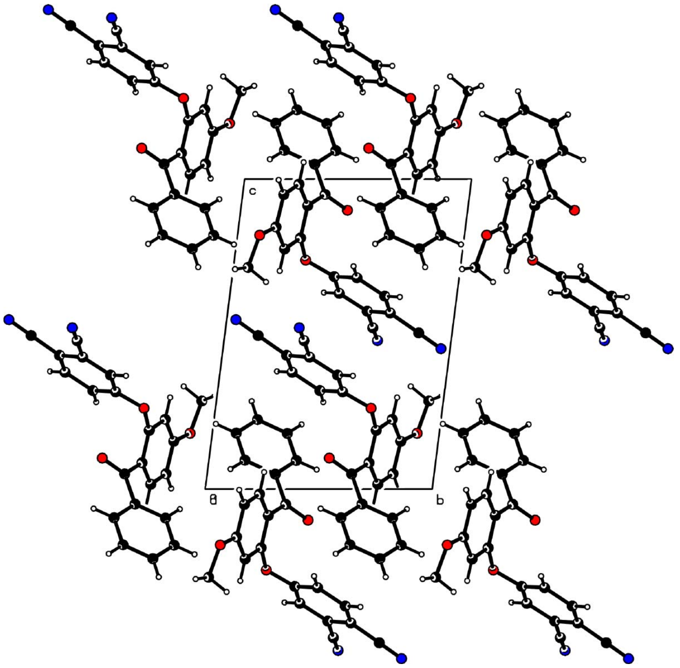


Figure 2
A plot of the crystal packing of (I), projected on the *bc* plane.

powdered potassium carbonate (1.2 g, 8.69 mmol) was added in portions (10 × 1 mmol) every 10 min. The reaction mixture was stirred for 48 h at 313 K and poured into ice–water (150 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 0.60 g (29.33%). Single crystals of (I) were obtained from absolute ethanol at room temperature by slow evaporation (m.p. 393 K). Elemental analysis, calculated for $C_{22}H_{14}N_2O_3$: C 74.57, H 3.98, N 7.91%; found: C 74.56, H 3.96, N 7.88%.

Crystal data

$C_{22}H_{14}N_2O_3$
$M_r = 354.35$
Triclinic, $P\bar{1}$
$a = 7.3142$ (9) Å
$b = 9.6929$ (11) Å
$c = 12.9986$ (16) Å
$\alpha = 81.233$ (9)°
$\beta = 83.004$ (10)°
$\gamma = 74.967$ (9)°
$V = 876.34$ (18) Å^3

$Z = 2$
$D_x = 1.343$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9968 reflections
$\theta = 2.2$–27.5°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Prism, light yellow
0.42 × 0.26 × 0.11 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.963$, $T_{\max} = 0.990$
10 703 measured reflections
3726 independent reflections

2453 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.046$
$\theta_{\max} = 27.1°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.085$
$S = 0.97$
3726 reflections
246 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.10$ e Å^{-3}
$\Delta\rho_{\min} = -0.11$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.034 (4)

Table 1
Selected geometric parameters (Å, °).

C7—O1	1.2149 (17)	C14—O3	1.3583 (15)
C11—O2	1.3610 (17)	C20—N1	1.134 (2)
C13—O3	1.3996 (15)	C21—N2	1.1406 (18)
O1—C7—C8	120.06 (14)	C11—O2—C22	118.01 (12)
O1—C7—C6	119.81 (13)	C14—O3—C13	119.99 (10)

All H atoms were placed in calculated positions and refined using a riding model. C—H distances were set to 0.93 (aromatic H) or 0.96 Å (methyl H). $U_{\rm iso}$(H) values were constrained to be 1.2 (1.5 for methyl H) times $U_{\rm eq}$ of the carrier atom.

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); software used to prepare material for publication: *WinGX* (Farrugia, 1999), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

The authors thank the Turkish Government and the University of Ondokuz Mayıs for research grant F343.

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