Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Benzyl 2-(3,4-dicyanophenoxy)benzoate

Şehriman Atalay[a]* and Ayşen Ağar[b]

[a]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey, and [b]Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey

Correspondence e-mail: atalays@omu.edu.tr

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.120
Data-to-parameter ratio = 14.4

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

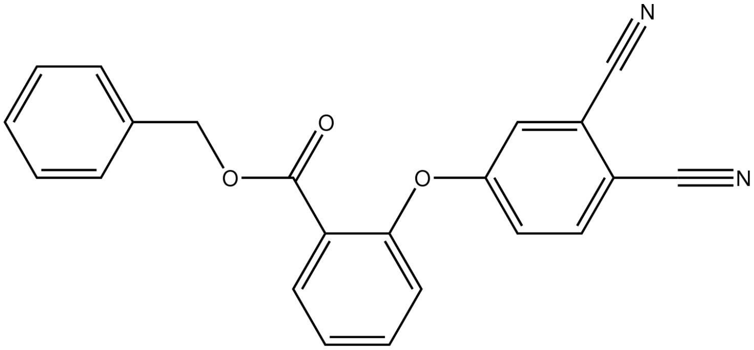
© 2005 International Union of Crystallography
Printed in Great Britain – all rights reserved

Received 18 April 2005
Accepted 6 May 2005
Online 21 May 2005

The title compound, $C_{22}H_{14}N_2O_3$, contains three planar aromatic rings arranged in a U-shaped conformation. There are weak intermolecular C—H···O hydrogen-bond interactions stabilizing the crystal structure.

Comment

Substituted phthalonitriles are generally used for preparing symmetrically and unsymmetrically peripherally substituted phthalocyanine complexes and subphthalocyanines. For many years, these compounds and their substituted analogues have attracted great interest in various research fields, such as chemical sensors, electrochromism, batteries, semiconductors, molecular metals, catalysts, photochemical hole burning, liquid crystals and non-linear optics (McKeown, 1998; Leznoff & Lever, 1989–1996).



(I)

The title compound, (I), contains three planar six-membered aromatic rings (A C1–C6, *B* C9–C14 and *C* C15–C20) arranged in a U-shaped conformation (Fig. 1). The dihedral angles formed by these rings are *A*/*B* = 74.28 (7), *A*/*C* = 10.03 (7) and *B*/*C* = 76.60 (5)°.

Selected bond lengths and angles are quoted in Table 1. The C≡N, C=O and C—O bond lengths are consistent with those found in similar compounds (Ocak *et al.*, 2004; Iskeleli & Ağar, 2005; Erdem, Atalay, Akdemir, Ağar & Kantar, 2004; Erdem, Atalay, Akdemir, Ağar & Özil, 2004).

The crystal structure is stabilized by weak intermolecular C—H···O hydrogen-bond interactions (Table 2).

Experimental

Benzyl 2-hydroxybenzoate (1.77 g, 7.75 mmol) and 4-nitrophthalonitrile (1.0 g, 5.78 mmol) were dissolved in dry dimethylformamide (50 ml). After stirring for 30 min at room temperature, dry fine-powdered potassium carbonate (2.40 g, 17.39 mmol) was added portionwise over 2 h with stirring. The reaction was stirred for 48 h at room temperature and poured into ice–water (200 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 1.70 g, 83.01%). Single crystals were obtained from absolute ethanol at room temperature *via* slow evaporation (m.p. 358 K); elemental analysis calculated for $C_{22}H_{14}N_2O_3$: C 74.57, H 3.98, N 7.91%; found: C 74.70 H 3.96 N 7.80%. IR (ν_{max}, cm^{-1}): 3045–3025 (Ar-CH), 2966–2842 (CH), 2225 (CN).

Crystal data

$C_{22}H_{14}N_2O_3$
$M_r = 354.35$
Monoclinic, $P2_1/c$
$a = 7.5535$ (5) Å
$b = 18.3764$ (9) Å
$c = 12.9216$ (9) Å
$\beta = 91.979$ (6)°
$V = 1792.53$ (19) Å^3
$Z = 4$

$D_x = 1.313$ Mg m$^{-3$}
Mo $K\alpha$ radiation
Cell parameters from 25 200 reflections
$\theta = 1.9$–28.0°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.56 × 0.42 × 0.22 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: by integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.989$, $T_{max} = 0.996$
25 200 measured reflections

3521 independent reflections
2557 reflections with $I > 2\sigma(I)$
$R_{int} = 0.168$
$\theta_{max} = 26.0°$
$h = -9 \rightarrow 9$
$k = -22 \rightarrow 22$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.120$
$S = 1.02$
3521 reflections
245 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.0771P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.078 (5)

Table 1
Selected geometric parameters (Å, °).

C7—O1	1.4659 (18)	C15—O3	1.3649 (17)
C8—O2	1.2023 (18)	C21—N1	1.135 (2)
C8—O1	1.3284 (19)	C22—N2	1.141 (2)
C14—O3	1.3963 (18)		
O2—C8—O1	124.08 (14)	C8—O1—C7	116.35 (13)
O2—C8—C9	122.12 (14)	C15—O3—C14	119.30 (11)
O1—C8—C9	113.80 (13)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O2^{i}	0.93	2.48	3.308 (2)	149
C17—H17···O2^{ii}	0.93	2.36	3.289 (2)	173

Symmetry codes: (i) $1 + x, y, z$; (ii) $-x, 1 - y, 1 - z$.

All H atoms were placed in calculated positions and refined using a riding model. C—H distances were set at 0.93 (aromatic H) and 0.97 Å (methylene H). U_{iso}(H) values were constrained to be 1.2 times U_{eq} of the carrier atom. The poor quality of the crystal may account for the rather high R_{int} value.

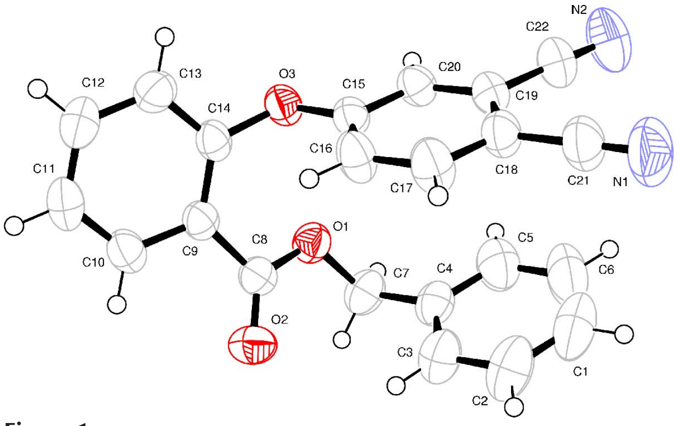


Figure 1
A view of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

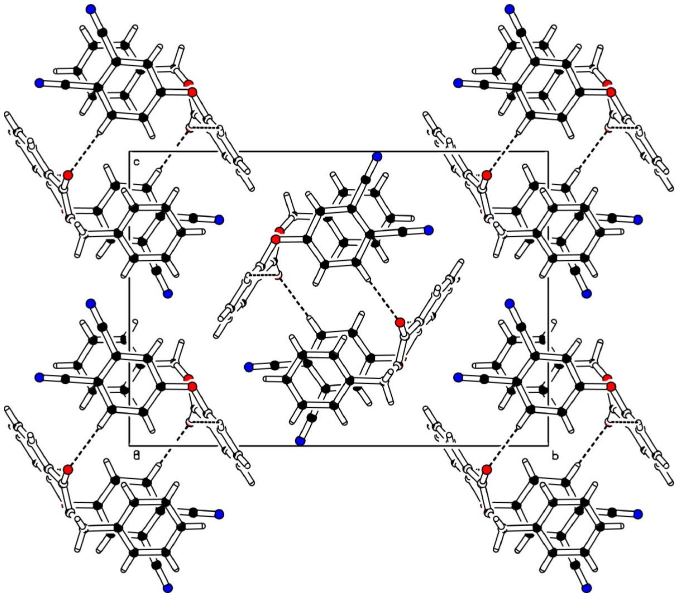


Figure 2
PLATON (Spek, 2003)/*PLUTON* (Spek, 1997) plot of the crystal packing, viewed along the *a* axis. Hydrogen bonds occurring between centrosymmetrically related molecules are shown as dashed lines.

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, 1997), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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

References

Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.

Erdem, T. K., Atalay, Ş., Akdemir, N., Ağar, E. & Kantar, C. (2004). *Acta Cryst.* E**60**, o1849–o1850.

Erdem, T. K., Atalay, Ş., Akdemir, N., Ağar, E. & Özil, M. (2004). *Acta Cryst.* E**60**, o1481–o1482.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Iskeleli, N. O. & Ağar A. (2005). *Acta Cryst.* E**61**, o158–o159.

Leznoff, C. C. & Lever, A. B. P. (1989–1996). *Phthalocyanines: Properties and Applications*, Vols. 1, 2, 3 & 4. Weinheim & New York: VHC Publishers Inc.

McKeown, N. B. (1998). *Phthalocyanine Materials: Synthesis, Structure and Function*. Cambridge University Press.

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.

Ocak, N., Işk, Ş., Akdemir, N., Kantar, C. & Ağar, E. (2004). *Acta Cryst.* E**60**, o361–o362.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Spek, A. L. (1997). *PLUTON*. University of Utrecht, The Netherlands.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Stoe & Cie (2002). *X-AREA* (Version 1.118) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.