Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

4-(Anthracen-9-ylmethoxy)phthalonitrile

Hande Petek,[a]* Şamil Işık,[b] Nesuhi Akdemir,[c] Cihan Kantar,[c] Erbil Ağar[c] and Ismet Şenel[b]

[a]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayís University, TR-55139, Kurupelit-Samsun, Turkey, [b]Ondokuz Mayıs University, Art and Science Faculty, Department of Physics, 55139 Samsun, Turkey, and [c]Ondokuz Mayıs University, Art and Science Faculty, Department of Chemistry, 55139 Samsun, Turkey

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

The title compound $C_{23}H_{13}N_2O_1$, consists of a benzene ring carrying two cyano groups linked to an anthracene moiety through an ether linkage.

Received 4 December 2003
Accepted 6 January 2004
Online 23 January 2004

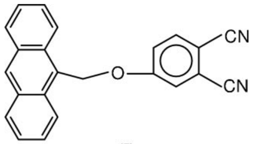
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.147
Data-to-parameter ratio = 13.1

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

Comment

Peripherally tetrasubstituted phthalocyanines are generally obtained from monosubstituted phthalonitriles (McKeown, 1998). For many years, phthalocyanines have attracted continued interest in various research fields, such as chemical sensors, catalysis, photodynamic therapy, semiconductor materials, liquid crystals and non-linear optics (Leznoff & Lever, 1989–1996). Taking into account the importance of phthalocyanines as outlined above, the X-ray study of the title compound, (I), has been carried out.



(I)

The C—C bonds and C—C—C angles in the anthracene fragment are comparable with reported values (Ramos Silva *et al.*, 2000). The benzene ring carries two cyano groups. The C1≡N1 and C2≡N2 bond lengths are 1.140 (3) and 1.141 (3) Å, respectively, typical of triple bonds. These values agree well with similar bonds reported in the literature (Öztürk *et al.*, 1999). The dihedral angle between the dicyanobenzene C1—C8 and the methylanthracene C9—C23 fragments is 66.34 (4)°.

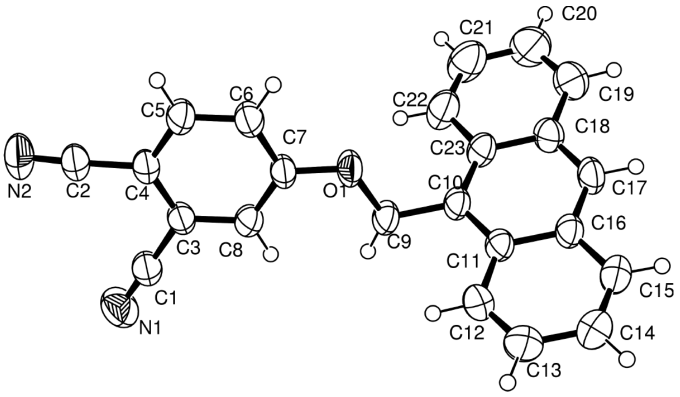


Figure 1
An *ORTEP*III (Burnett & Johnson, 1996) drawing of the molecule of the title compound, showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are shown at the 50% probability level.

DOI: 10.1107/S1600536804000285

Experimental

Anthracen-9-ylmethanol (1.20 g, 5.76 mmol) and 4-nitrophthalonitrile (0.95 g, 5.49 mmol) were dissolved in dry DMF (40 ml). After stirring for 30 min at room temperature, dry fine-powdered potassium carbonate (1.60 g, 11.6 mmol) was added portionwise over 2 h with stirring. The reaction was stirred for 24 h at room temperature and poured into ice–water (150 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 a yellow product (yield: 0.50 g; 27.3%). Single crystals were obtained from ethanol at room temperature *via* slow evaporation (m.p. 438 K). Elemental analysis, calculated for $C_{23}H_{14}N_2O$: C 82.62, H 4.22, N 8.38%; found: C 82.40, H 4.10, N 8.48%.

Crystal data

$C_{23}H_{13}N_2O$
$M_r = 333.35$
Monoclinic, $P2_1/n$
$a = 6.1396$ (4) Å
$b = 13.6929$ (12) Å
$c = 20.4225$ (13) Å
$\beta = 97.510$ (5)°
$V = 1702.2$ (2) Å^3
$Z = 4$
$D_x = 1.301$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11824 reflections
$\theta = 1.8$–29.3°
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.60 × 0.42 × 0.07 mm

Data collection

Stoe IPDS-2 diffractometer
φ scans
Absorption correction: by integration (*X-RED*; Stoe & Cie, 2002)
$T_{\min} = 0.944$, $T_{\max} = 0.994$
22331 measured reflections
3092 independent reflections
2028 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.146$
$\theta_{\max} = 25.3°$
$h = -7 \rightarrow 7$
$k = -16 \rightarrow 16$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.147$
$S = 0.96$
3092 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0862P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.51$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.014 (3)

Table 1
Selected geometric parameters (Å, °).

C9—C10	1.502 (3)	C10—C11	1.410 (3)
C23—C10	1.404 (3)		
O1—C9—C10	108.15 (15)	C23—C10—C9	118.95 (17)
C23—C10—C11	120.29 (17)		
C22—C23—C10—C9	−0.3 (3)	C9—C10—C11—C12	−3.3 (3)
O1—C9—C10—C23	−70.9 (2)	C10—C9—O1—C7	178.32 (16)
O1—C9—C10—C11	110.05 (19)		

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and $U_{\rm iso} = 1.2U_{\rm eq}$ of the parent atom. The high value of $R_{\rm int}$ is due to the poor quality of the crystal.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (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*III (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

References

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

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Leznoff, C. C. & Lever, A. B. P. (1989–1996). *Phthalocyanines: Properties & 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.

Ramos Silva, M., Matos Beja, A., Paixão, J. A., Alte da Veiga, L., Sobral, A. J. F. N., Rebanda, N. G. C. L. & d'A. Rocha Gonsalves, A. M. (2000). *Acta Cryst.* C**56**, 1136–1138.

Öztürk, S., Işık, Ş., Fun, H.-K., Kendi, E., Ağar,E., Şaşmaz, S. & İbrahim, A. R. (1999). *Acta Cryst.* C**55**, 395–397.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED* (Version 1.04). Stoe & Cie, Darmstadt, Germany.