

5-Benzylbenzene-1,2,4-tricarbonitrile

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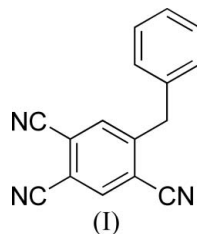
Key indicators

Single-crystal X-ray study
 $T = 288$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.052
 wR factor = 0.124
Data-to-parameter ratio = 14.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title compound, $\text{C}_{16}\text{H}_9\text{N}_3$, the phenyl ring makes a dihedral angle of $70.7(3)^\circ$ with the tricyanophenyl ring and there are intermolecular $\text{C}-\text{H}\cdots\text{N}$ interactions in the crystal structure.

Comment

Photo-induced electron-transfer (PET) reactions of cyanoarenes with alkenes have been the subject of active research (Mangion & Arnold, 2002). 1,2,4,5-Tetracyanobenzene (TCNB) is the strongest electron acceptor of all cyanoarenes (Mattes & Farid, 1982). In our ongoing research work on PET reactions between TCNB and different substrates, we have prepared the title compound, (I), which was obtained from the PET reaction of TCNB with styrene in a polar solvent mixture (acetonitrile–water = 85:15 v/v). As part of this study, we have undertaken an X-ray crystallographic analysis of (I) in order to elucidate its conformation and configuration.



The bond lengths and angles in (I) are in good agreement with expected values, except for the $\text{C}_{\text{ar}}-\text{C}(\equiv\text{N})$ bond lengths [$1.434(3)$ – $1.440(3)$ Å], which are slightly longer than the typical $\text{Csp}-\text{Csp}^2$ bond distance (Allen *et al.*, 1987). These $\text{C}_{\text{ar}}-\text{C}_{\text{CN}}$ bond lengths are comparable with those observed in the related compounds 1,2,4,5-benzenetetracarbonitrile–acridine (1/1) [$1.444(7)$ Å; Toupet *et al.*, 1989], 4-phenyl-1-(2,4,5-tricyanophenyl)-1,2,3,4-tetrahydronaphthalene [$1.442(4)$ – $1.446(4)$ Å; Zhang *et al.*, 2002] and 5-(1,4-dimethyl-4-phenyl-1,2,3,4-tetrahydro-1-naphthyl)-1,2,4-benzenetricarbonitrile [$1.440(4)$ – $1.446(4)$ Å; Usman *et al.*, 2002]. The dihedral angle formed between the phenyl and the tricyanophenyl rings is $70.7(3)^\circ$, with atom C7 lying on the intersection of the two planes. There are intermolecular $\text{C}-\text{H}\cdots\text{N}$ interactions in the crystal structure (Table 2).

Experimental

The title compound, (I), was prepared by the photo-induced reaction of 1,2,4,5-tetracyanobenzene with 1.5 equiv. of styrene in a polar solvent mixture (acetonitrile–water = 85:15 v/v), irradiated by light of wavelength longer than 300 nm for 120 h. It was isolated by column

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chromatography of the reaction mixture after evaporation of the solvent on silica gel. Single crystals of (I) were obtained by slow evaporation of a petroleum ether ethyl-acetate (3:1 v/v) solution (yield 25%).

Crystal data

C₁₆H₉N₃
M_r = 243.26
 Monoclinic, *P*2₁/*c*
a = 11.289 (2) Å
b = 8.6380 (17) Å
c = 14.193 (3) Å
 β = 113.42 (3)°
V = 1270.0 (4) Å³
Z = 4

D_x = 1.272 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 25 reflections
 θ = 10–13°
 μ = 0.08 mm⁻¹
T = 288 (2) K
 Block, colourless
 0.40 × 0.33 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: ψ scan (XCAD4; Harms & Wocadlo, 1995)
T_{min} = 0.954, *T_{max}* = 0.977
 2622 measured reflections
 2493 independent reflections

1560 reflections with *I* > 2σ(*I*)
R_{int} = 0.027
 θ_{max} = 26.0°
h = 0 → 13
k = 0 → 10
l = -16 → 16
 3 standard reflections every 200 reflections
 intensity decay: none

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.052
wR(*F*²) = 0.124
S = 1.00
 2493 reflections
 174 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2 + 0.8P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.006$
 $\Delta\rho_{max} = 0.20 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.25 \text{ e \AA}^{-3}$

Table 1 Selected geometric parameters (Å, °).

C4–C7	1.505 (3)	C11–C16	1.434 (3)
C7–C8	1.506 (3)	C12–C15	1.439 (3)
C9–C14	1.440 (3)		
C4–C7–C8	112.26 (17)		

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

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C1–H1...N2 ⁱ	0.93	2.73	3.621 (3)	161

Symmetry code: (i) *x* – 1, –*y* + $\frac{5}{2}$, *z* – $\frac{1}{2}$.

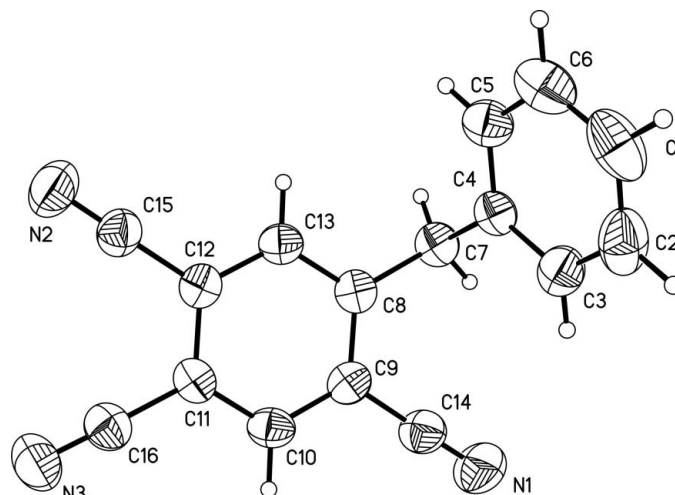


Figure 1 The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C–H distances in the range 0.93–0.97 Å and with *U_{iso}*(H) = 1.2*U_{eq}*(C).

Data collection: CAD-4 Software (Enraf–Nonius, 1989); cell refinement: CAD-4 Software; data reduction: XCAD4 (Harms & Wocadlo, 1995); program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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