

3-Phenyl-2-(2,4,5-tricyanophenylmethyl)-
1*H*-indeneJie-Qiong Huang^a and
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Key indicators

Single-crystal X-ray study

T = 293 KMean $\sigma(C-C)$ = 0.006 Å*R* factor = 0.046*wR* factor = 0.110

Data-to-parameter ratio = 8.5

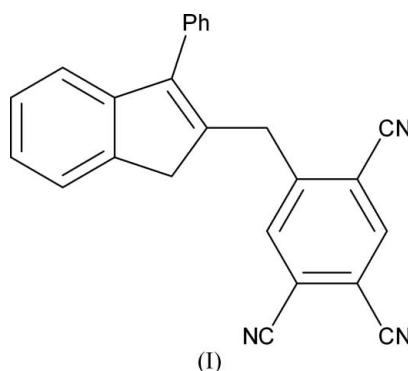
For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.In the title compound, C₂₅H₁₅N₃, the indene unit is essentially planar and there are intermolecular C—H··· π interactions in the crystal structure.

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Comment

Photo-induced electron-transfer (PET) reactions of cyanoarenes with alkenes have attracted much research interest in recent years (Mella *et al.*, 1998; Zhang *et al.*, 2006). 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, we have found that the PET reaction between TCNB and an excess amount of 1-phenyl-1,2,3,4-tetrahydronaphthalene in a polar solvent (acetonitrile) afforded the title compound, (I), as one of the products. As a 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) (Table 1) are in good agreement with expected values, except for the C_{ar}—C(≡N) bond lengths [1.435 (5)–1.439 (5) Å], which are slightly longer than the typical C_{sp}—C_{sp}² bond distance (Allen *et al.*, 1987). These C_{ar}—C_{CN} bond lengths are comparable with those observed in the related compounds 4-phenyl-1-(2,4,5-tricyanophenyl)-1,2,3,4-tetrahydronaphthalene [1.442 (4)–1.446 (4) Å; Zhang *et al.*, 2002], 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] and 5-benzylbenzene-1,2,4-tricarbonitrile [1.434 (3)–1.440 (3) Å; Wang *et al.*, 2005]. In the title structure (Fig. 1), the indene unit is essentially planar. The phenyl and the tricyanophenyl rings form dihedral angles of 77.7 (4) and 85.6 (4)°, respectively, with the mean plane through the indene unit.

In the crystal structure, the molecular packing is stabilized by intermolecular C—H··· π interactions (Table 2) involving the aromatic rings.

Experimental

The title compound, (I), was prepared by the photo-induced reaction of 1,2,4,5-tetracyanobenzene with 10 equivalents of 1-phenyl-1,2,3,4-tetrahydronaphthalene in an acetonitrile solution, irradiated by the light of wavelength longer than 300 nm for 60 h. It was isolated by column 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–acetone (1:1 v/v) solution (yield 7%).

Crystal data

$C_{25}H_{15}N_3$
 $M_r = 357.40$
 Orthorhombic, $P2_12_12_1$
 $a = 7.7190$ (15) Å
 $b = 10.155$ (2) Å
 $c = 24.316$ (5) Å
 $V = 1906.0$ (7) Å³

$Z = 4$
 $D_x = 1.245$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 293$ (2) K
 Block, colourless
 $0.45 \times 0.33 \times 0.30$ mm

Data collection

Enraf–Nonius CAD-4
 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: ψ scan
 (XCAD4; Harms & Wocadlo, 1995)
 $T_{\min} = 0.951$, $T_{\max} = 0.978$
 4216 measured reflections

2160 independent reflections
 1385 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$
 $\theta_{\text{max}} = 26.0^\circ$
 3 standard reflections
 every 200 reflections
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.110$
 $S = 1.00$
 2160 reflections
 254 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.02P)^2 + 0.765P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.16$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0339 (16)
 Absolute structure: Flack (1983)
 Flack parameter: -0.03 (7)

Table 1

Selected geometric parameters (Å, °).

C8–C9	1.362 (5)	C18–C23	1.437 (5)
C9–C10	1.488 (5)	C20–C24	1.435 (5)
C16–C17	1.498 (5)	C21–C25	1.439 (5)
C8–C7–C6	103.8 (3)	C17–C16–C8	114.0 (3)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C19–H19 \cdots CgA ⁱ	0.93	2.99	3.724 (4)	137

Symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$. Cg(A) denotes the centroid of the C1–C6 aromatic ring.

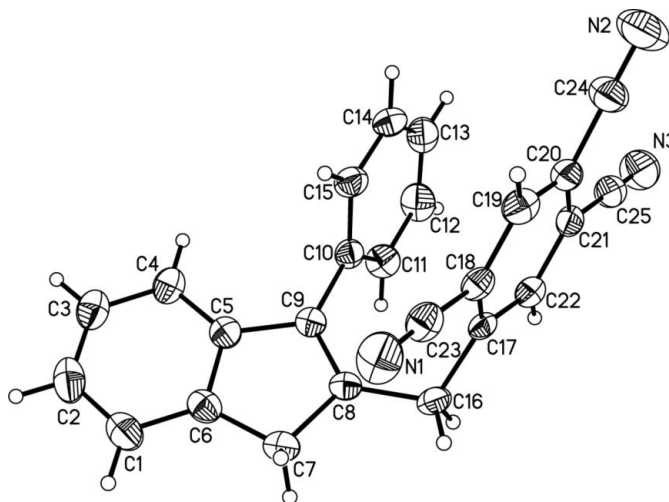


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are shown at the 30% probability level.

The H atoms were included in the riding-model approximation, with C–H distances of 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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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References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Enraf–Nonius. (1989). *CAD-4 Software*. Version 5. Enraf–Nonius, Delft, The Netherlands.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
- Mattes, S. L. & Farid, S. (1982). *Acc. Chem. Res.* **15**, 80–86.
- Mella, M., Fagnoni, M., Freccero, M., Fasani, E. & Albin, A. (1998). *Chem. Soc. Rev.* **27**, 81–89.
- Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Usman, A., Razak, I. A., Fun, H.-K., Chantrapromma, S., Zhang, M. & Xu, J.-H. (2002). *Acta Cryst.* **E58**, o467–o468.
- Wang, Y.-G., An, H.-Y., Lu, Z.-F., Wu, L. & Xu, J.-H. (2005). *Acta Cryst.* **E61**, o3543–o3544.
- Zhang, M., Lu, Z.-F., Liu, Y., Grampp, G., Hu, H.-W. & Xu, J.-H. (2006). *Tetrahedron*, **62**, 5663–5674.
- Zhang, M., Usman, A., Razak, I. A., Fun, H.-K., Chantrapromma, S. & Xu, J.-H. (2002). *Acta Cryst.* **E58**, o132–o133.