# organic papers

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# 4-Phenyl-1-(2,4,5-tricyanophenyl)-1,2,3,4-tetrahydro-naphthalene

In the title compound, $C_{25}H_{17}N_3$, the tetrahydrobenzene ring of the tetrahydronaphthalene moiety adopts a half-chair conformation. Both the phenyl and tricyanophenyl rings are oriented almost perpendicular to the tetrahydrobenzene ring. The crystal structure is stabilized by intermolecular C—H$\cdots\pi$ interactions.

## Comment

Photoinduced electron-transfer (PET) reactions have been receiving much research interest in recent years (Kavarnos & Turro, 1986). 1,2,4,5-Tetracyanobenzene (TCB) is one of the strongest electron acceptors used in PET reactions. In our recent research work on PET reactions between TCB and different substrates, we have prepared the title compound, (I), which is obtained from the PET reactions of TCB with styrene in a polar solvent (acetonitrile). As part of this study, we have undertaken the X-ray crystallographic analysis of (I) in order to elucidate the steric conformation and configuration of this cycloaddder product.



(I)
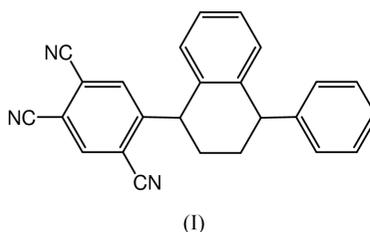
The bond lengths and angles in (I) are in good agreement with expected values, except for the $C_{ar}$—C bond lengths of the carbonitriles [1.442 (4)-1.446 (4) Å] which are slightly longer than the typical $Csp$—$Csp^2$ bond distance (Allen *et al.*, 1987). These $C_{ar}$—$C_{carbonitrile}$ bond lengths are comparable with those observed for 1,2,4,5-benzenetetracarbonitrile–acridine (1/1) (Toupet *et al.*, 1989).

In the title structure (Fig. 1), the tetrahydrobenzene ring adopts a half-chair conformation, with C1 and C2 deviating from the C3/C4/C9/C10 plane by 0.280 (3) and 0.495 (3) Å, respectively. The puckering parameters (Cremer & Pople, 1975) are $Q = 0.514$ (3) Å, $\theta = 50.1$ (3)° and $\varphi = 39.2$ (4)°. In the tetrahydronaphthalene moiety, the mean plane through the tetrahydrobenzene ring forms a dihedral angle of 5.0 (1)° with the benzene ring. The phenyl ring of the tricyanophenyl moiety is planar within ±0.01 Å. The phenyl and the tricyanophenyl rings form dihedral angles of 83.4 (1) and 85.4 (1)°, respectively, with respect to the mean plane through the tetrahydrobenzene ring.
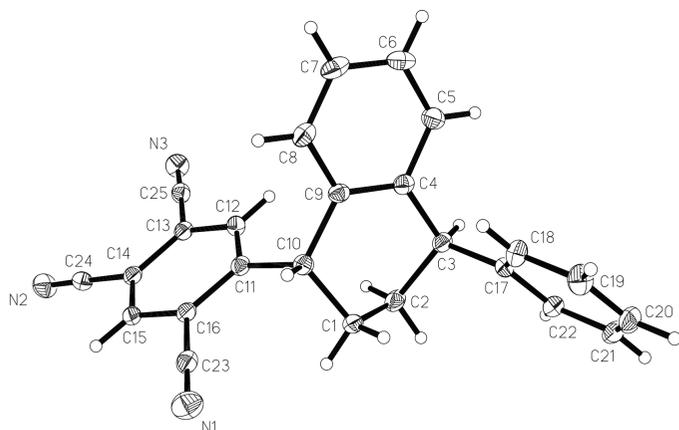
**Figure 1**
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

In the crystal, the molecular packing is stabilized by intermolecular C—H···$\pi$ interactions (Table 2) involving the aromatic rings. In Table 2, Cg($A$), Cg($B$) and Cg($C$) denote the centroids of the aromatic rings C17–C22, C4–C9 and C11–C16, respectively.

## Experimental

The title compound, (I), was one of the products of a photo-induced reactions between 1,2,4,5-benzenetetracarbonitrile and an excess amount of styrene in an acetonitrile solution. The title compound was isolated using column chromatography. Single crystals suitable for X-ray diffraction analysis were obtained from slow evaporation of a petroleum ether–ethyl acetate solution.

### Crystal data

| | |
|---|---|
| $C_{25}H_{17}N_3$ | Mo $K\alpha$ radiation |
| $M_r = 359.42$ | Cell parameters from 7065 |
| Orthorhombic, $Pna2_1$ | reflections |
| $a = 22.2686\ (3)$ Å | $\theta = 2.9–28.3°$ |
| $b = 9.2463\ (2)$ Å | $\mu = 0.08\ \text{mm}^{-1}$ |
| $c = 9.1349\ (2)$ Å | $T = 183\ (2)$ K |
| $V = 1880.9\ (1)$ Å$^3$ | Block, colorless |
| $Z = 4$ | $0.42 \times 0.30 \times 0.26$ mm |
| $D_x = 1.269$ Mg m$^{-3}$ | |

### Data collection

| | |
|---|---|
| Siemens SMART CCD area-detector diffractometer | 2435 independent reflections |
| | 1942 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int} = 0.086$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $\theta_{max} = 28.3°$ |
| $T_{min} = 0.969$, $T_{max} = 0.981$ | $h = -24 \rightarrow 29$ |
| | $k = -12 \rightarrow 11$ |
| 10933 measured reflections | $l = -12 \rightarrow 8$ |

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0483P)^2]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.047$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.104$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $S = 0.95$ | $\Delta\rho_{max} = 0.33$ e Å$^{-3}$ |
| 2435 reflections | $\Delta\rho_{min} = -0.22$ e Å$^{-3}$ |
| 254 parameters | Extinction correction: *SHELXTL* |
| H-atom parameters constrained | Extinction coefficient: 0.025 (3) |

**Table 1**
Selected interatomic distances (Å).

| | | | |
|---|---|---|---|
| C1—C2 | 1.522 (4) | C3—C17 | 1.521 (3) |
| C1—C10 | 1.543 (3) | C10—C11 | 1.520 (3) |
| C2—C3 | 1.541 (3) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C2—H2$A$···Cg($A^i$) | 0.97 | 3.35 | 3.943 (3) | 122 |
| C15—H15$A$···Cg($A^{ii}$) | 0.93 | 2.74 | 3.466 (3) | 135 |
| C18—H18$A$···Cg($B^{iii}$) | 0.93 | 3.39 | 4.160 (3) | 142 |
| C20—H20$A$···Cg($C^{iv}$) | 0.93 | 3.21 | 3.837 (3) | 126 |

Symmetry codes: (i) $1 - x, 2 - y, \frac{1}{2} + z$; (ii) $x - \frac{1}{2}, \frac{3}{2} - y, z$; (iii) $1 - x, 1 - y, z - \frac{1}{2}$; (iv) $1 - x, 2 - y, z - \frac{1}{2}$.

The H atoms were geometrically positioned and were treated as riding atoms on the parent C atoms, with C—H distances in the range 0.93–0.98 Å.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

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