

6-*tert*-Butylnaphthalene-2,3-dicarbonitrile

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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.036
 wR factor = 0.117
Data-to-parameter ratio = 13.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

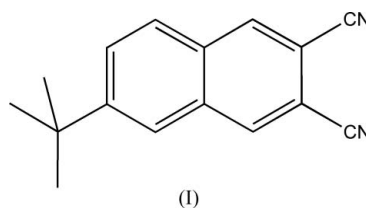
Molecules of the title compound, $\text{C}_{16}\text{H}_{14}\text{N}_2$, are located on a crystallographic mirror plane with one half-molecule in the asymmetric unit. The molecules are held together in the crystal structure by π - π stacking interactions.

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Comment

For many years, phthalocyanine derivatives have attracted attention because of their high thermal stability as well as their wide applications in many fields (Hanack *et al.*, 1994). Recently, there has been considerable interest in the synthesis and elucidation of the properties of structurally modified phthalocyanines.



Molecules of the title compound are located on a crystallographic mirror plane. The C—N bond lengths within each CN group are almost equal [1.138 (2) and 1.133 (2) Å]. The molecules in the crystal structure are held together by π - π stacking interactions. The closest centroid-centroid distance of two benzene rings is 3.821 Å [$\text{Cg}1 \cdots \text{Cg}1^i$ and $\text{Cg}1 \cdots \text{Cg}1^{ii}$ where $\text{Cg}1$ is the centroid of the C3–C8 ring; symmetry codes (i) $1 - x, 1 - y, 1 - z$; (ii) $1 - x, -y, 1 - z$].

Experimental

The title compound was synthesized according to a literature method (Chabach, *et al.*, 1995). Crystals were obtained by evaporation of an ethanol solution. Analysis calculated (%): C 82.02, N 11.96, H 6.02; found(%): C 82.00, N 12.01, H 6.07.

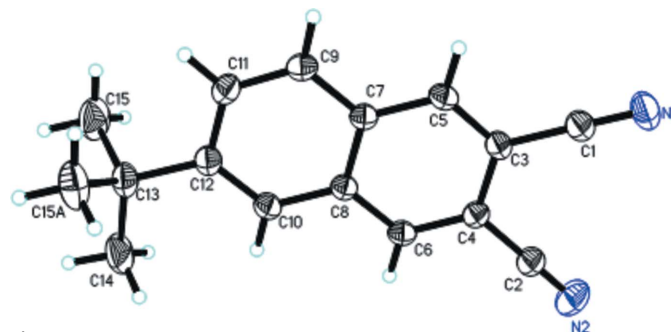


Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) $x, \frac{1}{2} - y, z$].

Crystal data

$C_{16}H_{14}N_2$
 $M_r = 234.29$
 Orthorhombic, *Pnma*
 $a = 11.1480$ (2) Å
 $b = 7.0072$ (2) Å
 $c = 16.7188$ (4) Å
 $V = 1306.01$ (5) Å³

$Z = 4$
 $D_x = 1.192$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹
 $T = 298$ (2) K
 Block, colourless
 $0.25 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART CCD diffractometer
 ω scans
 Absorption correction: multi-scan
SADABS (Bruker, 1997)
 $T_{\min} = 0.983$, $T_{\max} = 0.989$

10458 measured reflections
 1399 independent reflections
 1062 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 $\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.117$
 $S = 1.08$
 1399 reflections
 108 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.1377P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.14$ e Å⁻³
 Extinction correction: *SHELXL*
 Extinction coefficient: 0.008 (2)

H atoms were refined with fixed individual displacement parameters [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$] using a riding model with C–H = 0.93 (aromatic) or 0.96 Å (methyl). The C15 methyl group was allowed to rotate but not to tip.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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References

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