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3,3′,5,5′-Tetramethylbiphenyl-4,4′-dicarbonitrile

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Key indicators
Single-crystal X-ray study
T = 174 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.044
wR factor = 0.113
Data-to-parameter ratio = 14.9

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

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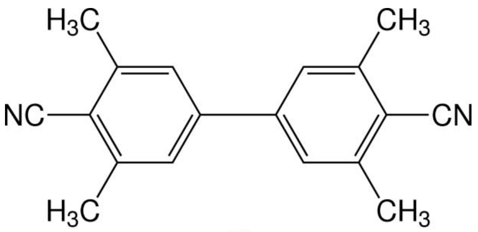
The title compound, $C_{18}H_{16}N_2$, crystallizes with $Z' = \frac{1}{4}$. The molecule exhibits 222 symmetry, with its centre at the intersection of three twofold axes, one of which traverses the molecule through the nitrile groups and the *ipso* and *para* ring atoms. The torsion angle between the rings is 50.3 (1)°. Adjacent molecules are involved in antiparallel CN···CN interactions and weak C—H···N hydrogen bonds.

Comment

The title compound, (I), was designed and prepared as part of an effort to develop efficient sensitizers for photoinduced electron-transfer reactions (Gassman & de Silva, 1991).



(I)

The atom labelling and the anisotropic displacement parameters are shown in Fig. 1. The molecule exhibits 222 symmetry, with its centre at the intersection of three twofold axes, one of which traverses the molecule through the nitrile groups and the *ipso* and *para* ring atoms. The bond lengths and angles are normal. The dihedral angle between the two rings is 50.3 (1)°. The methyl groups are disordered, with occupancy 0.87 (16) in the position shown in Fig. 1 and 0.13 (16) rotated by 60° around the C—C bond.

The intermolecular contacts are shown in Fig. 2. The C5—N7 nitrile group is next to two antiparallel groups at ($x \pm \frac{1}{2}$, y, $\frac{1}{4} - z$); the perpendicular distance to these groups is 3.735 (2) Å. The aromatic atom H3 is part of a weak C—H···*A* hydrogen bond, with C—H = 0.98 (2) Å and H···N7^{i} = 2.59 Å; the angles are C3—H3···N7^{i} = 161 (1) and H3···N7^{i}—C7^{i} = 101 (1)° [symmetry code (i): $x - \frac{1}{4}$, $y - \frac{1}{4}$, $z + \frac{1}{4}$]. For a discussion of C—H hydrogen bonds see Desiraju & Steiner (1999).

Experimental

The title compound was prepared by the Ullmann coupling of 4-bromo-2,6-dimethylbenzonitrile (Fuson *et al.*, 1941), using a procedure similar to that described by Colon & Kelsey (1986). The product was recrystallized from boiling toluene. Several other methods of preparation (Castle *et al.*, 1969; Inaba *et al.*, 1982) were unsatisfactory,

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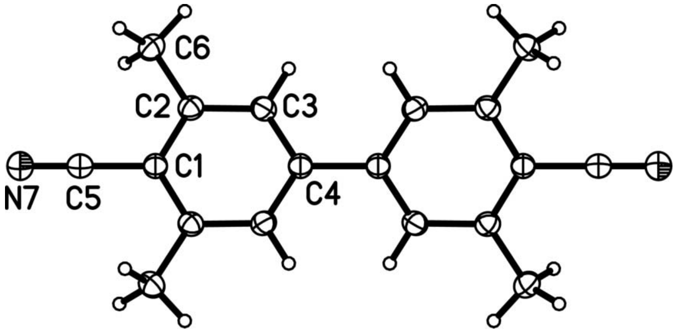

Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. The molecule has 222 symmetry and only the crystallographically independent atoms are labelled. The methyl groups are disordered; only the major component of the disorder is shown.

primarily owing to the low solubility of (I) in common organic solvents.

Crystal data

$C_{18}H_{16}N_2$
$M_r = 260.33$
Orthorhombic, *Fddd*
$a = 7.4694\ (19)$ Å
$b = 16.812\ (4)$ Å
$c = 22.514\ (6)$ Å

$V = 2827.2\ (12)$ Å^3
$Z = 8$
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 174\ (2)$ K
$0.25 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan [*SADABS* (Sheldrick, 2003; Blessing, 1995)]
$T_{\min} = 0.91$, $T_{\max} = 0.99$

7789 measured reflections
820 independent reflections
731 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.113$
$S = 1.11$
820 reflections
55 parameters

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.26$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

The methyl H atoms were placed in geometrically idealized disordered positions, rotated 60° around the C—C axis, with occupancies which refined to 0.87 (16) and 0.13 (16) (Fig. 1). They were constrained to ride on their parent C atoms, with C—H = 0.98Å and with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$. The ring atom H3 was found in a difference map and refined with a restrained C—H distance of 0.98 Å and free $U_{\rm iso}$(H).

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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*.

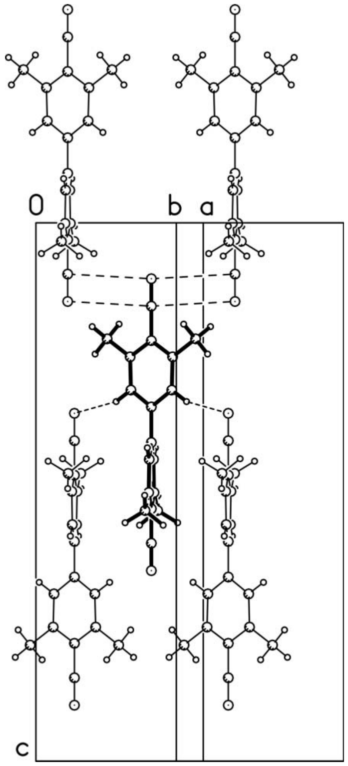

Figure 2
The intermolecular contacts in (I). The top part shows the CN···CN interactions (long-dashed lines). The bottom part shows the weak C—H···N hydrogen bonds (short-dashed lines).

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