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3,3′,5,5′-Tetramethylterphenyl

Jiyang Xu,[a] Adrien P. Côté[b] and Banglin Chen[c]*

[a]Department of Biochemistry, China Pharmaceutical University, Nanjing 210009, People's Republic of China, [b]Department of Chemistry, The University of Michigan, Ann Arbor, MI 48109, USA, and [c]Department of Chemistry, The University of Texas–Pan American, Edinburgh, TX 78541-2999, USA

Correspondence e-mail: banglin@panam.edu

Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.002 Å
R factor = 0.047
wR factor = 0.177
Data-to-parameter ratio = 18.2

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

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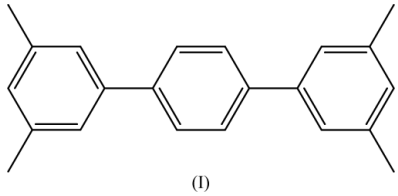
Molecules of the title compound, $C_{22}H_{22}$, crystallize in space group $P2_1/c$ and are located on crystallographic inversion centers. The structure reveals a twisted molecule with a dihedral angle of 31.9 (2)° between the central and outer benzene rings.

Comment

The title compound, (I), is used for the synthesis of 3,3′,5,5′-terphenyltetracarboxylic acid, which can be incorporated into porous metal–organic frameworks (MOFs) for their potential applications in gas storage, separation, molecular recognition, magnetism and catalysis (Eddaoudi *et al.*, 2001; Kitagawa & Kondo, 1998; Yaghi *et al.*, 2003; Janiak, 2003; Chen *et al.*, 2001).



(I)

The molecule of (I) is centrosymmetric, with no intermolecular π–π stacking interactions between benzene rings, and significantly twisted with a dihedral angle of 31.9 (2)° between the central and outer rings, as shown in Fig. 1. As expected, the C1—C7 bond distance of 1.489 (2) Å is longer than the aromatic C—C bond distances [1.387 (2)–1.402 (2) Å]. These structural features are normal and comparable to those found in *p*-terphenyl (Baudour *et al.*, 1986) and 3,3′-dimethylterphenyl (Avery *et al.*, 1998).

Experimental

The title compound was synthesized according to the modified procedure of Oh *et al.* (2002) by the reaction of 1,4-diiodobenezene and 3,5-dimethylphenylboronic acid at 323 K. Crystals of the title

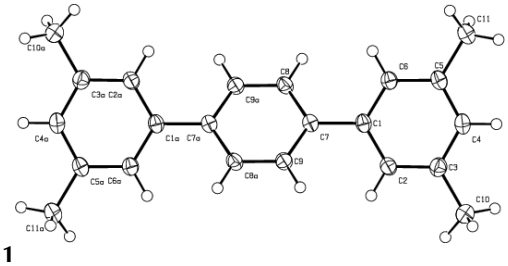


Figure 1
The structure of (I), showing the atom-numbering scheme and displacement ellipsoids at the 50% probability level. Atom labels having suffix A are related to their counterparts without A by the symmetry operation $2-x, -y, -z$.

compound were collected by recrystallization of the crude product from dichloromethane–hexane (1:2) in 56% yield.

Crystal data

$C_{22}H_{22}$	$D_x = 1.178$ Mg m^{-3}
$M_r = 286.42$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4518 reflections
$a = 11.9264$ (13) Å	$\theta = 2.2$–$27.6°$
$b = 9.2297$ (10) Å	$\mu = 0.07$ mm^{-1}
$c = 7.6075$ (8) Å	$T = 153$ (2) K
$\beta = 105.381$ (2)°	Prism, colourless
$V = 807.42$ (15) Å^3	0.40 × 0.10 × 0.09 mm
$Z = 2$	

Data collection

Bruker SMART APEX diffractometer	1574 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.073$
Absorption correction: none	$\theta_{max} = 27.6°$
7844 measured reflections	$h = -15 \rightarrow 15$
1854 independent reflections	$k = -11 \rightarrow 12$
	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.177$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.74$	$\Delta\rho_{max} = 0.35$ e Å^{-3}
1854 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
102 parameters	

H atoms were generated as spheres and constrained to riding the coordinates of their parent atoms.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2003); software used to prepare material for publication: *SHELXL*97.

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