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1,3,5-Tris(4-methylphenyl)benzene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.102
Data-to-parameter ratio = 18.9

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

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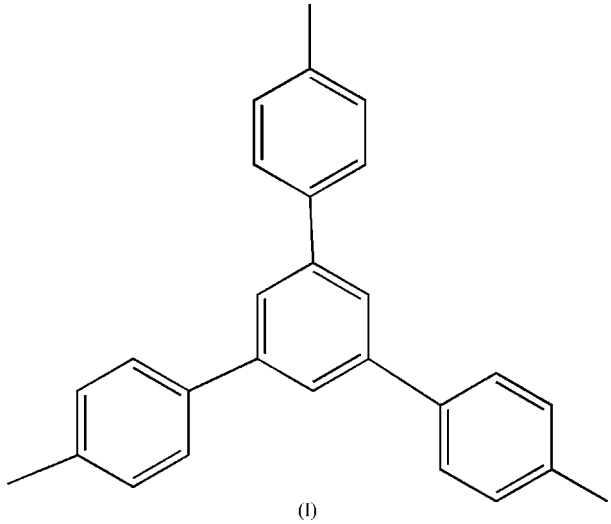
The title compound, $C_{27}H_{24}$, with a propeller-like shape, crystallizes with two crystallographically independent molecules in the asymmetric unit. Intermolecular π–π interactions are pronounced in the crystal structure.

Comment

Numerous small molecular propellers of approximate D_3 symmetry are known, but the vast majority of these compounds have the structure $(aryl)_3X$, where X is a single atom (Tong *et al.*, 1997). However, we present the structure of (I) where the central atom is replaced by a benzene ring (Weber *et al.*, 1988; Thallapally *et al.*, 2000; Elmorsy *et al.*, 1991; Grilli *et al.*, 2002; Lindeman *et al.*, 1984).



(I)

The crystal stucture of the title compound, (I), has two molecules (1 and 2) in the asymmetric unit (Fig. 1). Selected geometric parameters are shown in Table 1. In molecule 1, the central aromatic ring 1 (atoms C1–C6) is tilted with respect to the *p*-methylphenyl rings 2 (atoms C19–C24), 3 (C7–C12) and 4 (C13–C18), with dihedral angles of 42.93 (6), 35.15 (7) and 39.95 (8)°, respectively. In molecule 2, the dihedral angles of ring 1′ (atoms C28–C33) with rings 2′ (atoms C46–C51), 3′ (C34–C39) and 4′ (C40–C45) are 40.38 (8), 34.48 (7) and 47.99 (7)°, respectively. *p*-Methylphenyl ring 4 in molecule 1 is close to being perpendicular to ring 4′ in molecule 2, with a dihedral angle of 88.08 (6)°. However, rings 1, 2 and 3 are approximately parallel to the corresponding rings 1′, 2′ and 3′ in molecule 2, with dihedral angles of 11.15 (11), 14.57 (8) and 11.06 (6)°, respectively. π–π stacking interactions (with

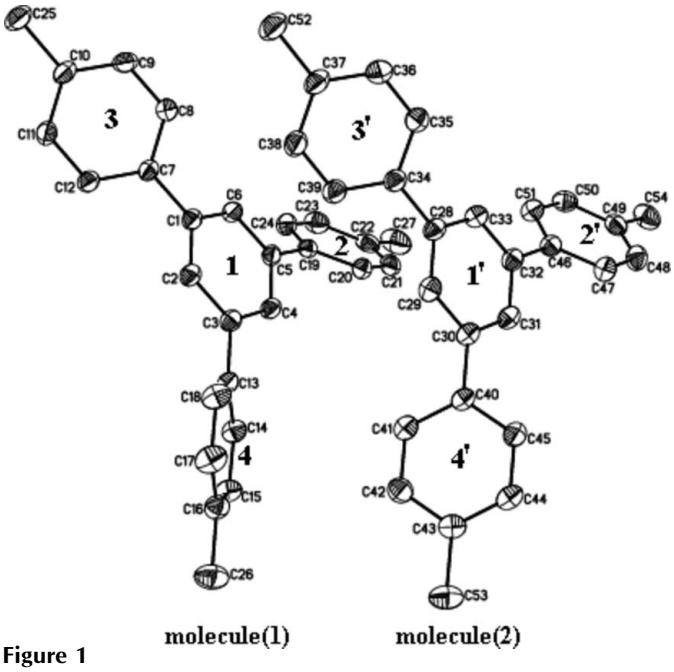


Figure 1
View of the asymmetric unit of (I), showing the atom-labelling scheme. All H atoms have been omitted for clarity.

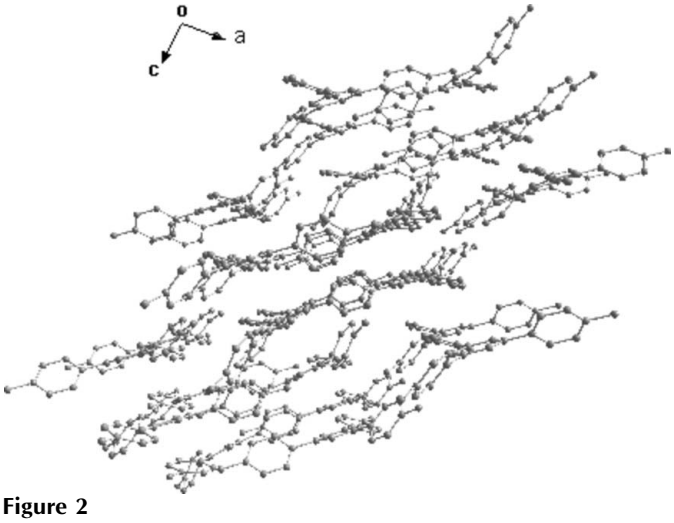


Figure 2
Packing diagram of (I), showing the π–π stacking along the *b* axis. All H atoms have been omitted for clarity.

centroid–centroid distances of 3.46–3.64 Å) support the crystal packing (Fig. 2).

Experimental

All reagents were of AR grade, available commercially and used without further purification. The title compound was prepared according to the procedure of Lyle *et al.* (1953). To 50 ml of absolute ethanol saturated with hydrogen chloride, 10 g of *p*-methylacetophenone was added. After standing for 30 d, the reaction mixture was filtered and the solid residue was washed with cold absolute ethanol, giving pure 1,3,5-tris(4-methylphenyl)benzene. A small amount of product was obtained by pouring the above filtrate into water and filtering the mixture. The crude oily product required washing with alcohol.

Crystal data

$C_{27}H_{24}$	D_x = 1.131 Mg m^{-3}
M_r = 348.46	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 9186 reflections
a = 13.1640 (6) Å	θ = 2.0–27.5°
b = 15.2531 (9) Å	μ = 0.06 mm^{-1}
c = 20.5554 (11) Å	T = 293 (2) K
β = 97.3083 (17)°	Prism, yellow
V = 4093.8 (4) Å^3	0.43 × 0.21 × 0.15 mm
Z = 8	

Data collection

Rigaku Weissenberg IP diffractometer	9186 independent reflections
Scintillation counter scans	3366 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*TEXSAN*; Molecular Structure Corporation, 1998)	R_{int} = 0.049
T_{min} = 0.899, T_{max} = 0.994	θ_{max} = 27.5°
31594 measured reflections	$h = 0 \rightarrow 16$
	$k = 0 \rightarrow 19$
	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.054	$w = 1/[\sigma^2(F_o^2) + (0.0251P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.102	$(\Delta/\sigma)_{max} < 0.001$
S = 0.99	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
9186 reflections	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
487 parameters	

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.486 (3)	C28—C34	1.477 (3)
C3—C13	1.489 (3)	C30—C40	1.490 (3)
C5—C19	1.477 (3)	C32—C46	1.487 (3)
C10—C25	1.513 (3)	C37—C52	1.520 (3)
C16—C26	1.520 (3)	C43—C53	1.513 (3)
C22—C27	1.524 (3)	C49—C54	1.516 (3)
C2—C1—C7	121.0 (2)	C29—C28—C34	119.9 (2)
C2—C3—C13	121.9 (2)	C29—C30—C40	120.4 (2)
C6—C5—C19	121.7 (2)	C33—C32—C46	121.1 (2)
C8—C7—C1	120.3 (2)	C35—C34—C28	120.9 (2)
C9—C10—C25	121.3 (2)	C36—C37—C52	121.6 (2)
C14—C13—C3	120.7 (2)	C41—C40—C30	120.8 (2)
C15—C16—C26	120.9 (2)	C42—C43—C53	120.8 (2)
C24—C19—C5	120.2 (2)	C51—C46—C32	121.0 (2)
C23—C22—C27	119.9 (3)	C50—C49—C54	121.2 (2)

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with aromatic C—H = 0.93 Å and methyl C—H = 0.96 Å, and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(C) for aromatic and methyl H atoms, respectively.

Data collection: *TEXSAN* (Molecular Structure Corporation, 1998); cell refinement: *TEXSAN*; data reduction: *TEXSAN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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