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[Tris(4-tolyl)methyl]benzene

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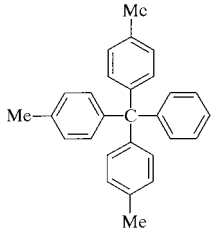
The crystal structure of the title compound, $C_{28}H_{26}$, in the monoclinic space group $C2/c$ has a columnar packing arrangement with a 7.20 Å axis, a feature common to several tetraphenylmethanes.

Comment

In the crystal structure of the title molecule, (I), translation-related molecules stack along [010] with the usual phenyl embrace-type packing forming a molecular column which is common in several tetraphenylmethanes (Kitaigorodskii, 1973).



(I)

Experimental

[Tris(4-tolyl)methyl]benzene was obtained as a by-product when 4-[tris(4-tolyl)methyl]aniline was diazotized with sodium nitrite and treated with KI solution (Grimm *et al.*, 1986). 4-[Tris(4-tolyl)-methyl]aniline was prepared by the alkylation of chlorotris(4-tolyl)-methane with aniline at 493 K (Su & Menger, 1997). Crystals of (I) suitable for single-crystal X-ray diffraction were grown by slow evaporation of a saturated solution of (I) from benzene.

Crystal data

$C_{28}H_{26}$	D_x = 1.135 Mg m^{-3}
M_r = 362.49	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 25 reflections
a = 17.843 (4) Å	θ = 1.5–27.5°
b = 7.2015 (14) Å	μ = 0.064 mm^{-1}
c = 33.176 (7) Å	T = 293 (2) K
β = 95.59 (3)°	Needle, colourless
V = 4242.6 (15) Å^3	0.60 × 0.40 × 0.36 mm
Z = 8	

Data collection

Enraf–Nonius CAD-4 diffractometer	θ_{max} = 27.47°
ω scans	$h = -23 \rightarrow 23$
9332 measured reflections	$k = -9 \rightarrow 0$
4864 independent reflections	$l = -42 \rightarrow 43$
3098 reflections with $I > 2\sigma(I)$	3 standard reflections every 100 reflections
R_{int} = 0.019	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 1.0945P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.057	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.173	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
S = 1.153	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
4864 reflections	Extinction correction: *SHELXL*97
254 parameters	Extinction coefficient: 0.0007 (3)
H-atom parameters constrained	

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *Xtal*3.5 (Hall *et al.*, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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