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2,4,6-Trimethylphenol

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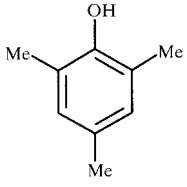
Crystals of the title compound, $C_9H_{12}O$, were formed as an unexpected by-product during the recrystallization of (2*R*,3*R*)-α,α,α′,α′-tetramesityl-1,4-dioxaspiro[4,5]decane-2,3-dimethanol from hexane/ethyl acetate (7:3). Strong hydrogen bonds between hydroxide groups connect the molecules around one set of four symmetry-equivalent 2_1 axes.

Comment

Crystals of the title compound, (I), were formed as an unexpected by-product during the recrystallization of (2*R*,3*R*)-α,α,α′,α′-tetramesityl-1,4-dioxaspiro[4,5]decane-2,3-dimethanol, (II), from hexane/ethyl acetate (7:3). Therefore, (I) seems to be a decomposition product of (II). Strong hydrogen bonds between hydroxide groups [the donor–acceptor distance is 2.790 (2) Å] connect the molecules around one set of four symmetry-equivalent 2_1 axes, forming rod-shaped subunits in the structure of (I). There



(I)

are no hydrogen bonds related to the other set of 2_1 axes. Perpendicular to [010], there are only weak van der Waals interactions. The dominant hydrogen bonds may be the reason for the very short *b* axis, which is in perfect accord with the concept of periodic bond-chain vectors (Hartmann & Perdock, 1955).

Experimental

Compound (II) was prepared as described in principle by Beck *et al.* (1991). Its decomposition to (I) occurs spontaneously in hexane/ethyl acetate.

Crystal data

$C_9H_{12}O$	D_x = 1.155 Mg m^{-3}
M_r = 136.19	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2000 reflections
a = 11.575 (3) Å	θ = 5.0–20.0°
b = 4.3655 (6) Å	μ = 0.073 mm^{-1}
c = 15.647 (4) Å	T = 180 (2) K
β = 97.94 (3)°	Prism, colourless
V = 783.1 (3) Å^3	0.60 × 0.20 × 0.20 mm
Z = 4	

Data collection

Stoe IPDS diffractometer	R_{int} = 0.028
φ-rotation scans, φ-incr. = 1.5°, 153 exposures	θ_{max} = 25.7°
4975 measured reflections	$h = -14 \rightarrow 14$
1412 independent reflections	$k = -4 \rightarrow 4$
1063 reflections with $I > 2\sigma(I)$	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$w = 1/[\sigma^2(F_o^2) + (0.0742P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.108	$(\Delta/\sigma)_{max}$ = 0.003
S = 0.995	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
1412 reflections	$\Delta\rho_{min}$ = −0.12 e Å^{-3}
139 parameters	

Refined C—H distances were in the range 0.91 (3)–0.98 (3) Å and the O1—H1*Y* distance was 0.89 (2) Å.

Data collection: *IPDS*-2.87 (Stoe & Cie, 1997); cell refinement: *IPDS*-2.87; data reduction: *IPDS*-2.87; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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