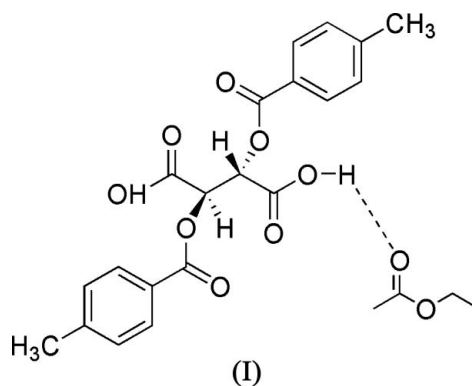
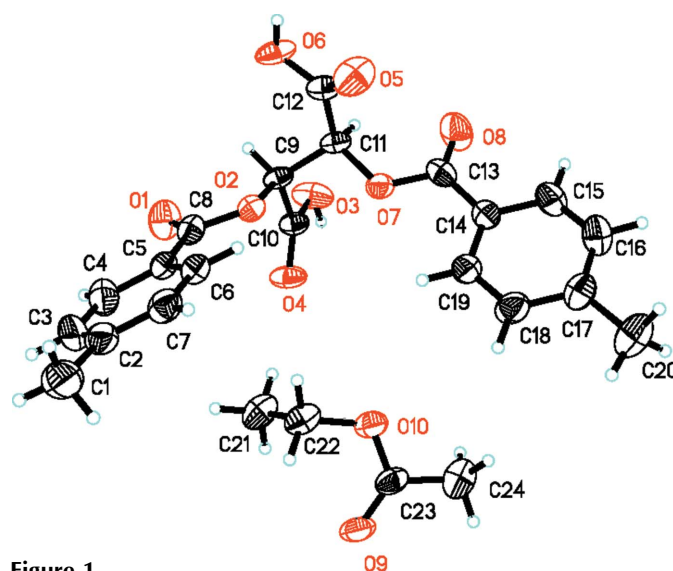


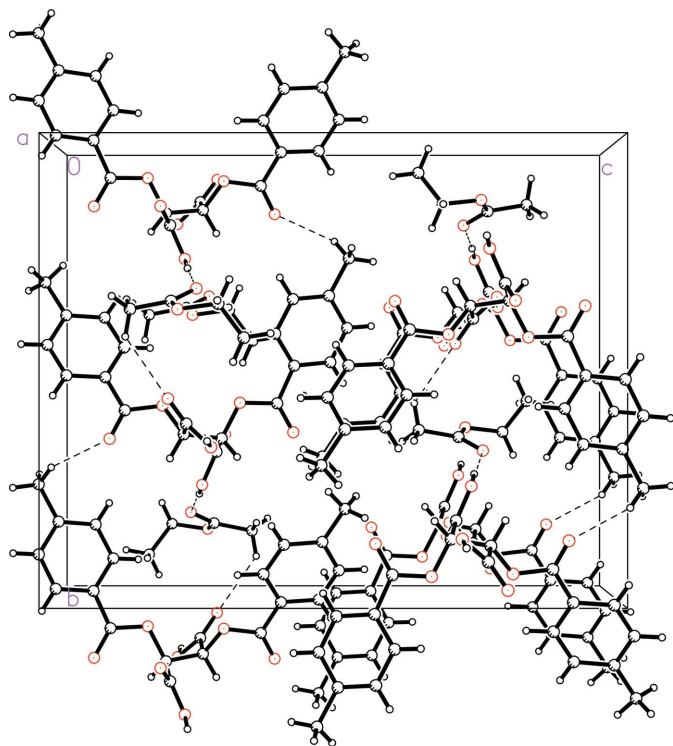
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## Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.046  
 $wR$  factor = 0.120  
Data-to-parameter ratio = 8.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.2,3-Di-*p*-toluoyl-(2*R*,3*R*)-tartaric acid  
ethyl acetate solvateIn the title compound,  $\text{C}_{20}\text{H}_{18}\text{O}_8 \cdot \text{C}_4\text{H}_8\text{O}_2$ , all bond lengths and angles in the di-*p*-toluoyltartaric acid molecule are normal. The structure is stabilized by  $\text{O}-\text{H} \cdots \text{O}$  and  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds in addition to van der Waals interactions.Received 27 February 2006  
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## Comment

2,3-Di-*p*-toluoyl-(2*R*,3*R*)-tartaric acid is an important chiral reagent and is widely used in chiral resolution of amines (Rogers *et al.*, 1989; Ward *et al.*, 1988). In this paper, we report the crystal structure of the title compound, (I).Fig. 1 shows the structure (I), which crystallizes in the orthorhombic space group  $P2_12_12_1$ . All bond lengths and angles in the di-*p*-toluoyltartaric acid molecule are normal**Figure 1**  
View of the title compound, (I), with displacement ellipsoids drawn at the 30% probability level.



**Figure 2**  
Packing diagram of (I), viewed along the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines.

(Table 1) and comparable to those found in published structures (Romanelli *et al.*, 1988; Chen *et al.*, 2003). The dihedral angle between the planes of the C2–C7 and C14–C19 benzene rings is 35.6 (3)°. The structure is stabilized by intra- and intermolecular O–H...O and C–H...O hydrogen bonds in addition to van der Waals interactions.

## Experimental

2,3-Di-*p*-toluoyl-(2*R*,3*R*)-tartaric acid was synthesized by reaction of (2*R*,3*R*)-tartaric acid (0.01 mol) and *p*-toluoyl chloride (0.02 mol) in toluene (20 ml) at 298 K over a period of 4 h in a yield of 86% (3.3 g). Crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethyl acetate solution at room temperature over a period of two weeks.

### Crystal data

$C_{20}H_{18}O_8 \cdot C_4H_8O_2$	$Z = 4$
$M_r = 474.45$	$D_x = 1.246 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_1$	Mo $K\alpha$ radiation
$a = 7.8516 (13) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$b = 16.140 (3) \text{ \AA}$	$T = 298 (2) \text{ K}$
$c = 19.951 (3) \text{ \AA}$	Block, colourless
$V = 2528.4 (7) \text{ \AA}^3$	$0.58 \times 0.36 \times 0.28 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer	12875 measured reflections
$\varphi$ and $\omega$ scans	2558 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2115 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.946$ , $T_{\max} = 0.973$	$R_{\text{int}} = 0.036$
	$\theta_{\text{max}} = 25.0^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.120$   
 $S = 1.06$   
 2558 reflections  
 317 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.1698P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.12 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O3–C10	1.296 (4)	O6–C12	1.320 (4)
O4–C10	1.187 (4)	C9–C10	1.522 (4)
O5–C12	1.184 (4)		
C8–O2–C9	115.6 (2)	C23–O10–C22	118.5 (3)
C13–O7–C11	116.2 (2)		

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O3–H3...O9 <sup>i</sup>	0.96 (5)	1.63 (5)	2.585 (3)	173 (4)
O6–H6...O4 <sup>ii</sup>	0.82 (4)	1.92 (5)	2.697 (3)	159 (4)
C24–H24C...O5 <sup>iii</sup>	0.96	2.57	3.328 (5)	136
C11–H11A...O3	0.98	2.53	2.872 (4)	100
C11–H11A...O8	0.98	2.23	2.618 (4)	102

Symmetry codes: (i)  $-x, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (ii)  $x + 1, y, z$ ; (iii)  $x - 1, y, z$ .

C-bound H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C–H = 0.93–0.98  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aryl and methine H atoms or  $1.5U_{\text{eq}}(\text{C})$  for methyl H atoms. H atoms of the OH groups were located in a difference Fourier map and refined freely. In the absence of significant anomalous dispersion effects, Friedel pairs were merged and the absolute configuration was assumed from the synthesis.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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