

(2*RS*,3*SR*)-Diethyl 2,3-bis(3,4,5-trimethoxybenzoyl)succinate**Xiang-Gao Meng* and An-Xin Wu***

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The title compound, $C_{28}H_{34}O_{12}$, is the *meso* isomer of a 2,3-disubstituted succinate derivative. Molecules are weakly linked *via* C—H $\cdots\pi$ interactions, forming layers parallel to the (100) plane.

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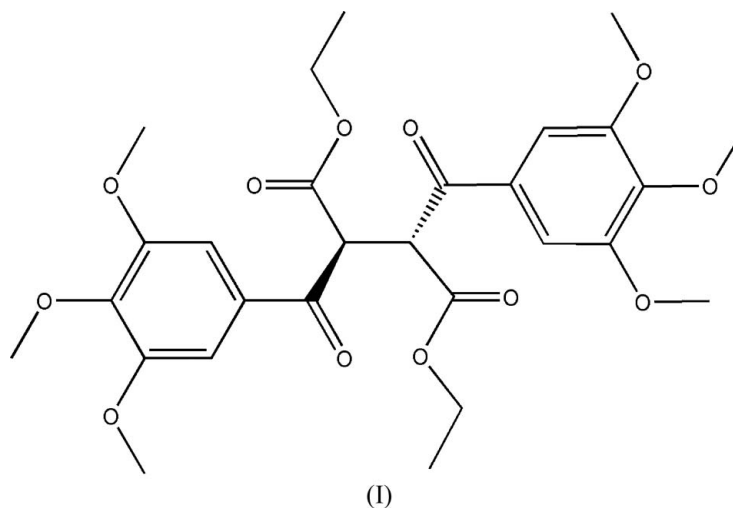
Comment

According to the literature (Wu *et al.*, 1998), we have synthesized the title compound, (I), and its crystal structure is reported here. The molecular structure of (I) is illustrated in Fig. 1, and selected geometric parameters are given in Table 1. The chiral atoms C11 and C15 possess different configurations, indicating that (I) is the *meso* isomer. *PLATON* (Spek, 2003) shows that intermolecular hydrogen bonds and π – π interactions are absent; however, molecules are weakly linked together by C—H $\cdots\pi$ interactions (Fig. 2 and Table 2).

Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.048
 wR factor = 0.125
Data-to-parameter ratio = 8.5

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

**Experimental**

Compound (I) was synthesized according to the literature procedure (Wu *et al.*, 1998). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{28}H_{34}O_{12}$
 $M_r = 562.55$
Orthorhombic, $Pca2_1$
 $a = 14.8730$ (14) Å
 $b = 7.9521$ (8) Å
 $c = 23.763$ (2) Å
 $V = 2810.5$ (5) Å³
 $Z = 4$
 $D_x = 1.330$ Mg m⁻³

Mo $K\alpha$ radiation
Cell parameters from 2977 reflections
 $\theta = 2.7$ – 22.3°
 $\mu = 0.10$ mm⁻¹
 $T = 292$ (2) K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART Apex CCD area-detector diffractometer
 ω scans
 Absorption correction: none
 18080 measured reflections
 3139 independent reflections

2404 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$
 $\theta_{\text{max}} = 27.0^\circ$
 $h = -19 \rightarrow 16$
 $k = -10 \rightarrow 10$
 $l = -30 \rightarrow 30$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.125$
 $S = 1.04$
 3139 reflections
 369 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.2925P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.005$
 $\Delta\rho_{\text{max}} = 0.19 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.14 \text{ e } \text{\AA}^{-3}$

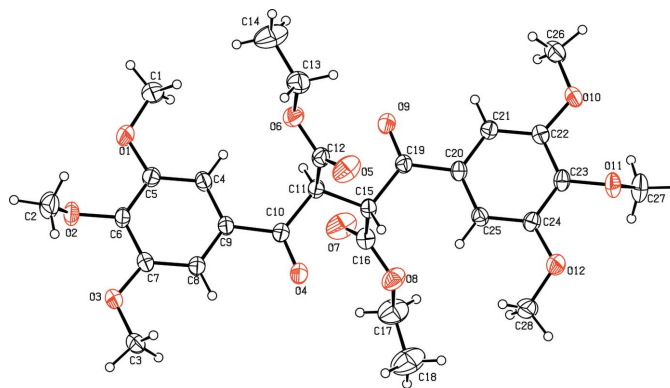


Figure 1 Molecular structure of (I), showing 30% probability displacement ellipsoids.

Table 1

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

C9—C10	1.481 (5)	C15—C16	1.514 (5)
C10—O4	1.220 (4)	C15—C19	1.532 (5)
C10—C11	1.527 (5)	C19—O9	1.206 (4)
C11—C12	1.521 (6)	C19—C20	1.491 (5)
C11—C15	1.537 (4)		
C9—C10—C11	121.0 (3)	C16—C15—C11	109.9 (3)
C12—C11—C10	109.2 (3)	C19—C15—C11	109.0 (3)
C12—C11—C15	108.4 (3)	C20—C19—C15	120.0 (3)
C10—C11—C15	109.8 (3)	C21—C20—C19	117.5 (3)
C16—C15—C19	108.7 (3)		
C4—C9—C10—C11	8.1 (6)	C16—C15—C19—O9	96.0 (4)
O4—C10—C11—C12	-98.9 (4)	C11—C15—C19—C20	158.1 (3)
C10—C11—C15—C19	-178.4 (3)	C15—C19—C20—C25	-2.9 (5)

Table 2

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

Cg_1 and Cg_2 are the centroids of the C4—C9 and C20—C25 phenyl rings, respectively.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C3—H3B \cdots Cg2 ⁱ	0.96	2.83 (1)	3.482 (1)	126
C17—H17B \cdots Cg2 ⁱⁱ	0.97	3.31 (1)	3.899 (1)	121
C18—H18B \cdots Cg2 ⁱⁱ	0.96	3.37 (1)	4.030 (1)	128
C27—H27B \cdots Cg1 ⁱⁱⁱ	0.96	3.23 (1)	3.718 (1)	114

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

All H atoms were placed in idealized positions [$C-H(\text{methyl}) = 0.96 \text{ \AA}$, $C-H(\text{methylene}) = 0.97 \text{ \AA}$, $C-H(\text{methine}) = 0.98 \text{ \AA}$, and $C-H(\text{aromatic}) = 0.93 \text{ \AA}$] and included in the refinement in the riding-model approximation, with $U_{\text{iso}}(\text{methyl H}) = 1.5U_{\text{eq}}(\text{C})$ and $U_{\text{iso}}(\text{methylene, methine and aromatic H}) = 1.2U_{\text{eq}}(\text{C})$. Friedel pairs were merged, since anomalous scattering effects were negligible.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to

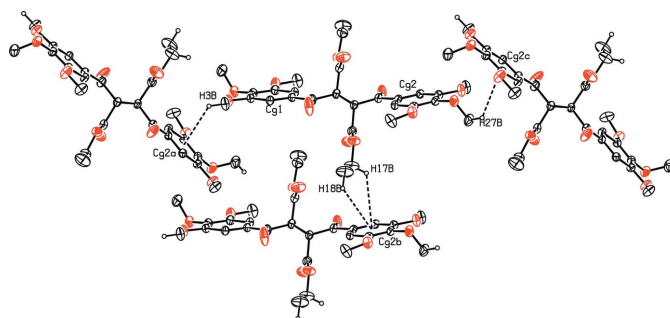


Figure 2

Plot of the crystal packing, showing the linkage of the molecules by $C-H \cdots \pi$ interactions (dashed lines). [Symmetry codes: (a) $1 - x, 1 - y, \frac{1}{2} + z$; (b) $x, y - 1, z$; (c) $1 - x, 2 - y, z - \frac{1}{2}$]

solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

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