# organic papers

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Key indicators

Single-crystal X-ray study
$T = 292$ K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.132
Data-to-parameter ratio = 12.9

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

(2RS,3SR)-Diethyl 2,3-bis(3,4-dimethoxy-benzoyl)succinate

The title compound, $C_{26}H_{30}O_{10}$, is the *meso* isomer of a 2,3-disubstituted succinic acid derivative and has inversion symmetry. The crystal structure is stabilized by intermolecular C—H···π and π–π stacking interactions.

Comment

1,4-Diketones are versatile intermediates for the synthesis of some natural products containing cyclopentanone and the furan ring system (McMurry & Meiton, 1971; Ito *et al.*, 1975, 1977). In the present paper, we report the crystal structure of the title compound, (I), which is a 1,4-diketone. The structure of a similar compound, (2RS,3SR)-diethyl 2,3-bis(3,4,5-trimethoxybenzoyl)succinate, has been reported previously (Meng & Wu, 2005).

(I)
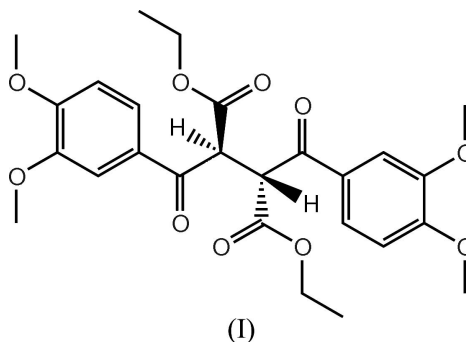
The asymmetric unit of (I) contains one half-molecule with the other half generated by a centre of inversion (Fig. 1 and Table 1). The crystal structure is stabilized by C—H···π intermolecular interactions (Table 2). A π–π stacking interaction is also observed, the $Cg1\cdots Cg1(1 - x, 1 - y, 1 - z)$ distance being 3.794 Å ($Cg1$ is the centroid of the benzene ring C3–C8).

Experimental

Compound (I) was synthesized as reported previously (Wu *et al.*, 1997). Crystals of (I) appropriate for data collection were obtained from a methanol–ethyl acetate solution by slow evaporation.

Crystal data

$C_{26}H_{30}O_{10}$	$Z = 1$
$M_r = 502.50$	$D_x = 1.351$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.5045$ (10) Å	Cell parameters from 2590
$b = 8.5868$ (10) Å	reflections
$c = 9.0850$ (11) Å	$\theta = 2.8$–25.2°
$\alpha = 80.306$ (2)°	$\mu = 0.10$ mm^{-1}
$\beta = 75.645$ (2)°	$T = 292$ (2) K
$\gamma = 75.245$ (2)°	Block, colourless
$V = 617.60$ (13) Å^3	$0.40 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	1851 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.014$
Absorption correction: none	$\theta_{max} = 25.0°$
3501 measured reflections	$h = -9 \rightarrow 10$
2140 independent reflections	$k = -8 \rightarrow 10$
	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.075P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.046$	$+ 0.1199P]$
$wR(F^2) = 0.133$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
2140 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
166 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C9—C10	1.540 (2)	C10—C10^i	1.528 (3)
C10—C11	1.525 (2)		
O3—C9—C7	121.36 (14)	C11—C10—C10^i	109.95 (16)
O3—C9—C10	118.22 (14)	C11—C10—C9	107.63 (13)
C7—C9—C10	120.41 (13)	C10^i—C10—C9	109.94 (15)
O3—C9—C10—C11	95.47 (19)	C7—C9—C10—C10^i	156.42 (17)
C7—C9—C10—C11	−83.84 (18)	C10^i—C10—C11—O4	46.7 (2)
O3—C9—C10—C10^i	−24.3 (3)	C9—C10—C11—O4	−73.1 (2)

Symmetry code: (i) $-x + 1, -y, -z + 2$.

Table 2
Hydrogen-bond geometry (Å, °).

$Cg1$ is the centroid of the benzene ring (C3–C8).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C13—H13$B\cdots Cg1^{ii}$	0.96	2.90	3.820	162

Symmetry code: (ii) $x - 1, y, z$.

The methyl H atoms were constrained to an ideal geometry, with C—H distances of 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å for benzene H and 0.97 Å for methine H, and with $U_{iso}(H) = 1.2U_{eq}(C)$.
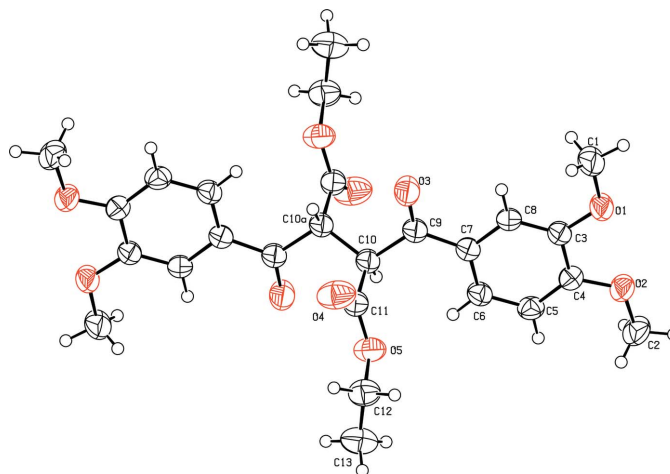

Figure 1
View of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. C10a and unlabelled atoms are related to C10 and other labelled atoms by the symmetry operation $(1 - x, -y, 2 - z)$.

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