Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

rac-Diethyl 2,3-bis(2-methoxybenzoyl)succinate

Xiang-Gao Meng* and An-Xin Wu*

Department of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

Correspondence e-mail: mengxianggao@mail.ccnu.edu.cn, chwax@mail.ccnu.edu.cn

Received 30 August 2005
Accepted 6 September 2005
Online 14 September 2005

Key indicators

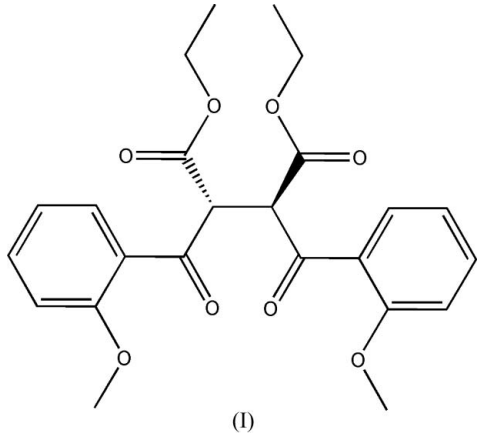
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
R factor = 0.065
wR factor = 0.177
Data-to-parameter ratio = 13.8

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

In the *rac* isomer mixture of the title compound, $C_{24}H_{26}O_8$, the molecules are weakly linked *via* C—H···O and π–π interactions, forming a three-dimensional network.

Comment

We synthesized the title compound, a 2,3-disubstituted succinate derivative, (I), according to the literature method of Wu *et al.* (1998), and report its crystal structure here.



(I)

The molecular structure of (I) is illustrated in Fig. 1, and selected bond lengths and torsion angles are given in Table 1.

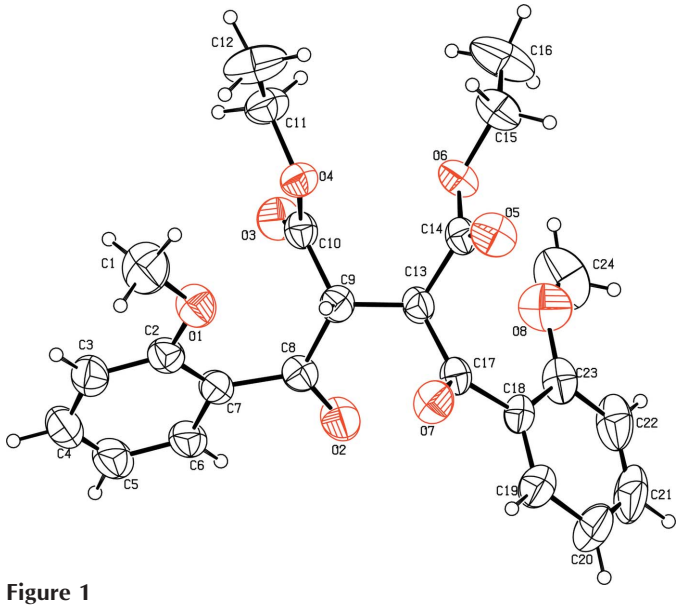


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

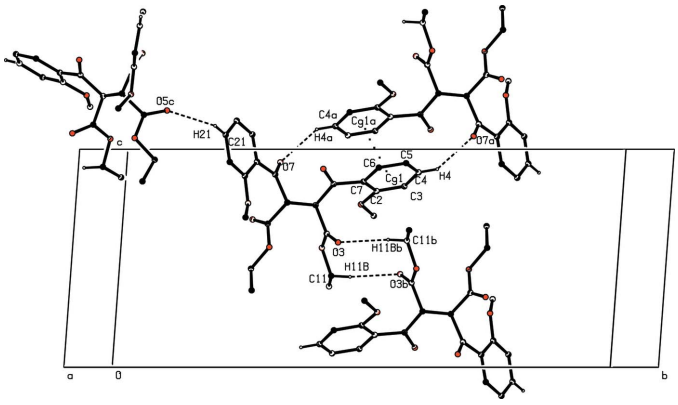


Figure 2
Plot of the crystal packing, showing the linking of the molecules by C—H···O hydrogen bonds and a π-π interaction (dashed lines). H atoms not involved in the hydrogen bonds have been omitted for clarity. [Symmetry codes: (ii) $1-x, 1-y, 2-z$; (iii) $1-x, 1-y, 1-z$; (iv) $1+x, \frac{1}{2}-y, \frac{1}{2}+z$]. *Cg*1 is the centroid of ring C2–C7. Labels having the suffix a indicate atoms at $(-x, 1-y, 2-z)$.

Chiral atoms C9 and C13 possess the same configuration. The central C8—C9—C13—C17 chain is in a *cis* configuration with a torsion angle of 53.0 (4)°. Analysis with *PLATON* (Spek, 2003) shows that no classical hydrogen bonds exist in the molecular structure, although C—H···O hydrogen bonds and a π–π interaction are present, forming a three-dimensional network in the crystal structure (Fig. 2 and Table 2). A π–π interaction is observed between the benzene rings [C2–C7 and C2^{v}–C7^{v}; symmetry code: (v) $-x, 1-y, 2-z$] with a centroid–centroid distance of 3.696 (2) Å.

Experimental

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

Crystal data

$C_{24}H_{26}O_8$
M_r = 442.45
Monoclinic, $P2_1/c$
a = 7.6510 (10) Å
b = 28.146 (4) Å
c = 10.9770 (14) Å
β = 103.214 (2)°
V = 2301.2 (5) Å^3
Z = 4
D_x = 1.277 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4946 reflections
θ = 2.4–21.7°
μ = 0.10 mm^{-1}
T = 292 (2) K
Block, colorless
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: none
16206 measured reflections
4040 independent reflections
2830 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°
$h = -8 \rightarrow 9$
$k = -33 \rightarrow 33$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.177
S = 1.09
4040 reflections
293 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0669P)^2 + 1.0101P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C7—C8	1.493 (4)	C13—C14	1.508 (4)
C8—C9	1.517 (4)	C13—C17	1.513 (4)
C9—C13	1.429 (4)	C17—C18	1.484 (4)
C9—C10	1.503 (4)		
C7—C8—C9—C13	−175.5 (3)	C8—C9—C13—C17	53.0 (4)
C7—C8—C9—C10	50.8 (4)	C9—C13—C17—C18	−136.3 (3)
C8—C9—C13—C14	−175.0 (3)	C13—C17—C18—C23	−14.3 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
C21—H21···O5^{i}	0.93	2.56	3.366 (5)	146
C4—H4···O7^{ii}	0.93	2.50	3.323 (4)	147
C11—H11*B*···O3^{iii}	0.97	2.49	3.448 (5)	169

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

All H atoms were located at idealized positions (methyl C—H = 0.96 Å, methylene C—H = 0.97 Å, methine C—H = 0.98 Å and aromatic C—H = 0.93 Å) and included in the refinement using the riding-model approximation, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and U_{iso}(H) = 1.2U_{eq}(C) for the other H atoms.

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*.

The authors are grateful to the Central China Normal University, the National Natural Science Foundation of China (grant No. 20472022) and the Hubei Province Natural Science Fund (grant Nos. 2004ABA085 and 2004ABC002) for financial support.

References

Bruker(2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wu, A.-X., Wang, M.-Y., Gan, Y.-H. & Pan, X.-H. (1998). *J. Chem. Res. (S)*, pp. 136–137.