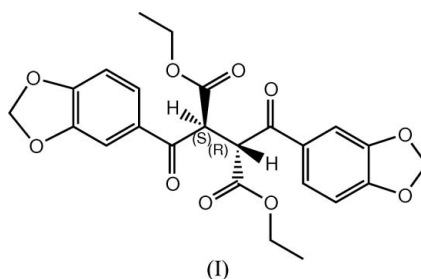
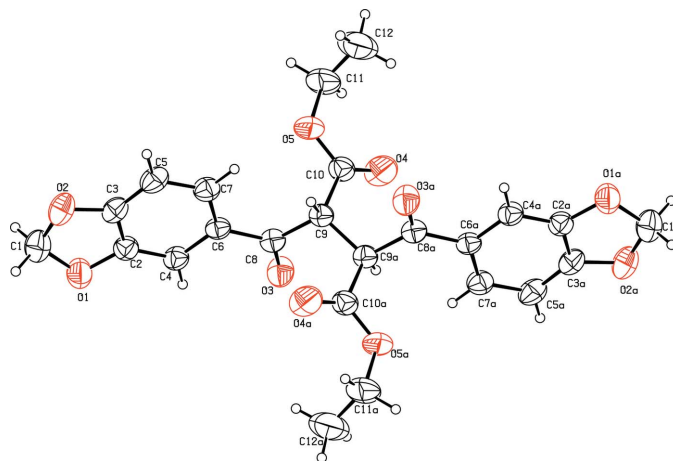


**(2*RS*,3*SR*)-Diethyl 2,3-bis(1,3-benzodioxole-5-carbonyl)succinate****Sheng-Li Hu,<sup>a,b</sup> Neng-Fang She<sup>a</sup>  
and An-Xin Wu<sup>a\*</sup>**<sup>a</sup>Key Laboratory of Pesticides & Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China, and <sup>b</sup>Hubei Key Laboratory of Bioanalytical Techniques (Hubei Normal University), Huangshi 435002, People's Republic of ChinaCorrespondence e-mail:  
chwuax@mail.ccnu.edu.cnIn the centrosymmetric title compound, C<sub>24</sub>H<sub>22</sub>O<sub>10</sub>, the two aromatic rings are parallel to each other. The crystal packing is stabilized mainly by van der Waals forces.Received 5 September 2005  
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Online 21 September 2005**Comment**1,4-Diketones are important intermediates for the synthesis of some natural products containing cyclopentanone and a furan ring system (Memurry & Meiton, 1971; Ito *et al.*, 1975, 1977). As part of a study of these compounds, we report here the crystal structure of (2*RS*,3*SR*)-diethyl 2,3-bis(1,3-benzodioxole-5-carbonyl)succinate, (I).**Key indicators**Single-crystal X-ray study  
 $T = 292$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.060  
 $wR$  factor = 0.177  
Data-to-parameter ratio = 14.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The asymmetric unit of (I) contains a half-molecule with the other half generated by inversion symmetry (Fig. 1 and Table 1). The two aromatic rings in (I) are parallel to each other and the aromatic ring is effectively coplanar with the five-membered C1/O1/C2/C3/O2 ring, making a dihedral angle of 1.06 (1)°. The crystal packing (Fig. 2) is stabilized mainly by van der Waals forces.

**Figure 1**  
View of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (a)  $-x, 2 - y, -z$ .]

Experimental

The title compound was synthesized according to the literature procedure of Wu *et al.* (1997). Crystals of (I) suitable for data collection were obtained by slow evaporation of a methanol–ethyl acetate solution.

Crystal data

$C_{24}H_{22}O_{10}$   
 $M_r = 470.42$   
 Monoclinic,  $P2_1/n$   
 $a = 8.0043$  (10) Å  
 $b = 9.5866$  (13) Å  
 $c = 14.6977$  (19) Å  
 $\beta = 96.778$  (2)°  
 $V = 1119.9$  (3) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.395$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 1024 reflections  
 $\theta = 2.8$ – $19.5$ °  
 $\mu = 0.11$  mm<sup>-1</sup>  
 $T = 292$  (2) K  
 Block, colorless  
 0.30 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.968$ ,  $T_{max} = 0.987$   
 5842 measured reflections

2189 independent reflections  
 1236 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.032$   
 $\theta_{max} = 26.0$ °  
 $h = -7 \rightarrow 9$   
 $k = -11 \rightarrow 11$   
 $l = -18 \rightarrow 18$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.060$   
 $wR(F^2) = 0.177$   
 $S = 1.03$   
 2189 reflections  
 155 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0815P)^2 + 0.1299P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.24$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.14$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

C1–O1	1.418 (4)	C8–O3	1.219 (3)
C1–O2	1.421 (4)	C8–C9	1.526 (4)
C2–O1	1.376 (3)	C9–C9 <sup>i</sup>	1.518 (5)
C3–O2	1.364 (4)	C10–O4	1.178 (3)
C6–C7	1.390 (3)	C10–O5	1.314 (4)
C6–C8	1.475 (4)	C11–O5	1.462 (4)
O1–C1–O2	107.8 (3)	C10–C9–C8	109.8 (2)
C4–C2–C3	122.5 (3)	O4–C10–O5	124.5 (3)
C5–C3–C2	121.5 (3)	O4–C10–C9	123.9 (3)
O2–C3–C2	109.8 (3)	O5–C10–C9	111.5 (3)
O3–C8–C9	117.9 (2)	C2–O1–C1	106.0 (2)
C6–C8–C9	121.4 (2)	C3–O2–C1	106.3 (2)
C9 <sup>i</sup> –C9–C10	109.6 (3)	C10–O5–C11	116.8 (3)
C9 <sup>i</sup> –C9–C8	110.2 (3)		
O1–C2–C4–C6	–178.1 (3)	C6–C8–C9–C9 <sup>i</sup>	138.6 (3)
C7–C6–C8–O3	–173.4 (3)	O3–C8–C9–C10	80.1 (3)
C4–C6–C8–C9	–171.9 (2)	C6–C8–C9–C10	–100.5 (3)
O3–C8–C9–C9 <sup>i</sup>	–40.7 (4)	C5–C3–O2–C1	176.4 (3)

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

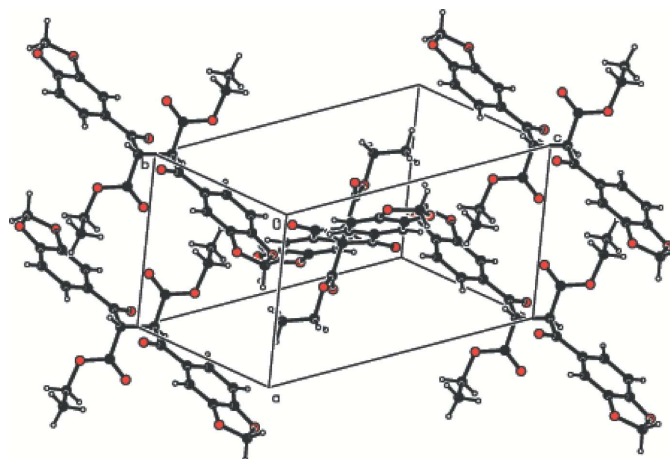


Figure 2  
 The packing of (I).

The methyl H atoms were constrained to an ideal geometry, with C–H = 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 = 0.93 Å for aromatic H atoms, 0.97 Å for methylene and methine H atoms and  $U_{iso}(H) = 1.2U_{eq}(C)$  for all 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.

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