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Ethyl 3-oxo-3-(3,4,5-trimethoxyphenyl)-propanoate

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, chwuax@mail.ccnu.edu.cn

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.057
wR factor = 0.168
Data-to-parameter ratio = 13.6

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

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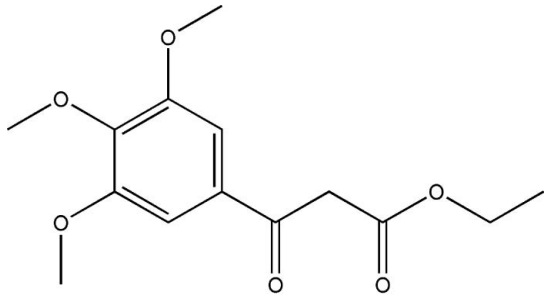
The molecules of the title compound, $C_{14}H_{18}O_6$, are linked into a three-dimensional network by a combination of C—H···O hydrogen bonds and C—H···π and π–π interacions

Comment

Recently published work forms part of our studies focused on structures and driving forces in solid-state packing involving C—H···π and π–π interactions (Hu & Wu, 2005; Meng & Wu, 2005). We present here the structural characterization of ethyl 3-oxo-3-(3,4,5-trimethoxyphenyl)propanoate, (I), the synthesis of which has been reported previously by Wu *et al.* (1997).



(I)

Compound (I) crystallizes in the space group $P2_1/c$ with Z' = 1. The 3- and 5-methoxy groups have their methyl C atoms essentially in the plane of the benzene ring, but the central methyl C atom at the 4 position is directed away from the ring (Fig. 1 and Table 1). There are no unremarkable bond lengths and angles.

The molecules are linked into a network by two C—H···O hydrogen bonds and one C—H···π interaction (Table 2). The second C—H···O interaction produces a centrosymmetric

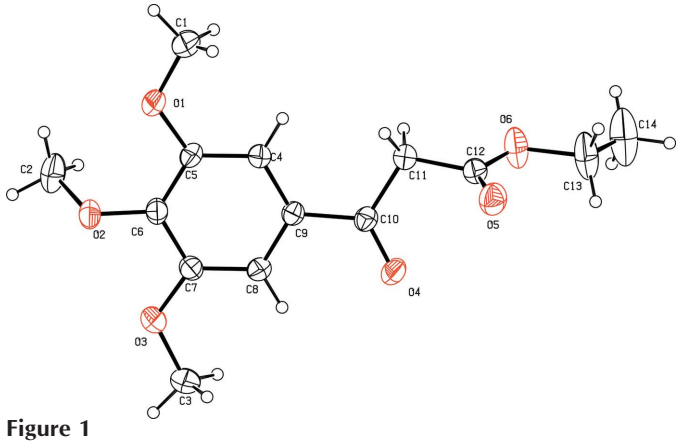


Figure 1
The molecular structure of the title compound, showing 30% probablity displacement ellipsoids.

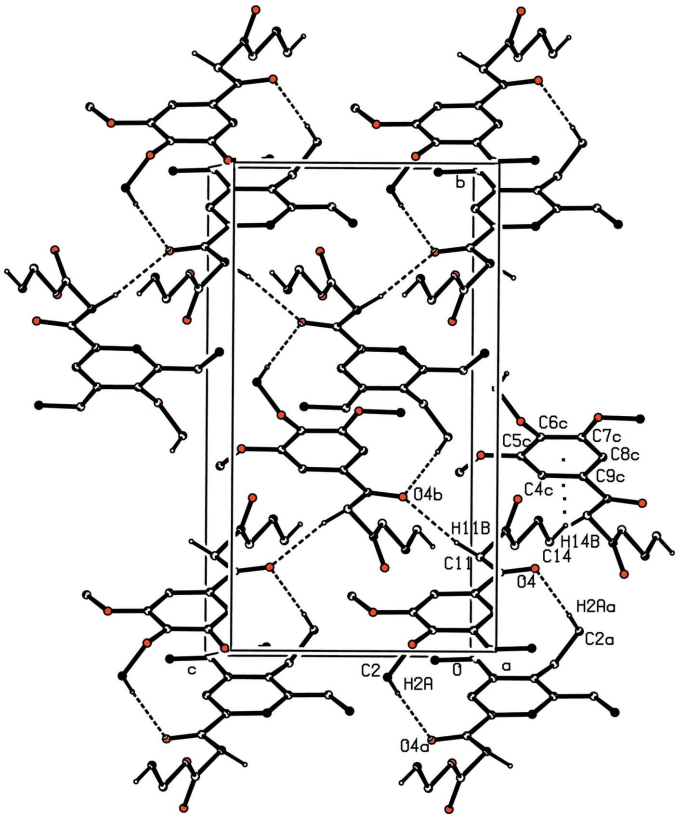


Figure 2
The crystal packing, showing C—H···O hydrogen bonds, C—H···π (dashed lines) and π–π interactions. H atoms not involved in the hydrogen bonds have been omitted for clarity. [Symmetry codes: (*a*) 1 − *x*, −*y*, −*z*; (*b*) *x*, $\frac{1}{2}-y$, $\frac{1}{2}+z$; (*c*) −1 + *x*, $\frac{1}{2}-y$, $-\frac{1}{2}+z$.]

dimer with an $R_2^2(9)$ ring, which is also stabilized by an aromatic π–π stacking interaction with a perpendicular separation of 3.60 (2) Å and a centroid–centroid distance of 4.096 (2) Å. These dimers are linked into a sheet in the *bc* plane, built from alternating $R_2^2(9)$ rings and C11—H11*B*···O4^{i} hydrogen bonds (Table 2 and Fig. 2). Adjacent sheets are linked into a network by means of a C—H···π interaction in which atom C14 acts as the hydrogen-bond donor to the benzene ring.

Experimental

Compound (I) was synthesized according to the literature procedure of Wu *et al.* (1997). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{14}H_{18}O_6$
M_r = 282.28
Monoclinic, $P2_1/c$
a = 9.7267 (13) Å
b = 16.584 (2) Å
c = 9.0476 (12) Å
β = 100.734 (2)°
V = 1433.9 (3) Å^3
Z = 4
D_x = 1.308 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1675 reflections
θ = 2.5–22.3°
μ = 0.10 mm^{-1}
T = 292 (2) K
Block, colorless
0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.970, T_{max} = 0.990
7110 measured reflections
2522 independent reflections
1815 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.0°
$h = -10 \rightarrow 11$
$k = -16 \rightarrow 19$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.168
S = 1.03
2522 reflections
185 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0853P)^2 + 0.459P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected torsion angles (°).

C4—C5—O1—C1	5.3 (4)	C7—C6—O2—C2	−118.6 (3)
C6—C5—O1—C1	−177.2 (3)	C8—C7—O3—C3	4.1 (4)
C5—C6—O2—C2	67.8 (3)	C6—C7—O3—C3	−175.5 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*B*···O4^{i}	0.97	2.49	3.450 (3)	172
C2—H2*A*···O4^{ii}	0.96	2.47	3.409 (4)	168
C14—H14*B*···*Cg*1^{iii}	0.96	2.80	3.600 (1)	141

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+1, -y, -z$; (iii) $x-1, -y-\frac{1}{2}, z-\frac{3}{2}$. *Cg*1 is the centroid of the benzene ring.

All the H atoms were placed in idealized positions (methyl C—H = 0.96 Å, methylene C—H = 0.97 Å and aromatic C—H = 0.93 Å) and included in the refinement in a riding-model approximation [U_{iso}(H) = 1.5U_{eq}(methyl C) or 1.2U_{eq}(other C)].

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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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