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Dimethyl fumarate

Huub Kooijman,[a]* Jeroen W. Sprengers,[b] Melvin J. Agerbeek,[b] Cornelis J. Elsevier[b] and Anthony L. Spek[a]

[a]Bijvoet Center for Biomolecular Research, Department of Crystal and Structural Chemistry, Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands, and [b]Van 't Hoff Institute of Molecular Sciences, Universiteit van Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands

Correspondence e-mail:
h.kooijman@chem.uu.nl

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.122
Data-to-parameter ratio = 10.3

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

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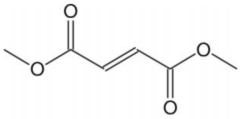
Dimethyl fumarate, $C_6H_8O_4$, crystallizes in the fully stretched planar conformation. The molecule is located on a crystallographic inversion centre and has local symmetry 2/m. The fumarate molecules aggregate in layers coinciding with the $(1\overline{1}1)$ lattice planes.

Comment

Dimethyl fumarate, (I), is frequently used as a coordinating ligand. The January 2004 update of the Cambridge Structural Database (CSD; Allen, 2002) contains 62 crystal structures of compounds with dimethyl fumarate acting as a ligand coordinated to a metal atom, mostly Ru and Pt. Knaggs & Lonsdale (1942) reported the unit-cell parameters of the crystal structure of the isolated molecule. Up until now, the full crystal structure determination of this compound has not been reported. The only other diester of fumaric acid reported in the CSD is diphenyl fumarate (Albano *et al.*, 2003).



(I)

Dimethyl fumarate adopts the fully stretched planar conformation in the crystal structure reported in this paper (Fig. 1). The molecule is located on a crystallographic inversion centre and has local symmetry 2/m, in contrast with diphenyl fumarate, which has neither crystallographic nor local symmetry. The intermolecular contact C3—H3$B\cdots$O2($1 + x$, $1 + y$, z) joins the molecules into chains running in the [110] direction (Fig. 2). The H$\cdots$O distance for this contact is 2.48 (3) Å, *i.e.* 0.24 Å shorter then the sum of the van der Waals radii. The orientations of groups within these chains suggest the presence of a close contact C1—H1$\cdots$O1($1 - x$, $1 - y$, $1 - z$). With an H$\cdots$O distance of 2.65 (2) Å, *i.e.* 0.07 Å shorter then the sum of the van der Waals radii, this contact is less pronounced. The chains of fumarate molecules are arranged into layers in such a way that all non-H atoms are more or less located on one of the $(1\overline{1}1)$ lattice planes (Fig. 3).

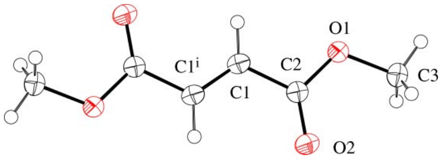


Figure 1
View of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. [Symmetry code: (i) $-x$, $-y$, $-z$.]

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Experimental

Crystals of the title compound were grown from a solution containing [platinum(dimethylfumarate)(norbornene)$_2$] and excess dimethyl fumarate in ether–pentane (2:1) at 253 K (Sprengers *et al.*, 2004). The dimethyl fumarate crystals in this batch were of highly irregular shape, but displayed reasonable extinction effects under crossed polarization filters.

Crystal data

$C_6H_8O_4$
$M_r = 144.12$
Triclinic, $P\bar{1}$
$a = 3.8680$ (14) Å
$b = 5.643$ (2) Å
$c = 8.364$ (3) Å
$\alpha = 100.843$ (16)°
$\beta = 100.289$ (18)°
$\gamma = 105.706$ (14)°
$V = 167.44$ (11) Å^3
$Z = 1$
$D_x = 1.429$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 530 reflections
$\theta = 2.0$–25.0°
$\mu = 0.12$ mm^{-1}
$T = 150$ K
Irregular block, colourless
0.3 × 0.2 × 0.2 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ scans, and ω scans with κ offsets
Absorption correction: none
1315 measured reflections
597 independent reflections
542 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.037$
$\theta_{\rm max} = 25.2$°
$h = -4 \rightarrow 3$
$k = -6 \rightarrow 6$
$l = -9 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.122$
$S = 1.11$
597 reflections
58 parameters
Only coordinates of H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0721P)^2 + 0.03P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.24$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.26$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1$^{\rm i}$	0.96 (2)	2.65 (2)	3.603 (2)	173.2 (14)
C3—H3B···O2$^{\rm ii}$	0.95 (3)	2.48 (3)	3.416 (2)	167 (2)

Symmetry codes: (i) $1-x, 1-y, -z$; (ii) $1+x, 1+y, z$.

The crystals diffracted poorly. Broad fuzzy reflections were observed and the mosaicity of the crystal refined to approximately 3.0°. H atoms were located in a difference Fourier map and their coordinates were refined [C—H = 0.94 (2)–0.96 (2) Å]. The isotropic displacement parameters of the H atoms were set at 1.5 or 1.2 times the equivalent isotropic displacement parameter of the carrier atom for methyl and alkene H atoms, respectively.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

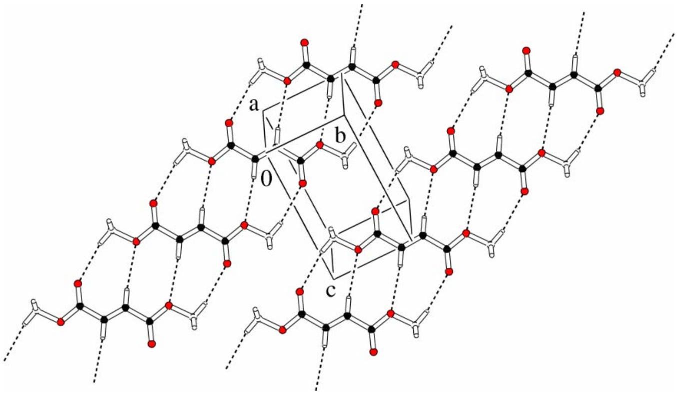

Figure 2
The title compound forms chains joined by close C—H···O contacts, running in the [110] direction.

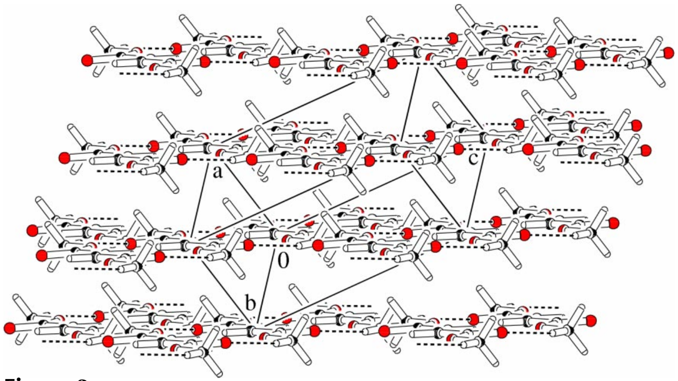

Figure 3
Arrangement of chains of dimethyl fumarate molecules into layers coinciding with the $(1\bar{1}1)$ lattice planes.

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