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(*RS*)-2-Methylglutaric acid

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.157
Data-to-parameter ratio = 17.6

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

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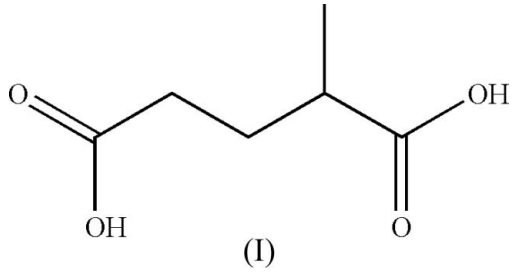
In the crystal structure of the title compound, $C_6H_{10}O_4$, the molecules form chains *via* centrosymmetrically related pairs of strong O—H···O hydrogen bonds.

Comment

2-Methylglutaric acid (2-MGA) is widely used to fabricate well-defined enantiomerically pure structures such as the synthesis of helical aromatics (Watanabe *et al.*, 2004) or chiral information transfer by solid–solid interaction (Tanaka *et al.*, 2003). A modern application of this compound concerns the analysis of the secondary organic aerosol (SOA) formation (Gao *et al.*, 2004). To be able to study and understand the solid-state properties of 2-MGA and its interactions with solvents or with other common reagents, it is essential to know the crystal structure of the compound. Since the structure of (*RS*)-2-MGA, (I), was unknown, we grew crystals. Fig. 1 shows the molecular structure of the title compound.



(I)

In the racemic crystal structure of (*RS*)-2-MGA, each *S* molecule is connected to two adjacent *R* molecules *via* hydrogen bonds and *vice versa* (Table 1 and Fig. 2).

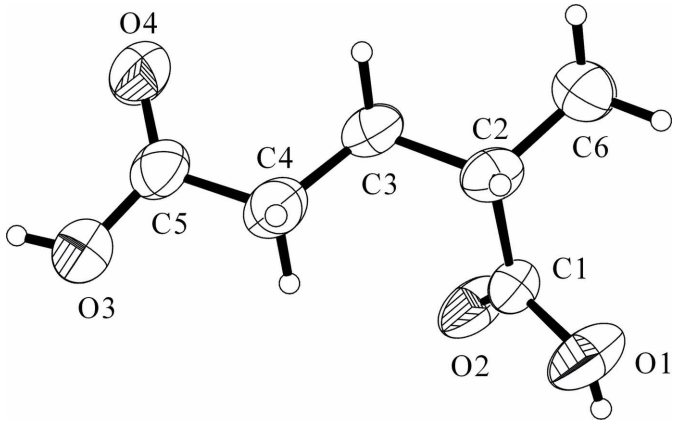


Figure 1
The molecular structure of (*S*)-2-MGA. Displacement ellipsoids are drawn at the 45% probability level.

Experimental

The title compound was purchased from Aldrich and was recrystallized from water and dried in air.

Crystal data

$C_6H_{10}O_4$
M_r = 146.14
Triclinic, $P\overline{1}$
a = 5.1765 (10) Å
b = 5.7929 (12) Å
c = 13.335 (3) Å
α = 80.92 (3)°
β = 83.54 (3)°
γ = 68.82 (3)°
V = 367.52 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
0.33 × 0.21 × 0.2 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.702, T_{max} = 0.776
(expected range = 0.885–0.978)
3517 measured reflections
1605 independent reflections
1007 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.157
S = 1.09
1605 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.84	1.84	2.671 (2)	167
O3—H3···O4^{ii}	0.84	1.83	2.661 (3)	171

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $-x+1, -y-1, -z+1$.

The C-bound H atoms were positioned geometrically, with C—H = 0.96–0.98 Å, and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). The O-bound H atoms were initially located in difference maps but were refined in the riding-model approximation, with O—H = 0.84 Å and U_{iso}(H) = 1.2U_{eq}(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

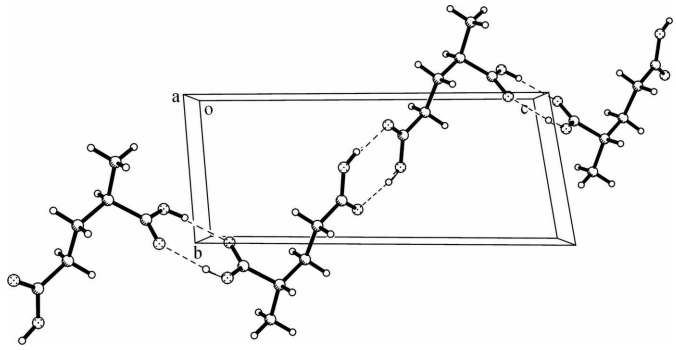


Figure 2
The zigzag chains formed by hydrogen bonds in (I). Hydrogen bonds are indicated by dashed lines.

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