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2-Mesitylacetic acid

Jiang-Sheng Li,^{a*} Qi-Xi He^b and Peng-Yu Li^a

^aSchool of Chemistry and Biological Engineering, Changsha University of Science & Technology, Changsha 410004, People's Republic of China, and ^bCollege of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, People's Republic of China

Correspondence e-mail: js_li@yahoo.com.cn

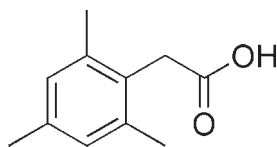
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Key indicators: single-crystal X-ray study; $T = 113$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.035; wR factor = 0.104; data-to-parameter ratio = 13.7.

In the title compound, $\text{C}_{11}\text{H}_{14}\text{O}_2$, the dihedral angle between the CCOO carboxyl unit and the benzene ring is $85.37(7)^\circ$. In the crystal, the molecules are linked into inversion dimers by pairs of $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For background to carboxylic acids as supramolecular synthons, see: Thalladi *et al.* (1996).



Experimental

Crystal data

 $\text{C}_{11}\text{H}_{14}\text{O}_2$ $M_r = 178.22$

Monoclinic, $P2_1/c$
 $a = 8.2312(16)$ Å
 $b = 15.366(3)$ Å
 $c = 7.5708(15)$ Å
 $\beta = 92.74(3)^\circ$
 $V = 956.4(3)$ Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 113$ K
 $0.32 \times 0.18 \times 0.12$ mm

Data collection

Rigaku Saturn CCD diffractometer
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku/MS, 2005)
 $T_{\min} = 0.974$, $T_{\max} = 0.990$

6163 measured reflections
 1681 independent reflections
 1259 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.104$
 $S = 1.03$
 1681 reflections

123 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.18$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2}\cdots\text{O1}^i$	0.82	1.84	2.6564 (15)	177

Symmetry code: (i) $-x + 1, -y + 2, -z$.

Data collection: *CrystalClear* (Rigaku/MS, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5261).

References

- Rigaku/MS (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Thalladi, V. R., Goud, B. S., Hoy, V. J., Allen, F. H., Howard, J. A. K. & Desiraju, G. R. (1996). *Chem. Commun.* pp. 401–402.

supplementary materials

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J.-S. Li, Q.-X. He and P.-Y. Li

Comment

Carboxylic acid is a supramolecular synthon, widely used to construct supramolecular array with one to three different dimensions *via* hydrogen bonds (Thalladi *et al.*, 1996). Herein the structure of the title compound (I) is reported.

In the title molecule, (Fig 1), the carbonyl moiety C1/C2/O1/O2 forms an angle of 85.3797) with the benzene ring. In the crystal packing, molecules are linked into dimers by strong O—H \cdots O H-bonding (Table 1 & Fig 2).

Experimental

The title compound was available from Hunan institute of Chemical Industry, received without further purification. Colourless blocks of (I) were obtained by evaporation from its solution of ethyl acetate/petroleum ether 1/4 (v/v).

Refinement

All H atoms were positioned geometrically and constrained to ride on their parent atoms [C—H distances are 0.93 and 0.97Å with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for aromatic and CH₂ H atoms, 0.82 and 0.96Å with $U_{\text{iso}} = 1.5 U_{\text{eq}}$ (O and C) for OH and CH₃ H atoms].

Figures

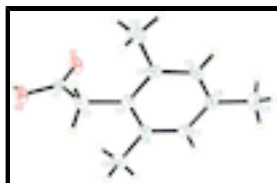


Fig. 1. The molecule of (I) showing displacement ellipsoids drawn at the 50% probability level.

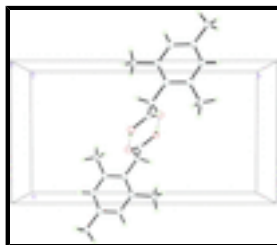


Fig. 2. The dimer formed *via* intermolecular O—H \cdots O hydrogen bonding.

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Crystal data

C₁₁H₁₄O₂

$F(000) = 384$

supplementary materials

$M_r = 178.22$	$D_x = 1.238 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Melting point: 440-442 K K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 8.2312 (16) \text{ \AA}$	Cell parameters from 2789 reflections
$b = 15.366 (3) \text{ \AA}$	$\theta = 2.5\text{--}27.9^\circ$
$c = 7.5708 (15) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 92.74 (3)^\circ$	$T = 113 \text{ K}$
$V = 956.4 (3) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.32 \times 0.18 \times 0.12 \text{ mm}$

Data collection

Rigaku Saturn CCD diffractometer	1681 independent reflections
Radiation source: rotating anode confocal	1259 reflections with $I > 2\sigma(I)$
Detector resolution: $7.31 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.040$
ω and ϕ scans	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.5^\circ$
Absorption correction: multi-scan (<i>CrystalClear</i> ; Rigaku/MSK, 2005)	$h = -9 \rightarrow 7$
$T_{\text{min}} = 0.974$, $T_{\text{max}} = 0.990$	$k = -18 \rightarrow 15$
6163 measured reflections	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
1681 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
123 parameters	$\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: <i>SHELXL</i> , $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.109 (9)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -

factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R - factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.36719 (12)	0.93504 (6)	0.08273 (12)	0.0294 (3)
O2	0.48038 (12)	1.05038 (6)	0.21730 (12)	0.0262 (3)
H2	0.5244	1.0548	0.1228	0.039*
C1	0.38084 (16)	0.98320 (8)	0.21106 (17)	0.0190 (3)
C2	0.29007 (17)	0.97161 (8)	0.37622 (17)	0.0232 (4)
H2A	0.2568	1.0284	0.4173	0.028*
H2B	0.3632	0.9467	0.4669	0.028*
C3	0.14180 (16)	0.91442 (8)	0.35423 (16)	0.0189 (3)
C4	0.14441 (17)	0.82764 (8)	0.41446 (17)	0.0205 (3)
C5	0.00572 (17)	0.77723 (8)	0.38957 (18)	0.0229 (4)
H5	0.0076	0.7201	0.4303	0.027*
C6	-0.13609 (17)	0.80882 (8)	0.30596 (17)	0.0231 (4)
C7	-0.13687 (17)	0.89545 (8)	0.25041 (17)	0.0235 (4)
H7	-0.2313	0.9183	0.1963	0.028*
C8	-0.00110 (17)	0.94838 (8)	0.27356 (16)	0.0198 (3)
C9	-0.00882 (18)	1.04182 (8)	0.21213 (18)	0.0270 (4)
H9A	-0.1139	1.0533	0.1566	0.040*
H9B	0.0736	1.0518	0.1289	0.040*
H9C	0.0090	1.0798	0.3119	0.040*
C10	0.29354 (18)	0.78874 (10)	0.50715 (19)	0.0316 (4)
H10A	0.2726	0.7291	0.5360	0.047*
H10B	0.3198	0.8207	0.6136	0.047*
H10C	0.3832	0.7916	0.4308	0.047*
C11	-0.28185 (19)	0.75097 (9)	0.2738 (2)	0.0340 (4)
H11A	-0.2606	0.7100	0.1821	0.051*
H11B	-0.3746	0.7858	0.2382	0.051*
H11C	-0.3035	0.7202	0.3805	0.051*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0363 (7)	0.0287 (6)	0.0241 (6)	-0.0128 (5)	0.0107 (5)	-0.0080 (4)
O2	0.0285 (6)	0.0279 (6)	0.0229 (6)	-0.0113 (4)	0.0080 (4)	-0.0047 (4)
C1	0.0194 (8)	0.0168 (6)	0.0207 (7)	0.0004 (6)	-0.0010 (6)	0.0015 (5)
C2	0.0284 (9)	0.0236 (7)	0.0178 (8)	-0.0039 (6)	0.0027 (6)	-0.0005 (5)
C3	0.0243 (8)	0.0199 (7)	0.0130 (7)	-0.0031 (6)	0.0064 (6)	-0.0029 (5)
C4	0.0250 (8)	0.0212 (7)	0.0159 (7)	0.0019 (6)	0.0061 (6)	-0.0016 (5)
C5	0.0330 (9)	0.0159 (6)	0.0206 (7)	-0.0011 (6)	0.0102 (6)	-0.0005 (5)
C6	0.0259 (9)	0.0253 (7)	0.0188 (7)	-0.0049 (6)	0.0094 (6)	-0.0048 (5)
C7	0.0228 (8)	0.0295 (8)	0.0185 (8)	0.0030 (6)	0.0044 (6)	-0.0018 (5)
C8	0.0270 (8)	0.0190 (7)	0.0141 (7)	0.0001 (6)	0.0073 (6)	-0.0014 (5)
C9	0.0343 (9)	0.0233 (7)	0.0237 (8)	0.0029 (6)	0.0055 (7)	0.0014 (5)

supplementary materials

C10	0.0317 (9)	0.0294 (8)	0.0336 (9)	0.0033 (6)	0.0022 (7)	0.0032 (6)
C11	0.0329 (10)	0.0366 (9)	0.0332 (9)	-0.0109 (7)	0.0080 (7)	-0.0040 (6)

Geometric parameters (Å, °)

O1—C1	1.2222 (15)	C6—C11	1.5037 (18)
O2—C1	1.3174 (15)	C7—C8	1.3865 (18)
O2—H2	0.8200	C7—H7	0.9300
C1—C2	1.4976 (19)	C8—C9	1.5096 (18)
C2—C3	1.5067 (17)	C9—H9A	0.9600
C2—H2A	0.9700	C9—H9B	0.9600
C2—H2B	0.9700	C9—H9C	0.9600
C3—C8	1.4000 (18)	C10—H10A	0.9600
C3—C4	1.4089 (18)	C10—H10B	0.9600
C4—C5	1.3850 (18)	C10—H10C	0.9600
C4—C10	1.5080 (19)	C11—H11A	0.9600
C5—C6	1.3885 (18)	C11—H11B	0.9600
C5—H5	0.9300	C11—H11C	0.9600
C6—C7	1.3959 (19)		
C1—O2—H2	109.5	C8—C7—H7	119.0
O1—C1—O2	122.43 (13)	C6—C7—H7	119.0
O1—C1—C2	124.14 (12)	C7—C8—C3	119.45 (11)
O2—C1—C2	113.42 (10)	C7—C8—C9	119.81 (12)
C1—C2—C3	114.26 (10)	C3—C8—C9	120.73 (12)
C1—C2—H2A	108.7	C8—C9—H9A	109.5
C3—C2—H2A	108.7	C8—C9—H9B	109.5
C1—C2—H2B	108.7	H9A—C9—H9B	109.5
C3—C2—H2B	108.7	C8—C9—H9C	109.5
H2A—C2—H2B	107.6	H9A—C9—H9C	109.5
C8—C3—C4	119.57 (12)	H9B—C9—H9C	109.5
C8—C3—C2	119.34 (11)	C4—C10—H10A	109.5
C4—C3—C2	121.09 (12)	C4—C10—H10B	109.5
C5—C4—C3	119.05 (12)	H10A—C10—H10B	109.5
C5—C4—C10	119.27 (12)	C4—C10—H10C	109.5
C3—C4—C10	121.68 (13)	H10A—C10—H10C	109.5
C4—C5—C6	122.41 (11)	H10B—C10—H10C	109.5
C4—C5—H5	118.8	C6—C11—H11A	109.5
C6—C5—H5	118.8	C6—C11—H11B	109.5
C5—C6—C7	117.54 (12)	H11A—C11—H11B	109.5
C5—C6—C11	120.94 (12)	C6—C11—H11C	109.5
C7—C6—C11	121.52 (13)	H11A—C11—H11C	109.5
C8—C7—C6	121.95 (13)	H11B—C11—H11C	109.5
O1—C1—C2—C3	-18.70 (18)	C4—C5—C6—C7	-1.7 (2)
O2—C1—C2—C3	162.26 (11)	C4—C5—C6—C11	177.16 (12)
C1—C2—C3—C8	-77.82 (15)	C5—C6—C7—C8	1.3 (2)
C1—C2—C3—C4	102.58 (14)	C11—C6—C7—C8	-177.55 (12)
C8—C3—C4—C5	1.12 (19)	C6—C7—C8—C3	0.3 (2)
C2—C3—C4—C5	-179.28 (12)	C6—C7—C8—C9	-179.59 (12)
C8—C3—C4—C10	-178.12 (12)	C4—C3—C8—C7	-1.50 (19)

C2—C3—C4—C10	1.48 (19)	C2—C3—C8—C7	178.89 (11)
C3—C4—C5—C6	0.5 (2)	C4—C3—C8—C9	178.36 (12)
C10—C4—C5—C6	179.77 (13)	C2—C3—C8—C9	-1.24 (19)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O2—H2 \cdots O1 ⁱ	0.82	1.84	2.6564 (15)	177

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

Fig. 1

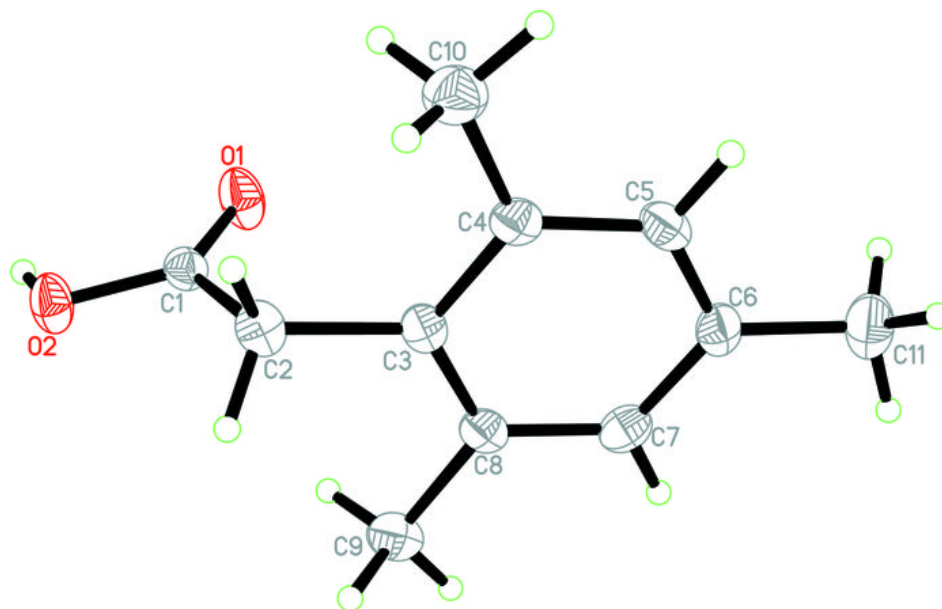


Fig. 2

