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2-Mesitylacetic acid

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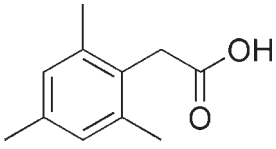
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.104; data-to-parameter ratio = 13.7.

In the title compound, $C_{11}H_{14}O_2$, the dihedral angle between the CCOO carboxyl unit and the benzene ring is 85.37 (7)°. In the crystal, the molecules are linked into inversion dimers by pairs of O—H···O hydrogen bonds.

Related literature

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



Experimental

Crystal data

$C_{11}H_{14}O_2$ M_r = 178.22
Monoclinic, $P2_1/c$
a = 8.2312 (16) Å
b = 15.366 (3) Å
c = 7.5708 (15) Å
β = 92.74 (3)°
V = 956.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 113 K
0.32 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.974, T_{max} = 0.990
6163 measured reflections
1681 independent reflections
1259 reflections with $I > 2\sigma(I)$
R_{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···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.84	2.6564 (15)	177

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

Data collection: *CrystalClear* (Rigaku/MSC, 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/MSC (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 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.

supporting information

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S1. 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···O H-bonding (Table 1 & Fig 2).

S2. 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*).

S3. 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_{iso}(H) = 1.2 U_{eq}(C) for aromatic and CH_2 H atoms, 0.82 and 0.96Å with U_{iso} = 1.5U_{eq} (O and C) for OH and CH_3 H atoms].

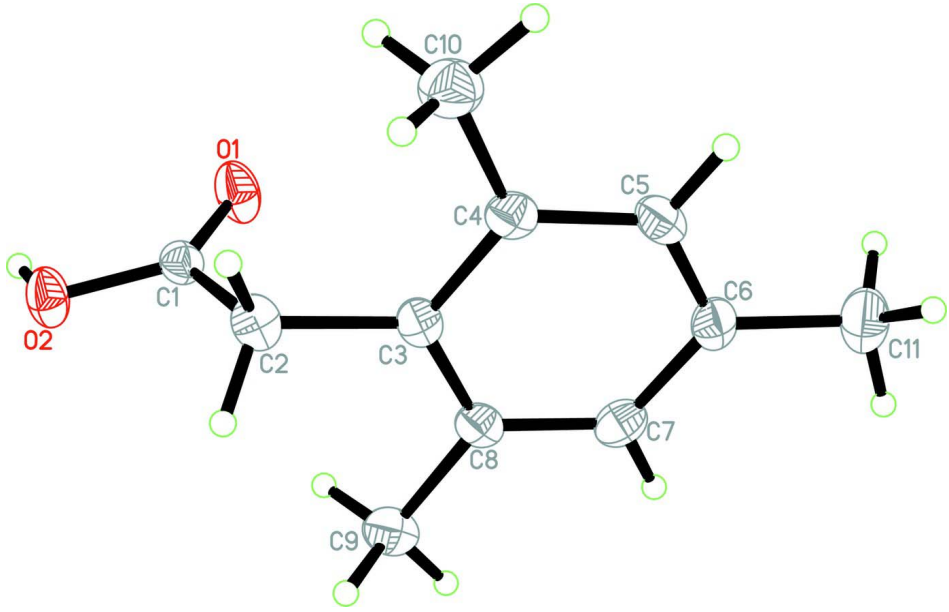

Figure 1

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

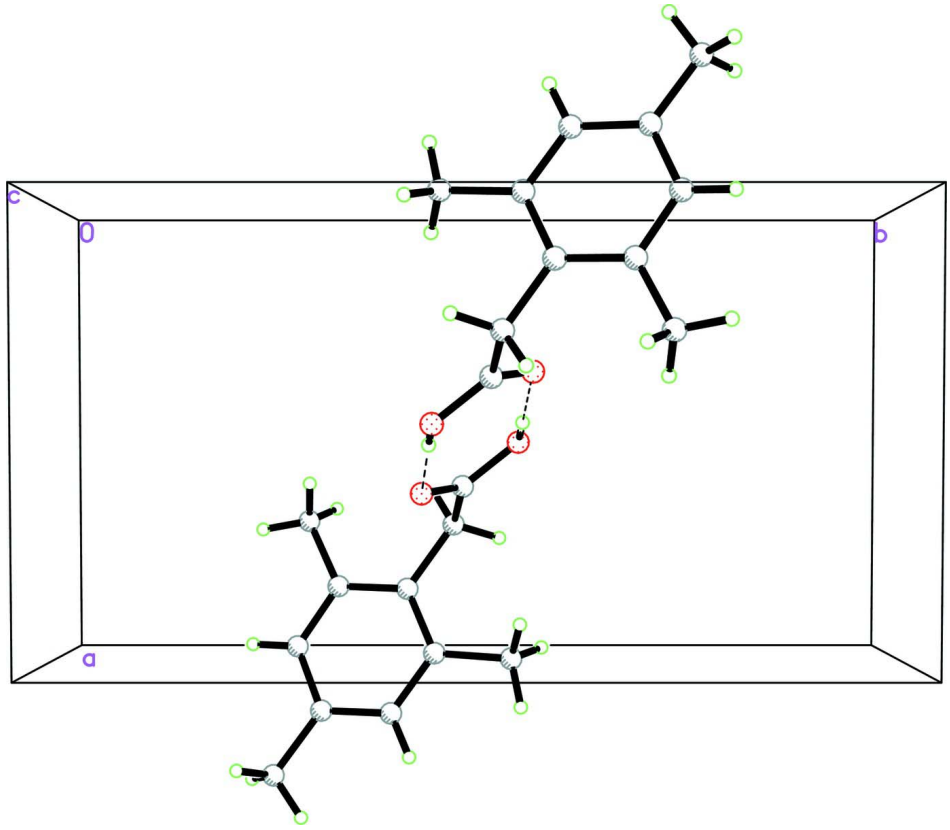

Figure 2

The dimer formed *via* intermolecular O—H···O hydrogen bonding.

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Crystal data

$C_{11}H_{14}O_2$
M_r = 178.22
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 8.2312 (16) Å
b = 15.366 (3) Å
c = 7.5708 (15) Å
β = 92.74 (3)°
V = 956.4 (3) Å^3
Z = 4

$F(000)$ = 384
D_x = 1.238 Mg m^{-3}
Melting point: 440-442 K K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2789 reflections
θ = 2.5–27.9°
μ = 0.08 mm^{-1}
T = 113 K
Block, colourless
0.32 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn CCD diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.974, T_{max} = 0.990

6163 measured reflections
1681 independent reflections
1259 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 25.0°, θ_{min} = 2.5°
h = −9→7
k = −18→15
l = −8→8

Refinement

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

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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)
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, º)

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, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.84	2.6564 (15)	177

Symmetry code: (i) −*x*+1, −*y*+2, −*z*.