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Sebacic acid

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The crystal structure of octane-1,8-dicarboxylic acid (sebacic acid), $C_{10}H_{18}O_4$, has been redetermined at 180 K. The molecular units are centrosymmetric and linked *via* the ubiquitous *syn–syn* carboxylic acid dimer to form infinite chains running along the $[\bar{1}01]$ vector.

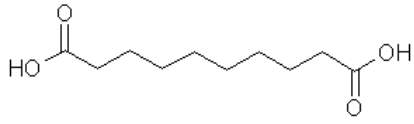
Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.002 Å
R factor = 0.051
wR factor = 0.139
Data-to-parameter ratio = 18.2

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

Comment

Crystal data for sebacic acid, (I), have been reported on four previous occasions, by Caspari (1928), Morrison & Robertson (1949) (SEBAAC01), Housty & Hospital (1966) (SEBAAC) and Haget *et al.* (1980) (SEBAAC02 in the Cambridge Structural Database; Allen & Kennard, 1993). All four studies essentially report the same structure in space group $P2_1/c$ with unit-cell dimensions *ca* a = 15.1, b = 5.0, c = 10.1 Å, β = 133.1°. [Morrison & Robertson (1949) describe the structure in the non-standard setting $P2_1/a$.] The most precise cell determination (SEBAAC02) to date is derived from powder X-ray diffraction data, and atomic coordinates were not determined. We have re-examined sebacic acid at 180 K and report the structure to significantly greater precision in $P2_1/c$ with β *ca* 92°. The previously reported structures in $P2_1/c$ with β *ca* 133.1° may be transformed to our structure by the matrix (101, 010, 001) followed by an origin shift of $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ to bring an entire molecule into the unit cell.



(I)

Experimental

Sebacic acid was obtained from Aldrich and recrystallized from ethanol.

Crystal data

$C_{10}H_{18}O_4$
M_r = 202.24
Monoclinic, $P2_1/c$
a = 10.9197 (7) Å
b = 4.9876 (6) Å
c = 9.964 (1) Å
β = 92.273 (6)°
V = 542.27 (9) Å^3
Z = 2
D_x = 1.239 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2040 reflections
θ = 1.0–27.5°
μ = 0.10 mm^{-1}
T = 180 (2) K
Plate, colourless
0.23 × 0.18 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Thin-slice ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.912, T_{max} = 0.995
3745 measured reflections
1241 independent reflections
796 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 27.5°
$h = -11 \rightarrow 14$
$k = -5 \rightarrow 6$
$l = -12 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.139
S = 1.05
1241 reflections
68 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O1^{i}	1.06 (3)	1.58 (3)	2.6406 (15)	175 (2)

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

All H atoms (apart from H1) were placed geometrically and allowed to ride during subsequent refinement with an isotropic displacement parameter fixed at 1.2 times that for the C atom to which they are attached. H1 was refined without restraint.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *SHELXL*97.

We thank the EPSRC for financial assistance with purchase of the CCD diffractometer.

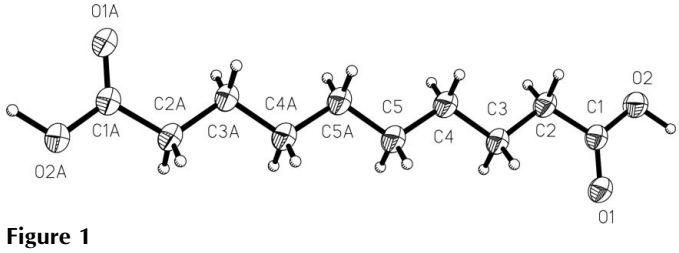


Figure 1
The molecular unit of the title compound showing displacement ellipsoids at the 50% probability level.

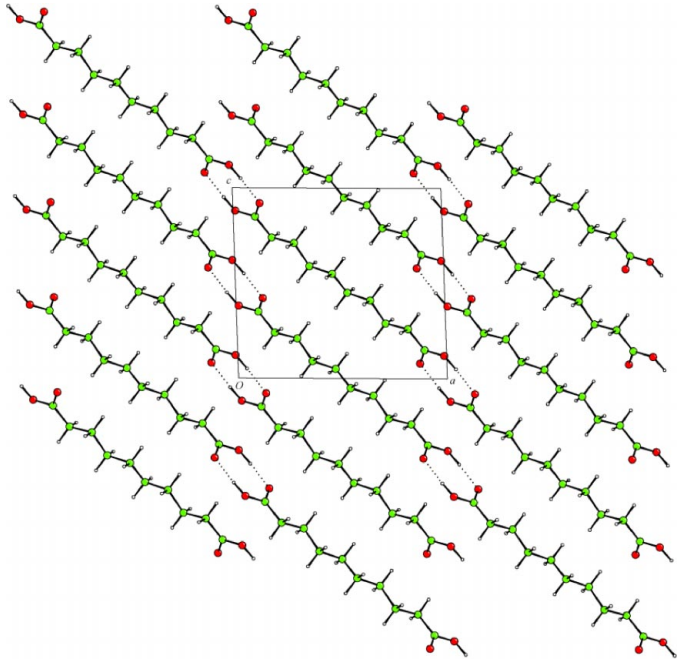


Figure 2
Projection onto (010) showing chains of sebacic acid running along the [$\bar{1}$01] vector.

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