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Azelaic acid

Andrew D. Bond,* Marc R. Edwards and William Jones

Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England

Correspondence e-mail: adb29@cam.ac.uk

Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.096
Data-to-parameter ratio = 17.0

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

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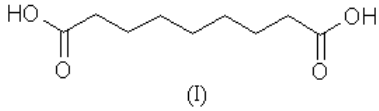
The crystal structure of heptane-1,7-dicarboxylic acid (azelaic acid), $C_9H_{16}O_4$, has been redetermined at 180 K. The molecular units have twofold symmetry and are linked *via* the ubiquitous *syn–syn* carboxylic acid dimer to form infinite chains running approximately along the [$\bar{4}$01] vector.

Comment

Two polymorphs of azelaic acid, (I), have been reported previously: the α form crystallizes in $P2_1/c$ (Caspari, 1928; Housty & Hospital, 1967) and the β form crystallizes in $C2/c$ (Housty & Hospital, 1967). For both polymorphs, the structures present in the CSD (AZELAC10 and AZELAC01; Allen & Kennard, 1993) are derived from room-temperature



(I)

data with R factors *ca* 10% and ambiguities in the treatment of H atoms. We have, therefore, re-examined azelaic acid and report here the structure of the β form measured at 180 K to significantly greater precision.

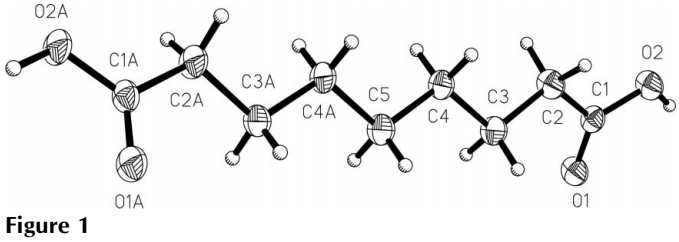


Figure 1
The molecular unit of the title compound showing displacement ellipsoids at the 50% probability level.

Experimental

Azelaic acid was obtained from Aldrich and recrystallized from ethanol.

Crystal data

$C_9H_{16}O_4$
M_r = 188.22
Monoclinic, $C2/c$
a = 22.622 (2) Å
b = 4.7348 (2) Å
c = 9.6864 (7) Å
β = 110.559 (3)°
V = 971.5 (1) Å^3
Z = 4
D_x = 1.287 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2161 reflections
θ = 1.0–27.5°
μ = 0.10 mm^{-1}
T = 180 (2) K
Plate, colourless
0.25 × 0.12 × 0.06 mm

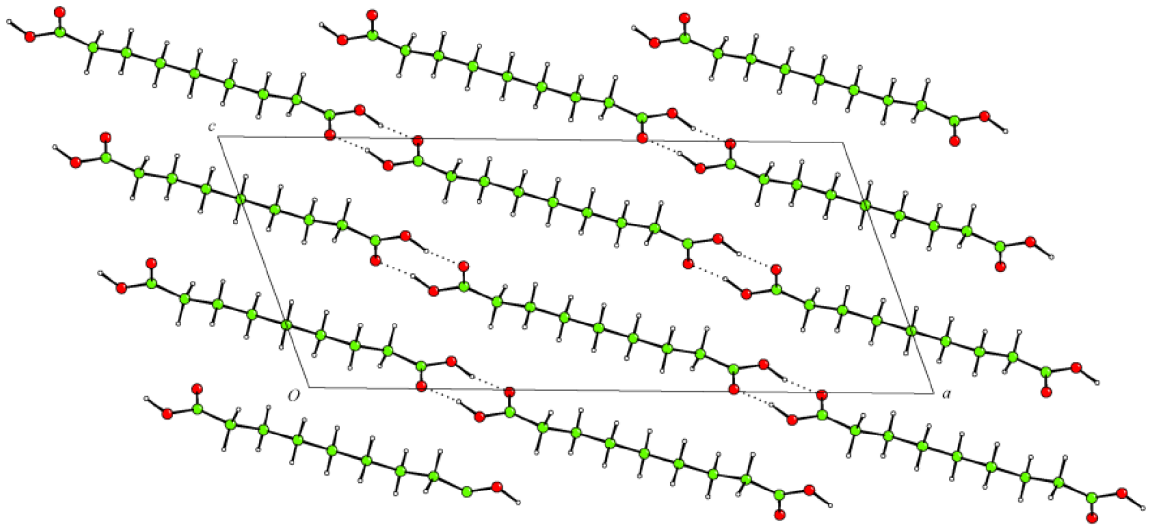


Figure 2
Projection onto (010) showing hydrogen-bonded chains running approximately along the [$\bar{4}$01] vector.

Data collection

Nonius KappaCCD diffractometer	913 reflections with $I > 2\sigma(I)$
Thin-slice ω and φ scans	$R_{int} = 0.039$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	$\theta_{max} = 27.4°$
$T_{min} = 0.907$, $T_{max} = 0.994$	$h = 0 \rightarrow 28$
3154 measured reflections	$k = -6 \rightarrow 6$
1085 independent reflections	$l = -12 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 0.5150P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.010$
$wR(F^2) = 0.096$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
$S = 1.09$	$\Delta\rho_{min} = -0.19$ e Å^{-3}
1085 reflections	
64 parameters	
H atoms: see below	

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O1^{i}	0.96 (2)	1.70 (2)	2.6576 (12)	173.5 (17)

Symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} - y, -z$.

The H atom of the carboxylic acid group was located in a difference Fourier map and refined without restraint. All other H atoms 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.

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.

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