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Elaidic acid (*trans*-9-octadecenoic acid)

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Key indicators

Single-crystal X-ray study
$T = 120$ K
Mean σ(C–C) = 0.005 Å
R factor = 0.102
wR factor = 0.256
Data-to-parameter ratio = 21.0

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

Elaidic acid, $C_{18}H_{34}O_2$, has an essentially linear alkyl chain. The double bond is twisted across the mean direction of the alkyl chain in a skew', *trans*, skew conformation. In the crystal structure, the molecules form centrosymmetric O—H⋯O hydrogen-bonded dimers (O⋯O = 2.684 Å).

Comment

The physical, biological and nutritional properties of fatty acids are largely determined by the number, position and configuration of their double bonds. These determine the shape of the molecules, the way molecules can pack together in solid phases, monolayers, bilayers *etc.*, and how individual molecules can interact with enzymes and receptors. Most natural unsaturated fatty acids have *cis* (*Z*) double bonds. Trans (*E*) fatty acids are present in dairy fats and are produced during the catalytic partial hydrogenation used in the production of hardened fats and during deodorization of commodity oils. The labelling of foods with *trans* content is increasingly required due to their undesirable nutritional properties. Alternative ways of producing hardened fats, such as interesterification or blending with fully saturated fats, and milder deodorization procedures, are being developed to reduce *trans* content. Trans fatty acids more closely resemble saturated acids in melting point and nutritional properties, sharing an essentially linear structure which allows closely aligned packing in condensed phases. In contrast, *cis* double bonds introduce a bend in the alkyl chain, making packing less stable and lowering the melting point. We have determined the structure of elaidic acid (*trans*-9-octadecenoic acid), (I), to enable a detailed comparison of a *trans* fatty acid with saturated and *cis*-unsaturated compounds.

(I)
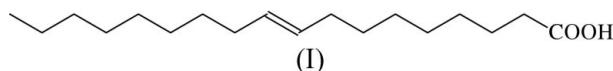
Relatively few crystal structures of fatty acids are available, as good crystals are difficult to obtain, often being thin plates and often crystallizing in several polymorphs. Most monoenes have low melting points and polyenes are liquids at room temperature. The crystal structures of the following saturated and monoene C_{18} fatty acids have been reported to date: stearic acid (octadecanoic acid) (Malta *et al.*, 1971; Kaneko *et al.*, 1990, 1994*a*,*b*), oleic acid (*cis*-9-octadecenoic acid) (Abrahamsson & Ryderstedt-Nahringbauer, 1962; Kaneko *et al.*, 1997) and petroselinic acid (*cis*-6-octadecenoic acid) (Kaneko *et al.*, 1992*a*,*b*). No *trans*-octadecenoic acid structure has been reported to date.
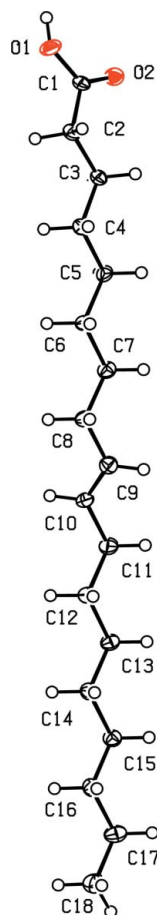
Figure 1
A view of (I), with displacement ellipsoids drawn at the 30% probability level.

Crystal data

$C_{18}H_{34}O_2$	$D_x = 1.075$ Mg m^{-3}
$M_r = 282.45$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3830
$a = 98.48$ (2) Å	reflections
$b = 4.9381$ (3) Å	$\theta = 3.3$–27.6°
$c = 7.1826$ (8) Å	$\mu = 0.07$ mm^{-1}
$\beta = 92.570$ (12)°	$T = 120$ (2) K
$V = 3489.4$ (8) Å^3	Plate, colourless
$Z = 8$	$0.20 \times 0.18 \times 0.01$ mm

Data collection

Bruker Nonius KappaCCD area-detector diffractometer	3830 independent reflections
	1679 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.150$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$\theta_{max} = 27.6°$
	$h = -126 \rightarrow 126$
$T_{min} = 0.987$, $T_{max} = 0.999$	$k = -6 \rightarrow 6$
17532 measured reflections	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0744P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.102$	$+ 7.8445P]$
$wR(F^2) = 0.256$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
3830 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
182 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected torsion angles (°).

C1—C2—C3—C4	−170.7 (3)	C9—C10—C11—C12	118.6 (4)
C2—C3—C4—C5	177.0 (3)	C10—C11—C12—C13	178.4 (3)
C3—C4—C5—C6	−176.6 (3)	C11—C12—C13—C14	−179.8 (3)
C4—C5—C6—C7	178.9 (3)	C12—C13—C14—C15	179.9 (3)
C5—C6—C7—C8	−179.1 (3)	C13—C14—C15—C16	179.8 (3)
C6—C7—C8—C9	−178.4 (3)	C14—C15—C16—C17	−179.6 (3)
C7—C8—C9—C10	−118.8 (4)	C15—C16—C17—C18	179.5 (3)
C8—C9—C10—C11	−179.9 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$\cdots$O2^i	0.87	1.86	2.684 (3)	158

Symmetry code: (i) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+1$.

Elaidic acid (I) has an essentially linear alkyl chain, with the torsion angle between saturated C atoms close to 180° (Table 1). The C7—C8—C9—C10, C8—C9—C10—C11 and C9—C10—C11—C12 torsion angles are −118.8 (4), −179.9 (4) and 118.6 (4)°, respectively, resulting in the double bond being twisted across the mean direction of the alkyl chain in a *skew'*, *trans*, *skew* conformation. The C1–C18 distance is 21.393 (6) Å, comparable with that in fully extended stearic acid structures (21.6 Å; Malta *et al.*, 1971; Kaneko *et al.*, 1990, 1994*b*). This contrasts with the *cis*-octa-decenoic acids, where the molecules are bent and the C1–C18 distance is reduced to between 17.8 and 19.7 Å (Abrahamsson & Ryderstedt-Nahringbauer, 1962; Kaneko *et al.*, 1997, 1992*a,b*).

In the crystal structure of (I), molecules related by inversion centres are linked by O—H$\cdots$O hydrogen bonds to form $R_2^2(8)$ dimers (Bernstein *et al.*, 1995) typical of carboxylic acids (Table 2).

Experimental

A commercial sample of (I) (Sigma, Poole, Dorset, UK) was re-crystallized from ethanol at room temperature. The crystals were composed of very thin stacked sheets which tended to be twisted. After many attempts, a crystal was found from which it was possible to obtain a data set.

H atoms were treated as riding, with C—H(aromatic) = 0.95 and C—H(CH$_2$) = 0.99 Å, with U_{iso}(H) = 1.2U_{eq}(C), C—H(methyl) = 0.98 Å, with U_{iso}(H) = 1.5U_{eq}(C), and O—H = 0.87 Å, with U_{iso}(H) = 1.5U_{eq}(O). The O-bound H atom was allowed to ride at its position as determined from a difference map. Although the best crystal was selected from many crystallization attempts, the higher than usual values for R, wR and R_{int} may be a result of the crystal quality. The possibilty that the crystal was twinned was investigated but this did not give any significant results.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

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