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The Crystal Structure of 13-Oxoisostearic Acid

BY BIRGITTA DAHLÉN

Crystallography Group, Swedish Medical Research Council Unit for Molecular Structure Analysis, University of Göteborg, Fack, S-400 33 Göteborg 33, Sweden

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13-Oxoisostearic acid (16-methyl-13-oxoheptadecanoic acid) is triclinic ($P\bar{1}$) with $a=4{\cdot}933$, $b=5{\cdot}623$, $c=34{\cdot}460$ Å, $\alpha=95{\cdot}65$, $\beta=94{\cdot}01$ and $\gamma=103{\cdot}60°$. The molecules are arranged in hydrogen-bonded dimers in which the chain axes are tilted 44° to the end-group planes to allow the methyl branches to be accommodated between the methyl ends of the chains. The keto oxygen is directly incorporated into the chain packing with a resulting strain at the sp^2 carbon atom. This leads to a bend of the chain axis *in* the zigzag plane of the molecule. The carboxyl group forms an angle of 13° with the chain plane.

Introduction

As a part of crystal structure investigations of compounds with long hydrocarbon chains at this research unit, branched-chain fatty acids have been studied (Abrahamsson, 1959*b*; Abrahamsson & Harding, 1966). The effect of a keto group along the carbon chain in an acid branched close to the carboxyl group (DL-2-methyl-7-oxododecanoic acid) was studied by O'Connell (1968). In connexion with work on the crystal structure of isostearic acid (Abrahamsson & Lundén, 1972) a single-crystal analysis of 13-oxoisostearic acid was performed to see the influence of the keto group on the molecular geometry and packing in the case of ω-branching.

Crystal data

Molecular formula	$C_{18}H_{34}O_3$, 16-methyl-13-oxoheptadecanoic acid
Unit cell:	
Triclinic	$a=4{\cdot}933$ (2), $b=5{\cdot}623$ (4), $c=34{\cdot}460$ (7) Å; $\alpha=95{\cdot}65$ (5), $\beta=94{\cdot}01$ (3), $\gamma=103{\cdot}60$ (5)°
V	920·25 Å^3
Molecular weight	298·47
Z	2
D_c	1·077 g.cm^{-3}
D_m	1·071 g.cm^{-3}
λ	1·54051 Å (Cu $K\alpha_1$ radiation)
Space group	$P\bar{1}$

The space group was assumed to be $P\bar{1}$ and this was not contradicted in the structure determination.

Experimental

13-Oxoisostearic acid was synthesized by Stenhagen & Tägtström-Eketorp (1944). The crystals grow from ether as soft thin plates. They have a melting point of 76·9–77·2 °C.

A single crystal with the dimensions $0{\cdot}07\times0{\cdot}59\times0{\cdot}24$ mm was mounted along the b axis and data were collected on a Picker four-circle automatic diffractometer using graphite monochromated Cu $K\alpha$ radiation. The $\theta/2\theta$ scanning mode was used to measure the reflexions at a scanning rate of 1°/min and with 10 sec background counts at the scan limits. 2758 reflexions having 2θ less than 120° were recorded. 458 of these intensities I, with $I\leq2\sigma(I)$ were considered to be unobservably weak and assigned an intensity of $2\sigma(I)$. The unobserved reflexions were not used in the least-squares refinement but included in the final SF-calculation.

The Lorentz and polarization corrections were applied to all reflexions, but no absorption correction was made as the linear absorption coefficient was small ($\mu=5{\cdot}63$ cm^{-1}).

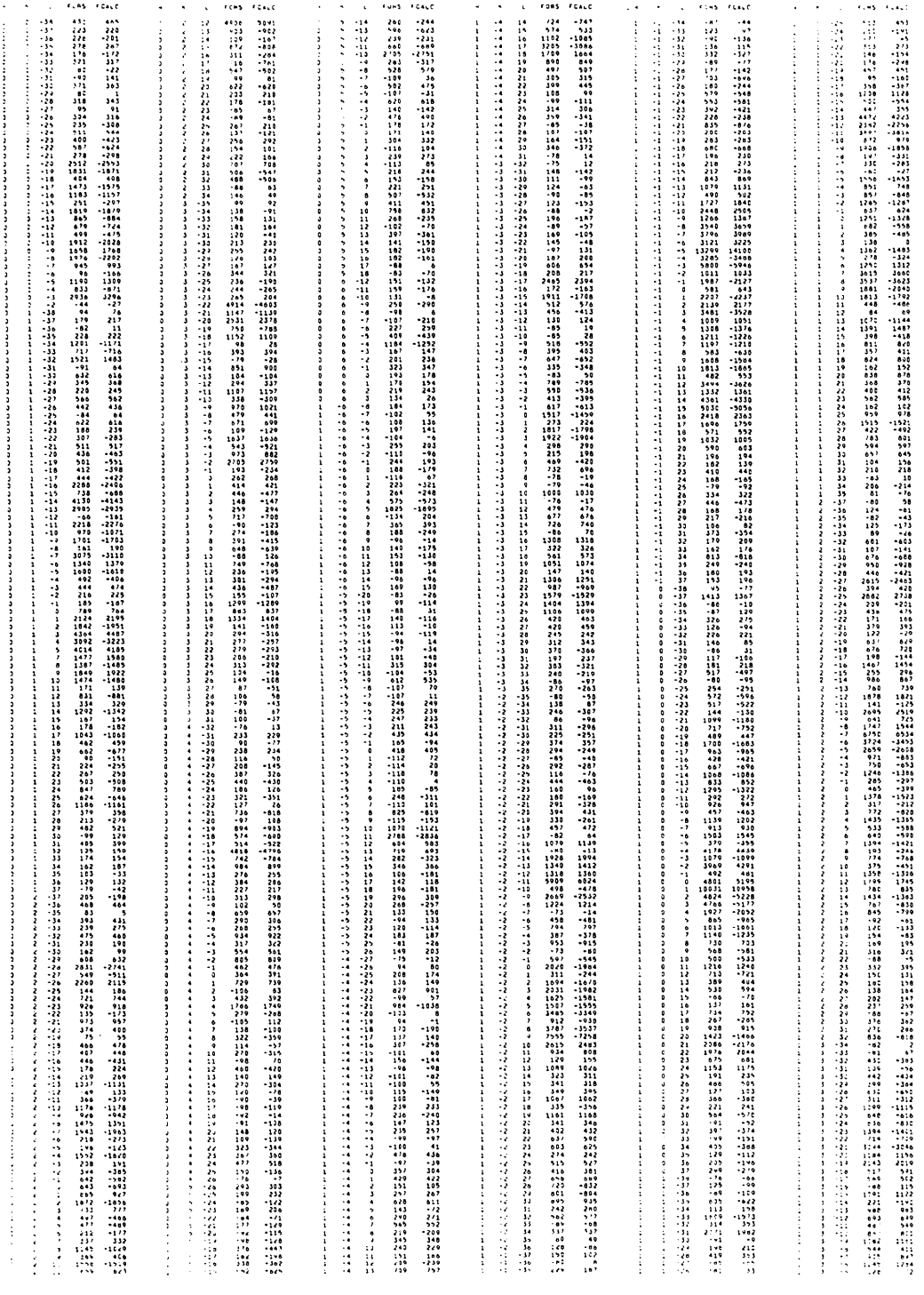
Structure determination and refinement

The carbon-chain direction was clearly shown in the three-dimensional sharpened Patterson function. The acid was considered to exist as hydrogen bonded dimers around centres of symmetry, as is usual for higher fatty acids. Therefore the assumption was made that the carbon atoms C(1) and C(2) and their symmetry-related equivalents were all on one line passing through the inversion centre. There were then two possible positions for the carboxyl carbon. The coordinates for the chain carbon atoms were calculated for the two different alternatives and from a calculation of distances and angles one of them seemed to be more plausible.

A structure-factor calculation including the 17 carbon atoms in the chain gave an R value of 0·8 for the 1237 reflexions whose F value exceeded 30. All these atoms appeared in the Fourier map but in addition there were fairly large peaks at a distance of about 1 Å from every odd-numbered carbon atom. The whole chain was therefore moved half the distance towards the 'ghost peaks' and after two cycles of structure-factor and Fourier calculation all carbon and oxygen atoms could be located. The resulting R value was then 0·36.

Table 1. *Observed and calculated structure factors* ($\times 100$)

The unobserved terms, indicated by a minus sign on F_{obs}, are included at the threshold values.



The structure was then refined with block-diagonal least-squares using isotropic temperature factors, to an R value of 0·18. The number of reflexions was now increased to include all the observed reflexions, and a calculated Fourier difference map revealed the positions of all hydrogen atoms except the hydrogen attached to the hydroxyl oxygen.

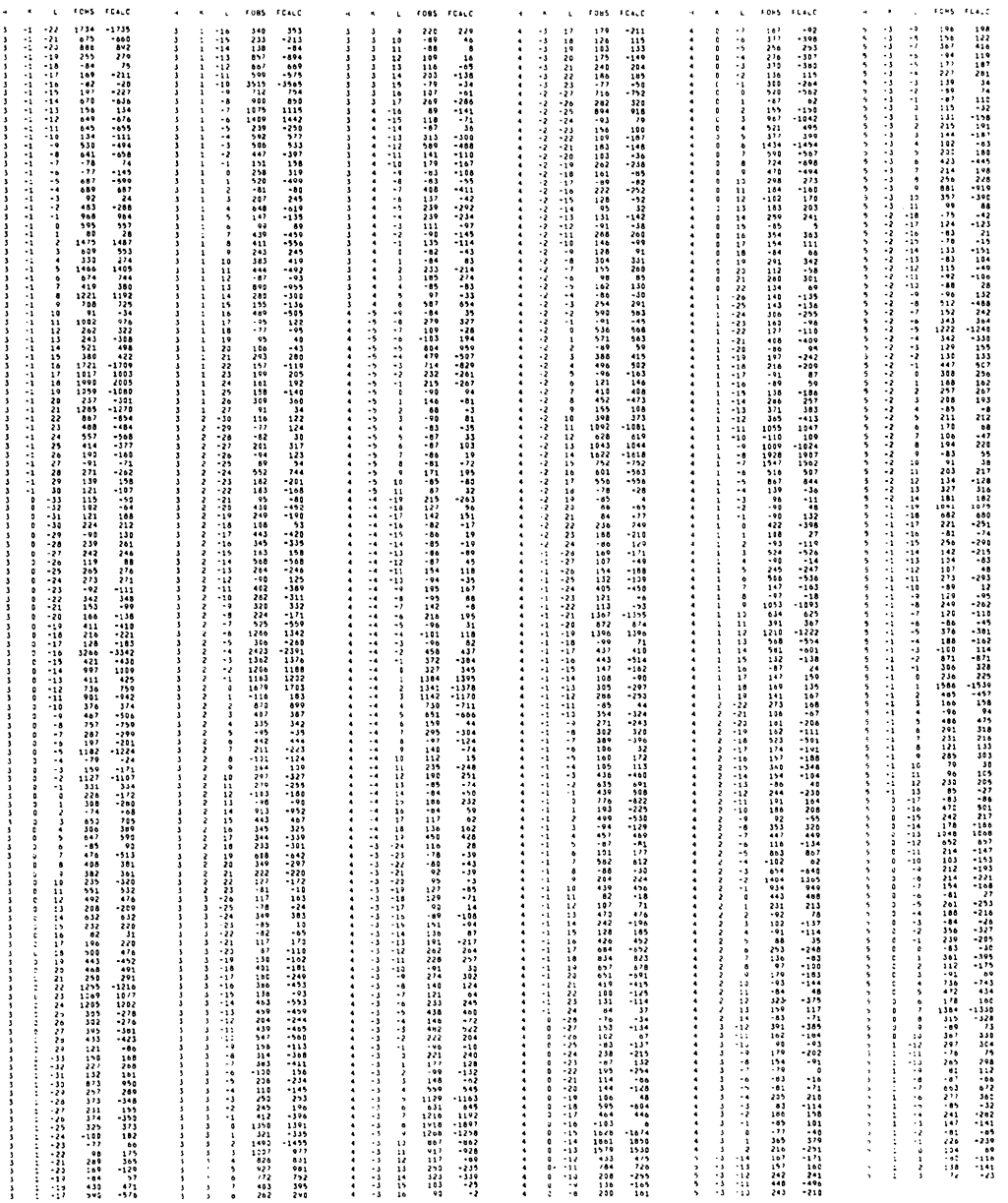
All the hydrogen atoms found were included in the structure-factor calculations with the same isotropic temperature factors as the parent atom. Full-matrix

Table 1 (*cont.*)

refinement was applied to the non-hydrogen atoms using anisotropic temperature factors and when the R value was 0·074 the remaining hydrogen atom could be located from a difference map. As the two largest reflexions showed poor agreement they were excluded from the refinement but included in the final structure-factor calculation.

Due to the relatively large number of parameters the hydrogen atoms were refined in separate runs. The final R index for the observed reflexions was 0·065.

Table 1 (*cont.*)



The weight assigned to each observation in the refinement was (Mills & Rollett, 1961)

$$w = 1/\left(1+\left[\frac{|F_o|-4\cdot3|F_{\min}|}{10\cdot2|F_{\min}|}\right]^2\right).$$

All calculations were performed on a Datasaab D21 computer with the program system of Abrahamsson, Aleby, Larsson, Nilsson, Selin & Westerdahl (1965). The X-ray atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1962) for carbon and oxygen and from Stewart, Davidson & Simpson (1965) for hydrogen.

Description of the structure

Observed and calculated structure factors are listed in Table 1, the final positional and thermal parameters in Tables 2, 3 and 4. The thermal ellipsoids are shown in Fig. 1. Interatomic distances and angles are given in Fig. 2 where the atomic numbering is also indicated and with standard deviations in Table 5. The standard deviations as calculated from the least-squares refinement appear to be somewhat small when compared with the differences in bond lengths and angles along the carbon chain.

Table 2. *Fractional atomic coordinates with standard deviations* ($\times 10^4$) *for the non-hydrogen atoms*

	x	*y*	*z*
C(1)	1·1154 (5)	0·8035 (4)	0·0378 (1)
C(2)	1·2182 (5)	0·6553 (5)	0·0667 (1)
C(3)	0·9980 (5)	0·4688 (5)	0·0828 (1)
C(4)	1·1211 (5)	0·3477 (4)	0·1149 (1)
C(5)	0·9104 (5)	0·1586 (5)	0·1326 (1)
C(6)	1·0358 (5)	0·0453 (4)	0·1655 (1)
C(7)	0·8301 (5)	−0·1390 (5)	0·1845 (1)
C(8)	0·9611 (5)	−0·2537 (5)	0·2165 (1)
C(9)	0·7582 (5)	−0·4361 (4)	0·2364 (1)
C(10)	0·8972 (5)	−0·5521 (4)	0·2675 (1)
C(11)	0·6942 (5)	−0·7337 (4)	0·2881 (1)
C(12)	0·8389 (5)	−0·8419 (5)	0·3193 (1)
C(13)	0·6537 (5)	−1·0260 (5)	0·3405 (1)
C(14)	0·7886 (5)	−1·1332 (5)	0·3726 (1)
C(15)	0·5899 (5)	−1·3223 (5)	0·3919 (1)
C(16)	0·7305 (5)	−1·4331 (5)	0·4242 (1)
C(17)	0·5170 (7)	−1·6428 (6)	0·4380 (1)
C(18)	0·8692 (7)	−1·2475 (6)	0·4581 (1)
O(1)	0·8768 (4)	0·7479 (4)	0·0220 (1)
O(2)	1·3036 (4)	0·9933 (4)	0·0308 (1)
O(3)	0·4024 (4)	−1·0873 (4)	0·3322 (1)

Table 3. *Anisotropic thermal parameters in the form*

$$\exp[-2\pi^2(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2klb^*c^*U_{23}+2lha^*c^*U_{31}+2hka^*b^*U_{12})]$$

Standard deviations are given in parentheses.
All values have been multiplied by 10^4.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{31}	U_{12}
C(1)	564 (15)	492 (14)	477 (14)	178 (11)	122 (12)	151 (12)
C(2)	568 (15)	607 (16)	530 (14)	284 (12)	72 (11)	151 (12)
C(3)	517 (14)	556 (15)	519 (14)	222 (12)	42 (11)	136 (12)
C(4)	495 (14)	499 (14)	506 (14)	196 (11)	26 (11)	119 (11)
C(5)	536 (14)	503 (14)	498 (14)	199 (11)	20 (11)	84 (11)
C(6)	500 (14)	479 (14)	541 (14)	203 (11)	21 (11)	80 (11)
C(7)	491 (14)	493 (14)	579 (15)	208 (12)	21 (11)	85 (11)
C(8)	522 (14)	498 (14)	526 (14)	210 (11)	34 (11)	84 (11)
C(9)	525 (14)	497 (14)	549 (15)	199 (12)	27 (11)	96 (12)
C(10)	518 (14)	497 (14)	522 (14)	162 (11)	13 (11)	102 (11)
C(11)	474 (13)	514 (14)	523 (14)	202 (12)	39 (11)	77 (11)
C(12)	445 (13)	570 (15)	544 (14)	226 (12)	36 (11)	110 (11)
C(13)	444 (14)	586 (15)	509 (14)	156 (12)	69 (11)	184 (11)
C(14)	489 (14)	565 (15)	573 (15)	275 (12)	55 (11)	86 (12)
C(15)	524 (14)	539 (15)	505 (14)	167 (12)	67 (11)	83 (12)
C(16)	634 (15)	504 (14)	520 (14)	248 (12)	131 (12)	137 (12)
C(17)	926 (23)	678 (19)	802 (20)	340 (16)	114 (17)	156 (17)
C(18)	1031 (24)	735 (20)	564 (17)	221 (15)	−90 (16)	49 (18)
O(1)	592 (12)	740 (13)	814 (14)	476 (11)	−30 (10)	105 (10)
O(2)	649 (12)	680 (12)	780 (13)	450 (10)	54 (10)	44 (10)
O(3)	425 (11)	979 (16)	949 (15)	572 (13)	27 (10)	72 (10)

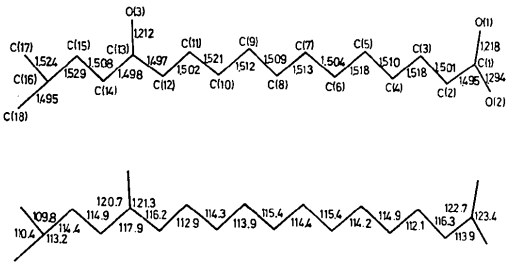


Fig. 2. Bond lengths and angles.

Table 4. *Fractional atomic coordinates and isotropic temperature factors with their estimated standard deviations for the hydrogen atoms*

The first appended number refers to that of the parent atom.

	x	*y*	*z*	*B*
H(21)	1·345 (6)	0·574 (6)	0·055 (1)	7·3 (7)
H(22)	1·313 (5)	0·754 (5)	0·087 (1)	4·8 (6)
H(31)	0·856 (5)	0·528 (5)	0·092 (1)	5·3 (6)
H(32)	0·898 (5)	0·343 (5)	0·061 (1)	5·1 (6)
H(41)	1·264 (5)	0·274 (5)	0·104 (1)	5·2 (6)
H(42)	1·219 (5)	0·472 (5)	0·136 (1)	5·1 (6)
H(51)	0·769 (5)	0·228 (5)	0·144 (1)	5·6 (6)
H(52)	0·818 (5)	0·026 (4)	0·110 (1)	4·4 (5)
H(61)	1·181 (6)	−0·028 (5)	0·155 (1)	5·6 (6)
H(62)	1·144 (6)	0·178 (5)	0·185 (1)	5·6 (6)
H(71)	0·685 (5)	−0·062 (5)	0·196 (1)	5·9 (6)
H(72)	0·734 (5)	−0·266 (5)	0·166 (1)	5·2 (6)
H(81)	1·102 (5)	−0·326 (4)	0·205 (1)	3·9 (5)
H(82)	1·062 (5)	−0·129 (5)	0·235 (1)	5·0 (6)
H(91)	0·627 (5)	−0·353 (5)	0·248 (1)	5·1 (6)
H(92)	0·665 (5)	−0·556 (5)	0·216 (1)	5·7 (6)
H(101)	1·034 (5)	−0·629 (5)	0·255 (1)	5·5 (6)
H(102)	1·006 (5)	−0·422 (5)	0·286 (1)	5·1 (6)
H(111)	0·551 (5)	−0·665 (5)	0·299 (1)	5·2 (6)
H(112)	0·586 (6)	−0·869 (5)	0·269 (1)	5·5 (6)
H(121)	0·976 (6)	−0·926 (5)	0·309 (1)	5·7 (6)
H(122)	0·932 (5)	−0·724 (5)	0·338 (1)	5·7 (6)
H(141)	0·926 (6)	−1·202 (5)	0·362 (1)	6·6 (7)
H(142)	0·870 (6)	−1·004 (5)	0·391 (1)	6·7 (7)
H(151)	0·449 (6)	−1·256 (6)	0·404 (1)	7·4 (7)
H(152)	0·479 (5)	−1·460 (5)	0·372 (1)	5·5 (6)
H(161)	0·896 (6)	−1·478 (5)	0·413 (1)	7·2 (7)
H(171)	0·447 (6)	−1·740 (5)	0·418 (1)	7·5 (7)
H(172)	0·355 (8)	−1·587 (7)	0·450 (1)	10·1 (10)
H(173)	0·592 (6)	−1·725 (5)	0·458 (1)	6·5 (7)
H(181)	0·707 (6)	−1·194 (5)	0·468 (1)	5·9 (6)
H(182)	1·018 (6)	−1·103 (5)	0·451 (1)	6·4 (7)
H(183)	0·938 (7)	−1·325 (6)	0·481 (1)	8·4 (8)
H(24)*	1·243 (8)	1·085 (7)	0·009 (1)	11·4 (11)

* Refers to the hydroxyl hydrogen.

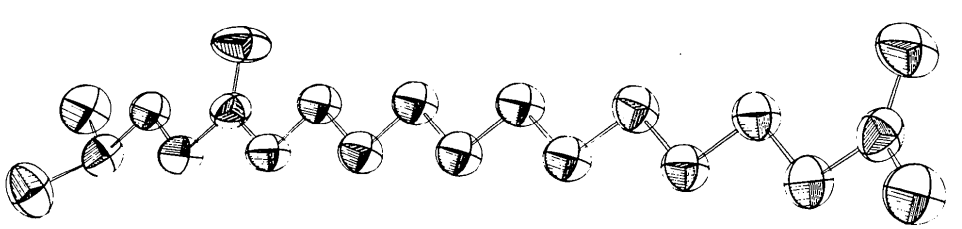


Fig. 1. Drawing of 13-oxoisostearic acid showing the thermal ellipsoids as viewed along the *b* axis.

Table 5. *Bond distances and angles and their estimated standard deviations for the non-hydrogen atoms*

C(1)—O(1)	1·218 (3) Å	O(1)—C(1)—O(2)	123·4 (3)°
C(1)—O(2)	1·294 (3)	O(1)—C(1)—C(2)	122·7 (2)
C(1)—C(2)	1·495 (4)	O(2)—C(1)—C(2)	113·9 (2)
C(2)—C(3)	1·501 (3)	C(1)—C(2)—C(3)	116·3 (2)
C(3)—C(4)	1·518 (4)	C(2)—C(3)—C(4)	112·1 (2)
C(4)—C(5)	1·510 (3)	C(3)—C(4)—C(5)	114·9 (2)
C(5)—C(6)	1·518 (4)	C(4)—C(5)—C(6)	114·2 (2)
C(6)—C(7)	1·504 (3)	C(5)—C(6)—C(7)	115·4 (2)
C(7)—C(8)	1·513 (4)	C(6)—C(7)—C(8)	114·4 (2)
C(8)—C(9)	1·509 (3)	C(7)—C(8)—C(9)	115·4 (2)
C(9)—C(10)	1·512 (4)	C(8)—C(9)—C(10)	113·9 (2)
C(10)–C(11)	1·521 (3)	C(9)—C(10)–C(11)	114·3 (2)
C(11)–C(12)	1·502 (4)	C(10)–C(11)–C(12)	112·9 (2)
C(12)–C(13)	1·497 (3)	C(11)–C(12)–C(13)	116·2 (2)
C(13)–C(14)	1·498 (4)	C(12)–C(13)–C(14)	117·9 (2)
C(13)–O(3)	1·212 (3)	C(12)–C(13)–O(3)	121·3 (2)
C(14)–C(15)	1·508 (3)	C(14)–C(13)–O(3)	120·7 (2)
C(15)–C(16)	1·529 (4)	C(13)–C(14)–C(15)	114·9 (2)
C(16)–C(17)	1·524 (4)	C(14)–C(15)–C(16)	114·4 (2)
C(16)–C(18)	1·495 (3)	C(15)–C(16)–C(17)	109·8 (2)
		C(15)–C(16)–C(18)	113·2 (2)
		C(17)–C(16)–C(18)	110·4 (2)

The mean C(sp^3)–C(sp^3) bond distance is 1·512 (4) Å and the mean C–C–C angle for the same carbon atoms is 113·9 (2)° (see, however, below). These values are in agreement with those found in other long hydrocarbon chains (Jensen & Mabis, 1966; O'Connell, 1968; O'Connell & Pascher, 1969). The systematically short bond lengths and large bond angles are most probably due to thermal motion and rotatory oscillations of the chain around the long axis. The distances and angles have not been corrected for thermal motion as this would require an analysis of the complete vibrational pattern of all the atoms. However, if a riding motion correction is considered applicable for the two C–C bonds in the iso-group the bond lengths should be increased by about 0·025 Å.

The equation of the best plane through C(2) to C(16) is given in Table 6 with the out-of-plane deviations as well as the in-plane deviations from the chain axis. From the Δ_1 and Δ_2 values it can be seen that the molecule is clearly bent in the zigzag plane. This is also shown by the interatomic angles where the C–C–C angle for the even-numbered carbon atoms are all somewhat larger than those of the odd-numbered atoms. This type of bending is rather unexpected but is a combined effect of the valence angles at the keto group and the molecular packing (Fig. 3). The keto oxygen atom is in the zigzag plane of the chain. The sp^2 carbon atom exerts a pressure on the chain to bend or twist locally to preserve the 120° valence angle. However, as the molecules are heavily tilted with respect to the end-group planes, each keto group is isolated in regions where normal carbon chain packing exists. The strain forces at the keto group are not strong enough to deform the chains locally. The strain is instead taken up by a successive bend of the chain axis. The C–C–C angle of the keto carbon atom has also decreased to 117·9°. In DL-2-methyl-7-oxodecanoic acid (O'Connell, 1968) the corresponding angle is 117·3°. Here the geometric requirements of the keto group resulted in a twist of 7·2° of the zigzag planes of the two chain parts on each side of the keto group. This is compatible with the less pronounced chain domination in the smaller molecule.

Table 6. *The best least-squares plane through* C(2) *to* C(16)

The equation is expressed in terms of the crystal axes.

$$-0{\cdot}0798X+0{\cdot}1873Y+0{\cdot}9791Z-0{\cdot}0886=0\,.$$

Δ_1 are the out-of-plane deviations, Δ_2 and Δ_3 are the in-plane distances from the chain axes and the 'worst' plane.

	Δ_1	Δ_2	Δ_3
C(2)	0·048	0·560	8·841 Å
C(3)	0·014	−0·358	7·655
C(4)	−0·009	0·405	6·343
C(5)	−0·036	−0·460	5·105
C(6)	−0·015	0·319	3·803
C(7)	−0·006	−0·516	2·552
C(8)	−0·018	0·284	1·267
C(9)	0·015	−0·532	−0·002
C(10)	−0·037	0·298	−1·264
C(11)	0·015	−0·513	−2·550
C(12)	−0·013	0·344	−3·783
C(13)	0·010	−0·382	−5·092
C(14)	0·022	0·435	−6·348
C(15)	0·008	−0·364	−7·627
C(16)	0·000	0·480	−8·901
*C(1)	0·214	−0·091	10·177
*C(17)	−0·187	−0·420	−10·116
*C(18)	1·226	1·322	−9·058
*O(1)	0·066	−1·287	10·349
*O(2)	0·508	0·734	11·131
*O(3)	0·018	−1·592	−5·141

* Atoms not included in the plane calculation.

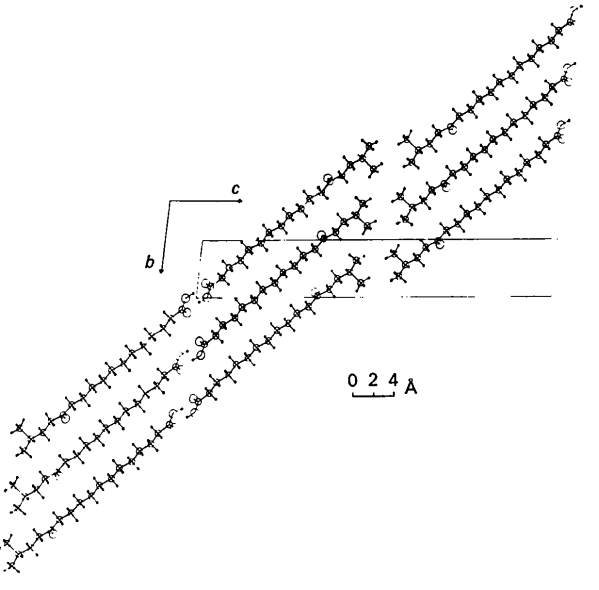


Fig. 3. Molecular arrangement of 13-oxoisostearic acid viewed along the *a* axis.

The closest intermolecular contacts between the keto oxygen and carbon atoms are 3·609, 3·403 and 3·387 Å to C(10), C(12) and C(14) respectively and the shortest keto oxygen–hydrogen distances are 2·67, 2·59 and 2·60 Å to H(102), H(121) and H(141) respectively. The corresponding values in DL-2-methyl-7-oxododecanoic acid for the oxygen–carbon contacts are 3·45, 3·50 and 3·52 Å and for oxygen–hydrogen contacts 2·76, 2·69 and 2·63 Å.

Fig. 3 shows the molecular packing which agrees in principle with that reported for 17-methyl-octadecanoic acid (Abrahamsson, 1959*a*). The molecules are arranged in layers but tilted by as much as 44° to the end-group planes to allow each branching methyl group to be accommodated in the space between two chain ends.

Some short contacts around the carboxyl group and at the end methyl groups are shown in Fig. 4. Table 7 gives all non-hydrogen intermolecular distances less than 3·8 Å. The molecules form hydrogen-bonded dimers and the two carboxyl groups are coplanar within the experimental errors. The perpendicular distance between the two carboxyl groups is thus only 0·016 Å. The hydroxyl hydrogen atom deviates from the plane by 0·083 Å. This hydrogen atom has a fairly large temperature factor and less definite positional parameters than the other hydrogen atoms which is often the case in O–H···O hydrogen bonds.

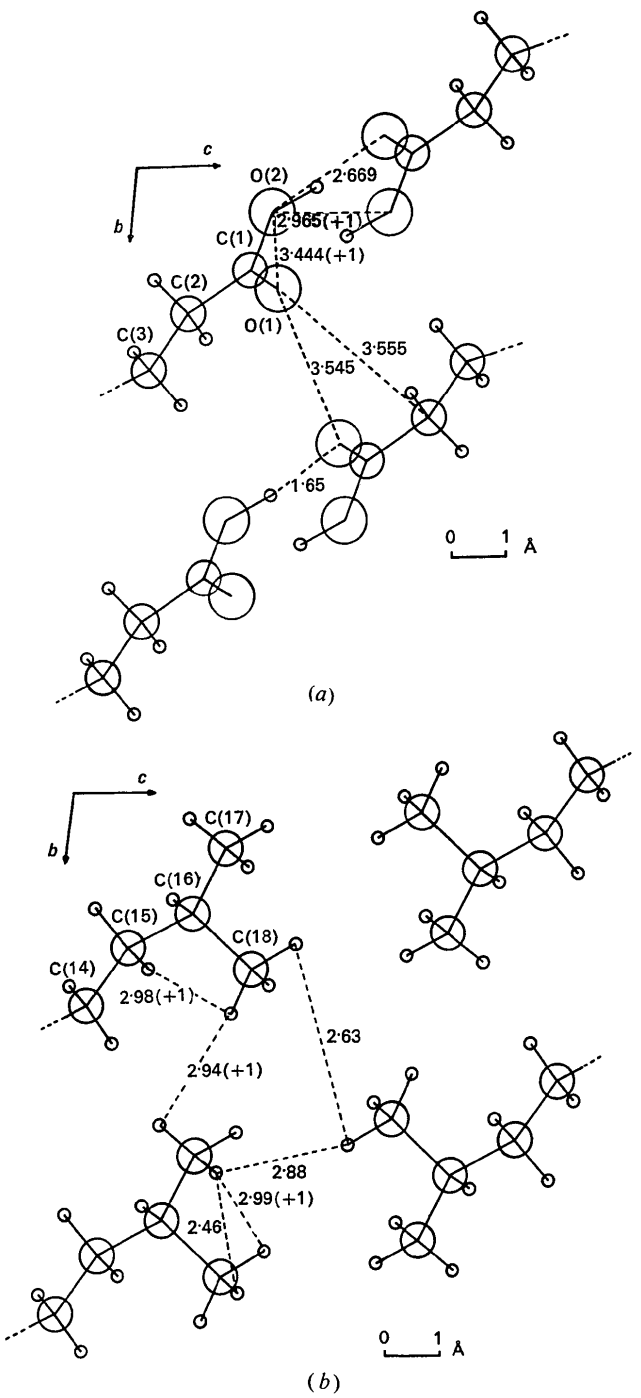


Fig. 4. (*a*) The carboxyl group contact planes as seen along the *a* axis with the shorter intermolecular distances indicated. (*b*) The methyl group contact planes as seen along the *a* axis with the shorter hydrogen contacts indicated.

Table 7. *Intermolecular distances less than* 3·8 Å

C(1)···O(1)	(2, 1, 0) 2*	3·560 (3) Å
C(1)···O(2)	(2, 2, 0) 2	3·406 (3)
C(1)···O(2)	(2, 2, 0) 2	3·481 (3)
C(2)···O(1)	(2, 1, 0) 2	3·555 (3)
C(2)···O(1)	(1, 0, 0) 1	3·641 (3)
C(3)···O(2)	(0, −1, 0) 1	3·737 (3)
C(4)···O(2)	(0, −1, 0) 1	3·641 (3)
C(10)···O(3)	(1, 1, 0) 1	3·609 (3)
C(12)···O(3)	(1, 0, 0) 1	3·403 (3)
C(14)···O(3)	(1, 0, 0) 1	3·387 (3)
C(18)···C(18)	(2, −2, 1) 2	3·737 (4)
O(1)···O(1)	(2, 1, 0) 2	3·545 (3)
O(1)···O(1)	(2, 2, 0) 2	3·363 (3)
O(1)···O(2)	(−1, 0, 0) 1	3·444 (3)
O(1)···O(2)	(2, 2, 0) 2	2·669 (3)
O(2)···O(2)	(2, 2, 0) 2	3·567 (3)
O(2)···O(2)	(3, 2, 0) 2	2·965 (3)

* Unit-cell translation of the second atom.

The carboxyl group has normal bond lengths and angles and is tilted 13° to the plane of the hydrocarbon chain. The O–H bond distance is 1·03 Å and the O···O and O···H distances are 2·669 and 1·65 Å respectively. The O···H–O angle is 171°. These values are in a good agreement with those found in neutron-diffraction studies of O–H···O bonded compounds (Hamilton & Ibers, 1968).

The closest interlayer van der Waals contact is 3·74 Å between branching methyl carbons. As shown in Fig. 4 the shortest hydrogen–hydrogen contacts between the layers are H(183)···H(183) and H(172)···H(183) which are 2·63 and 2·88 Å respectively.

The chains are arranged in the common triclinic subcell packing ($T\|\|$) (Abrahamsson, 1959*b*), illustrated

in Fig. 5, with the dimensions

$a_s = 4{\cdot}27$, $b_s = 5{\cdot}39$, $c_s = 2{\cdot}55$ Å
$\alpha_s = 73{\cdot}9$, $\beta_s = 108{\cdot}6$, $\gamma_s = 119{\cdot}6°$.

The volume of the CH_2 group is 23·9 Å^3.

The mean C–H bond distance in the subcell regions is 0·96 Å ($\sigma = 0{\cdot}04$ Å), where $\sigma = [\sum_N (X_N - \bar{X})^2/(N-1)]^{1/2}$ and the average value of the angles involving hydrogen atoms in the same part of the molecule is 108° ($\sigma = 3°$). The shortest H···H interatomic contacts are $H_A \cdots H_B$ 2·89 (6) Å, $H_A \cdots H_B$ (0,0,−1)* 2·77 (6) Å, $H_A \cdots H_C$ 2·98 (4) Å, $H_A \cdots H_C$ (0,0,1)* 2·88 (6) Å and $H_A \cdots H_D$ (0,0,1)* 2·73 (9) Å. (The standard deviations are calculated with the formula given above.)

A Fourier difference map was calculated in the plane of the molecule. Even if it showed the expected pattern of positive electron density in the middle of every carbon–carbon bond arising from the valence electrons these peaks were less than three standard deviations above the background level.

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* Subcell edge translation of the second atom.

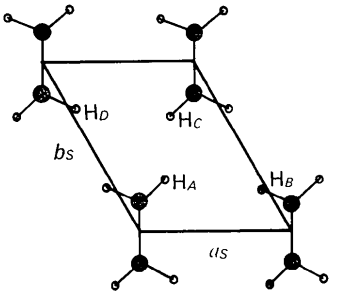

Fig. 5. The idealized subcell viewed down c_s.

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The Crystal Structure of Isostearic Acid

BY SIXTEN ABRAHAMSSON AND BRITT-MARIE LUNDÉN

Crystallography Group, Swedish Medical Research Council Unit for Molecular Structure Analysis, University of Göteborg, Fack, S-400 33 Göteborg 33, Sweden

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Crystals of isostearic acid, $C_{18}H_{36}O_2$, are triclinic ($P\bar{1}$) with $a = 4{\cdot}9356$, $b = 5{\cdot}6522$, $c = 34{\cdot}408$ Å, $\alpha = 95{\cdot}22$, $\beta = 95{\cdot}21$ and $\gamma = 103{\cdot}62°$. The molecules are, as is usual for long-chain fatty acids, held together by hydrogen bonds to dimers. The molecular packing is dominated by the space requirements of the methyl branches, which are accommodated between the ends of the carbon chains. The chain axes then become tilted 44° to the end group planes. The chain packing is of the common triclinic type $T_{\parallel}$.

The structures of branched-chain fatty acids have earlier been studied by this research group (Abrahamsson, 1959*a*; Abrahamsson & Harding, 1966). Two isoacids have so far been investigated by single-crystal methods. 17-Methyloctadecanoic acid (Abrahamsson, 1959*b*) had a superstructure of the carboxyl groups and was treated only in one projection. Isopalmitic acid was also studied only in projection (Stenhagen, Vand & Sim, 1952) and the reported structure is probably wrong as pointed out by Abrahamsson (1959*b*).