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.

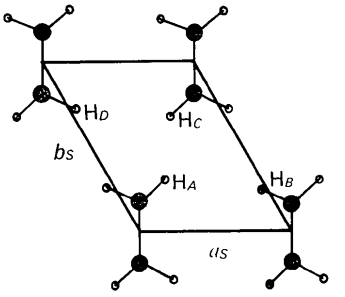

Fig. 5. The idealized subcell viewed down c_s.

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The Crystal Structure of Isostearic Acid

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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*).

It was, therefore, considered important to perform a three-dimensional single-crystal analysis of an ω-branched fatty acid.

Stenhagen, Vand & Sim (1952) reported that twinning was very common for isopalmitic acid crystals. We made several attempts to grow single crystals of isopalmitic acid but no suitable untwinned crystals for the X-ray work could be found. As isostearic acid gave good crystals and, judging from the cell dimensions, is structurally equivalent it was selected for the investigation.

Experimental

A sample of isostearic acid was kindly provided by Professor E. Stenhagen. Good crystals for the X-ray work were grown from hexane in a temperature-programmable thermostat. The crystals grow as thin plates and melt at 68·2 °C.

Crystal data

$C_{18}H_{36}O_2$ Isostearic acid (16-methylheptadecanoic acid)

Triclinic: $a = 4{\cdot}9356\ (29)$, $b = 5{\cdot}6522\ (45)$, $c = 34{\cdot}408\ (31)$ Å; $\alpha = 95{\cdot}22\ (4)$, $\beta = 95{\cdot}21\ (3)$, $\gamma = 103{\cdot}62\ (3)°$

$U =$ 922·7 Å^3

$Z =$ 2

$\varrho_c =$ 1·016 g.cm^{-3}

$\lambda =$ 1·54051 Å (Cu $K\alpha_1$)

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

H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC	H	K	L	FOBS	FCALC
4	-1	-2	197	260	2	-2	0	338	385	1	-2	27	487	709	0	2	-23	569	492	1	2	-8	2106	1977	2	0	13	937	809
4	-1	-1	220	435	2	-2	-2	702	796	1	-1	19	828	856	0	2	-21	637	674	1	2	-9	502	593	2	0	14	776	739
4	-1	0	660	689	2	-2	-4	691	750	1	-1	18	758	733	0	2	-13	331	390	1	2	-10	2068	1885	2	0	15	384	428
4	-1	1	294	529	2	-2	-5	465	497	1	-1	17	1596	1565	0	2	-11	519	558	1	2	-12	1683	1660	2	0	16	714	621
4	-2	1	323	297	2	-2	-6	687	720	1	-1	16	2467	2290	0	2	-10	422	413	1	2	-14	1261	1155	2	0	18	423	449
3	-4	0	1972	1905	2	-2	-7	931	983	1	-1	15	4711	4163	0	2	-9	1099	1152	1	2	-16	1005	1010	2	0	20	765	765
3	-4	2	584	767	2	-2	-8	2088	2234	1	-1	14	4625	4342	0	2	-8	831	840	1	2	-18	530	537	2	0	21	1790	1673
3	-3	13	298	323	2	-2	-9	3668	3565	1	-1	13	1049	914	0	2	-7	1171	1115	1	2	-23	533	568	2	0	23	2097	2048
3	-3	12	685	705	2	-2	-10	1428	1419	1	-1	12	2937	2764	0	2	-6	297	466	1	2	-24	269	422	2	1	16	248	339
3	-3	10	907	869	2	-2	-11	852	791	1	-1	10	2013	2088	0	2	-5	248	438	1	2	-25	2403	2366	2	1	14	209	250
3	-3	9	911	870	2	-2	-12	771	716	1	-1	9	745	698	0	2	-4	574	547	1	2	-26	664	876	2	1	12	378	404
3	-3	8	1117	1125	2	-2	-13	1036	920	1	-1	8	1128	1082	0	2	-2	440	438	1	2	-27	2279	2217	2	1	9	795	691
3	-3	7	603	648	2	-2	-14	624	603	1	-1	7	1161	1247	0	2	0	766	773	1	1	-16	496	502	2	1	6	376	416
3	-3	6	3147	3000	2	-2	-15	978	909	1	-1	6	265	300	0	2	2	1044	1030	1	1	-14	760	694	2	1	5	458	505
3	-3	5	410	397	2	-2	-16	456	491	1	-1	5	1738	1822	0	2	4	552	531	1	1	-13	3326	2882	2	1	4	433	507
3	-3	-12	793	727	2	-2	-17	552	595	1	-1	4	520	526	0	2	6	308	432	1	1	-12	2360	2133	2	1	3	616	619
3	-3	-14	1403	1237	2	-2	-18	385	388	1	-1	3	2034	2442	0	2	8	572	548	1	1	-11	3168	3008	2	1	2	1026	988
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3	-2	-6	993	966	2	-3	-21	341	418	1	-1	1	2339	2603	0	2	12	4649	4396	1	1	-7	903	980	2	1	0	1143	1141
3	-2	-4	745	633	2	-3	-19	384	410	1	-1	0	1423	1480	0	2	13	404	549	1	1	-5	837	1003	2	1	-1	586	590
3	-2	-2	565	546	2	-3	-18	388	469	1	-1	-1	2588	2699	0	2	15	835	784	1	1	-3	467	443	2	1	-2	1031	1111
3	-2	0	577	614	2	-3	-16	895	836	1	-1	-2	1066	1030	0	2	17	380	409	1	1	-2	509	586	2	1	-4	1136	1173
3	-2	2	667	682	2	-3	-15	1828	1693	1	-1	-3	4894	5092	0	2	18	323	376	1	1	0	925	926	2	1	-6	804	746
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3	-2	10	1082	1023	2	-3	-6	423	407	1	-1	-6	4498	4388	0	3	16	1209	1108	1	1	5	483	632	2	1	-11	5955	5397
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2	-1	3	730	720	1	-2	-12	2032	1951	0	1	8	779	877	1	3	0	1784	1913	2	0	-23	253	264	3	1	-9	692	645
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2	-1	5	552	587	1	-2	-10	1080	1175	0	1	6	13774	14567	1	3	5	995	781	2	0	-18	440	543	3	1	-7	716	739
2	-1	6	488	547	1	-2	-9	2040	1929	0	1	5	3952	4231	1	3	9	465	467	2	0	-17	2340	2437	3	1	-6	837	787
2	-1	7	872	922	1	-2	-8	985	921	0	1	4	2813	2771	1	2	16	405	471	2	0	-16	1029	1577	3	1	-4	231	348
2	-1	9	977	888	1	-2	-2	559	545	0	1	3	3619	3769	1	2	15	681	654	2	0	-15	613	571	3	1	8	259	438
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2	-1	22	237	295	1	-2	5	1534	1405	0	1	-9	2270	2338	1	2	6	591	648	2	0	-5	1123	1101	3	0	4	703	650
2	-1	23	1097	1063	1	-2	6	2674	2476	0	1	-10	163	227	1	2	5	701	749	2	0	-4	713	715	3	0	3	434	429
2	-1	25	812	760	1	-2	7	1501	1543	0	1	-11	2256	2149	1	2	4	834	858	2	0	-3	1162	1085	3	0	-2	469	490
2	-2	19	270	347	1	-2	8	3819	3593	0	1	-12	2275	2235	1	2	3	666	682	2	0	-2	520	527	3	0	-4	362	378
2	-2	17	488	465	1	-2	9	6734	5844	0	1	-14	4625	4185	1	2	2	944	966	2	0	-1	1011	965	3	0	-6	520	488
2	-2	12	1373	1231	1	-2	10	2452	2202	0	1	-15	1032	985	1	2	1	701	670	2	0	0	617	582	3	0	-8	356	355
2	-2	11	5589	5044	1	-2	11	866	868	0	1	-16	1618	1522	1	2	0	359	413	2	0	3	1275	1380	3	0	-7	345	420
2	-2	10	870	935	1	-2	12	398	556	0	1	-17	306	243	1	2	-1	353	340	2	0	4	268	354	3	0	-8	187	274
2	-2	9	2412	2263	1	-2	13	707	621	0	1	-18	675	685	1	2	-2	634	697	2	0	5	463	528	3	0	-9	474	477
2	-2	8	344	421	1	-2	15	629	665	0	1	-20	261	313	1	2	-3	599	610	2	0	7	1312	1391	3	0	-11	536	498
2	-2	7	1498	1442	1	-2	17	878	769	0	1	-27	297	264	1	2	-4	1013	952	2	0	9	1342	1279	3	0	-12	396	426
2	-2	5	1238	1259	1	-2	19	815	822	0	2	-28	2400	2379	1	2	-5	2193	1979	2	0	10	728	735	3	0	-14	1421	1538
2	-2	3	794	818	1	-2	21	448	527	0	2	-26	1910	1760	1	2	-6	3679	3361	2	0	11	1068	1045	3	0	-16	2998	2867
2	-2	1	546	536	1	-2	23	270	441	0	2	-24	479	495	1	2	-7	5771	5164	2	0	12	870	870	4	0	3	492	490

The space group was assumed to be $P\bar{1}$ which was confirmed by the structure analysis.

Reflexion data were collected on a Picker FACS I diffractometer using graphite-monochromated Cu $K\alpha$ radiation. The crystal used had the dimensions $0{\cdot}36\times0{\cdot}11\times0{\cdot}06$ mm. The $\theta/2\theta$ scanning mode was used with a scan speed of 1°/min. The background level was determined by 10 sec counts on each side of the reflexion. 1494 reflexions were measured with $2\theta\leq 85°$. 814 of these were considered unobserved ($I<2\sigma$).

The intensities were corrected for the Lorentz and polarization factors but not for absorption ($\mu=4{\cdot}92$ cm^{-1}) and extinction.

Structure refinement

The structure of 13-oxoisostearic acid had already been solved (Dahlén, 1972) when the reflexion data of isostearic acid were available. The cell dimensions of the oxo acid were very similar to those of isostearic acid, $a=4{\cdot}93$, $b=5{\cdot}62$, $c=34{\cdot}46$ Å, $\alpha=95{\cdot}65$, $\beta=94{\cdot}01$, $\gamma=103{\cdot}60°$. The two structures were therefore supposed to be isotypical, which was also supported by the Patterson analysis. The coordinates of corresponding atoms in the oxoacid were used in a structure-factor calculation which gave an R value of 0·32. Four rounds of block-diagonal least-squares refinement reduced R to 0·17. The hydrogen atoms (except that on the hydroxyl oxygen atom) were then included in the structure-factor calculation at their calculated positions after verification from a difference synthesis that the methyl groups had the normal staggered conformation. The refinement was continued using the full matrix and anisotropic thermal parameters for all non-hydrogen atoms. The hydrogen atoms were given isotropic temperature factors corresponding to those of the parent atoms. The B values were not varied.

Due to the relatively large number of parameters the hydrogen atoms and other atoms were refined separately in alternating cycles. After a few cycles a difference series was calculated in the plane of the carboxyl group. Positive density was found at the expected position of the hydroxyl hydrogen which was included in the following refinement. When the shifts for the non-hydrogen atoms were all less than $0{\cdot}25\sigma$ the refinement was terminated. The hydrogen parameter shifts were then less than $0{\cdot}60\sigma$. The final R value was 0·066.

The form factors used were those given in *International Tables for X-ray Crystallography* (1962) except for hydrogen where the values of Stewart, Davidson & Simpson (1965) were used. All calculations were performed on a Datasaab D21-PDP15 dual computer system with programs developed at this institute (Abrahamsson, Aleby, Larsson, Nilsson, Selin & Westerdahl, 1965). The weight assigned to each observation in the least-squares refinement was (Mills & Rollett, 1961)

$$w=1/\left(1+\left[\frac{|F_o|-0{\cdot}93\,.\,F_{\min}}{2{\cdot}17\,.\,F_{\min}}\right]^2\right).$$

Results

The final structure factors are given in Table 1 and the atomic parameters in Tables 2 and 3. The thermal ellipsoids are illustrated in Fig. 1.

Table 2. *Fractional atomic coordinates and hydrogen atom isotropic thermal parameters*

The estimated standard deviations are multiplied by 10^4 for C and O, and by 10^3 for H. For the hydrogen atoms the first appended number refers to that of the parent atom.

	x	y	z	B
O(1)	0·8785 (21)	0·7467 (18)	0·0224 (3)	
O(2)	1·3054 (19)	0·9873 (17)	0·0304 (2)	
C(1)	1·1181 (33)	0·7942 (29)	0·0381 (4)	
C(2)	1·2231 (23)	0·6560 (22)	0·0676 (3)	
C(3)	1·0018 (21)	0·4663 (20)	0·0822 (3)	
C(4)	1·1350 (21)	0·3519 (20)	0·1148 (3)	
C(5)	0·9217 (22)	0·1605 (21)	0·1321 (3)	
C(6)	1·0507 (20)	0·0440 (19)	0·1654 (3)	
C(7)	0·8402 (19)	−0·1453 (19)	0·1826 (3)	
C(8)	0·9759 (22)	−0·2574 (20)	0·2162 (3)	
C(9)	0·7722 (21)	−0·4441 (21)	0·2350 (3)	
C(10)	0·9087 (20)	−0·5518 (21)	0·2676 (3)	
C(11)	0·7061 (21)	−0·7436 (19)	0·2866 (3)	
C(12)	0·8426 (23)	−0·8485 (21)	0·3199 (3)	
C(13)	0·6360 (23)	−1·0395 (20)	0·3382 (3)	
C(14)	0·7835 (21)	−1·1401 (20)	0·3715 (3)	
C(15)	0·5832 (20)	−1·3220 (20)	0·3906 (3)	
C(16)	0·7154 (25)	−1·4377 (23)	0·4228 (4)	
C(17)	0·5094 (25)	−1·6387 (23)	0·4383 (4)	
C(18)	0·8600 (29)	−1·2468 (27)	0·4580 (4)	
H(21)	1·376 (19)	0·590 (17)	0·056 (3)	6·5
H(22)	1·357 (16)	0·728 (16)	0·085 (2)	6·5
H(31)	0·883 (20)	0·577 (18)	0·092 (3)	4·9
H(32)	0·872 (17)	0·312 (16)	0·053 (3)	4·9
H(41)	1·284 (16)	0·257 (15)	0·105 (2)	5·2
H(42)	1·248 (16)	0·485 (15)	0·138 (2)	5·2
H(51)	0·773 (17)	0·251 (16)	0·138 (2)	5·7
H(52)	0·856 (15)	0·031 (15)	0·116 (2)	5·7
H(61)	1·208 (16)	−0·040 (15)	0·155 (2)	4·9
H(62)	1·141 (16)	0·177 (16)	0·189 (2)	4·9
H(71)	0·681 (17)	−0·056 (16)	0·199 (2)	4·7
H(72)	0·709 (16)	−0·319 (16)	0·164 (2)	4·7
H(81)	1·122 (14)	−0·330 (14)	0·207 (2)	5·5
H(82)	1·068 (16)	−0·122 (15)	0·236 (2)	5·5
H(91)	0·621 (16)	−0·360 (14)	0·245 (2)	5·0
H(92)	0·680 (17)	−0·572 (17)	0·215 (2)	5·0
H(101)	1·062 (18)	−0·627 (15)	0·257 (2)	5·3
H(102)	1·003 (16)	−0·414 (15)	0·293 (2)	5·3
H(111)	0·537 (16)	−0·682 (16)	0·296 (2)	5·5
H(112)	0·586 (16)	−0·879 (14)	0·268 (2)	5·5
H(121)	0·986 (16)	−0·949 (15)	0·307 (2)	5·4
H(122)	0·956 (17)	−0·708 (16)	0·340 (2)	5·4
H(131)	0·402 (18)	−1·053 (16)	0·335 (2)	5·7
H(132)	0·455 (18)	−1·146 (17)	0·322 (3)	5·7
H(141)	0·975 (18)	−1·188 (16)	0·356 (3)	5·5
H(142)	0·903 (17)	−0·979 (16)	0·390 (3)	5·5
H(151)	0·396 (18)	−1·222 (17)	0·399 (3)	5·5
H(152)	0·457 (16)	−1·458 (15)	0·370 (2)	5·5
H(161)	0·888 (19)	−0·469 (17)	0·418 (3)	6·2
H(171)	0·375 (19)	−1·739 (17)	0·420 (3)	8·0
H(172)	0·359 (23)	−1·559 (21)	0·455 (3)	8·0
H(173)	0·596 (18)	−1·720 (16)	0·460 (3)	8·0
H(181)	0·718 (17)	−1·113 (15)	0·471 (2)	8·8
H(182)	0·994 (18)	−1·105 (17)	0·454 (2)	8·8
H(183)	0·937 (20)	−0·318 (18)	0·484 (3)	8·8
H(24)*	1·186 (20)	1·053 (20)	0·004 (4)	7·7

* Refers to the oxygen atom O(2).

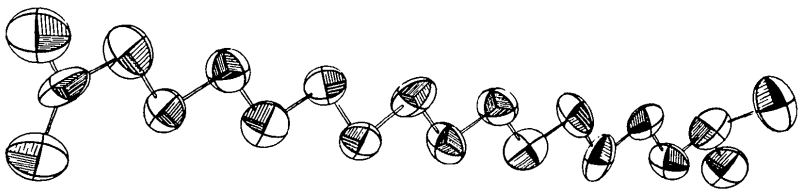

Fig. 1. Drawing of isostearic acid showing the thermal ellipsoids as viewed along the *b* axis.

Table 3. *Anisotropic thermal parameters in the form*
$\exp[-2\pi^2(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2klb^*c^*U_{23}+2lha^*c^*U_{31}+hka^*b^*U_{12})]$

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}
O(1)	757 (44)	1329 (63)	1057 (54)	608 (47)	51 (38)	272 (42)
O(2)	879 (50)	957 (60)	1087 (54)	485 (44)	73 (40)	151 (42)
C(1)	544 (64)	1110 (95)	733 (73)	271 (63)	283 (54)	141 (59)
C(2)	845 (73)	921 (91)	713 (72)	419 (62)	−28 (57)	399 (63)
C(3)	695 (63)	544 (72)	639 (63)	351 (50)	144 (48)	252 (52)
C(4)	651 (64)	625 (75)	710 (70)	215 (54)	118 (52)	93 (53)
C(5)	758 (68)	700 (78)	723 (69)	383 (55)	17 (53)	193 (56)
C(6)	630 (63)	643 (72)	600 (64)	291 (51)	73 (49)	108 (51)
C(7)	555 (59)	637 (72)	611 (62)	296 (52)	86 (47)	134 (51)
C(8)	649 (64)	722 (81)	738 (68)	351 (58)	133 (52)	183 (55)
C(9)	681 (66)	651 (70)	579 (60)	207 (50)	47 (49)	159 (53)
C(10)	671 (65)	831 (78)	572 (62)	191 (53)	12 (48)	295 (56)
C(11)	742 (70)	601 (76)	762 (69)	130 (56)	137 (55)	38 (57)
C(12)	823 (69)	817 (79)	488 (59)	195 (52)	−64 (49)	216 (58)
C(13)	1039 (77)	693 (78)	551 (63)	506 (53)	223 (54)	142 (58)
C(14)	727 (66)	672 (75)	716 (69)	519 (56)	114 (52)	−69 (54)
C(15)	733 (66)	756 (80)	636 (64)	353 (55)	−80 (50)	239 (57)
C(16)	932 (76)	647 (80)	811 (77)	223 (59)	198 (60)	78 (59)
C(17)	993 (87)	992 (99)	1043 (88)	573 (73)	138 (68)	249 (70)
C(18)	1534 (108)	1030 (104)	827 (84)	384 (74)	−188 (75)	86 (80)

Distances and angles are given in Fig. 2, where also the atomic numbering is indicated, and with standard deviations in Tables 3 and 4. The average C–C distance in the chain is 1·515 Å (σ=0·013 Å) and the average bond angle 113·3° (σ=0·69). They compare well with the values found in other long-chain structures. In 13-oxoisostearic acid (Dahlén, 1972) they are 1·512 Å and 113·9°. Though the hydrogen refinement proceeded normally in general, a few long distances involving hydrogen are found. As expected the hydroxyl hydrogen did not refine well and an O–H distance of 1·16 Å resulted. Excluding five long C–H distances, C(3)–H(32)=1·15, C(7)–H(71)=1·19, C(7)–H(72)=1·16, C(14)–H(141)=1·19, C(15)–H(151)=1·21 Å; an average C–H value of 1·01 is found.

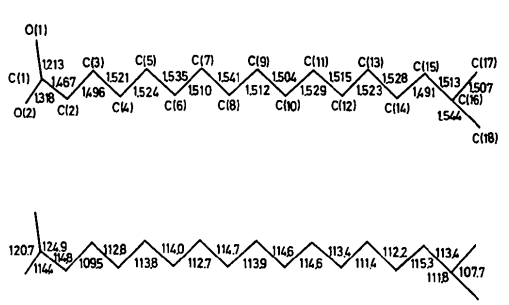

Fig. 2. Distances and angles of isostearic acid.

Table 4. *Bond distances and angles for the non-hydrogen atoms*

The estimated standard deviations for the distances are multiplied by 10^3, for the angles by 10.

C(1)—O(1)	1·213 (10) Å	O(1)—C(1)—O(2)	120·7 (9)°
C(1)—O(2)	1·318 (11)	O(1)—C(1)—C(2)	124·9 (8)
C(1)—C(2)	1·467 (14)	O(2)—C(1)—C(2)	114·4 (7)
C(2)—C(3)	1·496 (12)	C(1)—C(2)—C(3)	114·8 (7)
C(3)—C(4)	1·521 (13)	C(2)—C(3)—C(4)	109·5 (7)
C(4)—C(5)	1·524 (12)	C(3)—C(4)—C(5)	112·8 (7)
C(5)—C(6)	1·535 (13)	C(4)—C(5)—C(6)	113·8 (7)
C(6)—C(7)	1·510 (11)	C(5)—C(6)—C(7)	114·0 (7)
C(7)—C(8)	1·541 (13)	C(6)—C(7)—C(8)	112·7 (6)
C(8)—C(9)	1·512 (12)	C(7)—C(8)—C(9)	114·7 (7)
C(9)—C(10)	1·504 (13)	C(8)—C(9)—C(10)	113·9 (7)
C(10)–C(11)	1·529 (12)	C(9)—C(10)–C(11)	114·6 (7)
C(11)–C(12)	1·515 (13)	C(10)–C(11)–C(12)	114·6 (7)
C(12)–C(13)	1·523 (12)	C(11)–C(12)–C(13)	113·4 (7)
C(13)–C(14)	1·528 (13)	C(12)–C(13)–C(14)	111·4 (7)
C(14)–C(15)	1·491 (12)	C(13)–C(14)–C(15)	112·2 (7)
C(15)–C(16)	1·513 (14)	C(14)–C(15)–C(16)	115·3 (7)
C(16)–C(17)	1·507 (13)	C(15)–C(16)–C(17)	113·4 (8)
C(16)–C(18)	1·544 (13)	C(15)–C(16)–C(18)	111·8 (8)
		C(17)–C(16)–C(18)	107·7 (8)

The carbon chain is planar within 0·04 Å (Table 5). The zigzag plane forms an angle of 11·5° with the plane through the carboxyl group. This angle is 13° in 13-oxostearic acid. The molecules are held together to dimers over a centre of symmetry by hydrogen bonds. The O···O distance is 2·70 Å. The C–O···O angle is 115·7°. The two carboxyl groups of the dimer are coplanar with a maximum deviation from the plane of 0·007 Å. A detail of the polar group region is given in Fig. 3.

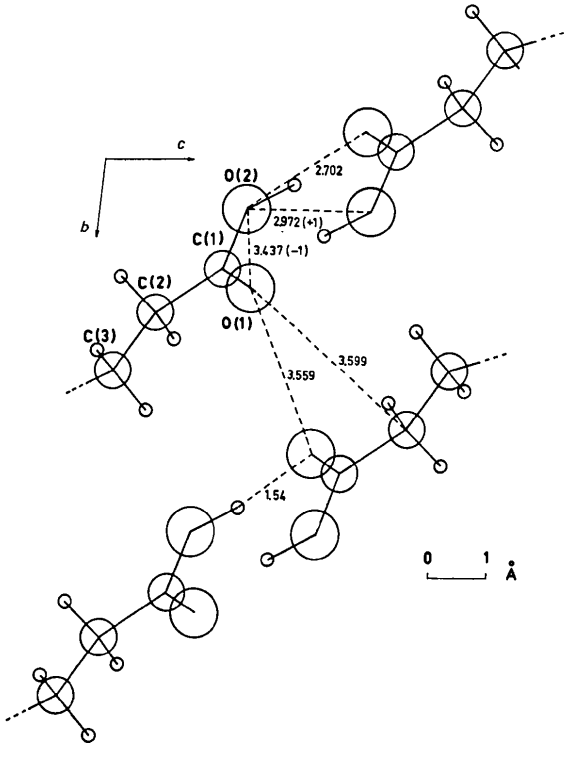

Fig. 3. Some packing contacts in the polar region of isostearic acid.

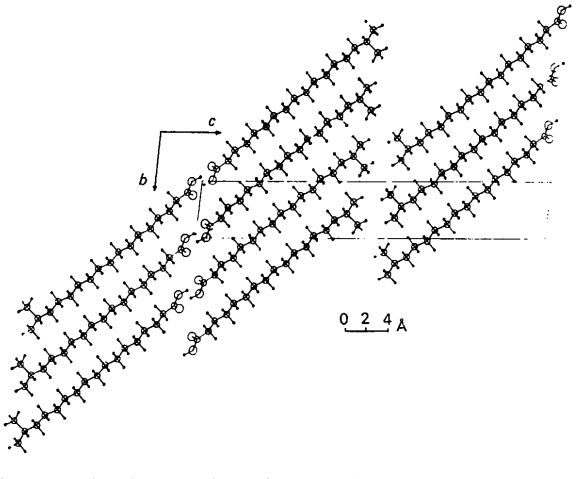

Fig. 4. Molecular packing of isostearic acid as seen along the *a* axis.

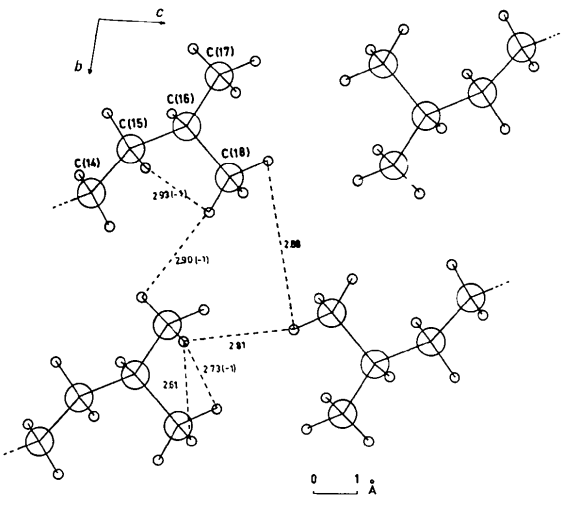

Fig. 5. Packing contacts in the methyl end-group planes.

Table 5. *Least-squares planes in the molecule*

The equations are expressed in terms of the crystal axes.

I $-0{\cdot}08664X+0{\cdot}18833Y+0{\cdot}97828Z-0{\cdot}07954=0$
II $0{\cdot}09146X-0{\cdot}13092Y-0{\cdot}98716Z+0{\cdot}03948=0$

	Deviations I		II
C(2)	0·055 Å	C(1)	0·007 Å
C(3)	0·025	O(1)	−0·006
C(4)	−0·014	O(2)	−0·004
C(5)	−0·008	C(11)	−0·006
C(6)	−0·037	O(11)	0·004
C(7)	−0·022	O(21)	0·005
C(8)	−0·042		
C(9)	−0·002		
C(10)	−0·025		
C(11)	−0·003		
C(12)	0·000		
C(13)	0·017		
C(14)	0·016		
C(15)	0·077		
C(16)	0·022		
C(17)	−0·061		
C(1)*	0·203		
C(18)*	1·244		

* Atoms not included in the plane calculation.

The packing of the dimers is shown in Fig. 4. The molecules have to slide along the chain axes relative to each other so that the methyl end of one chain just reaches the branch of another molecule. The branches are then accommodated between the methyl ends of the chains. This is one common way of accommodating the branch in monomethyl-substituted fatty acids (Abrahamsson, 1959*a*). The chain axes form an angle of 44° with the end-group planes. The corresponding value for 13-oxoisostearic acid is 44° and for isopalmitic acid (Stenhagen, Vand & Sim, 1952) 45°. In the latter structure the methyl group is reported to be accommodated *in* the chain packing which from the analysis of 13-oxoisostearic acid and the present work must be considered in error.

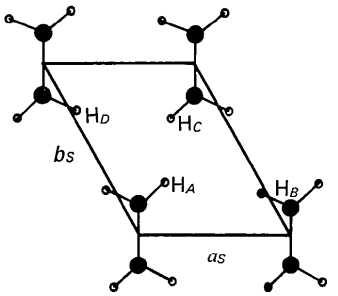

Fig. 6. Idealized triclinic subcell ($T\|\|$) of isostearic acid.

A packing detail of the methyl end group region is shown in Fig. 5. The H···H contacts agree very well with those in the oxo acid. The chains pack laterally in the common triclinic packing ($T\|\|$) Abrahamsson, 1959*a*). The subcell dimensions are

$a_s=4{\cdot}28$, $b_s=5{\cdot}37$, $c_s=2{\cdot}53$ Å,
$\alpha_s=72{\cdot}3$, $\beta_s=108{\cdot}8$, $\gamma_s=117{\cdot}2°$.

The corresponding dimensions for 13-oxoisostearic acid are

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

The closest subcell contacts to H_A are 2·89 Å to H_B and 2·72 Å to H_B translated one c_s distance, 2·94 Å to H_C and 2·70 Å to H_C translated one c_s and finally 2·72 Å to H_D (Fig. 6).

The carbon chain in isostearic acid is more regular than that of 13-oxoisostearic acid. Therefore, there are large regions in reciprocal space with very weak reflexions. Thus, only 45% of the measured reflexions of isostearic acid are more than two standard deviations above background whereas in 13-oxoisostearic acid, which has a bent chain and contains one more oxygen atom, the corresponding figure is 83%.

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The Crystal and Molecular Structure of Anhydrobromonitrocamphane

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Anhydrobromonitrocamphane crystals are orthorhombic, space group $P2_12_12_1$. The cell dimensions are $a=10{\cdot}364$, $b=9{\cdot}408$, $c=10{\cdot}499$ Å, $Z=4$. The crystals decompose quite rapidly when exposed to the atmosphere and X-rays. This results in a falling off of intensity with time. A method for correcting the intensity data for the above mentioned effects has been developed and used in the present study. The crystal structure has been solved using the heavy-atom method. The structure is highly disordered so that each type of site is statistically occupied by two optically isomeric forms of the molecule in two orientations. The disorder gives rise to an approximate (100) mirror. The bromine atom and one carbon atom lie on this pseudomirror, while the nitrogen atom and all other carbon atoms are distributed over two positions and the other oxygen atom over four positions. Some atomic positions were very close to their disordered counterparts and could not be refined by routine least-squares analysis. The final refinement was therefore done by the difference Fourier method. The final R value was 0·097. Bond lengths and angles in both orientations of the molecule are normal.

Introduction

The sulphuric acid transformation of bromonitrocamphane to anhydrobromonitrocamphane has been considered very unusual and fascinating (Goto, Hirata & Stout, 1968; Ranganathan, 1967). The proposed reaction mechanism is also very uncommon as it involves the initial loss of the nitro group and its subsequent