The Crystal and Molecular Structure of DL-3-Bromo-octadecanoic acid

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The crystal structure of DL-3-bromo-octadecanoic acid, $C_{18}H_{35}O_2Br$, has been determined from threedimensional X-ray diffraction data. The crystals are triclinic, with a = 5.68, b = 5.63, c = 32.8 Å; $\alpha = 101.8^{\circ}$, $\beta = 93.1^{\circ}$, $\gamma = 97.9^{\circ}$; space group *P*I. Positional and anisotropic thermal parameters have been refined by least-squares methods; the final *R* index is 8.5%.

The hydrocarbon chain is bent at C(3) to accommodate the bromine atom; the carbon chain from C(4) to C(18) is planar and regular; the packing of neighbouring chains is of the triclinic type observed in many other long-chain compounds; the carboxyl groups are joined in pairs, by hydrogen bonds, across centres of symmetry.

Introduction

We have earlier studied the effect on the molecular packing of a branching methyl group in different positions along a hydrocarbon chain (Abrahamsson, 1959a). A methyl group is either accommodated in the structure between the ends of straight chains or at the apices of V-shaped chains. In the series of racemic methyloctadecanoic acids all acids except DL-3-methyloctadecanoic acid were shown to belong to two main structure types. In order to determine the structure of the β -branched acid we have investigated DL-3-bromooctadecanoic acid. Compounds with a bromine atom substituted in place of a methyl group are often isotypical with the corresponding unsubstituted ones. This substitution technique is now used systematically in our lipid work to facilitate structure determinations.

The preliminary X-ray work on DL-3-bromo-octadecanoic acid showed, however, that the acid was not isotypical with the corresponding methyl branched acid but isostructural with DL-2-methyloctadecanoic acid (Abrahamsson, 1959b). As the latter acid was studied in projection only, we have carried out this analysis to determine the molecular conformation and packing in detail.

Experimental

DL-3-bromo-octadecanoic acid, $CH_3 \cdot [CH_2]_{14} \cdot CHBr \cdot CH_2 \cdot COOH$, was synthesized by Dr I. Pascher from gas-chromatographically pure stearic acid. The final product has a melting point of 53.7-53.8 °C. Crystallization from light petroleum gave lath-shaped crystals suitable for X-ray work.

The crystals are triclinic; rotation and Weissenberg photographs, taken with Cu K α radiation ($\lambda = 1.542$ Å) gave

$a = 5.68 \pm 0.03$ Å	$\alpha = 101 \cdot 8^{\circ}$
$b = 5.63 \pm 0.03$	$\beta = 93 \cdot 1$
$c = 32.80 \pm 0.2$	y = 97.9

The space group PI was assumed, and no indications of non-centrosymmetry have been observed. There are two molecules per unit cell. A subcell was evident from the distribution of intensities; the subcell parameters

$$a_s = 4.27$$
 Å
 $a_s = 80.4^{\circ}$
 $b_s = 5.29$
 $\beta_s = 105.9$
 $c_s = 2.55$
 $\gamma_s = 119.5$

have been calculated from the final atomic positions.

h0l to h2l and 0kl to 3kl intensities were estimated visually, and corrected for Lorentz and polarization effects, but not for absorption or spot shape effects. 1486 independent reflexions were recorded; the minimum plane spacing was 1.1 Å, and within this limit another 200 reflexions were too weak to be observed.

Determination and refinement of the structure

The bromine position was determined from sharpened (100) and (010) Patterson projections; most of the carbon and oxygen atom positions were found by superposition of these sharpened Patterson projections, and the remainder from electron-density projections. These parameters were first refined by two three-dimensional difference syntheses; in each of the structure factor calculations the coordinates of the carbon atoms C(4) to C(18) were constrained to be those of a planar, regular chain - deviations suggested by the difference syntheses were ignored. Hydrogen atom peaks appeared at all of the expected positions in the second difference synthesis. Eight cycles of block-diagonal leastsquares refinement were carried out, initially treating all atoms as isotropic. In the third and subsequent cycles hydrogen atoms at the stereochemically expected positions on C(2) to C(15), and on O(1) were included in F_c . Anisotropic vibration parameters were introduced for bromine at the fifth cycle, and for carbon and oxygen atoms at the seventh cycle. Reflexions with F < 30were given weight 1, and the others weight $(F/30)^2$ in

Table 1. Observed and calculated structure factors

A line is either hk or $l F_0 F_c$; F_0 and F_c are 5 times the absolute values for one unit cell.

	n	0	-26	65	64	-14	77	-71	-18	106	115	18	29	-20	-1	187	-167
3	29	62	-25	55	53	-11	56	66 247	-17	99 66	104	19	21 81	15 73	0	245 108	-251
4	226	-184	-23	34	-31	-9	74	85	-15	9	14	21	53	50	2	15	-20
6	263	-234	-22	80	-82	-7	49	-50	-14	60 84	-59	22	46	-24	3	184	265
8	19	19	-20	143	-144	-5	111 .	-122	-11	41	-40	24	63	-55	5	358	334
9	161	159	-19	125	-115	-4	106 -	-108	-10	10 88	88	25	94	-82	7	217	192
11	159	150	-17	53	44	-1	63	82	- 8	119	125	27	69	-63	8	84	67
12	59	58	-16	130	132	0	74	95 75	-7	139	139	28 33	29 41	-25	10	102	-106
13	31 91	-102	-14	31	40	4	69	-70	-5	35	-20				11	121	-119
15	109	-126	-13	25	-28	5	72	-80	-4	162	-155	-20	1 58	-72	12	21	-19
10	81 41	- 43	-12	125	-143	10	74	80	-2	212	-210	-28	84	-107	14	60	60
18	50	41	-10	152	-167	11	102	127	-1	78	-79	-24	60	63	15	63	64
19	72	79	-9	69	≈68	15	53	-75	Q	41	41	-23	63	67	16	124	125
20	117	128	- 8	9	6	16	58	-69	1	257	217	-22	60	69	17	208	207
21	223	256	-7	134	142	17	43	-51	23	294 391	399	-20	118	-124	19	145	-136
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26	29	-37	-4	97 150	99 -162	-7	112 .	-132 82	5	252	223	-16	118	-130	22	25	-19
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-23	74	56	9	121	-127	-13	63	63	17	125	-125	-6	504	450	-32	10	~10
-22	66	52	10	140	-151	-12	56 55	63 -58	18	131 109	-125	-5	313 226	301 199	-31 -30	10	23
-20	24	-34	11	63	-133	-8	81	-85	20	31	-19	- 3	335	349	-29	35	38
-18	161	-156	14	83	84	-7	88	-82	21	24	30	-2	158	177	-25	41 31	46
-17	78	-/0	15	109	110	-4	52	64	23	97	95	ō	117	- 92	-25	34	- 33
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-12	202	209	20	38	-45	ş	180	-190	27	27	-26	4	255	-230	-20	43 84	4 <u>1</u> 85
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-5	133	-147	31	24	-25	14	47	-61	34	59	29	11	130	-115	-13	145	-147
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13	229	-217	- 7	164	187	2	80	-78	-14	86	-80	-30	27	-50	07	139	-134
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-31	49	-40	-20	60	64	-23	28	-28	14	71	-72	-0	389	366	-26	56	-69
-29	19	-17	-19	43	45	-21	15	4	15	180	-167	- 4	816	806	-25	78	-70
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Table 1 (cont.)

-17	69 -5/	-21 55 59	22 86 -72	5 201 -187	3 108 101	3 -1
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-9	44 46	-15 108 -109	28 94 84	14 52 54	12 74 40	-20 74 -90
-7	102 -92	-14 105 -99	29 59 50	15 28 -28	14 65 70	-19 56 -60
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U	173 150	-7 74 -68	-25 35 44	21 50 55	-10 99 92	-13 16 14
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11	52 46	4 229 -211	-12 96 -101	-29 27 33	5 124 -128	-2 66 -64
15	49 -43	5 146 -130	-11 117 -136	-28 15 13	6 91 -95	-1 195 -200
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-17	133 -118	9 134 118	-7 53 58	-20 63 54	10 153 139	3 66 60
-15	55 6/	10 180 167	-6 112 115	-19 29 31	11 122 106	4 161 166
-14	93 90	11 145 131	-5 192 193			5 180 194
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-9	47 -50	1> 150 -153	-1 171 -187	-14 69 -64	-29 28 -24	9 80 -73
- 8	90 -80	16 112 -126	0 243 -247	-12 75 77	-28 34 -26	10 100 -102
- 4	14 - 14 14 64	1/ 80 -84 19 41 5n	1 198 -18/ 2 130 -108	-11 145 156 -10 147 145	-2/ 29 -24	11 117 -125 12 50 -45
- 3	90 91	20 88 106	4 117 120	-9 236 217	-25 15 10	14 71 67
-2	88 91	21 90 107	5 142 135	-8 229 207	-24 24 20	15 83 80
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5	38 45	28 19 26	10 119 -121	-2 71 63	-18 63 -76	20 152 -174
6	77 75	29 27 29	11 171 -180	-1 142 127	-17 56 -61	21 55 -60
	103 87	30 38 45	12 47 -53	0 155 146	-16 21 -21	22 13 4
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-14	96 85	2 -1	17 58 63	5 96 -96	-12 93 87	26 65 63
		-34 21 21	18 35 24	6 83 -69	-11 38 43	27 49 38
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-6	78 77	-20 38 37	21 65 -78	11 102 102	-8 158 -170	-21 55 58
-5	100 107	-24 58 55	22 50 -61	12 125 128	-7 143 -150	-20 96 112
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-/	146 153	-6 /5 -/9	-19 74 74	-4 97 89	10 12 -24	-2 117 -117
-4	136 -122	-4 150 134	-17 162 101	-2 88 82	12 155 -156	0 58 50
- 3	168 -156	-3 230 231	-16 53 49	1 87 -80	13 170 -181	1 153 155
-2	215 -209	-2 193 199	-14 94 -8/	2 109 -103	14 109 -122	2 46 66
-1	161 -159	-1 168 175	-13 94 -111	3 97 -96	15 63 -65	3 91 103
ĩ	/8 7u	2 198 -183	-11 156 -155		17 235 258	6 31 -38
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-27	25 - 29	10 49 53	3 263 253	-6 80 39	32 25 -22	23 47 57
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Table 1 (cont.)

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-17	145	-141	-6	71	70	-3	137	-136	-14	43	41	-9	46	45	-1	25	-24
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the refinement. The atomic scattering factors given in *International Tables for X-ray Crystallography* (1962), p. 202, were used for carbon, oxygen and hydrogen atoms; the bromine scattering factor on p. 211 (from a Thomas–Fermi–Dirac statistical wave function) was used, corrected for anomalous dispersion(p. 214). The final R index, for observed reflexions only, was 0.085. No shift in the last two cycles was greater than half the appropriate estimated standard deviation.

Observed and calculated structure factors are given in Table 1, positional and thermal parameters in Table 2, and bond lengths and angles in Table 3. The positional standard deviations were estimated from the reciprocals of the diagonal elements of the last least-squares matrix, and will therefore be slightly underestimated. The estimated standard deviations in bond lengths take account of the possible errors in cell dimensions, as well as the above positional errors (the former are only important in the C–Br bond).

Discussion of the structure

Hydrocarbon chain configuration

The mean C-C bond length is 1.526 Å and the mean C-C-C angle 113°. The conformation around the bond C(3)-C(4) is such that bromine is approximately *trans* to C(5) (so occupying the position that C(2) would have occupied in the absence of a branch); the dihedral angle Br-C(3)-C(4)-C(5) is 172°. The mean plane of the atoms C(4) to C(18) in terms of the orthogonal coordinates of Table 2(a) is

$$0.7013X + 0.2157Y - 0.6794Z - 0.652 = 0$$
.

Table 2(a). Fractional coordinates, x, y, z, and orthogonal coordinates, X, Y, Z, of atoms other than hydrogen, and their estimated standard deviations

The orthogonal coordinates refer to axes with X parallel to a^* , and Z parallel to c. σ is $\sigma(X)$ or $\sigma(X)$ or $\sigma(Z)$, which are equal.

	x	у	Ζ	X (Å)	Y (Å)	Z (Å)	σ (Å)
Br	0.2552	1.2491	0.09687	1.431	6.207	2.989	0.0015
O(1)	0.288	0.675	-0.0047	1.615	3.621	-0.588	0.008
O(2)	0.074	0.638	0.0486	0.414	3.222	1.525	0.008
C(1)	0.259	0.713	0.0359	1.452	3.583	1.029	0.012
C(2)	0.479	0.846	0.0626	2.686	3.988	1.782	0.012
C(3)	0.423	0.972	0.1054	2.370	4.453	3.184	0.011
C(4)	0.631	1.071	0.1368	3.537	4.642	4.093	0.011
C(5)	0.748	0.857	0.1491	4.191	3.261	4.431	0.013
C(6)	0.936	0·947	0.1862	5.248	3.371	5.535	0.012
C(7)	1.049	0.740	0.1974	5.878	2.042	5.839	0.011
C(8)	1.242	0.819	0.2341	6.960	2.094	6.926	0.012
C(9)	1.368	0.615	0.2442	7.668	0.774	7.189	0.012
C(10)	1.552	0.700	0.2812	8.697	0.861	8.292	0.012
C(11)	1.672	0.491	0.2910	9.374	-0.475	8.547	0.013
C(12)	1.861	0.567	0.3280	10.432	-0.440	9.646	0.013
C(13)	1.983	0.358	0.3382	11.116	-1.782	9.915	0.013
C(14)	2.170	0.437	0.3756	12.164	-1.734	11.028	0.014
C(15)	2.293	0.228	0.3860	12.853	- 3.081	11.305	0.012
C(16)	2.473	0.311	0.4239	13.864	-3.001	12.434	0.016
C(17)	2.594	0.094	0.4321	14.540	-4.381	12.642	0.017
C(18)	2.775	0.167	0.4694	15.554	-4.357	13.752	0.021

lable	2(0). An	isotropi	c therm	al vibr	ation par	ameters
ex	The term $(-b_{11}h^2)$	mperatur $^2 - b_{22}k^2$	re factor $-b_{33}l^2 -$	of each $b_{23}kl - b_{23}kl$	atom is b ₃₁ lh – b ₁₂	2hk)
1	$0_4 \times b_{11}$	b_{22}	b33	b23	b31	b_{12}
Br	401	379	17.7	41	-2	246
O(1)	498	546	10.4	11	-4	-30
0(2)	350	425	11./	15	-1	- 80
C(1)	423	342	12.2	22	1	170
C(2)	425	479	10.1	37	-21	118
C(3)	257	346	13.3	6	-16	161
C(4)	309	166	16.5	15	-26	79
C(5)	341	563	15.3	- 8	- 29	80
C(6)	415	349	14.5	33	-4	490
C(7)	291	401	11.5	23	- 39	- 184
C(8)	353	403	13.2	30	-12	114
C(9)	435	422	12.6	25	- 24	339
C(10)	478	357	17.5	46	-22	659
C(11)	362	637	13.6	-7	- 38	-118
C(12)	407	480	14.6	26	- 5	234
C(13)	468	458	12.5	22	-32	192
C(14)	435	616	17.3	53	-4	178
C(15)	502	539	16.7	42	- 34	437
C(16)	606	795	17.8	53	- 64	369
C(17)	817	867	21.6	85	- 101	522
C(18)	844	1314	26.5	96	- 99	502

• 1

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C(3) and Br are very significantly displaced from this plane, by 0.19 and 0.34 Å as shown in Fig. 1; C(4) and C(7) are displaced by small amounts which may just be significant.

There is a suggestion that, within its plane, the hydrocarbon chain is slightly curved. The odd carbon atoms deviate from collinearity by amounts just greater than three standard deviations, and in a systematic way; so do the even carbon atoms. This can be seen in their distances from the mean axis of the chain:

Carbon		Carbon	
atom no.	Distance	atom no.	Distance
3	-0.53 Å	4	0.35 Å
5	-0.49	6	0.39
7	-0.43	8	0.39
9	-0.42	10	0.43
11	-0.41	12	0.41
13	-0.43	14	0.40
15	-0.44	16	0.42
17	-0.48	18	0.32

Table 3. Bond lengths and angles

Bond		Angle	
C(3)–Br	2·00 Å	Br-C(3)-C(2)	106°
C(1) - O(1)	1.33	Br-C(3)-C(4)	108
C(1) - O(2)	1.21	O(1) - C(1) - O(2)	122
C(1) - C(2)	1.50	O(1) - C(1) - C(2)	113
C(2) - C(3)	1.51	O(2) - C(1) - C(2)	126
C(3) - C(4)	1.49	C(1) - C(2) - C(3)	112
C(4) - C(5)	1.56	C(2) - C(3) - C(4)	116
C(5) - C(6)	1.53	C(3) - C(4) - C(5)	110
C(6) - C(7)	1.50	C(4) - C(5) - C(6)	112
C(7) - C(8)	1.53	C(5) - C(6) - C(7)	112
C(8) - C(9)	1.52	C(6) - C(7) - C(8)	114
C(9) - C(10)	1.51	C(7) - C(8) - C(9)	115
C(10) - C(11)	1.52	C(8) - C(9) - C(10)	113
C(11) - C(12)	1.53	C(9) - C(10) - C(11)	112
C(12) - C(13)	1.53	C(10) - C(11) - C(12)	114
C(13) - C(14)	1.53	C(11) - C(12) - C(13)	115
C(14) - C(15)	1.54	C(12) - C(13) - C(14)	114
C(15) - C(16)	1.52	C(13) - C(14) - C(15)	114
C(16) - C(17)	1.54	C(14)-C(15)-V(16)	113
C(17) - C(18)	1.50	C(15)-C(16)-C(17)	110
$O(1)-H \cdots O($	2) 2.66	C(16) - C(17) - C(18)	112

Estimated standard deviations.

In bond lengths:

C-Br 0.014 Å

C–O 0.014

C-C	0.018
	0.021

0.028In bond angles 1° to 1.5° . between C(1) and C(12), rising to at C(15) and C(15)

Carboxyl group

The dimensions of the carboxyl group are in accord with those in other saturated fatty acids, for example with those collected by Higgs & Sass (1963). The mean plane of the atoms C(1), C(2), O(1), and O(2) is (in orthogonal coordinates)

-0.3186X + 0.9479Y - 0.0029Z - 2.922 = 0,

and none of these atoms is significantly displaced from the plane. The carboxyl group related by the symmetry centre at $0\frac{1}{2}0$ is joined to this one by two hydrogen bonds of length 2.66 Å. The two carboxyl groups are not coplanar, but are in planes 0.49 Å apart; Such a displacement of the planes is common in solid fatty acids and has been commented on by Jeffrey & Sax (1963).





Fig. 3. The mean square amplitudes of vibration of atoms (a) perpendicular to the plane of the carbon chain, (b) in the plane of the chain and perpendicular to the chain axis, (c) parallel to the chain axis.



Fig. 2. (100) projection showing the packing of the molecules. (b' and c' are the projections of b and c.)

Packing arrangement

Fig. 2 shows the packing of the molecules in the lattice. The straight portions of the hydrocarbon chains are arranged in the triclinic form found in many other long chain compounds. The dimensions of the triclinic subcell $(T \parallel)$ are given in the experimental section; they are close to those observed by Lomer (1963) in lauric acid.

There are two short intermolecular distances:

Br \cdots C(1) at 010 + xyz	3∙60 Å
Br \cdots O(2) at $010 \times xyz$	3.21

No others (except those between carboxyl groups) are less than 3.8 Å.

The angle of tilt of the chain axes to the end group planes is 36° as compared to 46° in DL-2-methylocta-decanoic acid.

Thermal vibrations

The anisotropic thermal parameters, b_{ij} , were converted to mean square amplitudes of vibration in the directions of the principal axes of the hydrocarbon chain [C(4)–C(18) portion], and these are shown in Fig. 3. Although the estimated standard deviations of the b_{ij} parameters suggest that variations between neighbouring atoms are not significant, the general pattern is physically sensible. The perpendicular vibrations [Fig. 3(a)] increase considerably towards the C(18) end of the chain; the increase is particularly marked

from about C(14) onwards, *i.e.* for that part of the chain which is not flanked on all sides by other chains (see Fig.2). The transverse vibrations [Fig.3(b)] also increase towards the C(18) end, while the longitudinal vibrations [Fig.3(c)] do not.

The initial calculations were done on the Saab D21 computer of the Institute of Medical Biochemistry, University of Göteborg. The remainder were done on the Atlas Computers at Manchester University and at the National Institute for Research in Nuclear Science in England. We are grateful to all these establishments and to the Edinburgh University Computer Unit for their cooperation, to Dr R.Diamand for his leastsquares refinement program, and to Dr L. Hodgson for a bond-length and angle program. We also thank Mrs M.Innes, Mr U.Lövås and Mr A. Westerdahl for technical assistance. Financial support has been obtained from the Swedish Natural Science and Swedish Medical Research Councils.

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An Experimental Determination of $\Delta f''$ for Iodine

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The imaginary component of the anomalous contribution to the scattering factor $(\Delta f'')$ of iodine for Cu K α radiation has been determined with the intensity data from the structure analysis of methyl melaleucate iodoacetate by Hall & Maslen (1965). The reliability of the calculation is shown to depend critically on the weighting of all terms, but particularly on those where the Bijvoet inequality is immeasurably small. A method for deriving the correct weighting scheme from an assessment of the errors is developed.

The results obtained are in reasonable agreement with those from theoretical calculations. The angular dependence of the $\Delta f''$ curve corresponds closely to that predicted. There is a small discrepancy in scale, but this may have resulted from an error in the experimental value.

Introduction

In recent years several experimental determinations of the anomalous dispersion corrections to the atomic scattering factors have been carried out. These were necessary both to confirm the theoretical values and to investigate the dependence of $\Delta f''$ on the presence of more than one anomalous scatterer in the unit cell. In general the experimental zero Bragg angle values are in good agreement with values calculated by James (1954) from the wave mechanical theory of Hönl (1933) and by Dauben & Templeton (1955) and Cooper (1963) from the work of Parratt & Hempstead (1954) and Eisenlohr & Muller (1954). Recently the corrections at zero Bragg angle have been re-evaluated with the

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