the D the methylene-group sites (Calvert, Shapley, Schultz, Williams, Suib & Stucky, 1978). The proton occupancies for D-QNA given in Table 11 are in accord with the observations cited above, and with simple energy considerations, which imply that the D atoms should prefer the sites with deepest potential wells. It is tempting to speculate that the slightly more equal distribution of protons at 298 K compared to that at the lower temperatures may be due to an entropy contribution. A similar tendency toward more equal H:D ratios at higher temperatures was observed in yttrium oxalate trihydrate where the sensitivity was enhanced owing to the use of an overall D fraction of 0·5. However, in the present study this temperature-dependent effect lies at the 1σ level and is of marginal significance.

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4-Octadecynoic Acid, a Largely Regular Structure in Space Group P1̄

By FRODE MO

Institutt for røntgenteknikk, Universitetet i Trondheim-NTH, N-7034 Trondheim-NTH, Norway

Abstract

$C_{18}H_{32}O_2$ is triclinic (P1̄) with $a = 8\cdot71$ (2), $b = 5\cdot475$ (10), $c = 45\cdot13$ (7) Å; $\alpha = 92\cdot55$ (15), $\beta = 93\cdot15$ (15), $\gamma = 123\cdot95$ (25)°, $Z = 4$. The structure which has some OD character was solved in two discrete steps by direct and Patterson methods. Full-matrix least-squares refinement based on 1155 F_o from visually estimated film intensities was terminated at $R = 0\cdot071$. In the ordered structure, neighbouring

carboxyl groups including the C^α atoms differ in relative orientation by about 82°. Atoms of both triple-bond fragments are displaced from the plane of the main chain, probably largely because of the packing requirements of one of the carboxyl groups. The zigzag chains are tilted 20° away from the perpendicular to the methyl end-group planes, and pack laterally according to a triclinic subcell. Molecules are linked together mainly as H-bonded dimers. The presence of stacking faults and possible disorder in one of the carboxyl groups suggests local alternative H-bond arrangements which would further stabilize the crystal structure.

Introduction

Long-chain fatty acids are constituents of lipids which serve important functions in a wide range of biological and technical systems. Presumably, the structures and functions of lipids and ordered aggregates of lipids such as are found in membranes of living organisms are closely related to the molecular properties of their components. X-ray diffraction studies of crystalline long-chain fatty acids therefore constitute one important source of information on these systems. Knowledge of fatty acid structures at the atomic level is also needed for the interpretation of other types of molecular experiments, e.g. studies of fatty acid monolayers in aqueous media which relate to the interfacial properties of complex lipids (Gaines, 1966).

Some 25–30 saturated normal and branched-chain fatty acids including members containing various substituents and functional groups have been investigated by single-crystal X-ray methods (von Sydow, 1956a; Abrahamsson, 1959a; Abrahamsson, Dahlén, Löfgren & Pascher, 1978). Data for unsaturated members are scarce by comparison. The analyses of the low-melting form of cis-9-octadecenoic (oleic) acid (Abrahamsson & Ryderstedt-Nahringbauer, 1962) and 4-octadecynoic acid, reported here, appear to be the only studies of fatty acids containing a double or triple bond.

The structure of 4-octadecynoic acid is an example of a more general type of crystallographic problem caused by the fact that part of the molecule conforms to a simple, repeating motif while the remainder does not; in 4-octadecynoic acid the non-regular fraction is about $\frac{1}{3}$ of the molecule. In cases like this, particular problems often arise in the course of structure solution and refinement requiring modifications of standard crystallographic techniques. Some details on the determination of this structure are given.

Experimental

Crystals of the acid were soft, thin plates with the longest dimension along a, the large face being (001). Faces (010) were also well developed. Crystal data are given in Table 1.

Two different crystals were used for data collection by the multiple-film equi-inclination Weissenberg technique. Intensities of layers $0kl$ to $6kl$ (set I) were recorded with crystal (I) rotating about a; crystal (II) was used for recording layers $h0l$ to $h3l$ (set II) about b. Intensities were estimated visually by comparison with a standard set of intensity spots; appropriate angular corrections (Grenville-Wells, 1955) of the normal-beam film factors were applied for the non-zero layers. Data reduction to structure factors included corrections for Lorentz and polarization factors but not for absorption. Interlayer scale factors obtained by least squares were used to bring all F's, 885 in set (I) and 783 in set (II), on to a common scale. 506 reflexions measured in both sets were averaged to give a final set of 1162 independent values of F. The discrepancy index for the averaged data, $D_F = \sum ||F_I| - |F_{II}||/\sum |F_{av}|$, was 0·040. About 90% of the intensities measured above background had $2\theta < 90°$; only 3% had $2\theta > 120°$.

Reflexions with h odd were generally weak, and diffuse tails between maxima in reciprocal space indicated partial disorder with period $a/2$ in the chain stacking (Dornberger-Schiff, 1966). Similar stacking faults have also been observed in other long-chain structures (Jensen, 1956; Lewis & Lomer, 1969).

Structure determination and refinement

A Patterson function showed the general orientation of the regular hydrocarbon chain; however, numerous attempts to solve the structure by Patterson methods failed. It was then assumed that the zigzag chains of the two crystallographically distinct molecules were approximately equivalent and related by a translation of $a/2$. Data with h even which include the subcell reflexions were reindexed in h, corresponding to a halving of a, and the symbolic-addition method (Karle & Karle, 1963) was used to develop the regular part of

Table 1. Crystal data

4-Octadecynoic acid, $C_{18}H_{32}O_2$

FW	280·45	Space group	$P\bar{1}$
a	8·71 (2) Å	λ (Cu $K\alpha$)	1·5418 Å
b	5·475 (10)	Z	4
c	45·13 (7)	D_x	1·049 Mg m^{-3}
α	92·55 (15)°	μ	0·479 mm^{-1}
β	93·15 (15)	M.p.	347·0–348·0 K*
γ	123·95 (25)	Crystal (I)	~0·42 × 0·14 × 0·05 mm
V	1775 Å^3	Crystal (II)	~0·40 × 0·12 × 0·05

* Gunstone & Ismail (1967).

one molecule. In symmorphic space groups like $P\bar{1}$ the most consistent set of phases based on the $\sum_2$ relation corresponds to a trivial solution which is most often incorrect (Schenk, 1972). In the present case, selection of the most probable models from E maps was based on several other criteria such as the height distribution of peaks along the chain, presence of ghost maxima and distribution of signs in a sequence of high-order 00l reflexions. E maps calculated from 50 terms gave atomic positions with ample accuracy. Considering the number of independent atoms in the subcell, smaller sets of E's involving subcell reflexions should be adequate and probably also preferable for two reasons. (1) The generation and subsequent propagation of incorrect signs through repeated use of the $\sum_2$ relation is less probable when only the largest E's are involved. This is a point of particular significance for highly regular structures in symmorphic space groups (Mo, Hjortås & Svinning, 1973). (2) Fewer symbols may be required, in which case a smaller number of phase models need be examined.

Six of the eight phase models could be rejected at this stage; identification of the correct arrangement required several cycles of refinement and considerations of the packing of methyl end groups. Calculation of 967 structure factors (both parities of h included) for the fragment C(6)–C(18) of the two molecules gave R $[=\sum||F_o| - K|F_c||/\sum |F_o|] = 0.65$, which was reduced to 0.49 following isotropic least-squares refinement. Further work to break the pseudosymmetry and locate the rest of the structure by means of ΔF syntheses and refinement was not successful.

In principle, the rest of the structure can be solved independently from data with no or very small contributions from the atoms of the regular fraction. For convenience, only reflexions with h odd were used in this work. A Patterson map calculated from 282 $|F|^2$ values with h odd showed two tentative arrangements of one of the O-atom pairs. Reasonable positions for the other pair were obtained from a ΔF map calculated for one of the arrangements with the same subset of F's. Least-squares refinement of the four O positions gave $R = 0.23$. With the O atoms added to the two zigzag chains, R for the set of 967 F's was 0.43, which decreased to 0.39 after three refinement cycles. Atoms C(1)–C(5), which connect the two fragments, were located successively from ΔF maps and included in the full-matrix least-squares refinement. The course of refinement had to be checked frequently by means of ΔF maps; scaling of data with h even and h odd was by separate scale factors.

At $R = 0.20$ about half of the F's left out due to possible indexing errors in l could be added to the data. Correlation was fairly high (0.5–0.65) between parent parameters of corresponding atoms in the two molecules and also between the x and y coordinates of the same atom. Despite pronounced anisotropy

features in the ΔF maps, maxima corresponding to H atoms were located near about half the C atoms in the zigzag chains. All H atoms bonded to C were added in their calculated positions assuming tetrahedral geometry and C–H = 1.0 Å. Temperature factors corresponding to those of the attached C atoms were used, but the H parameters were not refined. Isotropic refinement of the C and O atoms converged at $R = 0.164$.

In the anisotropic refinement each chain was refined separately, temperature factors and coordinates of the non-H atoms being treated in alternating cycles. On two separate occasions, the F's still omitted were added to the data, a few groups of high-order reflexions being corrected by ± 1 in l as required. Weighting was according to Hughes (1941) where $\sqrt{w} = 1.0$ if $F_o \leq 17$, $\sqrt{w} = 17/F_o$ if $F_o > 17$. Due to underestimation of the strongest intensities, seven large F's at low angles were given zero weight. Near the end of the refinement some problems remained in the carboxyl group and the sequence C(2′)–C(6′) of molecule B. Both O atoms showed very strong anisotropy in the direction normal to the O–C–O plane and a disorder model involving two arrangements of the O atoms about the C(1′)–C(2′) vector was attempted. The four O atoms were assigned variable isotropic temperature factors and a fixed population parameter of 0.5.

Refinement was carried out for both models, disordered and anisotropic O of molecule B, and terminated when no parameter shift exceeded 0.4σ. The final R based on 1155 values of F_o was 0.074 (disorder) and 0.071 (anisotropy). The magnitudes of residual features in the final ΔF maps were <0.2 e Å^{-3}. Common structure parameters of the two models do not differ significantly. Throughout these refinements correlation coefficients between variables of the same atom were: 0.5–0.75 for pairs U_{11}–U_{12}, U_{22}–U_{12}, U_{13}–U_{23} and 0.5–0.65 for pairs x–y. Final atomic parameters are listed in Table 2.* Scattering factors were those of Doyle & Turner (1968) except for H (Stewart, Davidson & Simpson, 1965). XRAY 76 (Stewart, 1976) was used for refinement and molecular-geometry calculations. Drawings of molecules were made with a slightly modified version of ORTEP II (Johnson, 1976).

Results and discussion

The two crystallographically different molecules of the acid are shown in Fig. 1. Atoms of molecule B are primed, as indicated by the numbering of the carboxyl-group atoms.

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* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34505 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The zigzag portion C(6)—C(18) is approximately planar in both molecules, with deviations ranging up to 0·07 Å. The major difference between A and B is in the orientation of the carboxyl group and C^α atoms relative to the main chain. In A, the carboxyl group makes an angle of 5° with the plane of the zigzag chain, in B this angle is about 83° (anisotropy model). Thus, the carboxyl ends define a superstructure with respect to the chain packing. Similar superstructures were observed in form A of lauric acid (von Sydow, 1956b) and in 17-methyloctadecanoic acid (Abrahamsson, 1959b).

Table 2. *Final atomic parameters*

Atoms with subscript D refer to the disorder model for carboxyl group B. The positional parameters are $\times 10^4$ for C, O and $\times 10^3$ for H. E.s.d.'s are in parentheses.

	x	y	z		x	y	z
O(1)	−1149 (11)	11225 (15)	95 (1)	O(1′)	4362 (10)	14135 (16)	345 (1)
O(2)	910 (9)	15569 (14)	354 (1)	O(2′)	6301 (12)	13570 (19)	108 (2)
C(1)	−74 (14)	12753 (24)	327 (2)	C(1′)	5436 (14)	13506 (20)	332 (2)
C(2)	−147 (12)	10998 (19)	584 (2)	C(2′)	5841 (15)	11934 (23)	576 (2)
C(3)	1057 (15)	12906 (22)	856 (2)	C(3′)	5256 (17)	12221 (26)	868 (2)
C(4)	897 (14)	11055 (19)	1109 (2)	C(4′)	5670 (17)	10647 (27)	1082 (2)
C(5)	866 (12)	9497 (16)	1288 (1)	C(5′)	5874 (16)	9430 (28)	1268 (2)
C(6)	998 (13)	7797 (19)	1503 (1)	C(6′)	5877 (15)	7666 (23)	1513 (2)
C(7)	2165 (13)	9560 (21)	1807 (2)	C(7′)	7148 (13)	9496 (17)	1774 (2)
C(8)	2028 (13)	7667 (19)	2053 (2)	C(8′)	7091 (12)	7671 (17)	2015 (2)
C(9)	3342 (14)	9441 (22)	2313 (2)	C(9′)	8232 (12)	9393 (16)	2323 (2)
C(10)	3139 (14)	7499 (21)	2561 (2)	C(10′)	8120 (12)	7589 (16)	2570 (1)
C(11)	4306 (13)	9188 (19)	2852 (2)	C(11′)	9395 (12)	9366 (17)	2852 (2)
C(12)	4139 (12)	7331 (17)	3101 (1)	C(12′)	9256 (13)	7522 (19)	3100 (2)
C(13)	5417 (11)	9113 (17)	3384 (1)	C(13′)	10429 (13)	9210 (20)	3386 (2)
C(14)	5298 (11)	7309 (17)	3630 (2)	C(14′)	10193 (13)	7275 (19)	3637 (2)
C(15)	6457 (13)	9009 (19)	3925 (2)	C(15′)	11499 (12)	9078 (17)	3914 (1)
C(16)	6317 (14)	7217 (18)	4176 (2)	C(16′)	11310 (12)	7143 (19)	4161 (2)
C(17)	7545 (13)	8913 (20)	4452 (2)	C(17′)	12470 (14)	8910 (19)	4455 (2)
C(18)	7375 (15)	7040 (23)	4703 (2)	C(18′)	12323 (15)	7070 (22)	4697 (2)
$O_D(11')$	4004 (19)	13403 (25)	325 (3)	H(181)	822	815	489
$O_D(21')$	6673 (22)	14346 (32)	148 (4)	H(182)	765	558	463
$O_D(12')$	4633 (17)	14778 (24)	365 (3)	H(183)	607	595	476
$O_D(22')$	5993 (18)	12939 (26)	79 (3)	H(21′)	723	1287	60
$C_D(1')$	5403 (15)	13545 (21)	334 (2)	H(22′)	519	981	51
H(21)	24	965	52	H(31′)	595	1436	94
H(22)	−148	973	63	H(32′)	389	1135	85
H(31)	237	1410	81	H(61′)	620	631	144
H(32)	66	1422	92	H(62′)	458	650	158
H(61)	162	688	141	H(71′)	844	1067	171
H(62)	−28	620	154	H(72′)	682	1084	185
H(71)	350	1090	177	H(81′)	763	655	194
H(72)	170	1080	188	H(82′)	578	623	205
H(81)	224	619	197	H(91′)	956	1075	229
H(82)	73	663	212	H(92′)	774	1059	239
H(91)	463	1044	225	H(101′)	843	620	250
H(92)	313	1095	239	H(102′)	681	645	263
H(101)	355	621	249	H(111′)	1072	1048	280
H(102)	181	627	260	H(112′)	912	1081	293
H(111)	563	1044	282	H(121′)	963	619	303
H(112)	388	1047	293	H(122′)	792	631	314
H(121)	444	592	303	H(131′)	1174	1035	335
H(122)	283	621	316	H(132′)	1006	1057	346
H(131)	674	1028	333	H(141′)	1042	577	357
H(132)	511	1051	346	H(142′)	888	625	370
H(141)	577	608	356	H(151′)	1281	1014	386
H(142)	399	599	367	H(152′)	1125	1053	399
H(151)	779	1032	389	H(161′)	1176	587	410
H(152)	602	1031	399	H(162′)	998	585	420
H(161)	659	579	410	H(171′)	1379	1027	442
H(162)	499	612	423	H(172′)	1199	1015	453
H(171)	886	997	440	H(181′)	1306	825	489
H(172)	727	1034	453	H(182′)	1278	586	463
				H(183′)	1099	574	473

Thermal parameters of the main-chain atoms are in general agreement with a physically reasonable picture of atoms vibrating with their largest amplitudes in planes normal to the chain direction. Excessive thermal motion in the fragment C(2')–C(6') could indicate disorder. Possible disorder is only one of several factors that might adversely affect the refinement of this structure. The number of variables is relatively large, (362 for the anisotropy model), and correlation was rather high between corresponding parameters of pairs of unprimed and primed atoms. Anomalies that occur in pairs in the two chains are probably in part due to correlation effects, *viz* unprimed and primed bonds C(6)–C(7) and C(8)–C(9), and C–C–C angles involving C(8), C(8') and C(9), C(9'). Intensities with *h* odd were weak, few in number and were measured with lower precision because of the weak diffuse streaks between maxima. Consequently, larger systematic errors may be deposited in the parameters of the carboxyl ends, as is also indicated by the fact that the final model with R (1155 F_o) = 0·071, has $R = 0·108$ for 290 F_o with *h* odd.

Bond lengths and angles uncorrected for thermal motion are given in Tables 3 and 4. The refined structure has a triple bond between C(4) and C(5) of average length 1·18 Å. The average C—C length in the two zigzag portions is 1·513 Å, the range excluding C(6)–C(7) and C(8)–C(9) of both chains is 1·48–1·54 Å. The average C—C—C angle is 114·6°, range 111–117°. Systematically short bond lengths and large bond angles have been observed in a number of long-chain structures (Jensen & Mabis, 1966; O'Connell, 1968; Dahlén, Lundén & Pascher, 1976) and were explained by Jensen & Mabis (1966) in terms of thermal anisotropy and possible libration of the chains about their long axes. Bonds involving C(3) of A and C(2') of B differ from expected values by 0·04–0·05 Å indicating small systematic errors in the positions of these atoms. Differences of this magnitude are also observed in both molecules at C(6) connecting the regular chain to the triple-bond fragment. Atoms C(3)–C(5) of each fragment are displaced to the same side of the regular-chain plane. In A the shifts are about 0·25–
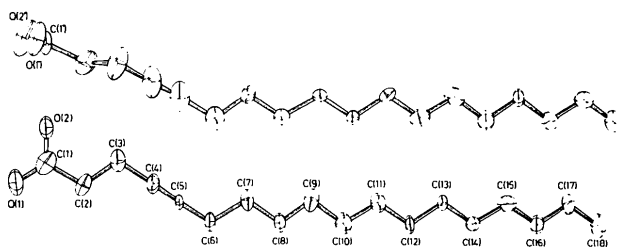
0·35 Å, in B 0·2–0·4 Å except for C(3') where Δ ~ 0·85 Å. Significant deviations from linearity of the triple-bonded C atoms are commonly observed in acetylenic compounds (Benghiat, Leiserowitz & Schmidt, 1972; Jones & Pauling, 1976); in 4-octadecynoic acid these deviations may be related largely to the accommodation of B carboxyl groups between adjacent A molecules.

Since the H atoms of the carboxyl groups were not located, the hydroxyl and carbonyl O atoms cannot be identified unambiguously. A synplanar sequence C^β—C^α—C=O is a typical feature of crystalline α,β-saturated carboxylic acids, however (Leiserowitz,

Table 3. *Bond lengths* (Å)

E.s.d.'s are about 0·015 Å except in bonds involving atoms C(1') to C(5') of molecule B where the e.s.d.'s are 0·015–0·02 Å.

C(1)–O(1)	1·27	C(1')–O(1')	1·17
C(1)–O(2)	1·27	C(1')–O(2')	1·28
C(1)–C(2)	1·52	C(1')–C(2')	1·57
C(2)–C(3)	1·49	C(2')–C(3')	1·47
C(3)–C(4)	1·52	C(3')–C(4')	1·48
C(4)–C(5)	1·19	C(4')–C(5')	1·16
C(5)–C(6)	1·42	C(5')–C(6')	1·50
C(6)–C(7)	1·57	C(6')–C(7')	1·46
C(7)–C(8)	1·52	C(7')–C(8')	1·49
C(8)–C(9)	1·46	C(8')–C(9')	1·58
C(9)–C(10)	1·53	C(9')–C(10')	1·50
C(10)–C(11)	1·52	C(10')–C(11')	1·52
C(11)–C(12)	1·51	C(11')–C(12')	1·51
C(12)–C(13)	1·53	C(12')–C(13')	1·50
C(13)–C(14)	1·49	C(13')–C(14')	1·53
C(14)–C(15)	1·53	C(14')–C(15')	1·52
C(15)–C(16)	1·50	C(15')–C(16')	1·52
C(16)–C(17)	1·48	C(16')–C(17')	1·54
C(17)–C(18)	1·52	C(17')–C(18')	1·48

Table 4. *Valency angles* (°)

E.s.d.'s are in the range 0·7–1·0° except for angles at atoms C(4) and C(5) of molecule A, and C(1') to C(5') of B where the e.s.d.'s are 1·0–1·5°.

O(1)–C(1)–O(2)	123	O(1')–C(1')–O(2')	128
O(1)–C(1)–C(2)	115	O(1')–C(1')–C(2')	125
O(2)–C(1)–C(2)	121	O(2')–C(1')–C(2')	107
C(1)–C(2)–C(3)	113	C(1')–C(2')–C(3')	113
C(2)–C(3)–C(4)	111	C(2')–C(3')–C(4')	109
C(3)–C(4)–C(5)	173	C(3')–C(4')–C(5')	173
C(4)–C(5)–C(6)	175	C(4')–C(5')–C(6')	173
C(5)–C(6)–C(7)	116	C(5')–C(6')–C(7')	113
C(6)–C(7)–C(8)	115	C(6')–C(7')–C(8')	112
C(7)–C(8)–C(9)	112	C(7')–C(8')–C(9')	117
C(8)–C(9)–C(10)	111	C(8')–C(9')–C(10')	117
C(9)–C(10)–C(11)	115	C(9')–C(10')–C(11')	115
C(10)–C(11)–C(12)	116	C(10')–C(11')–C(12')	114
C(11)–C(12)–C(13)	114	C(11')–C(12')–C(13')	116
C(12)–C(13)–C(14)	115	C(12')–C(13')–C(14')	114
C(13)–C(14)–C(15)	117	C(13')–C(14')–C(15')	112
C(14)–C(15)–C(16)	117	C(14')–C(15')–C(16')	112
C(15)–C(16)–C(17)	116	C(15')–C(16')–C(17')	114
C(16)–C(17)–C(18)	115	C(16')–C(17')–C(18')	115

Fig. 1. Structures of molecules A and B. The numbering of atoms in B is only shown for the carboxyl group. Thermal ellipsoids correspond to 40% probability.

1976); hence, the most probable assignments for the hydroxyl O atoms in A and B are O(1) and O(2'), respectively, which is also corroborated by the O—C—C$^\alpha$ angles.

The molecules are arranged in the pattern most frequently found for long-chain fatty acids with alternating polar and non-polar end-group layers (Fig. 2). The zigzag chains are tilted 70° relative to the methyl end-group planes and the lateral packing is according to a triclinic subcell $(T_{||})$ (Vand & Bell, 1951) with dimensions: $a_s = 4\cdot34$, $b_s = 5\cdot475$ $(\equiv b)$, $c_s = 2\cdot55$ Å; $\alpha_s = 74\cdot2$, $\beta_s = 108\cdot9$, $\gamma_s = 123\cdot8°$. Methyl contacts in the non-polar layers are normal with a shortest distance C(18)$\cdots$C(18')(2 − x, 1 − y, 1 − z): 3·69 Å. The shortest lateral contacts involve atoms near the carboxyl ends: C(1)$\cdots$C(2')(−1 + x, y, z): 3·58 Å, C(4)$\cdots$C(3') within the asymmetric unit: 3·72 Å. There are seven O$\cdots$O contacts in the normal van der Waals range. The molecules form H-bonded dimers over symmetry centres, O$\cdots$O distances for pairs $A\cdots A$ and $B\cdots B$ are: O(1)$\cdots$O(2)(−x, 3 − y, −z): 2·68 Å and O(2')$\cdots$O(1')(1 − x, 3 − y, z): 2·65 Å, respectively. This simple scheme where each type of carboxyl group forms separate dimers does not explain well why a structure with one single carboxyl orientation is not preferred. Considerations of possible stacking faults and disorder show that alternative arrangements of H-bonds may exist. In a system where the regular $ABAB...$ is broken by the sequence $ABBB...$ there are two O$\cdots$O contacts in the range 2·65–2·70 Å, suggesting a short sequence of H-bonds: O(1)(−x, 2 − y, −z)$\cdots$O(2'$_A$)$\cdots$O(1'); O(2'$_A$) denotes O(2') of carboxyl group B translated −a/2 within the asymmetric unit to simulate substitution of A by B. With the disorder model for carboxyl group B another possible H-bond is O(1)$\cdots$O$_D$(11')(−x, 2 − y, −z): 2·87 Å. These alternative H-bonds would mainly link molecules laterally. 4-Octadecynoic acid has a higher melting point than stearic acid and any of the isomeric octadecyn- and octadecenoic acids (Barve & Gunstone, 1971). Local, subsidiary H-bond patterns such as those discussed above presumably contribute to the observed stability of this crystal structure.
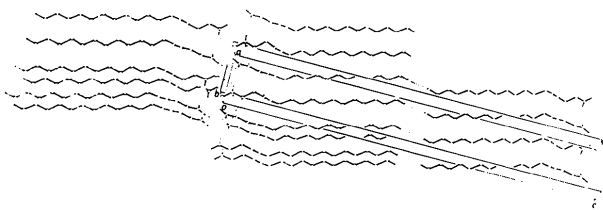
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Fig. 2. Packing of 4-octadecynoic acid molecules. H-bonds are shown as dashed lines, dotted lines indicate shortest C$\cdots$C contacts.