Conformation and packing of unsaturated chains in cholesteryl linolelaidate at 123 K[1]

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Abstract At 123 K, crystals of cholesteryl *trans*-9-*trans*-12-octadecadienoate (cholesteryl linolelaidate, $C_{47}H_{76}O_2$) are monoclinic, space group $P2_1$ with cell dimensions $a = 13.03(3)$, $b = 8.76(2)$, $c = 17.90(4)$ Å, $\beta = 89.7(2)°$, having two molecules per unit cell. The crystal structure has been determined from 2041 X-ray intensities with $\sin \theta/\lambda < 0.48$ Å^{-1}, of which 922 gave $I > 2\sigma(I)$. The hydrogen atoms were found in a difference Fourier synthesis. Block diagonal least squares refinement assuming isotropic thermal parameters has converged with $R_w = 0.13$. The molecule is fully extended (length 43.3 Å), except for a symmetric bowing in the linolelaidate chain segment which contains the two unconjugated *trans* ethylenic bonds. The torsion angles at the four C—C bonds adjacent to the C=C bonds are all in the preferred (±)-*skew* range. Chain packing is efficient, without having a regular subcell structure. There is a similarity with the overall conformation of the oleate chains in crystals of cholesteryl oleate. Although chemically disparate, the oleate and linolelaidate chains have similar crystal environments.—**Craven, B. M., and P. Sawzik.** Conformation and packing of unsaturated chains in cholesteryl linolelaidate at 123 K. *J. Lipid Res.* 1983. **24:** 784–789.

Supplementary key words chain conformation • unsaturated fatty acids • cholesteryl ester

We have undertaken a series of crystal structure determinations to study the effects of *cis* and *trans* unsaturation on the conformation of long fatty acid chains when they are incorporated in close-packed lipid systems. The crystal structures involve the alkenoate esters of cholesterol. These all appear to have one of two layer type crystal structures in which the arrangement of the cholesteryl ring systems has already been well characterized (1, 2). The differences from one crystal structure to another lie in the irregular packing of the fatty acid chains.

We have already determined the crystal structures of the oleate (3), palmitoleate (4), and nervonate (5) esters, which contain *cis* double bonds. The crystal structure determination of cholesteryl linolelaidate provides the first example of a long fatty acid chain containing two *trans* double bonds (**Fig. 1**). They are unconjugated, since the ethylenic groups are separated by a methylene group.

EXPERIMENTAL

Cholesteryl linolelaidate obtained from Sigma Chemical Co., St. Louis, MO, was crystallized with some difficulty by slow evaporation of a petroleum ether solution at 273 K. The crystals (mp 339.5 K) were thin blades with prominent {001} faces having their longest dimension in the *b*-axis direction. In a preliminary study (2), the crystal structure was found to be monoclinic, space group $P2_1$, with two molecules ($C_{47}H_{76}O_2$) in the unit cell.

The X-ray data were collected using an Enraf-Nonius CAD-4 diffractometer and Nb-filtered Mo K_α-radiation ($\lambda = 0.7109$ Å). The crystals were cooled to 123 K in a stream of dry nitrogen gas. Although cooling was slow (293 K to 123 K in 6 hr), crystals became strained due to anisotropic cell volume change, and tended to fracture unpredictably during data collection. Eventually the data were obtained using two crystals, measuring $0.61 \times 0.17 \times 0.07$ mm^3 and $0.67 \times 0.23 \times 0.03$ mm^3, that were mounted with *b* about 10° from the diffractometer Φ-axis. Lattice parameters were derived by least squares fitting of $\sin^2 \theta$-values for 25 reflections in the range $6 < \theta < 10°$, which were measured at $\pm\theta$. The following values for the crystal structure at room temperature (293 K) are more accurate than those previously obtained from X-ray photographs (2): $a = 12.855(12)$, $b = 8.984(18)$, $c = 18.726(17)$ Å, $\beta = 92.30(8)°$. At 123 K, the values are $a = 13.026(25)$, $b = 8.760(18)$, $c = 17.901(42)$ Å, $\beta = 89.68(16)°$. Cooling causes a net decrease in the unit cell volume from 2161(5) Å^3 to 2043(7) Å^3, although there is an increase $\Delta a = 0.17(3)$ Å in one of the lattice translations. There is a significant shearing of adjacent molecular layers (**Fig. 2**) and a contraction of the layer spacing, as shown

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Abbreviation: e.s.d., estimated standard deviation.

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by $\Delta\beta = -2.62(8)°$ and $\Delta d_{001} = -0.83(5)$ Å. The molecular basis for these changes has not been determined.

With the crystal at 123 K, X-ray integrated intensities were measured using $\theta/2\theta$ scans for reflections in the range $0.05 \leq \sin\theta/\lambda \leq 0.48$ Å^{-1}. At $\sin\theta/\lambda = 0.48$ Å^{-1}, corresponding to a resolution $d_{min} = 1.05$ Å, most reflections were so weak that data collection was not extended beyond this limit. There were 1230 reflections measured with the first crystal and 2179 with the second, which reduced to 2041 non-symmetry-related reflections. The variance in an integrated intensity was assumed to be $\sigma^2(I) = \sigma^2 + (0.021)^2$ where σ^2 is the variance due to counting statistics. It was found that only 922 reflections out of 2041 gave $I > 2\sigma(I)$. At first, the unusually high proportion of weak intensities was thought to be caused either by disorder or by large amplitude atomic thermal motion persisting at 123 K. However, the Wilson plot gave a value $B = 2.3$ Å^2 for the overall temperature factor, which is typical for an organic structure at low temperature. It was concluded that the observed intensities were weak because the available crystals were so thin along d_{001}, making them small in volume and hence in diffracting power. The X-ray intensities were not corrected for absorption.

The crystal structure was determined by making use of the close relationship with the structure of cholesteryl oleate (3). Atomic fractional coordinates for the 27 atoms, C(1) through C(23), C(28), C(29), O(1), and O(3) were transformed from their values in cholesteryl oleate into the linolelaidate unit cell, assuming a common direction for the *a*- and *b*-axes. The transformation matrix was

$$\begin{pmatrix} a_0/a_\ell & 0 & \left\{\dfrac{c_0 \cos\beta_0}{a_\ell} - \dfrac{c_0 \sin\beta_0}{c_\ell \tan\beta_\ell}\right\} \\ 0 & b_0/b_\ell & 0 \\ 0 & 0 & \dfrac{c_0 \sin\beta_0}{c_\ell \sin\beta_\ell} \end{pmatrix}$$

where the subscripts 0 and ℓ refer to the different structures. The initial structure factor calculation, using the Wilson plot scale and thermal parameters gave $R = 0.56$.[2] Atomic scattering factors were those of Cromer and Waber (6) for C and O atoms, and of Stewart, Davidson, and Simpson (7) for H atoms. After two cycles of Fourier refinement, all C and O atoms were located. The structure refinement was by a block-diagonal least squares procedure in order to minimize the residual $\sum_H w\Delta^2$ (see footnote 2). The weights were given by $w = 1/\sigma^2(F)$ where $\sigma^2(F) = \sigma^2(F^2)/4F^2$ except for the weakest reflections, $F^2 < \sigma(F^2)$ in which case, according to Rees (8), $\sigma^2(F) = \sigma(F^2)/4$.

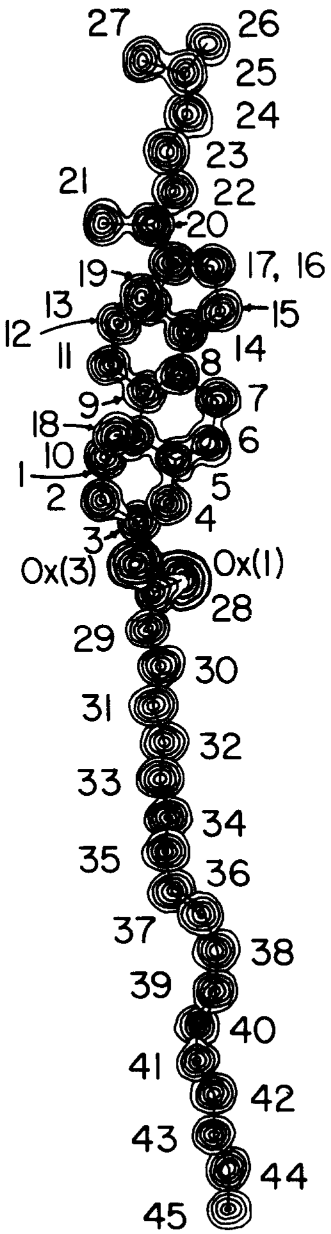

Fig. 1. The electron density and atomic nomenclature for cholesteryl linolelaidate. Contours are at intervals 1 eÅ^{-3} beginning at 1 eÅ^{-3}, except for the O-atoms, where the interval is 2 eÅ^{-3}.

Positional parameters for all H atoms were determined from a difference Fourier synthesis. They were included in the refinement with fixed parameters, in-

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[2]

$$R = \sum_H |\Delta| / \sum_H |F_0|; \quad R_w = \{\sum_H w\Delta^2 / \sum_H |F_0|^2\}^{1/2};$$

$$S = \{\sum_H w\Delta^2/(m-n)\}^{1/2},$$

where $\Delta = |F_0| - |F_c|$, m = number of reflections, n = number of parameters.

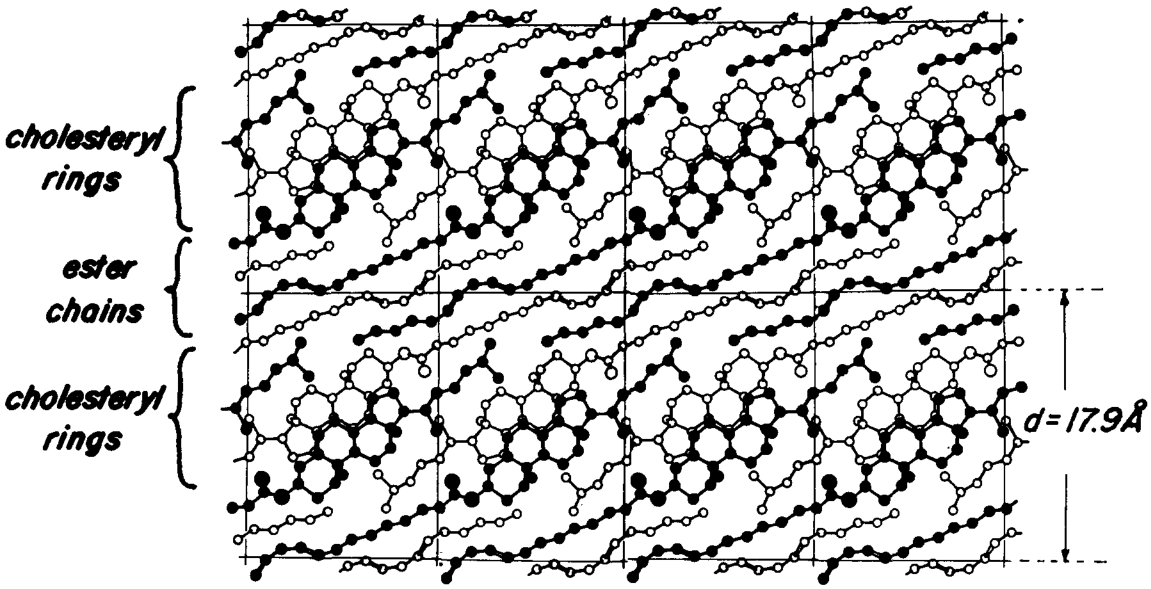

Fig. 2. The crystal structure of cholesteryl linolelaidate. Crystal axes are directed with *a* from left to right, *c* from top to bottom, and *b* into the page. Molecules with shaded atoms are close to y = ¼, and the others are close to y = ¾.

cluding a uniform thermal parameter, B = 6 Å^2. The C and O atoms were assumed to have individual isotropic temperature factors. Convergence was obtained with R = 0.23, R_w = 0.13, S = 1.54 for all reflections (see footnote 2), or R = 0.11, R_w = 0.10 for the 922 reflections with I > 2σ(I). Further refinement was begun, assuming anisotropic temperature factors, but this was not concluded. As was found qualitatively in the electron density distribution (Fig. 1) and also from considering differences in the principal values of the mean square atomic displacements in terms of their e.s.d.'s, the assumption of isotropic atomic thermal motion is adequate. The final atomic positional and thermal parameters from the isotropic refinement are in **Table 1.**[3]

RESULTS AND DISCUSSION

The molecular geometry

In this crystal structure, all atoms are well resolved (Fig. 1), so that the overall conformation of the molecule is clearly defined. However, the X-ray data necessary for a very accurate determination of bond lengths and angles were not available. The e.s.d.'s in the C—C and C—O bond lengths range from 0.020 to 0.028 Å, and in bond angles from 1.2 to 1.6°. Within these limitations, values obtained for cholesteryl linolelaidate (see footnote 1) agree with generally accepted values, and in particular, with corresponding values in the accurately determined crystal structure of cholesteryl acetate (9).

In the cholesteryl ring system and C(17) tail, C—C bond lengths range from 1.45(2) Å for C(3)–C(4) to 1.61(2) Å for C(13)–C(17). The C(5)=C(6) distance is 1.29(3) Å. The C—O(3) and C=O(1) distances are 1.49(2) and 1.17(2) Å. In the fatty acid chain, C—C bond lengths between tetrahedral C-atoms range from 1.52(3) to 1.62(3) Å, those between tetrahedral and trigonal C-atoms range from 1.49(2) to 1.52(2) Å, and the two C=C bond lengths are 1.33(3), 1.34(3) Å. Bond angles in the saturated regions of the chain range from 110(1) to 114(2)°. In the segment C(35)—C(36)=C(37)—C(38)—C(39)=C(40)—C(41), bond angles at C(36) through C(40) are 123(2), 127(2), 117(1), 126(2), and 126(2)°, respectively.

The molecule is almost fully extended (Figs. 1 and 2), with an overall length of 43.3 Å. The best least squares lines through atoms of the cholesteryl group C(1) through C(27) and the fatty acid chain O(1), O(3) and C(28) through C(45) make an angle of 12°. In **Table 2,** torsion angles are listed for the three ethylenic groups, which are planar within experimental error, and for the more flexible regions of the molecule. The most interesting are the torsion angles which describe the bowing of the fatty acid chain in the unsaturated region (**Figs. 1, 2, 3**). There is a (+)- or (−)-skewed conformation about each of the C—C bonds adjacent to a C=C bond, giving rise to an approximate local mirror plane normal to the fatty acid chain axis, and passing through the bridging methylene group at C(38). The

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[3] Tables of structure factors |F$_0$|, F$_c$, and σ(F), the H-atom positional parameters, and the bond lengths and angles for the molecular framework can be obtained as described in footnote 1.

observed torsion angles in the linolelaidate chain are consistent with previous tabulations of crystal structural data by Matuscelli (10) and Sundaralingam (11). These indicate that the preferred conformation at the C—C bonds adjacent to an unconjugated C=C bond is in the range ±(90° through 130°), regardless of whether the C=C bonds are in the *cis* or *trans* configuration.

The molecular packing

Cholesteryl linolelaidate belongs to the family of layer type crystal structure that we call type II. Other members are cholesteryl iodide (12), oleate (3), and octanoate (13). At the center of the layer there is an interlocking arrangement of antiparallel cholesteryl groups (Fig. 2) which has already been described (13). As a result, the molecular long axes make a large tilt angle with the layer planes. In the case of cholesteryl linolelaidate, the best least squares line through all C and O atoms in the molecule makes an angle 65.0° with c^* which is normal to the layers. This line is also at an angle 90.6° with respect to the crystallographic twofold screw axes which are along b.

The fatty acid chains project into the region between layers. In previously determined crystal structures of this type (3, 13) that were studied at room temperature, the chains were loosely packed and were subject to large amplitude thermal vibrations and possibly disorder. However, in cholesteryl linolelaidate at 123 K, cooling has resulted in considerably tighter packing for the cholesteryl groups and particularly for the fatty acid chains. Thus, isotropic thermal parameters for the C-atoms (Table 1) correspond to mean square amplitudes of vibration in the range 0.016(4) to 0.045(5) Å². These are an order of magnitude less than the values for cholesteryl oleate at 295 K. As expected, intermolecular distances are shorter for the low temperature structure. Thus, in both oleate and linolelaidate crystal structures, C(18)· · ·C(6) is the shortest distance between cholesteryl C-atoms. The values are 3.82(5) and 3.68(3) Å, respectively. Such comparisons cannot be made for the C· · ·C distances involving linolelaidate chains because no corresponding room temperature structure has been determined.[4] However, many of the C· · ·C distances in **Table 3** are less than the van der Waals distance between methylene groups (4.0 Å) which was proposed by Pauling (14) for crystal structures at room temperature.

TABLE 1. Atomic positional parameters (×10⁴) and thermal parameters for non-hydrogen atoms

Atom	x/a	y/b	z/c	B (Å²)[b]
C(1)	5416 (12)[a]	1509 (23)	7207 (9)	2.0 (4)
C(2)	6373 (12)	1854 (23)	7723 (9)	2.0 (4)
C(3)	7330 (11)	1828 (22)	7226 (8)	1.3 (3)
C(4)	7304 (12)	2903 (26)	6608 (9)	2.4 (4)
C(5)	6339 (12)	2810 (25)	6127 (9)	2.1 (4)
C(6)	6385 (11)	2794 (25)	5407 (8)	1.9 (4)
C(7)	5498 (11)	2651 (24)	4877 (8)	1.7 (3)
C(8)	4468 (13)	2978 (26)	5289 (10)	2.8 (4)
C(9)	4415 (12)	2114 (23)	6013 (9)	2.1 (4)
C(10)	5301 (12)	2703 (26)	6566 (9)	2.5 (4)
C(11)	3363 (13)	2181 (24)	6378 (9)	2.9 (4)
C(12)	2481 (14)	1684 (27)	5855 (10)	3.3 (4)
C(13)	2512 (12)	2676 (26)	5118 (9)	2.2 (4)
C(14)	3581 (11)	2387 (23)	4787 (8)	1.8 (3)
C(15)	3497 (11)	3057 (22)	3981 (8)	1.4 (3)
C(16)	2392 (12)	2604 (26)	3741 (9)	2.7 (4)
C(17)	1836 (11)	1993 (22)	4449 (8)	2.0 (4)
C(18)	2261 (14)	4335 (26)	5221 (10)	3.1 (4)
C(19)	5057 (13)	4316 (24)	6892 (10)	2.5 (4)
C(20)	674 (11)	2390 (22)	4436 (8)	1.3 (3)
C(21)	109 (14)	2031 (24)	5163 (10)	3.2 (4)
C(22)	165 (12)	1625 (23)	3738 (8)	1.7 (3)
C(23)	−838 (13)	2390 (27)	3526 (9)	3.4 (4)
C(24)	−1401 (13)	1661 (25)	2875 (9)	2.6 (4)
C(25)	−2326 (13)	2681 (27)	2566 (10)	3.1 (4)
C(26)	−2738 (14)	1828 (26)	1884 (10)	3.5 (5)
C(27)	−3127 (13)	2819 (28)	3144 (9)	2.9 (4)
C(28)	9131 (12)	1723 (24)	7548 (9)	2.3 (4)
C(29)	9897 (12)	2506 (25)	8037 (9)	2.6 (4)
C(30)	10899 (13)	1535 (25)	8139 (9)	2.6 (4)
C(31)	11706 (13)	2421 (25)	8604 (9)	3.0 (4)
C(32)	12682 (13)	1528 (25)	8745 (9)	2.6 (4)
C(33)	13470 (11)	2545 (24)	9143 (8)	1.9 (4)
C(34)	14509 (13)	1605 (25)	9323 (9)	2.9 (4)
C(35)	15269 (13)	2679 (28)	9694 (9)	3.2 (4)
C(36)	16246 (12)	1830 (23)	9887 (9)	2.4 (4)
C(37)	17162 (12)	2230 (23)	9624 (9)	2.3 (4)
C(38)	18169 (12)	1384 (24)	9737 (9)	2.2 (4)
C(39)	19024 (12)	2256 (22)	10089 (8)	2.0 (4)
C(40)	19583 (13)	1802 (24)	10676 (9)	2.5 (4)
C(41)	20434 (12)	2686 (26)	11024 (9)	2.4 (4)
C(42)	21440 (13)	1742 (25)	11024 (9)	2.7 (4)
C(43)	22341 (11)	2605 (24)	11417 (8)	1.7 (3)
C(44)	23316 (12)	1636 (24)	11455 (9)	2.2 (4)
C(45)	24244 (13)	2554 (28)	11799 (10)	3.6 (4)
O(1)	9257 (10)	782 (18)	7091 (7)	4.6 (3)
O(3)	8180 (8)	2271 (25)	7732 (6)	2.5 (2)

[a] Estimated standard deviations are given in parentheses.
[b] $B = 8\pi^2\langle u^2\rangle$.

The presence of the ethylenic bonds in the linolelaidate chain is a major factor in determining the nature of the molecular packing. Thus the molecule of cholesteryl stearate differs from the linolelaidate and oleate esters only in having a fully saturated ester chain. The crystal structure is quite different (15), being closely related to the crystal structure of cholesteryl myristate (16). For these long chain alkanoate esters, the crystal structure contains bilayers dominated by the packing together of saturated chains according to a highly reg-

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[4] In the X-ray intensity data for cholesteryl linolelaidate collected at 292 K, there are only 390 reflections with $I > 2\sigma(I)$ in the range $\sin\theta/\lambda < 0.5$ Å⁻¹. These are inadequate for a detailed structure determination. Other structures with type II layers such as cholesteryl oleate differ from the linolelaidate in chain conformation and packing (see Fig. 4).

TABLE 2. Torsion angles in cholesteryl linolelaidate

C(4)—C(5)=C(6))—C(7)	178 (2)°[a]	C(29)—C(30)—C(31)—C(32)	178 (2)
C(10)—C(5)=C(6)—C(7)	−1 (3)	C(30)—C(31)—C(32)—C(33)	175 (1)
C(13)—C(17)—C(20)—C(21)	−53 (2)	C(31)—C(32)—C(33)—C(34)	178 (1)
C(13)—C(17)—C(20)—C(22)	179 (1)	C(32)—C(33)—C(34)—C(35)	178 (1)
C(17)—C(20)—C(22)—C(23)	−159 (1)	C(33)—C(34)—C(35)—C(36)	−123 (2)
C(20)—C(22)—C(23)—C(24)	−177 (1)	C(34)—C(35)—C(36)=C(37)	121 (2)
C(22)—C(23)—C(24)—C(25)	−169 (2)	C(35)—C(36)=C(37)—C(38)	−175 (2)
C(23)—C(24)—C(25)—C(26)	176 (2)	C(36)=C(37)—C(38)—C(39)	−123 (2)
C(23)—C(24)—C(25)—C(27)	−65 (2)	C(37)—C(38)—C(39)=C(40)	129 (2)
C(2)—C(3)—O(3)—C(28)	153 (1)	C(38)—C(39)=C(40)—C(41)	180 (2)
C(4)—C(3)—O(3)—C(28)	−85 (2)	C(39)=C(40)—C(41)—C(42)	−123 (2)
C(3)—O(3)—C(28)=O(1)	−11 (2)	C(40)—C(41)—C(42)—C(43)	−177 (1)
C(3)—O(3)—C(28)—C(29)	170 (1)	C(41)—C(42)—C(43)—C(44)	177 (1)
O(3)—C(28)—C(29)—C(30)	155 (1)	C(42)—C(43)—C(44)—C(45)	176 (1)
C(28)—C(29)—C(30)—C(31)	176 (1)		

[a] Estimated standard deviations are given in parentheses.

ular subcell (17). Although it might appear that the *trans*-double bonds could be accommodated within such an arrangement, no cholesteryl ester with an unsaturated chain, *cis* or *trans*, has been found to crystallize with the bilayer type structure (1).

Variability and irregularity in unsaturated chain packing, as observed in the crystal structures of cholesteryl linolelaidate, oleate (3), and palmitoleate (4), appears to be derived from the greater flexibility of an unsaturated chain. As noted above, there are two preferred conformations (±)-*skew* at the C—C bonds adjacent to an unconjugated double bond (10, 11). The torsional barriers about such bonds have not been accurately determined. However, in 1-butene, the barrier for (+)- to (−)-*skew* conversion (1.75 kcal/mole, reference 18) is about half the value (3.5 kcal/mole) for the *trans* to *gauche* conversion in *n*-alkanes (19). The probability for chain-bending is enhanced where adjacent ethylenic centers are linked by methylene groups. In the linolelaidate structure, this methylene group C(38) is at the center of a symmetric bow in the chain (Figs. 1 and 3). The observed conformation provides a close molding of the chain to the A-ring and ester group of one neighbor molecule and to the projecting C(26) methyl group from the isoprenoid tail of another (Fig. 2). As seen in Table 3, the intermolecular distance C(37)• • •C(2) which occurs in this interaction is the shortest of any in the crystal structure, 3.58(2) Å.

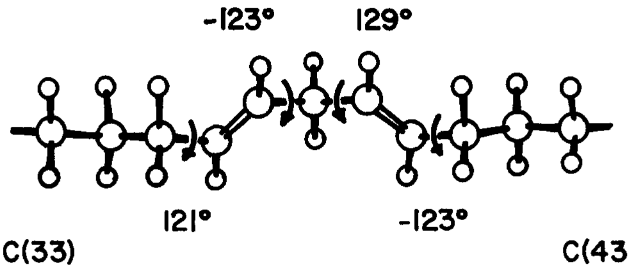

Fig. 3. Conformation of the linolelaidate chain in the unsaturated segment. Torsion angles are shown for the C—C bonds adjacent to C=C bonds.

It is noteworthy that in the crystal structure of cholesteryl oleate (3), the oleate chain also passes between the A-ring of one cholesteryl and the isoprenoid tail of another, and is bowed in the same region as the lino-

TABLE 3. Shortest intermolecular C• • •C distances involving linolelaidate chains[a]

Atoms	Symmetry	Distance
C(28)• • •C(38)	−1 + x, y, z	4.12 (3) Å
C(29)• • •C(39)	−1 + x, y, z	3.85 (3)
C(30)• • •C(25)	1 − x, −½ + y, 1 − z	4.05 (3)
C(31)• • •C(26)	1 − x, ½ + y, 1 − z	4.18 (3)
C(32)• • •C(25)	1 − x, −½ + y, 1 − z	4.13 (3)
C(33)• • •C(36)	3 − x, ½ + y, 2 − z	4.15 (3)
C(34)• • •C(2)	1 + x, y, z	3.75 (3)
C(35)• • •C(2)	1 + x, y, z	3.87 (3)
C(35)• • •C(34)	3 − x, ½ + y, 2 − z	3.87 (3)
C(36)• • •C(26)	2 + x, y, 1 + z	3.82 (3)
C(36)• • •C(2)	1 + x, y, z	3.88 (2)
C(37)• • •C(2)	1 + x, y, z	3.58 (2)
C(38)• • •C(29)	1 + x, y, z	3.90 (3)
C(38)• • •C(26)	2 + x, y, 1 + z	4.03 (3)
C(38)• • •C(41)	4 − x, −½ + y, 2 − z	3.95 (3)
C(39)• • •C(29)	1 + x, y, z	3.85 (2)
C(39)• • •C(26)	2 + x, y, 1 + z	3.96 (3)
C(40)• • •C(26)	2 + x, y, 1 + z	3.71 (3)
C(41)• • •C(38)	4 − x, ½ + y, 2 − z	3.95 (3)
C(42)• • •C(38)	4 − x, −½ + y, 2 − z	4.32 (3)
C(43)• • •C(38)	4 − x, ½ + y, 2 − z	3.96 (2)
C(44)• • •C(34)	1 + x, y, z	4.11 (2)
C(45)• • •C(1)	3 − x, ½ + y, 2 − z	3.92 (3)
C(45)• • •C(19)	3 − x, ½ + y, 2 − z	3.79 (3)
C(45)• • •C(35)	1 + x, y, z	3.99 (2)
C(45)• • •C(26)	3 − x, y, 1 + z	3.97 (3)

[a] The symmetry operations that are given, when applied to the fractional coordinates in Table 1, give rise to the atom at the right of each pair. Atoms at the left all belong to the same chain (Table 1). The shortest distance is given for every atom in the chain.

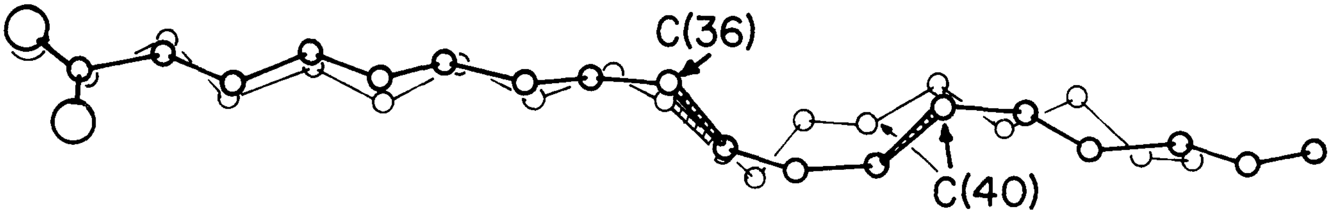

Fig. 4. Superposition of linolelaidate (heavy lines) on oleate chains, in the view down the crystal *b*-axes.

lelaidate chain (**Fig. 4**). This resemblance in gross conformation is accomplished although the two chains are chemically quite different in the segment C(36) through C(40). Thus the oleate chain has only one *cis*-ethylenic bond at C(36)=C(37), whereas in the linolelaidate chain, there are two *trans* bonds at C(36)=C(37) and C(39)=C(40). The complexity of the dislocation in the oleate chain, and its asymmetry with respect to the C(36)=C(37) bond are more readily understood by comparison with the conformation of the linolelaidate chain. In these two crystal structures there appears to be an expression of flexibility and adaptability of the two different chains to a similar crystal environment.

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