Solving a, b, c from equations (14) and (20), we obtain the following calculated lattice parameters of the orthorhombic cell:

$$a=3{\cdot}1460, \quad b=4{\cdot}7704, \quad c=4{\cdot}8510\,\text{kX}.$$

The correspondence between the calculated and measured (X-ray) lattice parameters of the orthorhombic cell is very good for the a and c axes and fair for the b axis. The comparison does not take into consideration any lattice readjustment, such as homogeneous contraction (or expansion) parallel to certain crystallographic directions, which might take place during transformation. Thus, a homogeneous contraction by 0·015 kX. along the b axis of the orthorhombic cell will bring almost exact agreement between the calculated and measured lattice parameters of the orthorhombic phase.

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References

BARRETT, C. S. & TRAUTZ, O. R. (1948). *Amer. Inst. Min. (Metall.) Engrs*, Tech. Paper No. 2346.

BURGERS, W. G. (1934). *Physica*, *'s Grav.*, **1**, 561.

BYSTROM, A. & ALMIN, K. E. (1947). *Acta Chem. Scand.* **1**, 76.

CHANG, L. C. & READ, T. A. (1950). *Amer. Inst. Min. (Metall.) Engrs*, Tech. Paper No. 2941–E.

COHEN, M. (1949). *Trans. Amer. Soc. Met.* **41**, 35.

GRENINGER, A. B. & TROIANO, A. R. (1949). *J. Metals*, **1**, 590.

GRENINGER, A. B. (1939). *Trans. Amer. Inst. Min. (Metall.) Engrs*, **133**, 204.

GRENINGER, A. B. & MOORADIAN, V. G. (1938). *Trans. Amer. Inst. Min. (Metall.) Engrs*, **128**, 337.

GRIDNEV, V. (1938). *J. Tech. Phys. (U.S.S.R.)*, **5**, 761.

JASWON, M. A. & WHEELER, J. A. (1948). *Acta Cryst.* **1**, 216.

KURDJUMOW, G. & SACHS, G. (1930). *Z. Phys.* **64**, 325.

MEHL, R. F. & DERGE, G. (1937). *Trans. Amer. Inst. Min. (Metall.) Engrs*, **125**, 482.

NISHIYAMA, Z. (1934). *Sci. Rep. Tôhoku Univ.* **23**, 637.

ÖLANDER, A. (1932). *Z. Krystallogr.* **83**, 145.

SMITH, G. V. & MEHL, R. F. (1942). *Trans. Amer. Inst. Min. (Metall.) Engrs*, **150**, 211.

SMITH, C. S. (1950). *Metal Progr.* **58**, 478.

TROIANO, A. R. & MCGUIRE, F. T. (1943). *Trans. Amer. Soc. Met.* **31**, 340.

TROIANO, A. R. & TOKICH, J. L. (1948). *Amer. Inst. Min. (Metall.) Engrs*, Tech. Paper No. 2348.

WASSERMANN, G. (1935). *Mitt. K.-Wilh.-Inst. Eisenforsch.* **17**, 149.

Acta Cryst. (1951). **4**, 324

The Crystal Structure of Lauric Acid

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Lauric acid (form C or α), $C_{12}H_{24}O_2$, is monoclinic with $a=9{\cdot}524$, $b=4{\cdot}965$, $c=35{\cdot}39$ A., $\beta=129°\ 13'$. The cell contains four molecules; density observed 1·032, calculated 1·034 g.cm.$^{-3}$. The space group is C_{2h}^5–$P2_1/a$. Fourier projections were prepared and atomic co-ordinates determined. The angle of tilt $\tau=54°\ 52'$.

Introduction

Lauric acid is known to exhibit polymorphism. Crystals of very pure lauric acid, prepared in these laboratories, were grown from ethanol solution. They proved to be in the form C of Francis & Piper (1939) or form α of Thibaud & Duprè de la Tour (1930a,b, 1932) with melting-point of 44·8° C. and setting-point 43·9° C.

Determination of X-ray data

The following data were determined from moving-film zero- and n-layer Weissenberg photographs about the a and b axes and powder photographs using Ni-filtered Cu $K\alpha$ radiation:

Molecular formula $C_{12}H_{24}O_2$.
Molecular weight = 200·31.
The crystal is monoclinic with

$$\begin{aligned} a&=9{\cdot}524\pm0{\cdot}02,\\ b&=4{\cdot}965\pm0{\cdot}01,\\ c&=35{\cdot}39\pm0{\cdot}07\ \text{A.},\\ \beta&=129°\ 13'\pm1',\\ c\sin\beta&=27{\cdot}42\pm0{\cdot}06\ \text{A.} \end{aligned}$$

Four molecules per unit cell.
Density calc. = 1·034, density meas. = 1·032 g.cm.$^{-3}$.
Absent reflexions: $(h0l)$ when h odd, $(0k0)$ when k odd.
Space group: C_{2h}^5–$P2_1/a$.

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Determination of the structure

The intensities of the reflexions were estimated by eye, using the multiple-film technique. During calculation of the observed structure factors, $|F_o|$, the normal Lorentz and polarization correction factors were applied, together with Tunell (1939) geometrical correction factors for non-equatorial reflexions. Absolute values were obtained at a later stage by comparison with the calculated structure factors, F_c.

Table 1. *Scattering curve for carbon and oxygen*

sin θ	0	0·05	0·10	0·15	0·20	0·25	0·30	0·35	
f	1·000	0·957	0·850	0·753	0·656	0·553	0·452	0·350	
sin θ	0·40	0·45	0·50	0·55	0·60	0·65	0·70	0·75	0·77
f	0·266	0·203	0·160	0·128	0·110	0·094	0·080	0·063	0·055

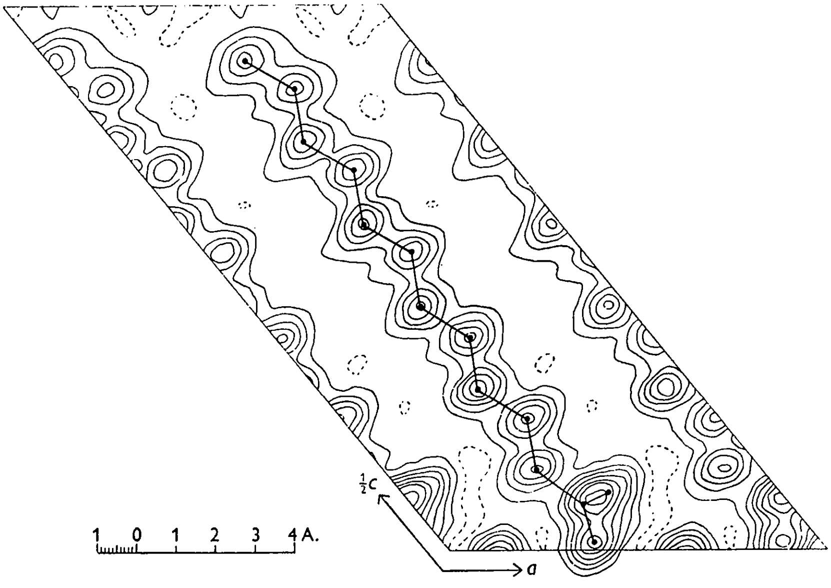

Fig. 1. Lauric acid. Fourier projection along the b axis.

In the refinement of the structure a scattering curve for carbon and oxygen (Table 1) was constructed from comparisons of $|F_o|$ and $|F_c|$ values, and used in the calculation of F_c's.

When calculating F_c values for zero-layer reflexions, with separate treatment of hydrogen atoms, the scattering curve of Morrison & Robertson (1949) was used.

Electron-density projections

A Fourier projection was made along the b axis, by addition of successive ripples starting with the strongest. Good resolution of the atoms was obtained and the z co-ordinates from this projection were used in the production of a projection along the a axis. Both were refined by the usual method of successive approximations. Line sections through some of the atoms, and a bounded projection along the a axis, were made, but the progress of refinement was slow.

Finally, difference maps, using (F_o-F_c) as Fourier coefficients, were tried and proved very informative. These projections revealed that the main cause of discrepancies between F_o's and F_c's had been the hydrogen atoms, which had not been included separately in the calculation of F_c's.

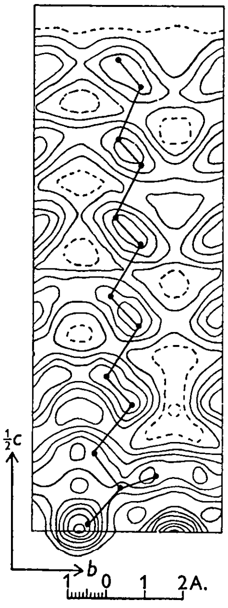

Fig. 2.

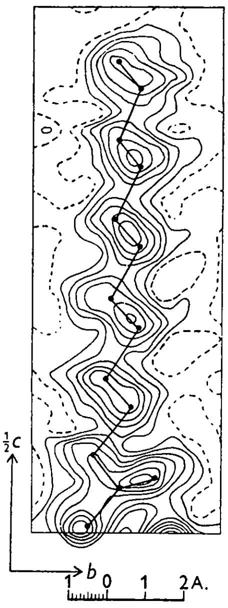

Fig. 3.

Fig. 2. Fourier projection along the a axis.

Fig. 3. A bounded section from $x=\frac{1}{4}$ to $x=\frac{3}{4}$ projected along the a axis.

Those hydrogen atoms not masked by carbon atoms in the projections appeared as positive peaks on the difference maps, and were then included in the structure-factor calculations, the remaining CH groups being assigned an effective atomic number of 7.

In the *a*-axis projection the carbon atoms were also moved in the directions of steepest ascent on a second difference map obtained with the new F_c values. The magnitude of the shifts was found by trial and error.

This treatment substantially reduced the figure of merit $\Sigma|F_o-F_c|\div\Sigma|F_o|$, from 26 to 21 % for the *b*-axis projection and from 49 to 29 % for the *a*-axis projection.

The final co-ordinates of the atoms are given in Table 2.

The hydrogen co-ordinates are those measured directly on the difference maps, and are much less accurate than the co-ordinates of the carbon atoms. No attempt was made to adjust the carbon–hydrogen distances to fit the accepted bond length, or to refine the hydrogen co-ordinates.

As each hydrogen atom was resolved in only one projection, either the *x* or the *y* co-ordinate remains undetermined, and, in the calculation of the general structure factors, hydrogen atoms could not be included.

In Tables 3 and 4, the observed and calculated structure factors are given for the zero-layer and *n*-layer reflexions respectively. The F_c values were calculated by treating each CH_2 group as a single scattering unit, whereas F_c(H) are structure factors calculated treating carbon and hydrogen atoms as separate.

Table 2. *Co-ordinates of the atoms*

Atom	*x/a*	*y/b*	*z/c*
OH	0·3933	0·3000	0·0067
C_1	0·4513	0·4667	0·0429
O	0·5457	0·6533	0·0538
C_2	0·4000	0·3300	0·0750
C_3	0·4900	0·5267	0·1208
C_4	0·4217	0·3917	0·1483
C_5	0·5167	0·5600	0·1958
C_6	0·4467	0·4100	0·2242
C_7	0·5433	0·5667	0·2739
C_8	0·4767	0·4333	0·2992
C_9	0·5690	0·5733	0·3483
C_{10}	0·4983	0·4567	0·3742
C_{11}	0·5867	0·5633	0·4237
C_{12}	0·5167	0·4533	0·4492

Atom	*x/a*	*z/c*
H_1	0·300	0·059
H_3	0·604	0·139
H_5	0·313	0·134
H_7	0·604	0·208
H_9	0·333	0·208
H_{11}	0·650	0·288
H_{13}	0·377	0·283
H_{15}	0·704	0·367
H_{17}	0·380	0·353
H_{19}	0·714	0·437
H_{21}	0·374	0·426
H_{23}	0·560	0·479

Atom	*y/b*	*z/c*
H_2	0·250	0·078
H_4	0·747	0·128
H_6	0·247	0·155
H_8	0·753	0·203
H_{10}	0·253	0·236
H_{12}	0·753	0·280
H_{14}	0·250	0·307
H_{16}	0·747	0·340
H_{18}	0·247	0·372
H_{20}	0·747	0·416
H_{22}	0·257	0·453
H_{23}	0·753	0·479

Table 3. (*h0l*) *and* (0*kl*) *reflexions*

hkl	$\|F_o\|$	F_c(H)	F_c
001	56·3	55·9	53·9
002	13·1	18·1	19·9
003	41·6	42·2	40·5
004	<1·4	0·1	−5·7
005	24·4	24·7	27·0
006	11·9	−8·9	−17·8
007	11·0	15.3	17·8
008	22·2	−22·1	−20·1
009	3·4	6·1	8·8
0,0,10	27·8	−21·2	−27·4
0,0,11	7·6	5·7	11·2
0,0,12	40·7	−34·0	−38·8
0,0,13	4·3	−2·8	−1·3
0,0,14	51·1	42·8	44·0
0,0,15	9·4	8·5	4·6
0,0,16	14·0	10·8	16·0
0,0,17	10·3	8·6	7·9
0,0,18	7·6	6·4	3·5
0,0,19	7·9	4·9	2·2
0,0,20	8·2	4·2	3·5
0,0,21	6·0	5·5	4·1
0,0,22	<4·3	3·7	7·7
0,0,23	<4·3	1·4	1·7
0,0,24	<4·4	2·8	0·4
0,0,25	<4·5	−0·1	1·4
0,0,26	12·7	12·3	11·4
200	190·5	184·9	212·5
201	37·5	19·7	19·2
202	47·3	41·2	47·6
203	7·0	10·3	3·6
204	7·4	12·8	11·3
205	<2·8	2·5	4·2
206	<2·8	1·5	−1·8
207	4·3	0·7	5·1
208	4·4	−5·7	−6·7
209	<3·3	3·6	2·9
2,0,10	3·5	−4·8	−7·6
2,0,11	<3·6	6·2	10·6
2,0,12	31·6	31·0	−40·8
2,0,13	<3·9	−6·5	0·0
2,0,14	14·1	20·8	23·4
2,0,15	5·9	5·5	4·0
2,0,16	6·1	11·3	16·3
2,0,17	<4·4	5·6	−4·6
$20\bar{1}$	11·6	9·4	2·0
$20\bar{2}$	68·0	−70·1	−86·9
$20\bar{3}$	20·9	13·8	17·8
$20\bar{4}$	23·6	−20·6	30·0
$20\bar{5}$	11·8	6·6	7·3
$20\bar{6}$	18·7	−17·6	28·8
$20\bar{7}$	<1·9	0·6	0·0
$20\bar{8}$	31·1	−24·2	−25·8
$20\bar{9}$	16·2	−15·2	−11·0
$2,0,\overline{10}$	30·9	−26·0	−33·5
$2,0,\overline{11}$	20·8	−15·6	−16·2
$2,0,\overline{12}$	34·5	−24·5	−25·9
$2,0,\overline{13}$	22·8	−18·7	−24·0
$2,0,\overline{14}$	20·6	−24·2	−15·4
$2,0,\overline{15}$	19·6	−12·5	−17·5
$2,0,\overline{16}$	8·4	−7·2	−4·2
$2,0,\overline{17}$	<3·1	−2·2	−4·0
$2,0,\overline{18}$	<3·2	2·2	−0·5
$2,0,\overline{19}$	<3·4	−0·3	−2·2
$2,0,\overline{20}$	7·1	4·3	8·0
$2,0,\overline{21}$	<3·8	3·3	2·0
$2,0,\overline{22}$	7·6	7·3	9·3
$2,0,\overline{23}$	<3·9	−1·2	−0·7
$2,0,\overline{24}$	5·8	5·3	1·9
$2,0,\overline{25}$	<4·2	−1·9	−0·9
$2,0,\overline{26}$	15·1	13·5	15·7
$2,0,\overline{27}$	<4·4	2·2	1·4
$2,0,\overline{28}$	25·5	−24·1	−24·7
$2,0,\overline{29}$	12·8	−6·2	−6·0
$2,0,\overline{30}$	12·7	−8·9	−10·6
$2,0,\overline{31}$	6·3	−4·6	−3·9
$2,0,\overline{32}$	<4·4	−3·2	−4·2
400	14·8	16·4	22·8
401	<3·4	−10·0	−7·5
402	<3·5	3·7	4·2
403	<3·6	−8·2	−12·2
404	5·3	−1·6	−0·8
405	<3·9	−7·5	−6·3
406	<4	−1·5	0·1
407	<4	−4·6	−2·4
408	6·0	−1·3	−1·5
409	<4	0	−1·3
4,0,10	<4·4	3·0	4·6
4,0,11	<4·5	5·4	6·5
4,0,12	15·6	−25·7	−29·6
$40\bar{1}$	9·1	−11·2	−14·8
$40\bar{2}$	44·0	−40·1	−50·2
$40\bar{3}$	<3·1	−3·8	−3·4
$40\bar{4}$	3·0	−10·3	−5·6
$40\bar{5}$	<2·9	−5·7	−4·0

Table 3 (*cont.*)

hkl	$\lvert F_o \rvert$	F_c(H)	F_c
$40\bar{6}$	2·9	−9·2	−10·7
$40\bar{7}$	2·8	−7·9	−7·4
$40\bar{8}$	17·8	−15·9	−13·2
$40\bar{9}$	17·8	−21·5	−13·6
$4,0,\overline{10}$	24·9	−22·6	20·8
$4,0,\overline{11}$	25·2	−20·7	−20·0
$4,0,\overline{12}$	44·0	−36·3	−31·6
$4,0,\overline{13}$	36·4	−24·4	−27·4
$4,0,\overline{14}$	90·6	−82·5	−76·3
$4,0,\overline{15}$	37·8	−22·2	−22·1
$4,0,\overline{16}$	8·6	19·7	13·6
$4,0,\overline{17}$	14·3	−8·0	−12·0
$4,0,\overline{18}$	4·6	7·7	8·1
$4,0,\overline{19}$	< 3·3	−3·4	−4·3
$4,0,\overline{20}$	4·9	6·1	−12·8
$4,0,\overline{21}$	< 3·5	0·1	−1·7
$4,0,\overline{22}$	5·1	9·2	7·8
$4,0,\overline{23}$	< 3·8	−2·8	−2·1
$4,0,\overline{24}$	5·5	5·4	4·2
$4,0,\overline{25}$	< 4·0	−0·7	−0·3
$4,0,\overline{26}$	5·8	4·0	8·3
$4,0,\overline{27}$	< 4·3	1·1	1·1
$4,0,\overline{28}$	69·9	−37·3	−40·8
$4,0,\overline{29}$	17·8	−8·5	−6·2
$4,0,\overline{30}$	< 4·5	−3·2	−5·8
$4,0,\overline{31}$	6·4	−5·4	−5·2
$6,0,\overline{12}$	< 3·7	−12·1	−16·1
$6,0,\overline{13}$	< 3·7	−4·5	−5·9
$6,0,\overline{14}$	28·5	−29·7	−35·7
$6,0,\overline{15}$	< 3·8	−0·7	−2·4
$6,0,\overline{16}$	31·3	24·6	40·3
$6,0,\overline{17}$	< 3·8	−0·1	−5·6
$6,0,\overline{18}$	< 3·8	8·3	10·2
$6,0,\overline{19}$	< 3·8	0·8	0·2
$6,0,\overline{20}$	< 3·9	6·1	8·1
$6,0,\overline{21}$	< 3·9	2·7	−0·3
$6,0,\overline{22}$	< 4·0	7·6	3·5
$6,0,\overline{23}$	< 4·0	4·2	2·5
$6,0,\overline{24}$	5·8	4·1	4·7
$6,0,\overline{25}$	5·9	4·9	6·8
$6,0,\overline{26}$	< 4·2	1·3	1·0
$6,0,\overline{27}$	6·1	6·0	6·4
$6,0,\overline{28}$	34·0	−23·7	−29·3
$6,0,\overline{29}$	< 4·4	0·4	1·5
$6,0,\overline{30}$	8·9	10·0	10·3
$6,0,\overline{31}$	< 4·5	−1·3	−1·7
$8,0,\overline{16}$	20·0	27·1	33·4
$8,0,\overline{29}$	6·4	3·2	4·8
010	0	0	0
011	10·3	−10·0	−8·1
012	20·5	−18·9	−8·3
013	12·2	−5·2	−2·5
014	2·9	0·2	3·0
015	< 1·9	0·4	0
016	< 2·2	4·8	8·7
017	< 2·5	2·7	1·0
018	< 2·5	3·5	3·6
019	11·7	−7·6	−7·8
0,1,10	< 2·7	0·3	−6·6
0,1,11	4·1	−6·8	−9·2
0,1,12	13·3	16·4	16·0
0,1,13	< 3·2	−4·1	−4·8
0,1,14	42·3	−40·2	−35·9
0,1,15	4·9	−9·0	−12·2
0,1,16	5·1	−11·1	−13·0
0,1,17	3·7	−6·4	−6·3
0,1,18	< 3·9	−3·7	−4·3
020	48·6	51·3	79·3
021	17·2	−30·1	−35·9
022	27·4	−25·1	−29·4
023	12·5	−9·2	−13·2
024	17·9	−18·5	−22·0
025	5·8	−0·5	0·9
026	8·3	−8·3	−8·8
027	3·0	5·1	8·1
028	4·4	−6·0	−5·8
029	< 3·1	1·0	3·1
0,2,10	4·7	−8·6	−11·8
0,2,11	3·4	−3·0	−0·7
0,2,12	29·7	−25·8	−29·9
0,2,13	19·4	−17·0	−16·8
0,2,14	< 3·8	−2·3	0·8
0,2,15	5·5	−8·3	−9·6
030	0		0
031	< 3·8	0·4	0
032	< 3·8	−1·0	−1·2
033	< 3·8	1·5	1·0
034	< 3·8	2·3	1·6
035	< 3·8	−0·5	−1·4
036	3·7	2·1	3·4
037	3·8	−2·1	2·2
038	< 3·8	−0·3	1·1
039	< 3·8	−5·4	−5·6
0,3,10	< 4·1	−0·3	−1·4
0,3,11	< 4·4	−3·4	−3·6
0,3,12	5·9	16·7	19·6
0,3,13	< 4·2	5·6	6·2
0,3,14	6·1	−19·3	−21·9
048	4·4	4·4	2·8
049	6·3	3·7	2·7
0,4,10	6·3	3·9	2·5
0,4,11	4·5	4·1	3·2

Table 4. *General reflexions*

hkl	$\lvert F_o \rvert$	F_c
110	152·3	233·5
111	10·1	1·7
112	< 1·3	17·6
113	< 1·8	1·8
114	1·9	−6·3
115	< 2·5	5·9
116	10·7	−8·0
117	< 2·5	10·7
118	12·1	−10·7
119	< 3·1	5·9
1,1,10	10·4	−14·8
1,1,11	< 3·1	8·5
1,1,12	33·1	−38·8
1,1,13	9·7	−6·3
1,1,14	10·2	21·1
$11\bar{1}$	< 1·2	0·7
$11\bar{2}$	22·5	−46·5
$11\bar{3}$	9·0	17·1
$11\bar{4}$	9·1	−24·8
$11\bar{5}$	5·9	13·4
$11\bar{6}$	10·5	−19·5
$11\bar{7}$	< 1·7	10·5
$11\bar{8}$	17·4	−19·7
$11\bar{9}$	4·2	−0·5
$1,1,\overline{10}$	25·0	−26·8
$1,1,\overline{11}$	11·0	−5·2
$1,1,\overline{12}$	37·2	−32·8
$1,1,\overline{13}$	19·8	−13·5
$1,1,\overline{14}$	12·9	16·4
$1,1,\overline{15}$	< 3·0	−2·8
$1,1,\overline{16}$	< 3·1	5·5
$1,1,\overline{17}$	4·7	2·3
$1,1,\overline{18}$	7·0	−3·8
$1,1,\overline{19}$	7·3	0·1
$1,1,\overline{20}$	5·4	3·4
$1,1,\overline{21}$	5·7	3·3
210	64·6	73·9
211	33·6	51·5
212	23·9	19·3
213	17·5	23·2
214	15·1	8·2
215	12·4	11·6
216	5·8	3·6
217	4·3	6·5
218	< 3·1	0·8
219	< 3·3	0·6
2,1,10	< 3·5	−4·0
2,1,11	< 3·8	−0·9
2,1,12	7·5	12·6
2,1,13	4·0	4·4
$21\bar{1}$	47·0	41·4
$21\bar{2}$	28·0	−12·8
$21\bar{3}$	30·8	24·2
$21\bar{4}$	7·5	1·2
$21\bar{5}$	10·6	6·9
$21\bar{6}$	< 1·9	−8·7
$21\bar{7}$	5·5	1·2
$21\bar{8}$	< 2·0	−5·7
$21\bar{9}$	9·4	9·6
$2,1,\overline{10}$	< 2·2	4·4
$2,1,\overline{11}$	12·3	11·8
$2,1,\overline{12}$	3·5	2·4
$2,1,\overline{13}$	7·4	19·4
$2,1,\overline{14}$	91·6	73·3
$2,1,\overline{15}$	20·6	20·0
$2,1,\overline{16}$	6·0	9·1
$2,1,\overline{17}$	10·8	10·4
$2,1,\overline{18}$	4·6	4·4
$2,1,\overline{19}$	6·8	4·3
$2,1,\overline{20}$	5·1	0·4
310	49·3	71·9
311	5·1	1·9
312	5·4	15·9
313	< 2·5	−8·2
314	< 3·1	2·7
315	3·1	2·8
316	< 3·1	1·9
3,1,12	14·3	30·5
$31\bar{1}$	< 2·7	−4·2
$31\bar{2}$	28·5	−54·5
$31\bar{3}$	12·1	7·7
$31\bar{4}$	< 2·3	−12·1
$31\bar{5}$	6·8	3·0
$31\bar{6}$	< 2·5	−12·4
$31\bar{7}$	< 2·5	−1·6
$31\bar{8}$	4·7	−11·5
$31\bar{9}$	6·8	−7·3
$3,1,\overline{10}$	12·9	−14·2
$3,1,\overline{11}$	13·2	−11·9
$3,1,\overline{12}$	16·2	−17·4
$3,1,\overline{13}$	7·6	−13·9
$3,1,\overline{14}$	32·5	−34·5
$3,1,\overline{15}$	4·0	−4·5
$3,1,\overline{16}$	10·2	11·8
$3,1,\overline{17}$	3·1	0·4
$3,1,\overline{18}$	11·1	8·5
$3,1,\overline{19}$	4·7	0·1
$3,1,\overline{20}$	6·9	8·3
$3,1,\overline{21}$	5·1	0·9
$3,1,\overline{22}$	5·3	7·6
$3,1,\overline{23}$	< 3·8	−1·2
$3,1,\overline{24}$	5·6	5·0
$3,1,\overline{25}$	< 4·1	−0·2
$3,1,\overline{26}$	11·8	14·3
$3,1,\overline{27}$	6·1	3·3
$3,1,\overline{28}$	27·8	−28·1
$3,1,\overline{29}$	6·3	−1·4

Table 4 (*cont.*)

hkl	$\vert F_o\vert$	F_o
410	22·1	29·3
411	11·9	12·8
412	12·2	14·3
413	5·2	7·7
$41\bar{1}$	11·3	10·1
$41\bar{2}$	< 3·2	−17·0
$41\bar{3}$	8·7	5·1
$41\bar{4}$	< 3·1	−4·3
$41\bar{5}$	< 3·1	−2·9
$41\bar{6}$	5·8	−9·1
$41\bar{7}$	8·1	−4·8
$41\bar{8}$	8·0	−7·4
$41\bar{9}$	5·6	−4·8
$4,1,\overline{10}$	4·0	3·3
$4,1,\overline{11}$	4·0	−5·6
$4,1,\overline{12}$	< 3·1	4·2
$4,1,\overline{13}$	< 3·1	1·7
$4,1,\overline{14}$	25·0	34·6
$4,1,\overline{15}$	< 3·1	−2·4
$4,1,\overline{16}$	20·4	−19·1
$4,1,\overline{17}$	< 3·1	−0·8
$4,1,\overline{18}$	< 3·1	−3·3
$4,1,\overline{19}$	< 3·4	−0·4
$4,1,\overline{20}$	< 3·4	−0·6
$4,1,\overline{30}$	6·3	−5·7
$5,1,\overline{14}$	27·9	−37·8
$5,1,\overline{16}$	25·0	32·3
$5,1,\overline{28}$	34·0	30·6
$61\bar{9}$	< 3·8	−6·9
$6,1,\overline{10}$	5·3	−5·8
$6,1,\overline{11}$	< 3·8	−10·1
$6,1,\overline{12}$	7·4	−5·5
$6,1,\overline{13}$	< 3·8	−8·5
$6,1,\overline{14}$	7·3	−3·3
$6,1,\overline{15}$	16·4	−10·5
$6,1,\overline{28}$	8·8	−13·6
$6,1,\overline{29}$	6·2	−8·1
$7,1,\overline{16}$*	18·6	32·9
$7,1,\overline{28}$	12·5	−17·9
120	24·7	40·4
121	4·0	6·1
122	< 3·1	−2·7
123	< 3·1	5·2
124	3·0	2·4
125	3·1	1·5
126	< 3·2	5·0
127	< 3·4	1·1
128	< 3·6	1·4
129	< 3·8	5·2
1,2,10	5·0	−6·1
1,2,11	< 3·8	−5·4
1,2,12	5·4	19·9
1,2,13	5·5	3·2
1,2,14	< 3·8	16·3
1,2,15	5·9	1·9
$12\bar{1}$	12·3	17·8
$12\bar{2}$	7·7	10·9
$12\bar{3}$	5·5	10·0
$12\bar{4}$	3·8	−4·4
$12\bar{5}$	3·9	3·7
$12\bar{6}$	8·0	−10·8
$12\bar{7}$	4·0	1·2
$12\bar{8}$	5·9	−6·6
$12\bar{9}$	< 3·1	7·0
$1,2,\overline{10}$	< 3·1	−1·0
$1,2,\overline{11}$	< 3·1	4·8
$1,2,\overline{12}$	18·6	−19·8
$1,2,\overline{13}$	6·8	1·3
$1,2,\overline{14}$	49·3	51·8
130	7·2	7·9
131	5·1	−19·2
132	7·3	−8·7
$13\bar{1}$	5·0	−13·7
$13\bar{2}$	7·1	−6·8

hkl	$\vert F_o\vert$	F_c
$13\bar{3}$	< 3·8	−2·1
$1,3,\overline{11}$	< 3·8	0·3
$1,3,\overline{12}$	8·0	−15·7
$1,3,\overline{13}$	5·7	−10·3
220	29·2	54·5
221	4·2	−17·5
222	8·6	1·5
223	14·0	−11·8
224	9·1	−5·3
225	4·7	−2·0
2,2,12	23·5	−22·7
2,2,13	4·2	−7·6
$22\bar{1}$	< 3·1	−7·4
$22\bar{2}$	17·9	−24·4
$22\bar{3}$	11·2	7·0
$22\bar{4}$	< 2·5	−12·9
$22\bar{5}$	7·8	4·9
$22\bar{6}$	< 2·5	−7·3
$22\bar{7}$	< 2·7	5·5
$22\bar{8}$	< 2·9	−3·8
$22\bar{9}$	< 3·1	0·6
$2,2,\overline{10}$	4·2	−6·2
$2,2,\overline{11}$	6·0	−2·4
$2,2,\overline{12}$	19·2	−16·3
$2,2,\overline{13}$	9·0	−7·8
$2,2,\overline{14}$	< 3·1	0·4
$2,2,\overline{15}$	6·7	7·1
$2,2,\overline{16}$	15·6	14·5
$2,2,\overline{17}$	12·5	6·7
$2,2,\overline{18}$	10·5	6·1
$2,2,\overline{19}$	5·4	2·0
$2,2,\overline{20}$	5·6	3·0
$2,2,\overline{21}$	< 3·8	0·1
$2,2,\overline{22}$	< 4·0	4·0
$2,2,\overline{23}$	< 4·2	−0·9
$2,2,\overline{24}$	< 4·4	3·8
$2,2,\overline{25}$	< 4·5	0·6
$2,2,\overline{26}$	8·9	8·5
$2,2,\overline{27}$	< 4·5	4·3
$2,2,\overline{28}$	8·9	−8·9
230	10·5	16·7
238	4·3	−1·6
239	5·2	−4·8
2,3,10	6·2	−7·9
2,3,11	4·4	−6·2
$23\bar{1}$	< 3·8	−4·3
$23\bar{2}$	7·3	−14·4
$23\bar{3}$	< 3·8	1·6
$23\bar{4}$	10·2	−6·4
$23\bar{5}$	10·1	2·7
$23\bar{6}$	10·1	−5·5
$23\bar{7}$	10·3	2·9
$23\bar{8}$	10·4	−4·2
$23\bar{9}$	5·2	1·9
$2,3,\overline{10}$	10·6	−5·9
$2,3,\overline{11}$	5·3	−5·7
$2,3,\overline{12}$	20·3	−17·1
$2,3,\overline{13}$	17·6	−12·4
$2,3,\overline{14}$	21·1	30·4
$2,3,\overline{15}$	< 4·4	−9·3
$2,3,\overline{16}$	16·5	−10·4
$2,4,\overline{19}$	4·4	−1·7
$2,4,\overline{20}$	4·4	−2·9
$2,4,\overline{21}$	4·3	−2·6
320	34·1	41·0
321	14·4	9·0
322	6·6	−11·6
3,2,10	4·2	−6·7
$32\bar{1}$	13·4	10·0
$32\bar{2}$	< 3·1	−18·8
$32\bar{3}$	8·2	6·9
$32\bar{4}$	< 3·1	−9·1
$32\bar{5}$	< 3·1	−0·3
$32\bar{6}$	5·5	−11·3

hkl	$\vert F_o\vert$	F_c
$32\bar{7}$	5·5	−1·1
$32\bar{8}$	9·9	−6·8
$32\bar{9}$	8·0	1·1
$3,2,\overline{10}$	8·0	−1·3
$3,2,\overline{11}$	5·8	−1·1
$3,1,\overline{12}$	5·9	0·7
$3,2,\overline{13}$	4·3	3·9
$3,2,\overline{14}$	27·8	58·5
$3,2,\overline{15}$	< 3·1	4·8
$3,2,\overline{16}$	11·4	−10·4
330	5·5	11·1
$3,3,\overline{15}$	4·0	14·5
$3,3,\overline{16}$	11·5	19·0
$3,4,\overline{11}$	< 4·4	−4·4
$3,4,\overline{12}$	8·7	−7·3
$3,4,\overline{13}$	8·7	−11·5
$3,4,\overline{14}$	8·8	17·2
$3,4,\overline{15}$	< 4·4	−7·8
$3,4,\overline{16}$	8·8	−9·5
420	15·5	20·8
421	3·6	2·8
$42\bar{1}$	6·7	6·5
$42\bar{2}$	< 3·1	−7·0
$42\bar{3}$	9·1	4·2
$42\bar{4}$	3·1	−4·1
$42\bar{5}$	4·3	0·3
$42\bar{6}$	4·3	−3·5
$42\bar{7}$	4·3	−3·2
$42\bar{8}$	4·3	1·0
$42\bar{9}$	4·2	3·1
$4,2,\overline{10}$	< 3·1	2·8
$4,2,\overline{11}$	< 3·1	5·4
$4,2,\overline{12}$	< 3·1	−1·8
$4,2,\overline{13}$	8·7	10·1
$4,2,\overline{14}$	< 3·1	−2·0
$4,2\ \overline{15}$	14·1	16·8
$4,2\ \overline{16}$	24·9	25·3
$4,2,\overline{17}$	11·4	4·9
$4,2,\overline{18}$	9·6	8·6
$4,2,\overline{19}$	< 3·8	0
$4,2,\overline{20}$	< 3·8	3·4
$4,2,\overline{21}$	< 3·8	2·8
$4,2,\overline{22}$	< 3·8	3·2
$4,2,\overline{23}$	< 3·8	−1·2
$4,2,\overline{24}$	5·6	4·3
$4,2,\overline{25}$	4·1	2·9
$4,2,\overline{26}$	11·7	7·6
$4,2,\overline{27}$	8·4	8·2
$4,2,\overline{28}$	17·0	−15·2
430	11·5	15·9
$43\bar{1}$	< 3·8	0·8
$43\bar{2}$	3·9	−20·0
$43\bar{3}$	3·9	9·1
$43\bar{4}$	< 3·8	0·5
$43\bar{5}$	< 3·8	3·2
$43\bar{6}$	< 3·8	−2·5
$43\bar{7}$	< 3·8	1·9
$43\bar{8}$	< 3·8	−1·1
$43\bar{9}$	< 3·8	−1·4
$4,3,\overline{10}$	< 3·8	−3·4
$4,3,\overline{11}$	3·8	−9·1
$4,3,\overline{12}$	3·8	−3·9
$4,3,\overline{13}$	3·8	−8·4
$4,3,\overline{14}$	10·9	24·7
$4,3\ \overline{15}$	< 3·8	−2·9
$4,3,\overline{16}$	13·6	−14·2
$4,3,\overline{17}$	< 3·8	4·3
$4,3,\overline{18}$	4·0	−3·4
$4,3,\overline{19}$	11·5	2·4
$4,3,\overline{20}$	8·2	1·7
$4,3,\overline{21}$	4·2	5·0
$4,4,\overline{18}$	8·5	−1·5
$4,4,\overline{19}$	8·5	−2·0
$4,4,\overline{20}$	8·5	−2·9

* May be $7,1,\overline{15}$

Discussion of the results

Closer examination of the projections revealed that in lauric acid the hydrocarbon chain is not quite straight. It is noticeably bent in the a-axis projection. The average vector between alternate carbon atoms has been calculated by the least-squares method; its components are given in Table 5, in which the linear term in the y component is due to the curvature of the chain.

Table 5. *Components of average vector between alternate carbon atoms*

Co-ordinate	Fractional components	Rectangular components (A.)
x	$0{\cdot}02473 \pm 0{\cdot}0005$	$-1{\cdot}4470 \pm 0{\cdot}006$
y	$(0{\cdot}0644 \pm 0{\cdot}005) - (0{\cdot}0068 \pm 0{\cdot}0006)\,N$	$(0{\cdot}319 \pm 0{\cdot}025) - (0{\cdot}0338 \pm 0{\cdot}003)\,N$
z	$0{\cdot}0752 \pm 0{\cdot}0001$	$2{\cdot}0617 \pm 0{\cdot}005$

The angles of constant direction, as defined by Vand, Aitken & Campbell (1949), are $\alpha_0 = 92^\circ\,28'$, $\beta_0 = 125^\circ\,1'$, and the angle of tilt $\tau = 54^\circ\,52'$.

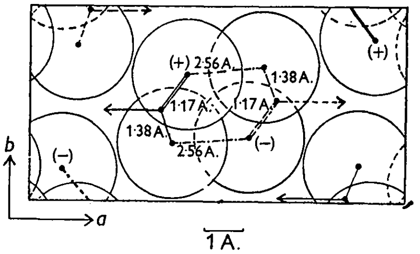

Fig. 4. Perpendicular projection of the oxygen atoms on the ab plane. The oxygen atoms marked (+) or (−) are 1.48 A. above or below the ab plane, the unmarked atoms approximately in that plane.

The average distance between alternate carbon atoms is $s = 2{\cdot}521 \pm 0{\cdot}007$ A. This is significantly shorter than the distance in soaps, namely, 2·610 A., found in strontium laurate by Morley & Vand (1949) and $2{\cdot}598 \pm 0{\cdot}007$ A. found in potassium caprate by Vand, Lomer & Lang (1949). One can thus conclude that this distance varies from compound to compound. It is probable that it depends on the compression forces within the crystal; a lateral compression would tend to elongate the zigzag hydrocarbon chains.

The co-ordinates of the atoms in the carboxyl group are not sufficiently accurate to warrant a detailed discussion of the bond lengths; however, it can be seen that, as in dicarboxylic acids recently studied by Robertson and co-workers, the two C—O and C=O bonds are of unequal length, being 1·38 and 1·17 A., respectively.

The molecules are joined in pairs by hydrogen bridges 2·56 A. in length between the double-bond oxygen of the upper molecule and the single-bond oxygen of the lower molecule and vice versa. The packing of the carboxyl groups is shown in Fig. 4.

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References

Francis, F. & Piper, S. H. (1939). *J. Amer. Chem. Soc.* **61**, 577.

Morley, W. M. & Vand, V. (1949). *Nature, Lond.*, **163**, 285.

Morrison, J. D. & Robertson, J. M. (1949). *J. Chem. Soc.* p. 933.

Thibaud, J. & Duprè de la Tour, F. (1930*a*). *C.R. Acad. Sci., Paris*, **190**, 945.

Thibaud, J. & Duprè de la Tour, F. (1930*b*). *C.R. Acad. Sci., Paris*, **191**, 200.

Thibaud, J. & Duprè de la Tour, F. (1932). *J. Chim. phys.* **29**, 153.

Tunell, G. (1939). *Amer. Min.* **24**, 448.

Vand, V., Aitken, A. & Campbell, R. K. (1949). *Acta Cryst.* **2**, 398.

Vand, V., Lomer, T. R. & Lang, A. (1949). *Acta Cryst.* **2**, 214.