Table 4 (cont.)

	1	2	3	4
C(26)			−0·008	
C(27)			−0·006	
C(28)			0·016	
C(29)			−0·021	
C(30)				0·019
C(31)				−0·013
C(32)				0·002
C(33)				0·010
C(34)				−0·018

Equations of planes. $lX+mY+nZ=p$
with $X=xa+zc\cos\beta$, $Y=yb$ and $Z=zc\sin\beta$.

1	0·8435	−0·4978	0·2020	3·666
2	0·8341	−0·5217	0·1791	3·472
3	0·9819	−0·0492	0·1827	8·806
4	−0·6070	0·7610	−0·2290	1·154
Mo(2)S(3)S(4)	0·8478	0·4884	0·2066	3·749
C₅H₅ normals	−0·1732	0·1546	0·9727	2·843

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The Crystal and Molecular Structure of Octa-cis-2,trans-6-diene-1,8-dioic Acid

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The crystal structure of octa-cis-2,trans-6-diene-1,8-dioic acid, $C_8O_4H_{10}$, has been determined from three-dimensional X-ray diffraction data. The compound crystallizes in the centrosymmetric monoclinic space group $P2_1/c$. The unit cell contains four molecules and has the dimensions $a=7·75\pm0·02$, $b=17·34\pm0·03$, $c=10·10\pm0·02$ Å; $\beta=138°52'\pm30'$. The molecules are associated in rows in the crystal lattice. The molecular rows lie in planes parallel to (10$\bar{1}$), alternately oriented along the $a+b+c$ and $a-b+c$ crystallographic directions. The values of the rotation angles around the single bonds C(5)–C(6) and C(3)–C(4) adjacent to the double bond in trans configuration and to the double bond in cis configuration are 126·6° and −97° respectively.

Introduction

The determination of the crystal and molecular structure of octa-cis-2,trans-6-diene-1,8-dioic acid,
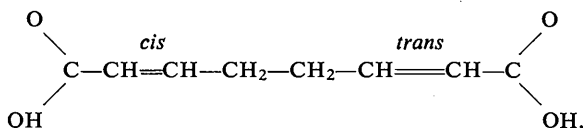
is part of a research programme whose aim is the determination of the values of internal rotation angles about single bonds adjacent to double bonds. As model compounds a series of aliphatic unsaturated bicarboxylic acids have been studied (Ganis & Martuscelli, 1966; Martuscelli, 1967). In fact, though the problem of hindered rotation around single bonds adjacent to double bonds has been extensively studied on simple molecules in the vapour and liquid phases by spectroscopic techniques (nuclear magnetic resonance, microwave and Raman spectroscopy; electron diffraction), only a few values of the conformational parameters determined by X-ray methods in the solid state are to be found in the literature.

Experimental and unit-cell parameters

Transparent plate-shaped crystals of octa-*cis*-2,*trans*-6-diene-1,8-dioic acid (melting point 113–114 °C) elongated along the **a** + **c** axis were grown by slow evaporation, at room temperature, of a saturated methanolic or benzenic solution. The space group and unit-cell dimensions were determined from oscillation and Weissenberg photographs taken about crystallographic axes with Cu *Kα* radiation. The density of the crystals was measured by the flotation method.

Crystal data

C$_8$O$_4$H$_{10}$ M.W. 170·18
Monoclinic $P2_1/c$
$a = 7·75 \pm 0·02$, $b = 17·34 \pm 0·03$, $c = 10·10 \pm 0·02$ Å,
    $\beta = 138° 52' \pm 30'$.

$U = 893·66$ Å^3
$Z = 4$

Density $\left\{ \begin{array}{l} \text{experimental} \\ \\ \text{X-ray} \end{array} \right.$ $\begin{array}{l} 1·28 \pm 0·01 \text{ g.cm}^{-3} \\ \\ 1·26 \quad \text{g.cm}^{-3} \end{array}$
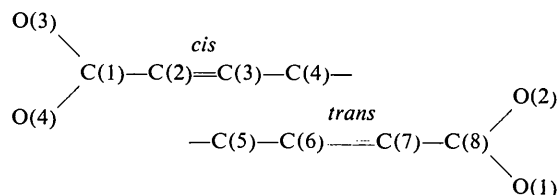
Intensity data were collected by nickel-filtered copper radiation with the use of multiple-film equi-inclination Weissenberg photographs about the **a** + **c** axis for layer lines 0 to 4. The zero layers about the *c* axis and about the *a* axis have been recorded to provide cross-correlation of the **a** + **c** axis data. The number of independent reflexions observed was 364. The intensities were evaluated by eye estimation, corrected for change of spot shape on upper layer equi-inclination photographs (Phillips, 1956) and reduced to structure amplitudes by a data reduction program written for an IBM 1620 computer (Damiani, De Santis, Giglio & Ripamonti, 1962). No absorption correction was applied.

Structure determination

In order to found a trial model of the structure of octa-*cis*-2,*trans*-6-diene-1,8-dioic acid, we followed a method that we had applied successfully to a series of dicarboxylic acids (Corradini, Ganis, Pedone, Sirigu & Temussi, 1967; Corradini, Ganis, Avitabile & Martuscelli, 1966; Ganis, Martuscelli & Avitabile, 1966; Martuscelli & Avitabile 1967; Martuscelli & Pedone, 1968). We supposed that the molecules of octa-*cis*-2, *trans*-6-diene-1,8-dioic acid were associated in rows through the formation of intermolecular hydrogen bonds between carboxylic groups related by crystallographic inversion centres. Assuming the internal parameters of Table 1 for the molecule (on the basis of the data reported in the literature for similar compounds) the periodicity of the molecular rows was found to be 18·44 Å. This periodicity is close to the crystallographic axis (**a** + **b** + **c**) (18·54 Å). Hence we assumed the molecular rows' direction was coincident with the **a** + **b** + **c** crystallographic axis in the crystals. Under this assumption

the only unknown parameter is the rotation angle, Φ, of the molecular rows around the **a** + **b** + **c** axis.

Table 1. *Internal coordinates assumed for the first trial model of octa-cis-2,trans-6-diene-1,8-dioic acid*

O(3)
\
C(1)—C(2)═C(3)—C(4)—   *cis*
/   O(2)
O(4)   *trans*   /
    —C(5)—C(6)═C(7)—C(8)
                                    \
                                    O(1)

Distance	
C–O	1·25 Å
C–C	1·54
C=C	1·33
O–H---O	2·70

Angles	
O–C–C	120°
C–C–C	110
C=C–C	120

Dihedral angles	
O–C(1)–C(2) ∧ C(1)–C(2)–C(3)	0 (180)°
O–C(8)–C(7) ∧ C(8)–C(7)–C(6)	0 (180)
C(2)–C(3)–C(4) ∧ C(3)–C(4)–C(5)	– 130
C(6)–C(5)–C(4) ∧ C(5)–C(4)–C(3)	180
C(8)–C(7)–C(6) ∧ C(5)–C(6)–C(7)	130

* The rotation angles are measured following Natta, Corradini & Bassi (1961).

The best orientation of the molecular rows was obtained by computing the reliability index,

$$R = \Sigma \, ||F_o| - |F_c||/\Sigma \, |F_o|,$$

for the $hk0$ and $0kl$ zones as a function of Φ. An absolute minimum of the R index is obtained for both zones for the same value of the rotation angle Φ ($R_{hk0} = 0·44$; $R_{0kl} = 0·41$). The relative fractional atomic coordinates were used as starting parameters for the refinement of the structure.

Refinement of the structure

The refinement was initially carried out for the (001) and (100) projections by successive Fourier synthesis calculations. The coordinates obtained in this way were used for the final three-dimensional refinement, which was carried out by the block-diagonal-matrix least-squares method. The minimized function was:

$$R_w = \underset{hkl}{\Sigma} \, w(hkl) \left[F_o(hkl) - \frac{1}{K} F_c(hkl) \right]^2,$$

giving a unit value to all the weighting factors $w(hkl)$. Thermal parameters were allowed to vary isotropically at the first stage up to the conventional R value of 0·20. The refinement was then continued by the use of anisotropic thermal parameters for the C and O atoms. In the last stage of the refinement the positions of the

hydrogen atoms were calculated (C–H = 1·10 Å) and introduced into the structure factor calculations with the same isotropic temperature factor ($B = 6$ Å^2). We have not taken into account the carboxylic hydrogen atoms. The scattering factors of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for carbon and oxygen atoms and of McWeeny (1951) for hydrogen atoms were used.

Table 2. *Final fractional atomic coordinates and their standard deviations* (Å × 10^{-2})

	x/a	y/b	z/c	σ(x)	σ(y)	σ(z)
C(1)	0·6282	0·4307	0·7043	3·1	1·8	2·8
C(2)	0·7572	0·3824	0·8829	3·4	2·1	3·1
C(3)	0·7800	0·3071	0·8924	3·6	2·0	3·1
C(4)	0·6798	0·2499	0·7272	3·4	2·1	3·1
C(5)	0·4294	0·2156	0·6186	3·3	2·3	3·3
C(6)	0·3101	0·1712	0·4306	3·4	1·9	3·5
C(7)	0·2388	0·1026	0·3960	3·4	2·2	3·4
C(8)	0·1449	0·0555	0·2228	3·4	2·0	3·1
O(1)	0·0834	0·0133	0·2131	2·4	1·4	2·2
O(2)	0·0869	0·0900	0·0833	2·2	1·3	1·9
O(3)	0·6480	0·5059	0·7389	2·3	1·3	1·9
O(4)	0·5468	0·4040	0·5537	2·4	1·3	1·9
H(2)	0·839	0·412	1·016			
H(3)	0·884	0·281	1·036			
H(4a)	0·826	0·204	0·769			
H(4b)	0·659	0·280	0·620			
H(5a)	0·457	0·176	0·718			
H(5b)	0·293	0·261	0·571			
H(6)	0·287	0·202	0·323			
H(7)	0·244	0·074	0·496			

Table 3. *Comparison between observed* (F_o) *and calculated* (F_c) *structure factors of octa-cis-2,trans-6-diene-1,8-dioic acid*

The refinement was considered complete when the coordinate shifts were less than the corresponding standard deviations. The final value of the reliability index, R was 0·131. The final atomic coordinates, together with the corresponding standard deviations, (Cruickshank, 1949) are reported in Table 2. In Table 3 observed and calculated structure factors are listed.

Table 4 shows the coefficients B_{ij} of the temperature factor in the form:

$$\exp\left[-\tfrac{1}{4}(h^2a^{*2}B_{11}+k^2b^{*2}B_{22}+l^2c^{*2}B_{33}+2hka^*b^*B_{12}\right.$$
$$\left.+2hla^*c^*B_{13}+2klb^*c^*B_{23})\right],$$
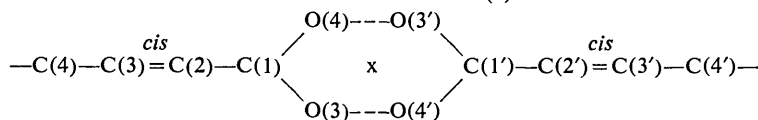
with the corresponding standard deviations.

A composite projection of the electron density distribution is shown in Fig. 1.

The fading out of the intensities with sin θ and the shape of the spots are responsible for the relatively high value of the R index.

Description of the structure

Molecules of octa-cis-2,trans-6-diene-1,8-dioic acid are linked together to form chains by a double hydrogen-bonding system between adjacent carboxylic groups, related by a centre of symmetry. The molecular rows, as in the case of deca-trans-3,trans-7-diene-1,10-dioic acid (Martuscelli, 1967), are not parallel but oblique. In fact, the molecular rows lie in planes parallel to (10$\bar{1}$), alternatively oriented along **a** + **b** + **c** and **a** − **b** + **c** crystallographic directions.

The main feature of the octa-cis-2,trans-6-diene-1,8-dioic crystalline structure is the planarity of the atomic groups:
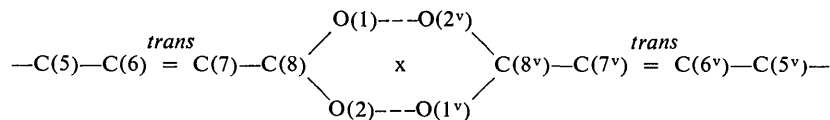
The corresponding least-squares mean planes equations, calculated by the method of Schomaker, Waser, Marsh & Bergman (1959), attributing a unit weight factor to all atoms are:

$$7\cdot13X+1\cdot13Y-4\cdot44Z=1\cdot91,$$
$$6\cdot39X-4\cdot25Y-2\cdot90Z=0\cdot00.$$

The equations are referred to the axes of the unit cell, X, Y, Z being fractional coordinates. The two planes make an angle of 19°.

In Tables 5 and 6 the distances of the atoms from the relative plane are compared with their standard deviations. As already pointed out above the molecular rows are contained in the (10$\bar{1}$) plane, and the packing of the rows in this plane can be seen in Fig. 2, where all the shortest intermolecular contacts are reported. In this layer the structure is made up by an infinite succession of the two molecular planes described above, one containing the cis double bond ('cis' plane) and the other containing the trans double bond ('trans' plane.) The relative packing of the layers can be seen in Fig. 3, and it is characterized by the interlocking of the 'cis' plane of one layer with the 'trans' plane of the neighbouring layers, and vice versa.

Table 5. *Distances* (Å × 10⁻²) *of atoms*
C(4), C(3), C(2), C(1), O(3), O(4), C(4′), C(3′),
C(2′), C(1′), O(3′), O(4′)
from the least-square mean plane of equation:
$$7\cdot13X+1\cdot13Y-4\cdot44Z=1\cdot91$$
and their atomic standard deviations (Å × 10⁻²)

	Distance	σ(x)	σ(y)	σ(z)
C(4)	−0·7	3·4	2·1	3·1
C(3)	3·8	3·7	2·0	3·1

and

Table 4. *Final temperature parameters*

Temperature factors are given in the form:

$$\exp\left[-\tfrac{1}{4}(h^2a^{*2}B_{11}+k^2b^{*2}B_{22}+l^2c^{*2}B_{33}+2hka^*b^*B_{12}+2hla^*c^*B_{13}+2klb^*c^*B_{23})\right].$$

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}	σ(B_{11})	σ(B_{22})	σ(B_{33})	σ(B_{12})	σ(B_{13})	σ(B_{23})
C(1)	11·739	7·782	7·168	−3·039	7·076	−3·420	1·511	1·165	1·330	1·116	1·313	1·007
C(2)	12·930	8·314	9·375	1·633	8·216	0·962	1·668	1·286	1·492	1·235	1·451	1·134
C(3)	16·225	8·280	9·107	0·546	10·129	0·812	1·882	1·271	1·481	1·286	1·527	1·092
C(4)	13·862	9·771	9·483	−4·367	9·068	−1·669	1·654	1·313	1·406	1·374	1·407	1·279
C(5)	11·279	14·520	11·981	−4·770	9·141	−8·456	1·606	1·892	1·731	1·397	1·541	1·524
C(6)	13·048	6·930	14·168	−0·369	11·020	0·061	1·683	1·220	1·859	1·218	1·655	1·216
C(7)	12·437	9·669	13·014	0·754	10·357	0·744	1·623	1·417	1·734	1·299	1·561	1·353
C(8)	13·317	10·164	8·600	0·035	8·610	−1·229	1·688	1·349	1·438	1·297	1·440	1·181
O(1)	16·482	8·302	12·220	−0·120	11·209	0·379	1·332	0·869	1·112	0·920	1·119	0·871
O(2)	13·654	7·983	8·661	0·856	8·060	1·237	1·176	0·826	1·000	0·834	1·003	0·720
O(3)	16·859	7·358	8·280	−3·622	9·282	−3·940	1·243	0·785	0·864	0·873	0·944	0·752
O(4)	15·707	7·452	7·677	−0·412	8·739	−2·302	1·204	0·784	0·938	0·837	0·989	0·685

Table 5 (*cont.*)

	Distance	σ(x)	σ(y)	σ(z)
C(2)	3·2	3·4	2·1	3·1
C(1)	−7·0	3·1	1·8	2·8
O(3)	0·2	2·3	1·3	1·9
O(4)	−1·2	2·4	1·3	1·9
C(4′)	0·7	3·4	2·1	3·1
C(3′)	−3·8	3·7	2·0	3·1
C(2′)	−3·2	3·4	2·1	3·1
C(1′)	7·0	3·1	1·8	2·8
O(3′)	−0·2	2·3	1·3	1·9
O(4′)	1·2	2·4	1·3	1·9

Table 6. *Distances* (Å × 10⁻²) *of atoms*
C(5), C(6), C(7), C(8), O(1), O(2), C(5ᵛ), C(6ᵛ),
C(7ᵛ), C(8ᵛ), O(1ᵛ), O(2ᵛ) *from the least-square
mean plane of equation*:
$$6·39X + -4·25Y - 2·90Z = 0 \text{ and}$$
their atomic standard deviations (Å × 10⁻²)

	Distance	σ(x)	σ(y)	σ(z)
C(5)	3·6	3·3	2·3	3·3
C(6)	0·7	3·4	1·9	3·5
C(7)	−5·7	3·4	2·2	3·4
C(8)	4·4	3·4	2·0	2·1
O(1)	−2·8	2·4	1·4	2·2
O(2)	−6·8	2·2	1·3	1·9
C(5ᵛ)	−3·6	3·3	2·3	3·3
C(6ᵛ)	−0·7	3·4	1·9	3·5
C(7ᵛ)	5·7	3·4	2·2	3·4
C(8ᵛ)	−4·4	3·4	2·0	3·1
O(1ᵛ)	2·8	2·4	1·4	2·2
O(2ᵛ)	6·8	2·2	1·3	1·9

Table 7. *Intramolecular distances and angles
with standard deviations*

Distances

C(1)–C(2)	1·496 Å	0·045 Å
C(2)–C(3)	1·311	0·030
C(3)–C(4)	1·555	0·043
C(4)–C(5)	1·455	0·066
C(5)–C(6)	1·552	0·049
C(6)–C(7)	1·246	0·035
C(7)–C(8)	1·530	0·046
C(8)–O(1)	1·261	0·029
C(8)–O(2)	1·261	0·036
C(1)–O(3)	1·329	0·023
C(1)–O(4)	1·217	0·036
C(4)···O(4)	2·925	0·029
O(4)···O(3′)	2·595	0·030
O(2)···O(1)	2·554	0·030

Angles

C(1)–C(2)–C(3)	125·2°	1·5°
C(2)–C(3)–C(4)	128·7	1·2
C(3)–C(4)–C(5)	112·0	1·6
C(4)–C(5)–C(6)	110·6	1·5
C(5)–C(6)–C(7)	123·1	1·8
C(6)–C(7)–C(8)	124·0	1·1
C(7)–C(8)–O(1)	114·9	1·3
C(7)–C(8)–O(2)	119·1	1·2
O(1)–C(8)–O(2)	124·5	1·1
O(4)–C(1)–C(2)	122·7	1·2
O(3)–C(1)–C(2)	113·1	0·9
O(3)–C(1)–O(4)	123·4	1·1

Table 7 (*cont.*)

Dihedral angles

O(4)–C(1)–C(2) ∧ C(1)–C(2)–C(3)	−5·1°
O(3)–C(1)–C(2) ∧ C(1)–C(2)–C(3)	−175·5
C(1)–C(2)–C(3) ∧ C(2)–C(3)–C(4)	−1·1
C(2)–C(3)–C(4) ∧ C(3)–C(4)–C(5)	−97·9
C(3)–C(4)–C(5) ∧ C(4)–C(5)–C(6)	169·4
C(4)–C(5)–C(6) ∧ C(5)–C(6)–C(7)	126·6
C(5)–C(6)–C(7) ∧ C(6)–C(7)–C(8)	−174·0
C(6)–C(7)–C(8) ∧ C(7)–C(8)–O(1)	179·3
C(6)–C(7)–C(8) ∧ C(7)–C(8)–O(2)	−14·2

The lengths of the two independent hydrogen bonds between carboxylic groups of two centrosymmetrically related molecules are 2·595 ± 0·030 and 2·554 ± 0·030 Å respectively, between O(4)---O(3′) and O(2)---O(1ᵛ).

Molecular conformation

Fig. 4 shows a drawing of the molecular model of octa-*cis*-2, *trans*-6,diene-1,8-dioic acid, and the conformational parameters are listed in Table 7, together with their extimated standard deviations. Each carboxylic group lies, within the experimental errors, in the plane of the neighbouring double bond. The C(8)–O(1) and C(8)–O(2) bond lengths are practically equal, while in the other carboxylic group the C(1)–O(3) and C(1)–O(4) distances are rather different. The values of the rotation angles around the single bonds C(5)–C(6) and C(3)–C(4) adjacent to the double bond in *trans* configuration and to the double bond in *cis* configuration are 126·6° and −97·0° respectively.

In Table 8 a comparison with the values which the same parameters assume in a series of low-molecular weight and macromolecular compounds is given. As can be deduced from the Table, in the solid state the skew conformation is more frequently found than the *cis* conformation, and the value of the rotation angle is nearer to 130° than to the assumed value of 120°. The value of −97° for the rotation angle C(2)–C(3)–C(4) ∧ C(3)–C(4)–C(5) is not very unusual. In fact, in geranyl-amine hydrochloride (Jeffrey, 1944) and in poly-t-butyl-butadiene (Cesari, 1964) the rotation angles about the –CH₂–C and CH₂–C bonds assume the values of 99°

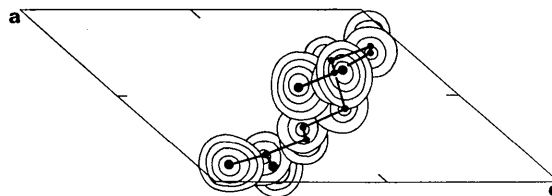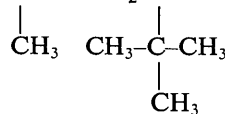$$\begin{array}{cc} | & | \\ CH_3 & CH_3\!-\!C\!-\!CH_3 \\ & | \\ & CH_3 \end{array}$$

Fig. 1. Composite drawing of the final electron-density series viewed along the *b* axis. Contours are at intervals of 2 eÅ⁻³. starting with 2 e.Å⁻³.
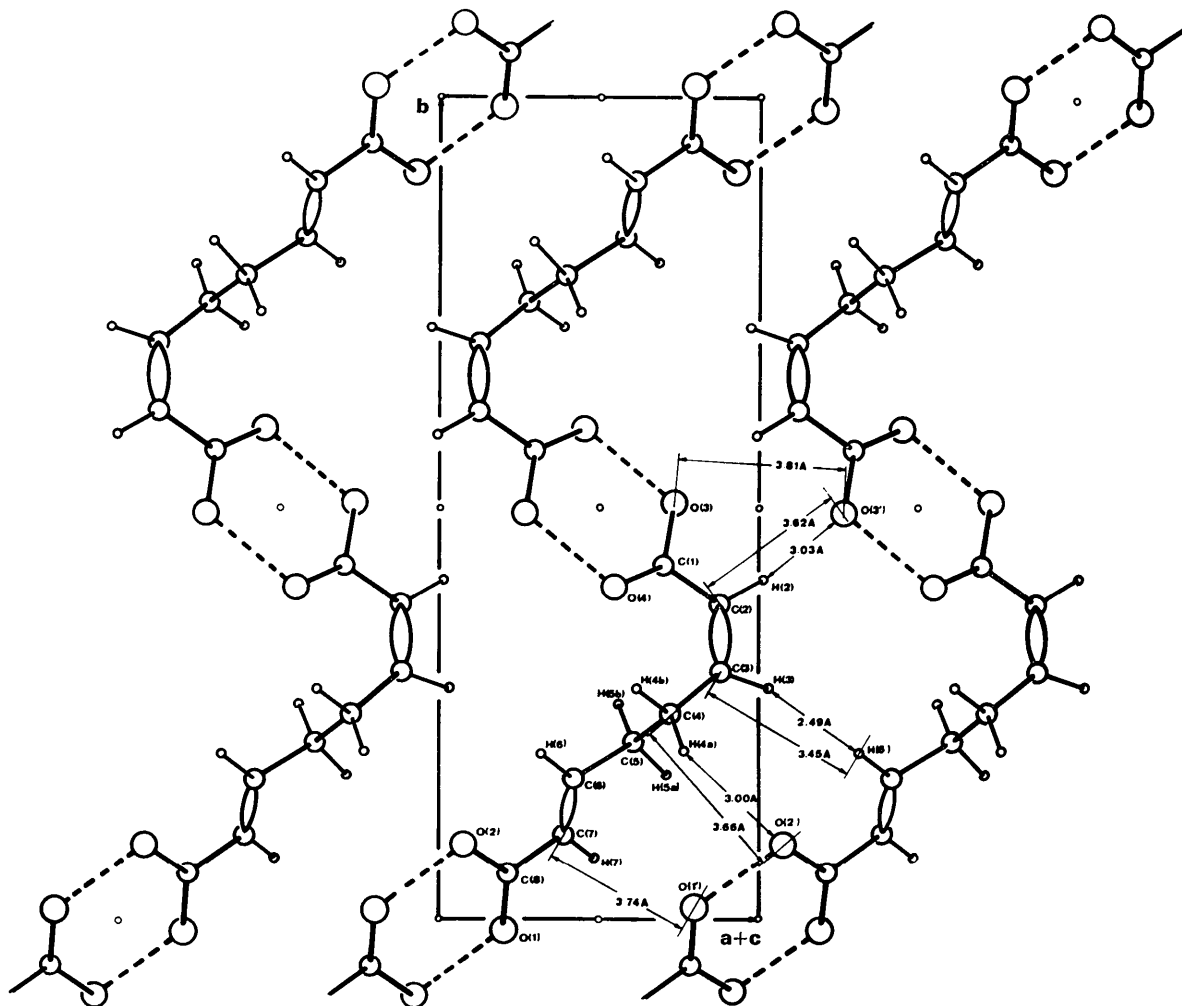
Fig. 2. Projection of the structure on the (10T) plane. Only the molecular rows oriented along the a + b + c crystallographic axis are reported.
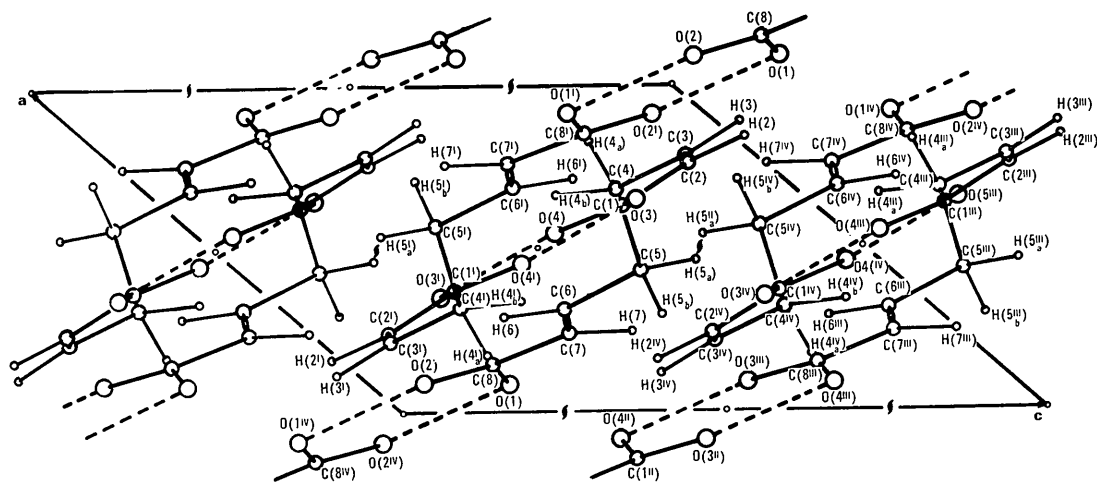
Fig. 3. Projection of the structure along [010].

Table 8. *Rotation angles about single bonds adjacent to double bonds in a series of low-molecular weight and macromolecular compounds*

Compound	Chemical formula	Rotation angles	Reference
Geranylamine hydrochloride	CH_3—$\overset{\sigma_3\ trans}{C}$ = CH—CH_2—CH_2—$\overset{\sigma_2\ trans}{C}$ = CH—$\overset{\sigma_1}{C}H$—CH_2NH_2Cl (with CH_3 branches)	$\sigma_1 = -117°$ $\sigma_2 = 99$ $\sigma_3 = 132$	Jeffrey, 1944.
Oleic acid	HO—$\overset{O}{C}$—$(CH_2)_6$—$\overset{\sigma_1}{C}H_2$—$CH = CH$ (*cis*)—$\overset{\sigma_2}{C}H_2$—$(CH_2)_6$—CH_3	$\sigma_1 = 132°$ $\sigma_2 = -127$	Abrahamsson, Ryderstedt & Nahringbauer, 1962.
Poly-t-butylbutadiene	—$\overset{\sigma_1\ cis}{C}H_2$—$\overset{\sigma_2}{C}$=CH—$CH_2$—$CH_2$—$\overset{cis}{C}$=CH—$CH_2$— (with CH_3—C—CH_3 / CH_3 t-butyl groups)	$\sigma_1 = 90°$ $\sigma_2 = 90°$	Cesari, 1964.
Hexa-*trans*-3-ene-1,6-dioic acid	HO—$\overset{O}{C}$—CH_2—$\overset{\sigma}{C}H$ = CH—CH_2—C (*trans*) $\overset{OH}{\underset{O}{C}}$	$\sigma = 130°$	Ganis & Martuscelli, 1966.
trans-Polyalkenamers	—$CH_2$$\left[—\overset{\sigma_1}{C}H = \overset{\sigma_2}{C}H—(CH_2)_n \right]_p$—CH=CH—$(CH_2)_n$— (*trans*)	$\sigma_1 = 130°$ $\sigma_2 = -130$	Natta & Bassi, 1967.
Deca-*trans*-3,*trans*-7-diene-1,10-dioic acid	$\overset{O}{\underset{HO}{C}}$—$\overset{\sigma_1}{C}H_2$—CH = CH—$CH_2$—$CH_2$—$CH_2$—$\overset{\sigma_2}{C}H$ = CH—CH_2—C $\overset{OH}{\underset{O}{}}$ (*trans*, *trans*)	$\sigma_1 = -125·5°$ $\sigma_2 = -1·6$	Martuscelli, 1967.
Octa-*cis*-2,*trans*-6-diene-1,8-dioic acid	$\overset{O}{\underset{HO}{C}}$—$\overset{\sigma_1}{C}H$ = CH—CH_2—CH_2—$\overset{\sigma_2}{C}H$—CH=CH—C $\overset{O}{\underset{OH}{}}$ (*trans*, *cis*)	$\sigma_1 = 126·6°$ $\sigma_2 = -97·0$	Present work.

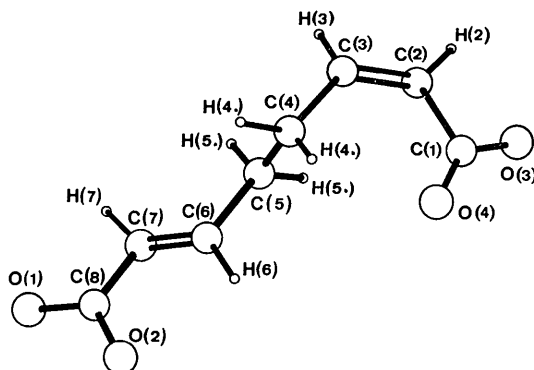valence angles O(4)–C(1)–C(2) (122·7°); C(1)–C(2)–C(3) (125·2°), C(2)–C(3)–C(4) (128·7°).

Fig.4. Molecular model of octa-cis-2,trans-6-diene-1,8-dioic acid.

and 90° respectively. These deformations are evidently induced by the presence of a bulk side group on the double bond.

In the case of octa-cis-2,trans-6-diene-1,8-dioic acid the deviation from the skew conformation is probably a result of both intermolecular and intramolecular interactions. In fact, a skew conformation would further decrease the distance between O(4) and H(4b) which is already unusually short (2·22 Å). The short intramolecular contacts C(4)---O(4) (2·925 Å) and O(4)---H(4b) (2·22 Å) are also responsible for the large values of the

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Affinement de la Structure Cristalline du Composé Pyridinoxyde Dibrome, Chlorure Mercurique

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The refinement of the crystal structure of dibromopyridine oxide–mercuric chloride has clearly shown a bending of the mercuric chloride molecule. The structure is made up of mercuric chloride chains linked together by the organic molecules.

$C_5NOH_3Br_2$–$HgCl_2$
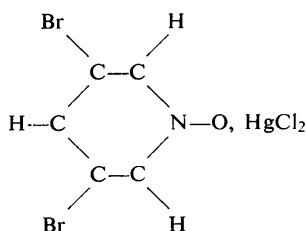
L'étude de ce composé a été entreprise dans le cadre général d'une étude de la liaison aminoxyde et, dans ce cas, de chlorure mercurique au voisinage d'une liaison polaire: la liaison azote–oxygène du pyridinoxyde.

Le cristal appartient au système monoclinique, les paramètres sont les suivants (Bompoint, 1962) $a=9,2\pm0,1$, $b=27,1\pm0,1$, $c=4,08\pm0·05$ Å, $\beta=97°\pm1°$.

L'application de la méthode de l'atome lourd a permis d'obtenir une représentation approchée de la struc-