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The Crystal and Molecular Structure of the High Temperature Stable Conformer of Deca-*trans*-3, *trans*-7-diene-1,10-dioic acid

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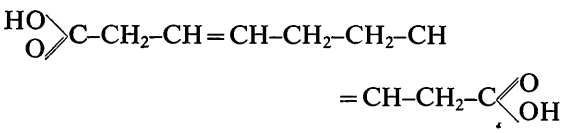
The crystal and molecular structure of the high temperature stable conformer of deca-*trans*-3,*trans*-7-diene-1,10-dioic acid has been solved using the conformational and close packing principles previously applied in the structural analysis of crystalline polymers. Two molecules are contained in the monoclinic unit cell, which has space group symmetry $P2_1/c$. The unit-cell parameters are: $a=11{\cdot}11 \pm 0{\cdot}02$, $b=4{\cdot}66 \pm 0{\cdot}01$, $c=10{\cdot}45 \pm 0{\cdot}02$ Å; $\beta=97°\,12' \pm 30$. Three-dimensional X-ray diffraction data were collected by the photographic method. Refinement was carried out by least-squares methods. The aliphatic chain $-CH_2-CH=CH-CH_2-CH_2-CH=CH-CH_2$ between the two terminal carboxylic groups has the conformation (skew+) (*trans*) (skew−) (T) (skew+) (*trans*) (skew−). The molecules are associated in parallel rows in the crystal lattice.

Introduction

Deca-*trans*-3-*trans*-7-diene-1,10-dioic-acid:



undergoes a reversible, enantiotropic transition in the crystalline state at 193°C ($\Delta H=7{\cdot}9$ cal.g^{-1}; $\Delta S=0{\cdot}022$ cal.g^{-1}deg^{-1}) (Corradini, Frasci & Martuscelli, 1969). The structure of the low-temperature modification (henceforth called deca-I) has been reported by one of us (Martuscelli, 1967). The present work is relative to the crystal and molecular structure of the high temperature modification of deca-*trans*-3,*trans*-7-diene-1,10-dioic acid (henceforth called deca-II).

Experimental

Single crystals of the high temperature modification grow from the melt. Attempts to fasten the crystals on the goniometer head and adjust it (in spite of preheating) were for the most part unsuccessful, since phase transformation (Form II – Form I) took place at some stage of these operations.

In three cases, however, the crystals remained in the high temperature modification for two days at room temperature; the X-ray studies were carried out at room temperature with these crystals.

From Weissenberg photographs taken with Cu $K\alpha$ radiation the unit-cell parameters of deca-II are: $a=11{\cdot}11 \pm 0{\cdot}02$, $b=4{\cdot}66 \pm 0{\cdot}01$, $c=10{\cdot}45 \pm 0{\cdot}02$ Å; $\beta=97°\,12' \pm 30'$. The space group indicated by the systematic absences is the centrosymmetric $P2_1/C$ with four equivalent units per unit cell. Two molecules per unit cell give a calculated density of 1·22 g.cm^{-3} in agreement with the experimental value (1·24 g.cm^{-3}). The molecules of deca-II must be characterized by a symmetry centre on the central $-CH_2-CH_2-$ bond. In Table 1 the unit-cell parameters of the high and low-temperature modifications are compared.

Intensity data were collected with nickel-filtered copper radiation with the use of multiple-film equi-

Table 1. *Comparison between the unit-cell parameters of the low and high temperature modifications of deca-trans-3-trans-7-diene-1,10-dioic acid*

		Form I	Form II
a	(Å)	$21{\cdot}74 \pm 0{\cdot}02$	$11{\cdot}20 \pm 0{\cdot}02$
b		$4{\cdot}66 \pm 0{\cdot}01$	$4{\cdot}66 \pm 0{\cdot}01$
c		$10{\cdot}40 \pm 0{\cdot}01$	$10{\cdot}45 \pm 0{\cdot}02$
α	(°)	90°	90°
β		$106° \pm 30'$	$97°\,12' \pm 30'$
γ		90°	90°
V	(Å^3)	1013·08	541·02
Density	X-ray (g.cm^{-3})	1·296	1·216
	Experimental (g.cm^{-3})	$1{\cdot}30 \pm 0{\cdot}01$	$1{\cdot}24 \pm 0{\cdot}02$
Space group		$C2/c$	$P2_1/c$
Number of molecules per unit cell		4	2

inclination Weissenberg photographs about the *b* axis for layer lines 0 to 2. The zero layers about the *c* axis have been recorded to provide cross correlation of the *b* axis data. Because of the instability of the crystals at room temperature the number of observed reflexions was low (225). The shape of the reflexions also turned out to be poor because of the impossibility of growing morphologically well defined crystals from the melt.

The intensities were evaluated by eye-estimation, corrected for change of spot shape on upper layer equi-inclination photographs (Phillips, 1954) 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

The method employed to determine the atomic coordinates resembles that which has been used in the structural analysis of crystalline polymers (Corradini, Diana, Ganis & Pedone, 1963) and successfully applied by us to a series of dicarboxylic acids (Corradini, Ganis, Pedone, Sirigu & Temussi, 1967; Avitabile, Corradini, Ganis & Martuscelli, 1966; Ganis, Martuscelli & Avitabile, 1966; Martuscelli & Avitabile, 1967; Martuscelli & Mazzarella, 1969). The method is based essentially on a prediction of the packing of long hydrogen-bonded rows of molecules similar to polymer chains.

Assuming for the molecule the internal parameters of Table 2 (on the basis of data reported in the literature for similar compounds) it is found that the repetition period to be expected along the hydrogen-bonded rows is 14·2 Å. This periodicity is close to the crystallographic axis **a**+**c** (14·26 Å) which was assumed to be coincident with the molecular row direction in the crystal. Under this assumption the only unknown parameter is the rotation angle (φ) of the molecular rows around the **a**+**c** axis. The best orientation of the molecular rows was obtained by computing the reliability index R, $R=\Sigma||F_o|-|F_c||/\Sigma|F_o|$, for the *h0l* zone as a function of φ. An absolute minimum of R is obtained for $\varphi=0$ as shown in Fig. 1. The corresponding fractional atomic coordinates of the first trial model are reported in Table 3; they were used as starting parameters for the refinement of the structure.

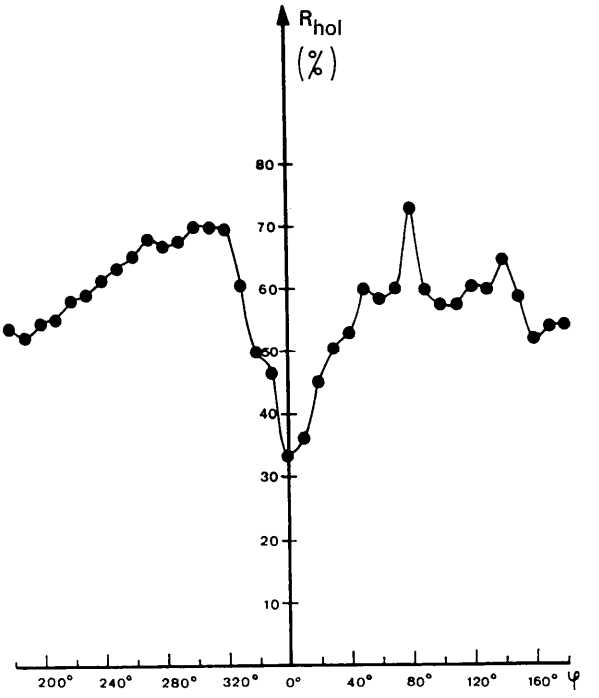


Fig. 1. The R value for *h0l* reflexions of DECA-II is plotted *versus* φ (φ is the internal rotation angle of the molecular rows around the crystallographic axis **a**+**c**). The internal coordinates of the molecular model are in Table 2.

Table 2. *Internal coordinates assumed for the first trial model of deca-trans-3-trans-7-diene-1,10-dioic acid, high temperature modification*

O(1)/O(2) > C(1)–C(2)–C(3)=C(4)–C(5)–C(5′)–C(4′)=C(3′)–C(2′)–C(1′) < O(2′)/O(1′)

Distances	
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°)*
C(1)—C(2)–C(3) ∧ C(2)–C(3)–C(4)	125
C(2)—C(3)–C(4) ∧ C(3)–C(4)–C(5)	180
C(3)—C(4)–C(5) ∧ C(4)–C(5)–C(5′)	−125
C(4)—C(5)–C(5′) ∧ C(5)–C(5′)–C(4′)	180

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

Table 3. *Fractional atomic coordinates of the* C *and* O *atoms of the first trial model relative to* $\varphi=0$

(φ is the rotation angle of the molecular rows around the crystallographic axis **a** + **c**).

	x/a	y/b	z/c
C(1)	0·106	$0\cdot\overline{174}$	0·137
C(2)	0·186	$0\cdot\overline{314}$	0·248
C(3)	0·303	$0\cdot\overline{157}$	0·280
C(4)	0·344	$0\cdot\overline{054}$	0·396
C(5)	0·457	0·103	0·443
O(1)	0·002	$0\cdot\overline{274}$	0·100
O(2)	0·143	0·043	0·086

Refinement of the structure

The refinement was initially carried out for the (010) and (001) 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.

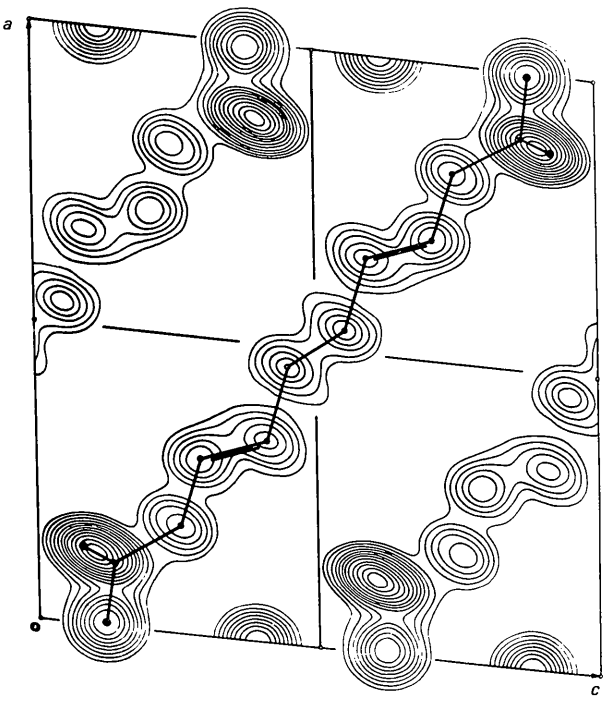


Fig. 2. Projection of the electron density on the (010) plane. Levels are drawn at intervals of 1 e.Å^{-2} starting from 1 e.Å^{-2}.

The function minimized was:

$$R_w=\sum_{hkl} W(hkl)\left[F_o(hkl)-\frac{1}{K}F_c(hkl)\right]^2$$

with a unit value for 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 using 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 ($B=5$ Å^2). We did not take the carboxylic hydrogen atoms into account. 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. The refinement was considered complete when the coordinate shifts were less than the corresponding standard deviations. The final value of the reliability R index was 0·129.

The final atomic coordinates together with the corresponding standard deviations (Cruickshank, 1949) are reported in Table 4. In Table 5 observed and calculated structure factors are listed. Table 6 shows the coefficients B_{ij} of the temperature factor of the form:

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

with the corresponding standard deviations.

A projection of the electron density distribution on the (010) plane is shown in Fig. 2.

Description of the molecular packing

Molecules of the high temperature stable modification of deca-*trans*-3-*trans*-7-diene-1,10-dioic acid are linked by means of paired hydrogen bonds (broken lines in Figs. 3 and 4), between the carboxylic groups located on crystallographic symmetry centres, into parallel

Table 4. *Final fractional atomic coordinates and their standard deviations*

	x/a	y/b	z/c	$\sigma(x/a)$	$\sigma(y/b)$	$\sigma(z/c)$
C(1)	0·1048	$\overline{0\cdot1558}$	0·1489	0·002	0·005	0·002
C(2)	0·1829	$\overline{0\cdot2972}$	0·2552	0·002	0·005	0·002
C(3)	0·2985	$\overline{0\cdot1189}$	0·2946	0·002	0·006	0·002
C(4)	0·3411	$\overline{0\cdot0660}$	0·4062	0·002	0·008	0·003
C(5)	0·4601	0·1039	0·4540	0·002	0·007	0·003
O(1)	0·0037	$\overline{0\cdot2917}$	0·1175	0·001	0·004	0·002
O(2)	0·1322	0·0565	0·0846	0·001	0·004	0·001
H(2*a*)	0·133	$\overline{0\cdot322}$	0·339			
H(2*b*)	0·208	$\overline{0\cdot512}$	0·224			
H(3)	0·346	$\overline{0\cdot033}$	0·217			
H(4)	0·290	$\overline{0\cdot147}$	0·482			
H(5*a*)	0·438	0·295	0·508			
H(5*b*)	0·507	0·158	0·371			

molecular rows extending in the **a**+**c** direction as illustrated in Fig. 3. On the other hand in deca-I crystals, the molecular rows were shown to be oblique (Martuscelli, 1967).

The projection of the structure on the (001) plane is shown in Fig. 4. In order to clarify the packing between molecular rows contained in the ($\bar{1}01$) plane, the rows lying in the ($20\bar{2}$) and ($\bar{2}02$) planes have been

Table 5. *Comparison between observed* (F_o) *and calculated* (F_c) *structure factors*

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
1	0	0	39.0	31.4	1	0	8	7.0	3.5	$\bar{3}$	1	5	12.0	14.1	6	1	6	10.9	-10.8
2	0	0	15.2	9.2	$\bar{1}$	0	8	9.6	7.9	5	1	5	4.6	4.9	7	1	6	8.6	-10.8
3	0	0	5.5	-3.9	2	0	8	8.0	7.2	$\bar{1}$	1	6	11.0	-10.2	3	1	7	5.4	5.0
4	0	0	13.6	-10.6	3	0	8	2.8	2.9	$\bar{2}$	1	6	7.0	-8.6	5	1	7	8.0	-8.8
5	0	0	11.8	-11.8	4	0	8	8.0	8.5	$\bar{3}$	1	6	11.6	-12.7	4	1	8	5.7	-8.0
6	0	0	10.7	8.6	5	0	8	9.2	8.6	4	1	6	8.1	-11.0	$\overline{10}$	1	2	3.8	4.8
9	0	0	13.3	13.2	$\bar{5}$	0	8	5.0	7.1	$\bar{1}$	1	7	5.0	-7.2	$\bar{4}$	1	5	2.9	4.3
10	0	0	5.2	3.6	$\bar{7}$	0	8	5.0	0.7	$\bar{5}$	1	7	3.6	2.3	$\bar{3}$	1	8	3.7	-3.6
11	0	0	3.2	3.1	9	0	8	3.4	4.7	$\bar{7}$	1	7	5.6	-2.1	$\bar{1}$	1	9	4.3	-6.3
1	0	2	17.6	-19.1	10	0	8	3.6	3.7	$\bar{2}$	1	8	5.1	-6.4	$\bar{7}$	1	0	3.2	-3.4
$\bar{1}$	0	2	16.1	-15.6	1	1	0	39.0	37.0	$\bar{8}$	1	8	4.2	-1.4	$\overline{11}$	1	0	3.8	-1.9
2	0	2	30.0	-22.9	2	1	0	12.9	12.9	$\bar{2}$	1	10	4.7	6.7	8	1	3	3.8	4.4
$\bar{2}$	0	2	103.0	53.6	3	1	0	9.4	-7.0	9	1	0	5.7	5.6	3	1	6	3.7	-3.7
3	0	2	28.5	-26.3	4	1	0	13.2	14.2	0	1	1	5.0	-8.2	8	1	6	2.8	-3.4
$\bar{3}$	0	2	25.0	21.5	5	1	0	11.8	-11.2	0	1	2	16.9	19.9	4	1	7	4.1	4.2
4	0	2	10.5	-6.1	6	1	0	5.5	6.5	0	1	4	4.6	3.8	7	1	7	4.2	-4.3
5	0	2	4.9	3.1	1	2	0	20.5	-20.3	0	1	5	8.5	-8.6	5	1	9	3.6	-1.8
$\bar{5}$	0	2	15.3	-11.8	2	2	0	15.2	-16.0	0	1	6	12.2	-13.3	0	2	1	1.3	1.2
6	0	2	8.4	6.0	3	2	0	11.0	-9.8	0	1	8	4.9	6.9	2	2	1	9.4	-9.9
$\bar{6}$	0	2	10.5	-10.5	4	2	0	15.4	-13.0	1	1	1	4.8	6.9	$\bar{2}$	2	1	8.4	-11.7
7	0	2	19.6	19.0	5	2	0	19.3	19.3	2	1	1	3.4	-3.2	3	2	1	16.9	17.1
$\bar{7}$	0	2	11.0	-10.2	2	3	0	12.3	-14.1	3	1	1	30.0	-33.3	$\bar{3}$	2	1	7.8	8.0
8	0	2	4.0	4.0	3	3	0	6.7	6.7	4	1	1	35.0	-38.0	4	2	1	17.0	-15.2
$\bar{8}$	0	2	10.1	11.0	4	3	0	12.0	12.4	5	1	1	4.9	4.1	5	2	1	7.0	-6.2
9	0	2	9.2	9.3	0	2	0	8.0	-10.4	6	1	1	10.0	9.4	$\bar{5}$	2	1	29.0	-26.1
10	0	2	13.0	-12.6	6	0	0	27.5	27.7	7	1	1	8.6	9.4	6	2	1	11.0	-9.1
11	0	2	4.2	-5.1	7	0	0	19.0	19.4	8	1	1	7.5	8.5	0	2	2	13.7	14.1
0	0	4	23.5	-21.5	$\bar{1}$	1	1	56.5	63.0	2	1	2	21.2	25.6	$\bar{1}$	2	2	5.1	6.8
1	0	4	41.5	-39.2	$\bar{2}$	1	1	9.2	-9.3	3	1	2	6.6	5.7	2	2	2	16.5	16.1
$\bar{1}$	0	4	18.7	-19.7	$\bar{3}$	1	1	18.2	-13.8	4	1	2	28.5	28.8	$\bar{2}$	2	2	4.5	3.9
2	0	4	44.0	-41.4	$\bar{4}$	1	1	11.3	-9.7	5	1	2	9.5	11.5	$\bar{3}$	2	2	18.3	-13.9
$\bar{2}$	0	4	9.6	-8.6	$\bar{5}$	1	1	15.6	-13.2	6	1	2	8.5	9.4	$\bar{3}$	2	2	14.0	-11.0
3	0	4	11.4	-9.8	6	1	1	22.7	-22.6	8	1	2	4.7	5.6	$\bar{4}$	2	2	20.0	-16.4
$\bar{3}$	0	4	24.8	-20.1	$\bar{7}$	1	1	5.2	5.4	9	1	2	9.6	9.5	5	2	2	5.2	4.8
4	0	4	7.3	6.3	$\bar{8}$	1	1	6.3	6.4	10	1	2	5.3	6.1	6	2	2	11.5	9.7
5	0	4	12.2	12.3	$\bar{1}$	1	2	53.8	55.1	1	1	3	23.0	-23.5	0	2	3	11.5	-11.0
$\bar{5}$	0	4	5.6	-5.5	$\bar{2}$	1	2	45.0	44.2	2	1	3	22.0	-20.9	$\bar{1}$	2	3	6.3	-4.5
6	0	4	14.0	-15.2	$\bar{3}$	1	2	16.8	15.7	3	1	3	3.0	-2.5	2	2	3	22.0	-21.3
7	0	4	4.1	-2.4	$\bar{4}$	1	2	9.6	9.6	4	1	3	12.6	16.5	$\bar{2}$	2	3	11.0	5.4
$\bar{7}$	0	4	9.6	-9.6	$\bar{5}$	1	2	10.6	8.7	5	1	3	14.0	15.8	$\bar{3}$	2	3	7.2	5.8
8	0	4	30.5	-26.2	$\bar{7}$	1	2	11.0	11.1	6	1	3	11.6	12.6	5	2	3	11.1	10.7
$\bar{8}$	0	4	3.6	-4.6	$\bar{8}$	1	2	7.0	4.7	9	1	3	7.9	-8.4	1	2	4	9.0	7.3
9	0	4	5.4	-8.3	$\bar{9}$	1	2	4.0	2.8	2	1	4	8.5	5.8	$\bar{1}$	2	4	11.6	11.2
$\bar{9}$	0	4	8.7	-6.5	$\overline{11}$	1	2	4.9	5.6	3	1	4	8.3	-7.0	$\bar{2}$	2	4	30.0	24.0
$\overline{10}$	0	4	4.4	1.5	$\bar{1}$	1	3	23.9	24.3	4	1	4	3.5	4.8	$\bar{3}$	2	4	20.0	16.7
0	0	6	18.4	-19.0	$\bar{2}$	1	3	5.6	9.6	6	1	4	4.3	6.7	3	2	4	12.5	11.5
1	0	6	5.3	3.0	$\bar{3}$	1	3	30.3	26.3	7	1	4	7.6	8.7	$\bar{4}$	2	4	11.7	10.7
$\bar{1}$	0	6	15.4	-15.3	$\bar{5}$	1	3	11.4	-9.6	9	1	4	4.2	-3.8	$\bar{7}$	2	4	12.0	8.9
2	0	6	6.2	6.0	$\bar{6}$	1	3	4.3	-4.6	1	1	5	9.8	-10.3	7	2	4	12.4	8.2
3	0	6	10.0	8.4	$\bar{7}$	1	3	9.0	3.1	2	1	5	10.0	10.5	0	2	5	11.7	-9.2
4	0	6	6.8	6.5	$\bar{8}$	1	3	4.5	-5.0	3	1	5	6.6	5.6	$\bar{3}$	2	5	21.3	21.2
$\bar{4}$	0	6	5.3	3.0	$\overline{10}$	1	3	5.4	4.6	4	1	5	7.6	5.2	$\bar{4}$	2	5	13.2	10.7
5	0	6	5.0	-6.3	$\bar{1}$	1	4	15.4	-12.8	5	1	5	7.0	5.5	$\bar{5}$	2	5	10.0	9.6
6	0	6	21.0	-19.5	$\bar{2}$	1	4	18.5	18.6	6	1	5	7.0	7.5	1	2	7	10.0	14.1
7	0	6	9.7	-4.3	$\bar{4}$	1	4	18.6	16.0	7	1	5	9.6	-11.1					
12	0	6	1.2	1.0	$\bar{5}$	1	4	8.4	8.9	5	1	6	14.0	-6.2					
0	0	8	3.5	3.7	$\bar{6}$	1	4	5.7	-8.1	1	1	6	12.0	-13.1					

Table 6. *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}	$\sigma(B_{11})$	$\sigma(B_{22})$	$\sigma(B_{33})$	$\sigma(B_{12})$	$\sigma(B_{13})$	$\sigma(B_{23})$
C(1)	4·46	0·52	6·31	0·81	−0·88	0·48	0·99	2·04	1·37	1·24	0·97	1·47
C(2)	5·71	0·70	5·14	−1·70	−1·97	1·25	1·15	1·76	1·28	1·34	1·01	1·47
C(3)	6·20	3·91	5·03	−3·79	−1·36	0·85	1·23	2·20	1·28	1·51	1·04	1·68
C(4)	5·78	8·72	8·51	−4·26	−0·29	2·33	1·33	2·65	1·74	1·76	1·23	2·14
C(5)	5·38	8·24	11·20	−4·47	−3·77	5·65	1·35	2·98	2·11	1·77	1·27	2·25
O(1)	4·24	2·69	6·13	−0·76	−0·64	−2·89	0·69	1·31	0·88	0·85	0·65	1·06
O(2)	2·72	5·20	4·50	−1·10	0·13	0·92	0·59	1·30	0·77	0·88	0·55	1·03

omitted. The most significant intermolecular contact distances are indicated in Figs. 3 and 4.

The molecular packing is dominated by O···O, O···C, O···H, H···H and H···C interactions. All the C···C intermolecular distances are larger than 3·90 Å. The length of the hydrogen bridges connecting the carboxylic groups of adjoining molecules in the **a**+**c** direction is 2·68 Å (2·62 Å in deca-I crystals).

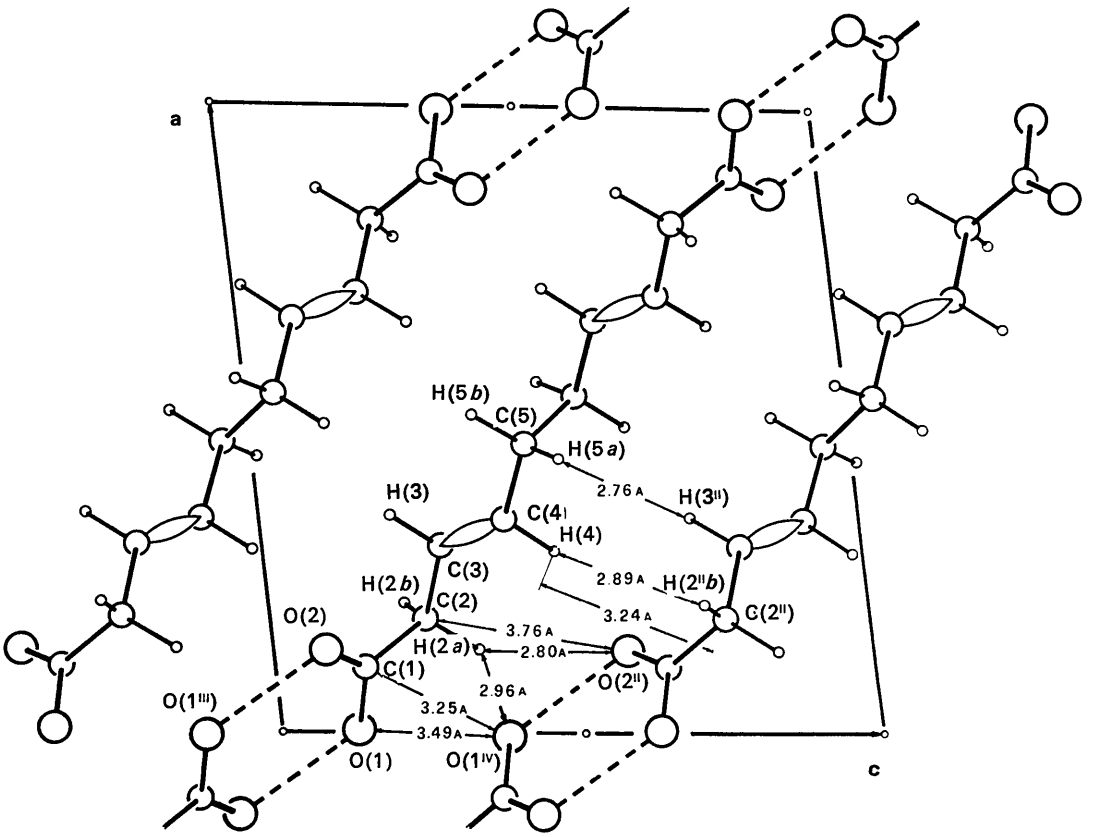


Fig. 3. Projection of the structure along [010].

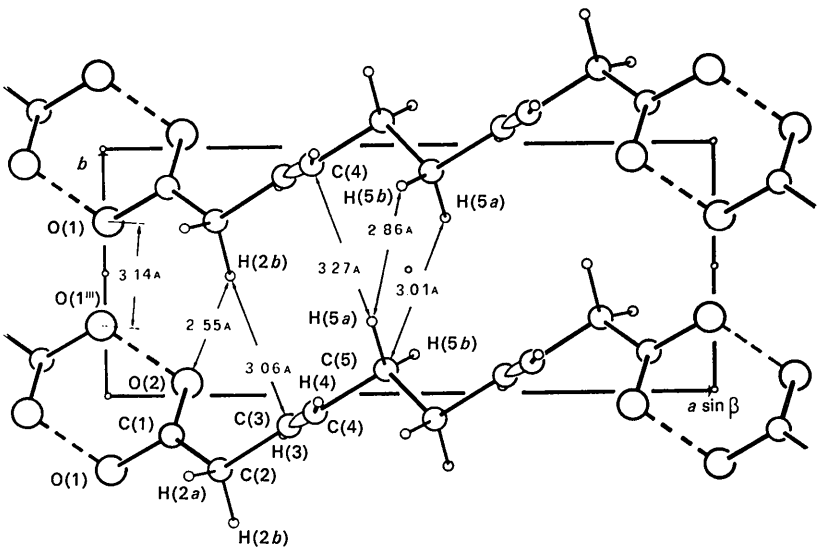


Fig. 4. Projection of the structure along [001]. Molecular rows contained in the ($\bar{2}02$) and ($20\bar{2}$) planes have been omitted.

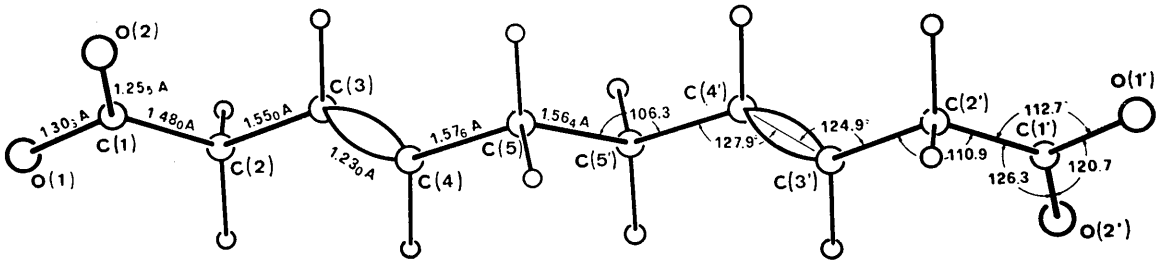


Fig. 5. Molecular model of the high temperature stable modification of deca-*trans*-3,*trans*-7-diene-1,10-dioic acid.

Molecular conformation

A drawing of the molecular model of deca-II is shown in Fig. 5. The corresponding conformational parameters are listed in Table 7, together with their estimated standard deviations.

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

Distances		
C(1)—O(1)	$1{\cdot}30_3$ Å	0·03 Å
C(1)—O(2)	$1{\cdot}25_5$	0·03
C(1)—C(2)	$1{\cdot}48_0$	0·03
C(2)—C(3)	$1{\cdot}55_0$	0·03
C(3)—C(4)	$1{\cdot}23_0$	0·04
C(4)—C(5)	$1{\cdot}57_6$	0·04
C(5)—C(5′)	$1{\cdot}56_4$	0·04
O(2)···O(1‴)	$2{\cdot}67_8$	0·04
Angles		
O(1)–C(1)–C(2)	112·7°	0·8°
O(2)–C(1)–C(2)	126·3	0·9
O(1)–C(1)–O(2)	120·7	0·9
C(1)–C(2)–C(3)	110·9	0·9
C(2)–C(3)–C(4)	124·9	1·6
C(3)–C(4)–C(5)	127·9	1·1
C(4)–C(5)–C(5′)	106·3	1·0
Dihedral angles		
O(1)–C(1)–C(2) ∧ C(1)–C(2)–C(3)		−177°
O(2)–C(1)–C(2) ∧ C(1)–C(2)–C(3)		9
C(1)–C(2)–C(3) ∧ C(2)–C(3)–C(4)		135
C(2)–C(3)–C(4) ∧ C(3)–C(4)–C(5)		178
C(3)–C(4)–C(5) ∧ C(4)–C(5)–C(5′)		−123
C(4)–C(5)–C(5′) ∧ C(5)–C(5′)–C(4′)		180

The conformation of the carboxylic groups in deca-I and deca-II is very similar, in fact the values of the rotation angles around the bond C(1)–C(2) are −177° and −175° respectively for the high and low temperature stable modifications (Martuscelli, 1967). The values of the torsional angles around the C(2)–C(3) and C(4)–C(5) are 135°(skew+) bonds and −123° (skew−) in the high temperature stable modification, −126° (skew−) and −2° (*cis*) in the low temperature stable modification respectively (Martuscelli, 1967). The aliphatic chain –C(1)–C(2)–C(3)=C(4)–C(5)–C(5′)–C(4′) = C(3′)–C(2)–C(1′)– comprised between the two terminal carboxylic groups has the conformation: (skew+) (*trans*) (skew−) (*T*) (skew+) (*trans*) (skew−) in the deca-II molecule and the conformation: (skew−) (*trans*) (*cis*) (*T*) (*cis*) (*trans*) (skew+) in the deca-I molecule. Thus the dimorphism of deca-*trans*-3-*trans*-7-diene-1,10-dioic acid is of the '*conformational*' type and is due to the existence of two rotation isomers of the compound. The atomic groups

$$C(2)\text{–}C(1)\left\langle\begin{matrix}O(1)\\O(2)\end{matrix}\right. \text{ and } C(2)\text{–}C(3)\text{=}C(4)\text{–}C(5)$$

are planar within experimental error.

The shortness of the double bond C(3)=C(4) (1·23 Å) is not real but the result of experimental error.

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