

C(5) and C(6) relatively large ones. The anisotropic parameters of the ruthenium atom correspond to values of B ranging from 2.8 (in a direction approximately parallel to c) to 2.0 (approximately along a).

The disordered modification

Visual intensity data for the $hk0$ reflections of the disordered modification of bisindenylruthenium (see *Experimental*) were obtained from a set of Weissenberg photographs prepared with $\text{Cu K}\alpha$ radiation. The Patterson projection onto (001) could be interpreted on the basis of four ruthenium atoms, each of half weight, in the unit cell; phases calculated from these ruthenium positions led to the electron-density projection shown in Fig. 4. Since this projection is down a relatively short (6.2 Å) axis, separate molecules must be resolved. Accordingly, it seems quite clear that each molecule can assume either of two orientations with equal probability, one orientation being related to the other by a twofold rotation about an axis perpendicular to the rings and passing approximately through the centers of the two C(8)–C(9) bonds. A similar sort

of disorder was proposed by Trotter (1958) for bisindenyliron.

In view of the near equality of the lengths of the c axes in the two modifications, there appears to be a simple relationship between the ordered and the disordered structures. This relationship is shown in Fig. 5.

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The Crystal Structure of Terephthalic Acid

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X-ray diffraction photographs of terephthalic acid have shown the existence of two polymorphic forms which have closely related triclinic unit-cell dimensions. The crystal structures of both these forms have been determined from two-dimensional data, and a full three-dimensional analysis, including the calculation of anisotropic temperature factors, has been carried out for one of these forms. The R index over 470 $F(hkl)$ was 7.5%. The bond lengths indicated a small amount of quinonoid character in the benzene ring, and a slight departure from planarity between the ring and the carboxyl groups. The molecules pack together in the crystal in systems of infinite chains linked together by double hydrogen bonds of length 2.608 Å.

Introduction

In the course of examining samples of terephthalic acid, $\text{HOOC}\cdot\text{C}_6\text{H}_4\cdot\text{COOH}$, by X-ray powder photographs, two slightly different patterns were found to occur, suggesting the possibility of more than one polymorph. Single-crystal photographs showed that terephthalic acid does in fact crystallize with two different triclinic structures, both of which have been determined. In both forms, the molecules are hydrogen-bonded into infinite chains parallel to an axis of length 9.54 Å, the difference between them being in the relative longitudinal displacement of these chains, as shown in Fig. 1.

Neighbouring chains in form I pack with the benzene rings of one chain adjacent to the carboxyl groups of the next chain, whereas in form II the benzene rings of adjacent chains are in line. For successive layers, however, the reverse is true; in form I layers pack with benzene rings almost in line with each other, while for form II, benzene rings pack alternately with carboxyl groups.

Experimental

Pure terephthalic acid was recrystallized from water in a glass tube in a Carius furnace at about 150°. The resulting crystals were mostly highly twinned, but by

examining the extinction effects in polarized light, a number of single untwinned specimens of suitable size and shape were collected. They were found to occur in more than one habit from the same crystallization; needles, thin plates and more equidimensional parallelepipeds were all present. The extinction direction was parallel to a strongly marked cleavage plane which was diagonally across the needles, but parallel to one set of edges in the plates and parallelepipeds.

Sets of oscillation and Weissenberg photographs were taken about several axes of each kind of crystal. For the collection of intensity data, multiple films were used in the Weissenberg camera, and the intensities of the spots were estimated by comparison with a time-exposure calibrated film strip. The usual corrections were applied and the approximate scale and temperature factors found from Wilson's statistical method.

Determination of the structures

Preliminary unit-cell measurements were made from rotation and Weissenberg photographs. All the crystals were found to have one common axis length of 9.54 Å parallel to the cleavage direction, but whereas the needles and plates were found to have identical unit cells (the needle axis of 3.749 Å corresponding to an axis in the plates parallel to the other set of edges), the parallelepipeds had a different unit cell, the shortest axis of which was 5.02 Å. The original unit cells, referred to unconventional directions, but retaining the common 9.54 Å were:

Form I (needles and plates)

$$a=9.54, b=7.73, c=3.74 \text{ \AA}, \\ \alpha=109^{\circ}9', \beta=73^{\circ}36', \gamma=137^{\circ}46'.$$

Form II (parallelepipeds)

$$a=9.54, b=5.34, c=5.02 \text{ \AA}, \\ \alpha=86^{\circ}57', \beta=134^{\circ}39', \gamma=94^{\circ}48'.$$

A trial structure for form I was obtained by placing the length of the molecule along $a=9.54$ Å, which is exactly the calculated length of one unit of a hydrogen-bonded molecular chain, and also taking into consideration strong $\{hk0\}$ reflexions of spacing 1.16 and 2.26 Å. Approximate z coordinates were obtained from a sharpened $[a]$ Patterson projection. The coordinates obtained in this way were refined rapidly by successive electron density projections along b and c , resulting in R values of 19.5 and 11.6% respectively. The $[a]$ projection was of little use owing to overlapping of atoms. When the Pegasus computer became available, two-dimensional least-squares refinement was carried out with a program written by Milledge (1961). The best electron density projection along c is shown in Fig. 2.

Similarly a trial structure for form II was obtained by consideration of the close relationship to form I. The final R values for this were 16.4% for $\{hk0\}$ and 18.0% for $\{h0l\}$.

Unit-cell dimensions

Before commencing further refinement, the unit-cell measurements were reduced to conventional triclinic descriptions.

Form I (needles and plates) Form II (parallelepipeds)

$a=7.730 \text{ \AA}$	$a=7.452 \text{ \AA}$
$b=6.443$	$b=6.856$
$c=3.749$	$c=5.020$
$\alpha=92.75^{\circ}$	$\alpha=116.6^{\circ}$
$\beta=109.15$	$\beta=119.2$
$\gamma=95.95$	$\gamma=96.5$

Table 1. Atomic parameters

Form I, relative to the 7.730, 6.443, 3.749 Å axes
The components of the thermal ellipsoid are defined by the expression

$$\exp[-\frac{1}{2}(h^2a^2B_{11} + 2hka^*b^*B_{12} + \dots)]$$

used in the structure amplitude calculations.

	x/a	y/b	z/c	B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	B_{13}
C(1)	0.1454	0.1460	0.0063	2.86	2.68	3.69	0.26	0.09	0.92
C(2)	-0.0361	0.1895	-0.1615	3.02	2.77	3.73	0.44	0.32	1.20
C(3)	0.1801	-0.0442	0.1687	2.81	3.01	3.81	0.41	0.34	1.30
C(4)	0.3012	0.3017	0.0078	2.89	3.01	2.99	0.08	0.09	1.07
O(1)	0.4633	0.2614	0.1856	2.72	3.85	5.14	-0.08	1.13	1.10
O(2)	0.2681	0.4638	-0.1660	3.06	3.13	4.56	0.07	0.98	1.28
H(1)	0.5746	0.3752	0.1775						
H(2)	-0.0624	0.3362	-0.2842						
H(3)	0.3205	-0.0758	0.2994						

Mean isotropic $B=7.90$

Form II, relative to the 9.54, 5.34, 5.02 Å axes

	x/a	y/b	z/c	B
C(1)	0.147	-0.002	0.000	3.00
C(2)	0.175	0.217	-0.184	3.00
C(3)	0.031	-0.224	0.186	3.00
C(4)	0.301	-0.007	0.003	3.00
O(1)	0.461	-0.196	0.181	3.00
O(2)	0.275	0.209	-0.158	3.00

Table 2. Observed and calculated structure amplitudes

H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)	H	K	L	F(OBS)	F(CAL)
0	0	1	36.0	+36.0	1	3	-1	8.4	+9.1	2	5	0	8.2	+9.1	4	-5	0	1.9	+2.0	5	-1	2	4.9	-5.0	7	-5	0	2.0	-2.1
0	0	2	3.1	-3.4	1	3	0	6.6	-6.3	2	5	2	2.2	-2.1	4	-5	2	0.9	-0.9	5	0	-2	2.6	-2.6	7	-5	1	2.5	-2.2
0	1	-2	1.3	+1.5	1	3	1	15.4	-14.4	2	6	-2	1.7	-1.4	4	-4	-2	3.7	-3.5	5	0	-1	2.8	-2.5	7	-4	-1	2.8	+2.5
0	1	-1	0.9	+0.8	1	4	-1	3.8	-3.3	2	6	-1	2.0	-1.9	4	-4	0	11.0	+11.1	5	0	0	5.0	-4.5	7	-4	0	1.7	+1.9
0	1	0	1.7	+1.2	1	4	-2	3.0	-3.2	2	6	1	0.9	+0.7	4	-4	1	12.7	+13.6	5	0	1	3.9	-3.6	7	-4	1	0.8	-0.6
0	1	1	0.9	+1.0	1	4	0	2.0	-2.0	2	7	-2	2.0	-1.6	4	-4	2	5.4	+5.2	5	0	2	1.3	-1.3	7	-4	2	1.3	-1.3
0	1	2	2.0	+1.8	1	4	1	2.3	-1.8	2	7	-1	2.6	-1.6	4	-3	-2	0.8	-1.0	5	1	-2	1.7	+2.2	7	-3	-2	0.9	+1.2
0	2	-2	4.6	-5.4	1	4	2	2.9	-2.6	3	-8	-1	1.0	-1.6	4	-3	-1	3.8	+3.1	5	1	-1	4.6	+4.4	7	-3	0	3.2	-3.0
0	2	-1	9.6	-10.3	1	5	-2	1.2	+1.0	3	-8	0	1.0	-1.0	4	-3	0	4.5	+4.4	5	1	0	5.4	+5.0	7	-3	1	4.9	-5.3
0	2	0	7.3	-7.9	1	5	-1	2.4	+2.2	3	-7	-1	2.3	-2.4	4	-3	1	1.0	+1.0	5	1	1	4.5	+4.0	7	-3	1	2.1	-2.2
0	2	1	1.1	-1.0	1	5	0	4.6	+4.4	3	-7	0	3.0	-3.8	4	-2	-2	5.4	-5.6	5	1	2	1.2	+1.6	7	-2	-2	2.5	-2.4
0	3	-2	5.3	-5.2	1	5	1	3.5	+3.7	3	-7	1	1.6	-1.7	4	-2	-1	9.3	-8.2	5	2	-2	5.9	-6.9	7	-2	0	2.3	-2.5
0	3	-1	15.9	-15.7	1	6	-2	2.7	-2.5	3	-7	2	1.0	+0.8	4	-2	0	5.3	-5.9	5	2	-1	5.9	-5.2	7	-2	1	0.6	-0.7
0	3	0	6.3	-6.0	1	6	-1	4.9	+4.7	3	-6	-2	2.9	-1.7	4	-2	1	1.8	-1.3	5	2	0	7.8	+7.9	7	-1	-2	3.5	+2.9
0	3	1	6.4	+6.8	1	6	0	9.4	+10.5	3	-6	0	2.0	+2.2	4	-2	0	4.2	+4.2	5	2	1	11.1	+11.6	7	-1	-1	1.4	+1.3
0	3	2	5.4	+5.0	1	6	1	6.8	+6.9	3	-6	1	2.8	+2.7	4	-1	-2	6.4	+5.3	5	2	2	5.0	+5.2	7	-1	-1	1.4	+1.3
0	4	-2	1.3	-1.3	1	6	-2	2.7	-2.5	3	-5	-2	2.8	-3.2	4	-1	-1	1.4	-1.1	5	3	-1	2.0	+1.6	7	0	-2	8.7	+8.9
0	4	-1	7.4	+7.2	1	7	-1	1.9	-1.6	3	-5	-1	2.8	-3.2	4	-1	1	4.2	+3.9	5	3	1	1.4	-1.4	7	0	-1	11.1	+11.4
0	4	0	8.2	+7.7	1	7	0	1.9	-1.8	3	-5	0	0.7	-0.6	4	-1	2	2.4	+2.3	5	3	0	3.2	-3.6	7	0	0	2.0	-1.9
0	4	1	2.2	-2.3	1	8	-1	1.8	-1.6	3	-5	1	1.4	-1.2	4	0	-2	11.8	-11.7	5	4	0	2.9	-3.6	7	0	1	1.3	-1.4
0	4	2	7.5	-6.1	1	8	0	1.1	-0.8	3	-5	2	2.1	-1.8	4	0	-1	4.6	+4.6	5	4	1	0.8	-0.9	7	1	-2	1.2	+1.1
0	5	-2	3.0	-3.4	2	-8	0	0.9	+0.9	3	-4	-2	2.3	-1.7	4	0	0	9.3	+9.5	5	5	-2	2.3	+2.5	7	1	0	2.1	-2.4
0	5	-1	4.3	-3.9	2	-8	1	1.8	+1.8	3	-4	-1	2.6	+2.2	4	0	1	7.8	+7.2	5	5	-1	2.0	-1.0	7	1	1	1.2	+1.2
0	5	0	3.1	-2.9	2	-8	2	1.1	+1.1	3	-4	0	2.2	+2.2	4	0	2	0.9	-1.0	5	5	0	2.6	-2.6	7	1	2	1.2	+1.2
0	6	-2	0.9	+0.9	2	-7	-2	1.1	-1.2	3	-4	1	2.2	+2.2	4	1	-2	5.4	-5.2	5	5	1	0.9	-0.9	7	2	-2	2.2	-1.9
0	6	0	1.6	+1.7	2	-7	-1	2.7	-2.8	3	-4	2	0.9	+0.8	4	1	-1	4.5	-4.2	5	5	0	2.6	-2.6	7	2	0	1.4	+1.7
0	6	1	3.4	+3.5	2	-7	0	2.3	-2.6	3	-3	-2	2.1	-2.1	4	1	0	3.5	-3.4	5	6	-2	3.8	-4.5	7	3	-2	2.8	-2.9
0	6	2	3.4	+2.8	2	-7	1	0.9	-1.1	3	-3	-3	2.1	+2.4	4	1	1	4.0	+3.7	5	6	-1	3.1	-3.3	7	3	0	2.2	+2.0
0	7	-2	1.9	-1.8	2	-6	-1	1.1	+1.3	3	-3	-1	0.5	-0.3	4	2	-2	1.2	+1.3	6	-7	-1	0.9	-1.1	7	4	-2	2.0	+2.1
0	7	-1	2.8	-2.7	2	-6	0	3.0	-3.1	3	-3	0	9.4	+10.3	4	2	-1	2.5	+2.7	6	-6	-2	4.8	+4.9	7	4	-1	1.9	+1.7
0	7	0	2.0	+2.0	2	-6	1	5.7	-5.5	3	-3	1	13.0	+12.8	4	2	0	3.3	+3.2	6	-6	-1	5.0	+5.3	7	4	0	2.7	+1.9
0	7	1	4.6	+5.5	2	-6	2	2.8	-2.4	3	-2	-1	1.7	-1.1	4	2	1	4.7	+4.1	6	-6	-2	1.5	+1.6	7	4	1	1.9	+1.7
0	7	2	3.7	+4.1	2	-5	-2	2.6	-2.3	3	-2	0	4.6	+2.2	4	2	2	3.5	+3.7	6	-6	0	1.5	+1.6	7	4	2	2.7	+1.9
0	8	0	1.8	-1.4	2	-5	-1	5.9	-5.2	3	-2	1	1.1	-1.4	4	2	2	4.8	+4.8	6	-6	1	1.6	-1.4	7	5	-2	1.2	-1.0
1	-8	0	2.0	-1.7	2	-5	2	4.8	+4.6	3	-1	-2	2.9	-2.2	4	3	-1	6.9	+7.4	6	-5	-2	2.3	+2.5	7	5	-1	1.4	-1.4
1	-7	-2	2.1	+2.1	2	-4	-2	3.9	-3.5	3	-1	-1	11.4	-11.5	4	3	0	6.3	+6.5	6	-5	-1	1.3	+1.4	8	-5	-2	1.1	+1.3
1	-7	-1	0.9	+0.9	2	-4	-1	6.6	-6.0	3	-1	1	9.0	-8.1	4	3	2	7.3	+6.8	6	-5	1	1.1	-1.1	8	-5	0	1.0	-0.9
1	-7	0	0.8	+0.9	2	-4	0	4.8	-4.1	3	-1	2	2.4	-2.1	4	4	-2	1.7	-1.3	6	-4	1	2.1	-1.7	8	-4	-2	2.2	-1.9
1	-7	1	2.0	+1.6	2	-4	1	1.8	-1.4	3	-1	3	2.4	-2.1	4	4	1	1.1	+1.1	6	-4	2	1.8	-2.1	8	-4	-1	1.2	-1.3
1	-6	-1	1.8	-1.9	2	-4	2	1.2	-1.1	3	0	-2	11.4	+10.7	4	4	0	1.1	+1.1	6	-4	2	1.8	-2.1	8	-4	0	1.2	-1.3
1	-6	0	3.7	-3.6	2	-3	0	5.8	-5.0	3	0	0	5.8	-5.0	4	4	2	1.4	-1.2	6	-3	-2	3.9	-3.9	8	-3	-2	2.7	-2.6
1	-6	1	3.2	-3.4	2	-3	1	12.1	+12.1	3	0	1	12.1	+12.1	4	5	-2	1.2	+1.1	6	-3	-1	0.9	-0.6	8	-3	-1	2.2	-2.0
1	-6	2	2.0	+2.0	2	-3	2	2.0	-2.0	3	0	2	3.0	-3.4	4	5	0	2.5	-2.7	6	-3	0	4.0	+3.7	8	-3	0	2.2	-2.0
1	-5	-1	4.4	+4.8	2	-3	0	4.1	+3.7	3	1	-2	9.1	-8.6	4	5	1	2.8	-2.7	6	-3	1	2.8	+2.7	8	-2	1	1.4	+1.5
1	-5	0	4.5	+4.3	2	-3	1	4.0	+3.8	3	1	-1	22.3	-22.8	4	6	-2	2.3	+2.6	6	-2	-2	3.7	+3.9	8	-2	-2	7.6	+7.5
1	-5	1	2.8	-2.8	2	-3	2	2.4	+2.3	3	1	0	9.8	-9.2	4	6	-1	2.1	+2.5	6	-2	-1	4.8	+3.7	8	-2	-1	2.8	+2.4
1	-5	2	4.9	-5.6	2	-2	-2	20.5	+21.1	3	1	1	7.7	+6.7	4	6	1	1.4	-1.3	6	-2	0	2.6	-2.4	8	-1	0	2.9	-2.7
1	-4	-2	2.5	+1.9	2	-2	-1	11.7	+10.7	3	1	2	5.5	+4.8	4	6	2	1.4	-1.3	6	-2	1	2.1	-1.1	8	-1	1	1.3	-1.4
1	-4	-1	5.1	-4.6	2	-2	0	16.7	-15.5	3	2	-2	4.0	-4.0	4	7	-2	2.4	-2.3	6	-2	2	2.1	-2.1	8	0	-1	2.4	-2.5
1	-4	0	10.9	-11.4	2	-2	1	11.1	-10.4	3	2	-1	6.0	-6.2	4	7	0	1.1	+1.1	6	-2	1	1.1	-1.5	8	0	0	1.8	-1.5
1	-4	1	4.6	+3.9	2	-1	2	6.5	+6.0	3	2	0	5.5	-5.1	4	7	1	2.4	+2.3	6	-1	-2	4.6	-3.7	8	0	1	1.1	+1.1
1	-4	2	4.4	+4.3	2	-1	-1	0.9	-1.4	3	2	1	4.2	-3.6	4	7	2	1.6	+1.6	6	-1	0	4.1	-4.3	8	1	-2	1.1	+1.1
1	-3	-2	1.3	-1.0	2	-1	0	1.0	-1.2	3	2	2	2.4	-2.3	5	-7	-1	0.9	-0.9	6	-1	1	2.5	-2.4	8	1	-1	1.4	+1.4
1	-3	-1	6.2	-5.8	2	-1	1	5.1	+4.8	3	3	-2	3.0	+2.3	5	-7	0	2.1	+2.1	6	0	-2	3.8	+4.0	8	1	0	1.1	+1.1
1	-3	0	9.4	-9.9	2	-1	2	1.9	+1.7	3	3	-1	3.6	+3.2	5	-6	-2	1.5	+2.1	6	0	-1	5.1	+4.4	8	2	-2	2.7	+2.6
1	-3	1	6.2	-5.9	2	0	-2	1.7	-1.5	3	3	0	2.2	+2.2	5	-6	-1	1.6	+1.2	6	0	0	3.3	+3.0	8	2	-1	1.8	+1.7
1	-3	2	2.7	-2.2	2	0	-1	2.0	-1.7	3	3	1	1.3	+1.4	5	-6	0	0.9	-0.9	6	0	1	0.9	+1.0	8	2	0	1.8	+1.7
1	-2	-1	3.2	-3.6	2	0	0	7.2																					

The space group in each case was assumed to be $P\bar{1}$, with the centre of the molecule lying on the centre of symmetry of the unit cell. For one molecule of molecular weight 166 per unit cell, the calculated specific gravity of form I is 1.577, and that of form II 1.522; the experimental value for form I found by flotation in sodium iodide solution was 1.568, while that for form II was not determined as suitable crystals were no longer available. As the density of the form II parallelepipeds was the lower, and because they tended to become rarer on storage, it was thought probable that form II might be more stable at higher temperatures, but experiments to test this have not been carried out.

The $[110]$ axis of these revised cell descriptions is 9.54 Å, which was originally taken as a . The similarity of the a , b and γ dimensions suggests that the molecules have a similar disposition in this plane, and the similarity of the spacing $d(001)$ for the two forms (3.50 and 3.45 Å) indicates a very close relationship between the polymorphs; in fact, c of either form corresponds to $[112]$ of the other. This implies that (001) layers stack differently in the two forms; if one is regarded as primitive with the origin of an adjacent layer at $(0,0,1)$, then the other may be regarded as centred with the origin of an adjacent layer at $(\frac{1}{2}, \frac{1}{2}, 1)$.

Three-dimensional refinement of form I

Three-dimensional intensity data were obtained from c Weissenberg photographs (zero and two layers) for form I only and these were used in a series of least-squares refinements and structure factor calculations on the computer, using a program written by Cruickshank & Pilling (1961). The coordinates of the hydrogen atoms were included in these at calculated positions, assuming C-H and O-H = 1.08 Å, but they were not refined. For H(2) and H(3) the C-H bond direction was taken as bisecting the external angles of the benzene ring, but H(1) could be bonded directly to either O(1) or O(2). Preference was shown to O(1) since the C(4)-O(1) bond was slightly longer than C(4)-O(2), although there might actually be random disorder in the hydrogen position.

Anisotropic temperature factors were calculated for the carbon and oxygen atoms, and after four cycles of refinement, the value of the residual R over all the 470 $F(hkl)$ was reduced to 7.5%. As the shifts for both the positional and thermal parameters were less than a quarter of their standard deviations, the refinement was considered to be complete. The final values of the atomic coordinates and the anisotropic temperature factors are listed in Table 1, and the observed and calculated structure amplitudes are compared in Table 2.

Description of the structure

The crystal structure consists of continuous chains of terephthalic acid molecules linked by double hydrogen

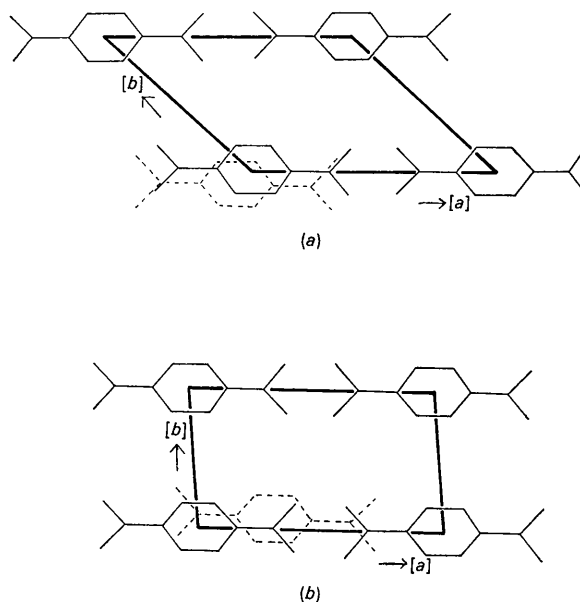


Fig. 1. The relationship between the packing of the two polymorphs. $[c]$ projections: (a) Form I (needles and plates), $c = 3.74$ Å. (b) Form II (parallelepipeds), $c = 5.02$ Å. The dashed lines represent the molecule lying immediately above that at the origin.

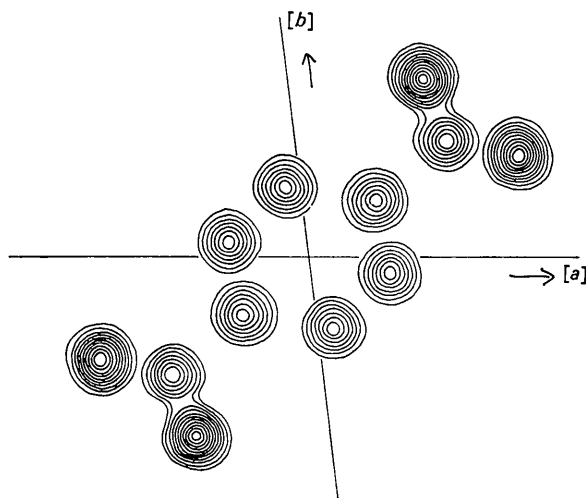


Fig. 2. $[c]$ electron density projection. The contours are at intervals of approximately $1 \text{ e.}\text{\AA}^{-2}$.

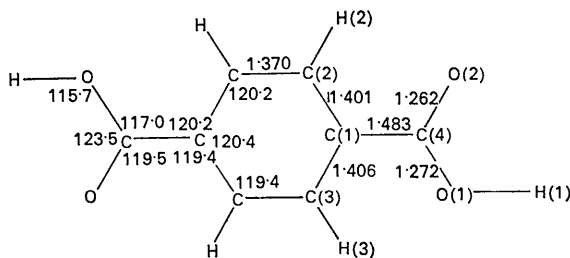


Fig. 3. Bond lengths and inter-bond angles (form I).

bonds in the manner which is usual in carboxylic acids, e.g. phthalic acid (Nowacki & Jaggi, 1957), benzoic acid (Sim, Robertson & Goodwin, 1955), acrylic acid (Higgs & Sass, 1963) and fumaric acid (Brown, 1966). A fuller list of structures of carboxylic acids is given in the paper by Higgs & Sass. There are no bonds, other than van der Waals, between neighbouring chains, which pack together slightly differently in the two forms. The reasons for this, and the conditions under which the two polymorphs crystallize, have not yet been elucidated. The bond lengths and inter-bond angles obtained are shown in Table 3, and the values for form I only are shown in Fig. 3.

Table 3. *Bond lengths and inter-bond angles*

Form I			
C(1)–C(2)	1.401 Å	C(1)–C(2)–C(3')	119.4°
C(1)–C(3)	1.406	C(1)–C(3)–C(2')	120.2
C(2)–C(3')	1.370	C(2)–C(1)–C(3)	120.4
C(1)–C(4)	1.483	C(2)–C(1)–C(4)	119.4
C(4)–O(1)	1.272	C(3)–C(1)–C(4)	120.2
C(4)–O(2)	1.262	C(1)–C(4)–O(1)	117.0
O(1)–H(1)–O(2')	2.608	C(1)–C(4)–O(2)	119.5
C–H (assumed)	1.08	O(1)–C(4)–O(2)	123.5
O–H (assumed)	1.08	C(4)–O(1)–H(1)	115.7
Mean standard deviation for bonds 0.0030 Å			
Mean standard deviations for angles 0.3°			
Form II			
C(1)–C(2)	1.38 Å	C(1)–C(2)–C(3')	121°
C(1)–C(3)	1.42	C(1)–C(3)–C(2')	120
C(2)–C(3')	1.39	C(2)–C(1)–C(3)	119
C(1)–C(4)	1.47	C(2)–C(1)–C(4)	120.5
C(4)–O(1)	1.28	C(3)–C(1)–C(4)	120.5
C(4)–O(2)	1.25	C(1)–C(4)–O(1)	118.5
		C(1)–C(4)–O(2)	119.5
		O(1)–C(4)–O(2)	122

The molecule is not quite planar; the equation of the mean plane through the benzene ring lying on the origin, in terms of standard orthogonal axes (for definition, see Truter, 1961) is

$$0.2972 X - 0.3753 Y - 0.8780 Z = 0$$

and that through atoms C(1), C(4), O(1) and O(2) is

$$0.3287 X - 0.4480 Y - 0.8314 Z = -0.0235.$$

The normals to these two planes are inclined at 5.25°. The carbon atoms of the benzene ring are all 0.0017 Å out of their mean plane, alternately above and below, which is within the limits of experimental error.

Intermolecular distances range from 3.32 Å upwards, the shortest being between oxygen atoms and carbon atoms of neighbouring molecules. The length of the hydrogen bond, 2.608 Å, compares with 2.64 Å in benzoic acid, and 2.68 Å in phthalic acid. The mean C–C length in the benzene ring (1.392 Å) is identical with that found in benzene (Cox, Cruickshank & Smith, 1958) after correcting for thermal vibrations, but there is evidence of a certain amount of quinonoid character in the ring, the C–C bonds parallel to the substituent groups being 0.034 Å shorter than the mean of the other four bonds in the ring. It would be interesting to relate this quinonoid character to the strength and reactivity of terephthalic acid.

The only temperature parameters which show any particular anisotropy are those of the two oxygen atoms which have a higher amplitude along c^* (see Table 1); this could be accounted for by a large oscillatory motion about the C(1)–C(4) bond.

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