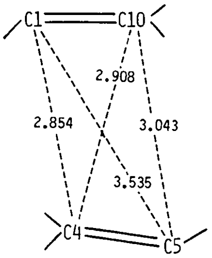

Fig. 4. Interatomic distances (Å) between the C–C double bonds in molecule (I). The mean e.s.d. of the values shown is $\sigma(\mathrm{C}\cdots\mathrm{C}) = 0{\cdot}009$ Å.

The three condensed six-membered rings of (II) adopt slightly deformed boat forms, the centered six-membered ring is a chair, and the γ-lactone ring shows an envelope form, while the γ-lactone ring of (I) is much more planar than that of (II). The junctions between the ten-membered ring and the γ-lactone ring, for (I), and the six-membered ring and the γ-lactone ring, for (II), are all *trans*. In both crystals, the molecules are packed together mainly by van der Waals forces and there are no hydrogen bonds.

The authors wish to express their thanks to Professor T. Inoue and Dr M. Nagai of Hoshi College of Pharmacy, Tokyo, Japan, for their helpful advice.

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Acta Cryst. (1982). **B38**, 1662–1663

Diethyl Terephthalate

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(*Received* 6 *October* 1981; *accepted* 4 *January* 1982)

Abstract. $C_{12}H_{14}O_4$, $M_r = 222{\cdot}24$, monoclinic, $P2_1/n$ (systematic absences: $h0l$, $h + l$ odd; $0k0$, k odd), $a = 9{\cdot}140\,(1)$, $b = 15{\cdot}450\,(3)$, $c = 4{\cdot}225\,(6)$ Å, $\beta = 92{\cdot}89\,(1)^\circ$, $U = 595{\cdot}9$ Å^3; $Z = 2$, $D_x = 1{\cdot}238$, $D_m = 1{\cdot}243$ Mg m^{-3}, m.p. = 317 K. $R = 0{\cdot}065$ for 922 counter reflexions. C(4)=O(8) = 1·206 (2) Å and the ethyl C(6)—C(7) = 1·467 (2) Å.

Introduction. This work is a continuation of our investigation of the model compounds of poly(ethylene terephthalate) (Hašek, Ječný, Langer, Huml & Sedláček, 1980). The structure of diethyl terephthalate was determined by Bailey (1949) with a relatively high $R = 0{\cdot}28$. In order to obtain more reliable results for the discussion of IR spectra, we redetermined this structure.

The unit-cell parameters were obtained by refinement of 19 reflexions with $23 < 2\theta < 112^\circ$ measured with a Syntex $P2_1$ diffractometer. X-ray intensities were collected by θ–2θ scans at room temperature using monochromated Cu $K\alpha$ radiation. 1005 independent reflexions were measured up to $\sin\theta/\lambda = 0{\cdot}59$ Å^{-1}; 83 of them were classified as unobserved with $I < 1{\cdot}96\sigma_I$, where σ_I was calculated from counting statistics.

No correction was made for absorption or extinction [μ(Cu $K\alpha$) = 0·73 mm^{-1}, crystal dimensions 0·1 × 0·1 × 0·2 mm]. Other measurement details are the same as in Hašek, Hlavatá & Huml (1977).

The structure was redetermined by direct methods with *MULTAN* 78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and refined by least squares in the block-diagonal approximation. The function minimized was $\sum w\Delta^2$, where $w = [\sigma_F^2 + (0{\cdot}02F)^2]^{-1}$ and $\Delta = ||F_o| - |F_c||$. Atomic scattering factors were taken from *International Tables for X-ray*

Table 1. *Final fractional coordinates* ($\times 10^4$) *and* B_{eq} *values* (Å^2) *of the non*-H *atoms with e.s.d.'s in parentheses*

	x	y	z	B_{eq}
C(1)	1503 (2)	−102 (1)	9883 (4)	6·42 (4)
C(2)	−689 (2)	703 (1)	8576 (4)	6·49 (4)
C(3)	811 (2)	615 (1)	8426 (4)	5·85 (4)
C(4)	1643 (2)	1280 (1)	6715 (4)	6·19 (4)
O(5)	3068 (1)	1106 (1)	6724 (3)	6·90 (3)
C(6)	3998 (2)	1718 (1)	5110 (5)	7·42 (5)
C(7)	5484 (3)	1357 (2)	5184 (7)	9·69 (8)
O(8)	1082 (2)	1901 (1)	5419 (4)	8·34 (4)

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Table 2. *Final fractional coordinates* ($\times 10^3$) *and* $B_{\rm iso}$ *values* (Å^2) *of the* H *atoms with e.s.d.'s in parentheses*

	x	y	z	$B_{\rm iso}$
H(1)	248 (2)	−21 (1)	966 (4)	6·6 (4)
H(2)	−110 (3)	118 (2)	784 (6)	9·4 (5)
H(61)	394 (3)	224 (1)	628 (5)	8·6 (5)
H(62)	356 (3)	178 (2)	276 (6)	10·9 (6)
H(71)	536 (2)	94 (1)	377 (4)	7·8 (5)
H(72)	590 (4)	126 (2)	790 (7)	12·6 (7)
H(73)	615 (3)	175 (2)	374 (7)	11·4 (6)

Crystallography (1974), those for H being taken as a spherical approximation of the bonded atom in the hydrogen molecule.

The refinement (all non-H atoms with anisotropic and H atoms with isotropic temperature factors) was stopped when the shifts of all parameters were $<0·2\sigma$. The final agreement factors are: $R_1 = \sum \Delta / \sum |F_o| = 0·065$, $R_2 = (\sum \Delta^2 / \sum |F_o|^2)^{1/2} = 0·088$, $wR_2 = (\sum w\Delta^2 / \sum w|F_o|^2)^{1/2} = 0·093$ for 922 observed reflexions. The residual electron density on the final difference map did not exceed 0·13 e Å^{-3}. The coordinates of all non-H atoms with $B_{\rm eq}$ values (Hamilton, 1959) are in Table 1 and those of the H atoms with $B_{\rm iso}$ values are in Table 2.*

Discussion. The numbering scheme, bond distances and selected bond angles and torsion angles are shown in Fig. 1. Angles not in Fig. 1 have been deposited.*

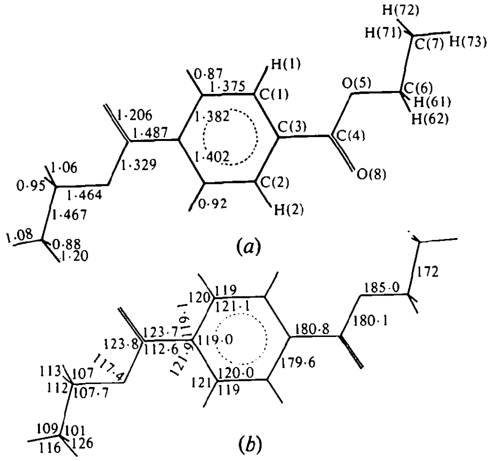

Fig. 1. (*a*) Numbering scheme and interatomic distances (Å); (*b*) Bond and torsion angles (°). E.s.d.'s for non-H and H atoms are: for distances 0·002 and 0·03 Å; for bond angles 0·2 and 1·0°; and for torsion angles not involving H 0·5°.

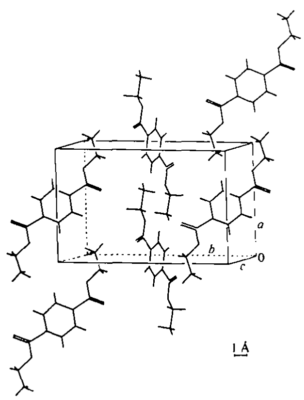

Fig. 2. Projection of the unit-cell contents perpendicular to the mean plane of the benzene ring.

Distances C(4)—O(8) and C(6)—C(7) were measured by Bailey (1949) as 1·28 (5) and 1·55 (5) Å. We have found significantly different values: 1·206 (2) and 1·467 (2) Å, respectively, in good agreement with those expected for this type of structure (Hašek, Ječný, Langer & Sedláček, 1980).

A projection of the structure perpendicular to the mean plane of the benzene ring is shown in Fig. 2. No significant intermolecular contact was observed. A list of the shortest distances has been deposited.*

The authors thank Dr P. Sedláček, CHEMOPETROL, SILON, Planá nad Lužinci, Czechoslovakia, for kindly supplying the crystal and for valuable discussions.

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* Lists of structure factors, anisotropic thermal parameters, additional bond- and torsion-angle data, and intermolecular distances have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36633 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

* See deposition footnote.