

Table 2. Bond distances (Å), bond angles (°) and selected torsion angles (°)

O(1)–C(1)	1.363 (9)	C(2)–H(1)	0.82 (8)
O(1)–C(5)	1.390 (9)	C(2)–H(2)	0.93 (10)
O(2)–C(1)	1.199 (10)	C(3)–H(3)	1.09 (8)
O(3)–C(5)	1.175 (9)	C(3)–H(4)	0.95 (7)
C(1)–C(2)	1.493 (13)	C(4)–H(5)	0.79 (7)
C(2)–C(3)	1.519 (13)	C(7)–H(6)	1.01 (8)
C(3)–C(4)	1.475 (14)	C(8)–H(7)	0.93 (6)
C(4)–C(5)	1.513 (12)	C(9)–H(8)	1.14 (9)
C(4)–C(6)	1.536 (12)	C(10)–H(9)	1.04 (9)
C(6)–C(7)	1.372 (10)	C(11)–H(10)	1.07 (5)
C(6)–C(11)	1.373 (13)		
C(7)–C(8)	1.419 (12)		
C(8)–C(9)	1.364 (14)		
C(9)–C(10)	1.364 (11)		
C(10)–C(11)	1.388 (11)		
C(1)–O(1)–C(5)	124.5 (6)	O(1)–C(5)–O(3)	116.6 (7)
O(1)–C(1)–O(2)	116.6 (7)	O(1)–C(5)–C(4)	115.6 (7)
O(1)–C(1)–C(2)	119.3 (8)	O(3)–C(5)–C(4)	127.7 (8)
O(2)–C(1)–C(2)	124.1 (8)	C(4)–C(6)–C(7)	124.0 (8)
C(1)–C(2)–C(3)	113.2 (8)	C(4)–C(6)–C(11)	116.4 (7)
C(2)–C(3)–C(4)	110.9 (8)	C(7)–C(6)–C(11)	119.4 (8)
C(3)–C(4)–C(5)	109.0 (8)	C(6)–C(7)–C(8)	119.7 (7)
C(3)–C(4)–C(6)	117.5 (7)	C(7)–C(8)–C(9)	119.5 (8)
C(5)–C(4)–C(6)	110.1 (6)	C(8)–C(9)–C(10)	120.6 (9)
		C(9)–C(10)–C(11)	119.9 (8)
		C(6)–C(11)–C(10)	120.7 (8)
C(6)–C(4)–C(3)–C(2)	173.5 (8)	O(2)–C(1)–O(1)–C(5)	171.8 (7)
C(6)–C(4)–C(5)–O(3)	10.5 (13)	C(5)–O(1)–C(1)–C(2)	7.7 (12)
C(6)–C(4)–C(5)–O(1)	–173.5 (7)	O(1)–C(1)–C(2)–C(3)	10.5 (13)
C(1)–O(1)–C(5)–C(4)	9.1 (11)	C(1)–C(2)–C(3)–C(4)	–44.9 (12)
C(1)–O(1)–C(5)–O(3)	–174.3 (7)	O(2)–C(1)–C(2)–C(3)	–170.0 (9)

molecule with the arbitrary numbering scheme used in the analysis. As expected, the molecule as a whole is not planar. The angle formed by the two mean ring planes is 50.9 (3)°. The phenyl ring is planar within the errors and the bond distances and angles are normal.

The cyclohexane ring shows a half-boat conformation. Atom C(4) is out of the plane formed by the other ring atoms by 0.57 (8) Å. The ring-puckering parameters calculated following Cremer & Pople (1975) are $Q = 0.49$ Å, $\theta = 56.0$ and $\varphi = 208.6$ °.

Both carbonyl oxygens occupy an equatorial position and the angles formed by the two C=O bonds

with the normal to the mean ring plane are 96.2 (3) and 100.7 (4)°.

None of the intermolecular contacts are shorter than 3.41 Å; consequently the molecules are held in the crystal by van der Waals forces.

The work is a part of an International Project supported by CNR and CNRS (ERA 895).

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Structure of 1,4-Butanediyl Dibenzoate*

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Abstract. C₁₈H₁₈O₄, $M_r = 298.3$, triclinic, $P\bar{1}$, $a = 115.3$ (2), $\beta = 90.2$ (2), $\gamma = 83.7$ (1)°, $V = 12.591$ (3), $b = 8.555$ (2), $c = 7.854$ (3) Å, $\alpha = 759.4$ (2) Å³, $D_x = 1.30$ Mg m⁻³, $\mu(\text{Cu } K\alpha) = 0.71$ mm⁻¹. The structure was solved by direct methods and refined to $R = 0.057$ for 2725 collected reflections. A

* Stereochemical Studies of Oligomers. I.

significant shortening is present in the $C_{sp^3}-C_{sp^3}$ bonds of the 'glycol' part of the molecule which shows a *trans-trans-gauche* conformation. The two carboxylic groups are tilted with respect to the aromatic rings.

Introduction. In the past years a great number of studies on the conformation of polyethylenes, polypeptides, polynucleotides and polysaccharides have been made *via* the conformations of small molecules which are very close, in the solid state, to those of the polymers. The problem was tackled by numerous theoretical techniques and in some cases (Sundararajan & Marchessault, 1975; Sundararajan, Labrie & Marchessault, 1975) encouraging results were obtained when the repeat distance and the screw symmetry of the polymer helix were known from X-ray analysis.

The difficulties in the analysis of these derivatives by NMR spectroscopy methods suggested that more extensive studies with X-ray techniques would be useful and the first of these analyses is reported in this paper.

Single crystals of the compound were recrystallized from a benzene solution as white prisms. Preliminary cell constants were obtained from rotation and Weissenberg photographs. The crystal ($0.6 \times 0.4 \times 0.3$ mm) was then transferred to a Siemens AED single-crystal diffractometer. The orientation matrix and precise cell constants resulted from a least-squares calculation performed using the setting angles of 27 accurately measured reflections ($17.7 < \theta < 55.5^\circ$). The diffraction intensities for 2725 reflections ($2 < \theta < 70^\circ$) were collected with nickel-monochromated Cu $K\alpha$ radiation ($\lambda = 1.5418 \text{ \AA}$) using a method which collects the outline of any peak (Belletti, Ugozzoli, Cantoni & Pasquinelli, 1979); 247 of these, having $I < 2\sigma(I)$, were considered unobserved and excluded from the refinement. The intensity of a check reflection, periodically monitored during the data collection, showed no appreciable decomposition of the specimen. No absorption correction was made.

The structure was solved by direct methods using the *SHELX* system (Sheldrick, 1976). Refinement of all the non-hydrogen atoms gave an R of 0.33. Isotropic full-matrix refinement of these atoms lowered the R to 0.162 and with anisotropic thermal parameters $R = 0.116$. A difference-Fourier synthesis calculated at this stage showed all the hydrogen atoms as the highest peaks of the map. The final R value was 0.0567 for all the reflections. Twelve reflections, for which the difference $|F_o - F_c|$ was large, were omitted in the last cycles of refinement.

The function minimized was $\sum w|\Delta F|^2$ with unit weights as the weighting scheme $w^{-1} = [\sigma^2(F_o) + k(F_o)^2]$ attempted with different k values gave unsatisfactory results.

Scattering-factor curves were taken from *International Tables for X-ray Crystallography* (1974). A ΔF synthesis calculated at the end of the refinement

Table 1. Atomic coordinates ($\times 10^4$ for O and C, $\times 10^3$ for H atoms), B_{eq} (\AA^2) and isotropic U ($\text{\AA}^2 \times 10^3$) for H

	x	y	z	B_{eq}^*/U_{iso}
O(1)	744 (1)	4424 (2)	-2250 (2)	5.82 (11)
O(2)	-822 (1)	5542 (1)	-2660 (2)	4.48 (10)
O(3)	-4364 (1)	8120 (1)	704 (1)	4.07 (10)
O(4)	-6010 (1)	7532 (1)	297 (2)	5.51 (11)
C(1)	547 (1)	7183 (2)	-2350 (2)	4.24 (12)
C(2)	-115 (1)	8401 (2)	-2683 (2)	4.89 (13)
C(3)	257 (2)	9887 (3)	-2604 (3)	6.16 (15)
C(4)	1271 (2)	10163 (3)	-2184 (3)	6.80 (15)
C(5)	1919 (2)	8996 (3)	-1800 (3)	6.79 (14)
C(6)	1565 (1)	7492 (3)	-1891 (3)	5.48 (13)
C(7)	191 (1)	5578 (2)	-2417 (2)	4.20 (11)
C(8)	-1275 (1)	4089 (2)	-2582 (3)	4.52 (12)
C(9)	-2435 (1)	4489 (2)	-2563 (2)	4.24 (11)
C(10)	-2866 (1)	6177 (2)	-893 (2)	4.14 (10)
C(11)	-4023 (1)	6439 (2)	-842 (2)	4.08 (11)
C(12)	-5379 (1)	8489 (2)	1139 (2)	3.83 (11)
C(13)	-5640 (1)	10211 (2)	2776 (2)	3.74 (11)
C(14)	-6670 (1)	10778 (2)	3414 (2)	4.90 (12)
C(15)	-6928 (2)	12366 (3)	4969 (3)	5.81 (12)
C(16)	-6161 (2)	13376 (2)	5858 (2)	5.58 (13)
C(17)	-5141 (2)	12825 (2)	5222 (3)	4.48 (12)
C(18)	-4879 (1)	11233 (2)	3679 (2)	4.07 (11)
H(1)	-84 (2)	825 (3)	-297 (3)	68 (5)
H(2)	-9 (2)	1061 (3)	-288 (3)	83 (7)
H(3)	147 (2)	1119 (4)	-210 (4)	100 (8)
H(4)	267 (2)	923 (3)	-142 (3)	76 (6)
H(5)	202 (2)	667 (3)	-166 (3)	75 (6)
H(6)	-99 (1)	307 (3)	-361 (3)	61 (5)
H(7)	-106 (1)	403 (2)	-142 (3)	57 (5)
H(8)	-263 (2)	466 (3)	-371 (3)	79 (6)
H(9)	-282 (1)	356 (3)	-256 (2)	58 (5)
H(10)	-263 (2)	719 (3)	-96 (3)	75 (6)
H(11)	-264 (1)	619 (2)	39 (2)	52 (4)
H(12)	-425 (2)	656 (3)	-213 (3)	75 (5)
H(13)	-429 (1)	559 (2)	-66 (2)	51 (4)
H(14)	-717 (1)	1005 (2)	291 (2)	52 (4)
H(15)	-763 (2)	1275 (4)	528 (4)	107 (8)
H(16)	-625 (2)	1439 (4)	678 (4)	101 (8)
H(17)	-459 (2)	1357 (3)	586 (3)	71 (5)
H(18)	-421 (2)	1086 (2)	319 (3)	63 (5)

* Defined according to Hamilton (1959).

process gave no peaks of magnitude greater than $0.2 e \text{ \AA}^{-3}$.

The final positional and thermal parameters are listed in Table 1.*

All the calculations were performed on the General Automation SPC/16 computer using a local set of programs and on the CDC CYBER 76 computer of the Centro di Calcolo Interuniversitario dell'Italia Nord-Orientale, Casalecchio, Bologna, with financial support from the University of Parma.

* Lists of structure factors, anisotropic thermal parameters and equations of least-squares planes of the molecule have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36749 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. Bond distances, bond angles and selected torsion angles are listed in Table 2. A drawing of the molecule is depicted in Fig. 1.

The two phenyl rings show normal geometries, 1.363 (6), 1.359 (8) Å and 120.0 (4), 119.5 (5)° for the mean $C_{sp^2}-C_{sp^2}$ bond distances and the mean internal angles for the two rings respectively. These two distances are rather short if compared with the values

Table 2. Bond distances (Å), bond angles (°), and selected torsion angles (°)

O(1)—C(7)	1.199 (3)	C(2)—H(1)	0.95 (3)
O(2)—C(7)	1.292 (2)	C(3)—H(2)	0.82 (3)
O(2)—C(8)	1.448 (3)	C(4)—H(3)	0.92 (4)
O(3)—C(11)	1.450 (4)	C(5)—H(4)	1.01 (3)
O(3)—C(12)	1.293 (2)	C(6)—H(5)	0.94 (3)
O(4)—C(12)	1.189 (3)	C(8)—H(6)	0.93 (2)
C(1)—C(2)	1.374 (3)	C(8)—H(7)	0.97 (2)
C(1)—C(6)	1.354 (2)	C(9)—H(8)	1.00 (3)
C(1)—C(7)	1.470 (3)	C(9)—H(9)	0.98 (2)
C(2)—C(3)	1.379 (3)	C(10)—H(10)	0.97 (3)
C(3)—C(4)	1.340 (4)	C(10)—H(11)	1.04 (2)
C(4)—C(5)	1.352 (4)	C(11)—H(12)	1.09 (3)
C(5)—C(6)	1.380 (4)	C(11)—H(13)	0.90 (2)
C(8)—C(9)	1.462 (2)	C(14)—H(14)	0.90 (1)
C(9)—C(10)	1.521 (5)	C(15)—H(15)	0.90 (2)
C(10)—C(11)	1.448 (2)	C(16)—H(16)	0.86 (3)
C(12)—C(13)	1.487 (5)	C(17)—H(17)	0.98 (2)
C(13)—C(14)	1.352 (3)	C(18)—H(18)	0.89 (2)
C(13)—C(18)	1.354 (3)		
C(14)—C(15)	1.389 (5)		
C(15)—C(16)	1.352 (4)		
C(16)—C(17)	1.338 (4)		
C(17)—C(18)	1.388 (4)		
C(7)—O(2)—C(8)	116.4 (7)	C(8)—C(9)—C(10)	112.7 (5)
C(11)—O(3)—C(12)	116.4 (5)	C(9)—C(10)—C(11)	110.7 (4)
C(6)—C(1)—C(7)	118.3 (6)	O(3)—C(11)—C(10)	107.2 (5)
C(2)—C(1)—C(7)	123.0 (7)	O(3)—C(12)—O(4)	122.4 (5)
C(2)—C(1)—C(6)	118.7 (7)	O(4)—C(12)—C(13)	125.4 (7)
C(1)—C(2)—C(3)	120.8 (7)	O(3)—C(12)—C(13)	112.1 (6)
C(2)—C(3)—C(4)	120.0 (7)	C(12)—C(13)—C(18)	122.4 (6)
C(3)—C(4)—C(5)	119.6 (7)	C(12)—C(13)—C(14)	119.3 (5)
C(4)—C(5)—C(6)	121.3 (7)	C(14)—C(13)—C(18)	118.4 (4)
C(1)—C(6)—C(5)	119.6 (7)	C(13)—C(14)—C(15)	120.2 (7)
O(2)—C(7)—C(1)	111.8 (7)	C(14)—C(15)—C(16)	120.9 (6)
O(1)—C(7)—C(1)	126.1 (8)	C(15)—C(16)—C(17)	119.1 (4)
O(1)—C(7)—O(2)	122.2 (7)	C(16)—C(17)—C(18)	120.1 (7)
O(2)—C(8)—C(9)	106.1 (6)	C(13)—C(18)—C(17)	121.3 (7)
C(1)—C(7)—O(2)—C(8)	174.8 (6)	C(9)—C(10)—C(11)—O(3)	-176.2 (5)
O(1)—C(7)—O(2)—C(8)	-4.4 (9)	C(10)—C(11)—O(3)—C(12)	171.0 (6)
C(7)—O(2)—C(8)—C(9)	170.4 (6)	C(11)—O(3)—C(12)—C(13)	178.2 (6)
O(2)—C(8)—C(9)—C(10)	-59.3 (7)	C(11)—O(3)—C(12)—O(4)	-2.0 (9)
C(8)—C(9)—C(10)—C(11)	-175.0 (6)		

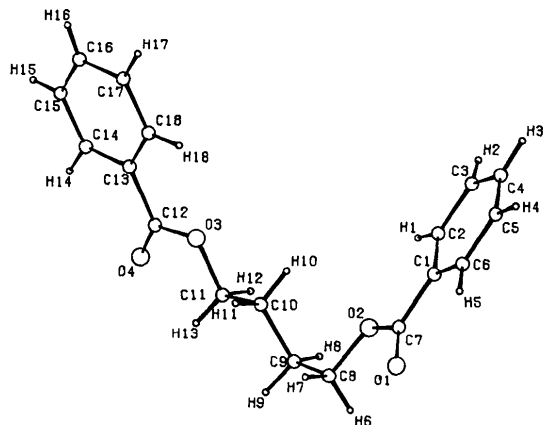


Fig. 1. Projection of the molecule.

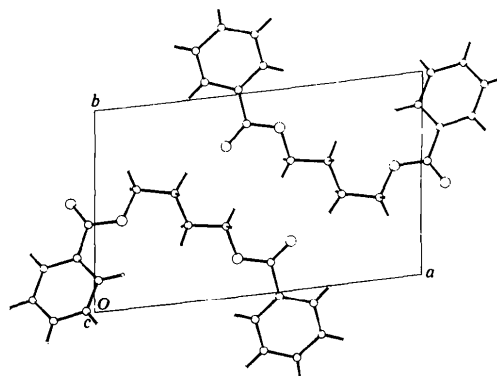


Fig. 2. Packing of the molecules viewed down the *c* axis.

indicated by Sutton (1965) [1.395 (5) Å] or by Brisse & Sygusch (1974) [1.379 Å] but they are not extraordinary. The angles formed by the two aromatic-ring planes is 58.5 (4)°.

It was systematically found in other structures with a 'glycol' part (Pérez & Brisse, 1975, 1976*a,b*, 1977; Flippin, 1977; Hašek, Ječný, Langer, Huml & Sedlacek, 1980) that there was a significant shortening of the $C_{sp^2}-C_{sp^2}$ distances, which range between 1.464 and 1.504 Å, very far from the expected value of 1.537 Å (Sutton, 1965). Thus in the present compound the C(8)—C(9) and the C(10)—C(11) distances are 1.462 (2) and 1.448 (2) Å respectively, while the third one [C(9)—C(10) = 1.521 (5) Å] is nearer to the expected value. A relative lengthening of the $C_{sp^2}-C_{sp^2}$ distance in 'glycol' derivatives when the carbons are not attached to oxygens was previously observed in 'hexamethylene glycol dibenzoate' (Pérez & Brisse, 1977).

The two carboxylic groups present geometries as expected for these molecular fragments and the two planes are tilted by 6.3 (3) and 1.1 (3)° respectively from the phenyl-ring planes.

Two of the torsion angles of the tetramethylene part are near to 180° [176.2 (5), 175.0 (6)°] while the third one is 59.3 (7)° and, consequently, this part shows a *trans-trans-gauche* conformation. The departure from the *trans* conformation is also notable in the torsion angles involving the O(2) and O(3) atoms [170.4 (6) and 171.0 (6)°].

The molecules, as shown in Fig. 2, are held in the crystal by van der Waals forces.

This work is a part of an International Project supported by CNR and CNRS (ERA 895).

Soon after this paper was submitted for publication a communication appeared (Palmer & Brisse, 1981) in which the resolution of the structure of the title compound is announced.

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Structure de la Di(thyminy1-1)-1,8 Dioxa-3,6 Octane

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(Reçu le 27 octobre 1981, accepté le 15 février 1982)

Abstract. $C_{16}H_{22}N_4O_6$, triclinic, space group $P\bar{1}$, $a = 12.356$ (1), $b = 9.341$ (2), $c = 8.524$ (2) Å, $\alpha = 116.08$ (2), $\beta = 96.10$ (1), $\gamma = 92.58$ (1)°, $V = 874$ Å³, $D_c = 1.39$ Mg m⁻³, $Z = 2$. Final $R = 0.041$ for 2704 observed reflections. The triethylenedioxy chain does not appreciably disturb the stacking capacity of the thymine groups.

Introduction. La préparation de la di(thyminy1-1)-1,8 dioxa-3,6 octane a été réalisée dans le cadre d'une série de trois composés du type $A-E_3-B$ où A et B représentent l'un des groupes thymine ou psoralène (furo[3,2-g]coumarine) et E_3 une chaîne triéthylène-oxy. Cette série a été synthétisée en vue de l'étude dans le cristal des interactions s'établissant entre psoralène et thymine et de l'influence de la présence de la chaîne E_3 sur ces interactions. C'est précisément afin de tester les contraintes induites par cette chaîne sur l'organisation des groupes thymine dans le cristal que l'étude radiocristallographique du présent composé a été entreprise.

Le cristal étudié a été obtenu par lente évaporation d'une solution dans l'acétate d'éthyle. Les intensités de diffraction de Bragg ont été mesurées sur un diffractomètre automatique CAD-4 Enraf-Nonius à la température ambiante avec la radiation $K\alpha$ du cuivre mono-

chromatisée. Le cristal étudié, de forme prismatique, a des dimensions de $0,2 \times 0,2 \times 0,2$ mm. Sur 3444 réflexions indépendantes, 2704 ont une intensité supérieure à 3σ pour $1^\circ < 2\theta < 110^\circ$. Les intensités ont été corrigées du facteur de Lorentz-polarisation mais non de l'absorption ni de l'extinction.

La structure de départ a été déterminée par méthode directe à l'aide du programme *MULTAN* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). Les cartes de densité électronique ont permis de localiser les atomes non hydrogène. Les atomes d'hydrogène ont été situés géométriquement à l'exception de ceux des groupes méthyles qui ont été localisés par synthèses différence. L'affinement par moindres carrés des paramètres atomiques par la méthode des blocs diagonaux a conduit à la valeur final $R = 0,041$ du facteur d'accord. Les valeurs des paramètres atomiques sont reportées dans le Tableau 1, le dessin de la molécule est donné dans la Fig. 1.*

* Les listes des facteurs de structure, des facteurs d'agitation thermique anisotrope et des coordonnées atomiques des atomes d'hydrogène ont été déposées au dépôt d'archives de la British Library Lending Division (Supplementary Publication No. SUP 36757: 24 pp.). On peut en obtenir des copies en s'adressant à: The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.