Related literature. Structures containing the carbamoyl moiety have been reported by Baggio, Becka, Amzel, Avey & Poljak (1973) and Ganis, Avitabile, Migdal & Goodman (1971).

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Stereochemical Studies of Oligomers. XVI.* 2,3-Butanediyl Bis(*m*-chlorobenzoate)

BY GABRIELE BOCELLI

Centro di Studio per la Strutturistica Diffrattometrica del CNR, Via M. D'Azeglio 85, 43100 Parma, Italy

AND MARIE-FLORENCE GRENIER-LOUSTALOT

Institut Universitaire de Recherche Scientifique, ERA 895, Avenue Philippon, 6400 Pau, France

Abstract. $C_{18}H_{16}Cl_2O_4$, $M_r = 367.2$, triclinic, $P\bar{1}$, $a = 8.327$ (3), $b = 7.874$ (2), $c = 7.645$ (3) Å, $\alpha = 61.89$ (4), $\beta = 91.46$ (3), $\gamma = 93.02$ (3)°, $V = 441.5$ (3) Å³, $Z = 1$, $D_x = 1.38$ g cm⁻³, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 35.23$ cm⁻¹, $F(000) = 190$, room temperature, $R = 0.059$ for 983 observed reflections. The conformation of the molecule is *trans* in the central part of the aliphatic chain while the rest differs noticeably from this arrangement, the C(7)–O(2)–C(8)–C(8') torsion angle being 149.9 (4)°. The carboxylic groups are tilted by 12.2 (2)° with respect to the aromatic ring planes. The two methyls are *trans* with respect to the C(8)–C(8') bond.

Experimental. Prismatic specimen $0.2 \times 0.4 \times 0.4$ mm, lattice parameters refined by least squares by use of 19 $(\theta,\chi,\varphi)_{hkl}$ accurate measurements on a Siemens AED single-crystal diffractometer on line to a General Automation Jumbo 220 computer. Intensities collected $(2 < \theta < 70°)$ with a modified version (Belletti, Ugozzoli, Cantoni & Pasquinelli, 1979) of the Lehmann & Larsen (1974) procedure, one check reflection recorded every 50 counts, only statistical variation in intensity, 983 observed reflections [$I >$

$2\sigma(I)$] retained out of a total of 1486 measured independent reflections, $-10 \leq h \leq 10$, $-7 \leq k \leq 8$, $0 \leq l \leq 8$, data corrected for Lorentz and polarization effects but not for absorption. Direct methods with *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), atomic coordinates of heavy atoms refined by full-matrix least squares first with isotropic temperature factors and then with anisotropic ones using *SHELX*76 (Sheldrick, 1976), H atoms found in a difference Fourier map and refined isotropically; $R = 0.059$ and $wR = 0.061$ where $w = 0.3972/(\sigma^2 F + 0.02812F^2)$, $\sum w(F_o - F_c)^2$ minimized, final difference electron density map did not show peaks >0.26 e Å⁻³, $(\Delta/\sigma)_{max} = 0.288$, scattering factors those of *SHELX*.

All calculations performed on a Gould Sel 32/77 computer.†

Table 1 gives the atom parameters and Table 2 bond lengths, angles and selected torsion angles. Fig. 1 shows the molecule and numbering scheme.

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* Part XV: Bocelli, Ugozzoli & Grenier-Loustalot (1985).

† Lists of structure factors, thermal parameters, H coordinates and bond lengths involving H have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42610 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates* $(\times 10^4)$ *and* U_{eq} $(\text{Å}^2 \times 10^4)$

	x	y	z	U_{eq}*
Cl	1826 (1)	10496 (2)	2470 (2)	880 (8)
O(1)	6378 (4)	5586 (4)	6373 (5)	720 (15)
O(2)	8547 (3)	6793 (4)	4431 (4)	600 (12)
C(1)	6278 (4)	8655 (6)	3514 (5)	476 (16)
C(2)	4636 (5)	8743 (6)	3653 (7)	542 (20)
C(3)	3895 (5)	10399 (6)	2335 (7)	573 (20)
C(4)	4758 (6)	11944 (7)	911 (8)	683 (24)
C(5)	6398 (6)	11876 (7)	800 (7)	715 (23)
C(6)	7167 (5)	10216 (6)	2101 (6)	575 (21)
C(7)	7034 (5)	6859 (6)	4940 (6)	527 (19)
C(8)	9426 (5)	5087 (6)	5715 (6)	591 (18)
C(9)	10305 (8)	5417 (10)	7306 (9)	810 (33)

* Hamilton (1959).

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

Cl—C(3)	1·736 (4)	C(2)—C(3)	1·382 (6)
O(1)—C(7)	1·201 (5)	C(3)—C(4)	1·372 (6)
O(2)—C(7)	1·339 (5)	C(4)—C(5)	1·376 (7)
O(2)—C(8)	1·459 (5)	C(5)—C(6)	1·392 (6)
C(1)—C(2)	1·382 (6)	C(8)—C(9)	1·522 (9)
C(1)—C(6)	1·385 (5)	C(8)—C(8')	1·528 (7)
C(1)—C(7)	1·480 (5)		

C(7)—O(2)—C(8)	117·4 (3)	C(4)—C(5)—C(6)	121·3 (5)
C(6)—C(1)—C(7)	122·0 (4)	C(1)—C(6)—C(5)	119·8 (4)
C(2)—C(1)—C(7)	117·6 (4)	O(2)—C(7)—C(1)	112·0 (4)
C(2)—C(1)—C(6)	120·4 (4)	O(1)—C(7)—C(1)	124·8 (4)
C(1)—C(2)—C(3)	118·9 (4)	O(1)—C(7)—O(2)	123·2 (4)
Cl—C(3)—C(2)	119·0 (4)	C(2)—C(8)—C(8')	103·2 (3)
C(2)—C(3)—C(4)	121·3 (5)	O(2)—C(8)—C(9)	109·3 (5)
Cl—C(3)—C(4)	119·7 (4)	C(9)—C(8)—C(8')	112·6 (4)
C(3)—C(4)—C(5)	119·9 (5)		

C(2)—C(1)—C(7)—O(1)	−11·0 (7)	O(1)—C(7)—O(2)—C(8)	−0·8 (5)
C(2)—C(1)—C(7)—O(2)	168·0 (4)	C(7)—O(2)—C(8)—C(9)	−90·0 (5)
C(6)—C(1)—C(7)—O(1)	168·1 (5)	C(7)—O(2)—C(8)—C(8')	149·9 (4)
C(6)—C(1)—C(7)—O(2)	−13·0 (6)	O(2)—C(8)—C(8')—C(9')	−62·3 (5)
C(1)—C(7)—O(2)—C(8)	−179·7 (4)	C(9)—C(8)—C(8')—C(9')	180·0
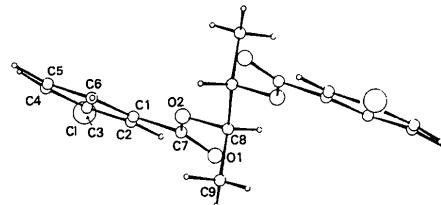
Fig. 1. Projection of the molecule viewed down **a**.

Related literature. Bocelli, Ugozzoli & Grenier-Loustalot (1985).

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Stereochemical Studies of Oligomers. XVII.* Dibenzyl Phthalate

By GABRIELE BOCELLI

Centro di Studio per la Strutturistica Diffrattometrica del CNR, Via M. D'Azeglio 85, 43100 Parma, Italy

AND MARIE-FLORENCE GRENIER-LOUSTALOT

Institut Universitaire de Recherche Scientifique, ERA 895, Avenue Philippon, 6400 Pau, France

Abstract. $C_{22}H_{18}O_4$, $M_r = 346\cdot4$, orthorhombic, $P2_12_12_1$, $a = 15\cdot731$ (3), $b = 10\cdot932$ (3), $c = 10\cdot646$ (2) Å, $V = 1830\cdot8$ (7) Å^3, $Z = 4$, $D_x = 1\cdot26$ g cm^{-3}, $\lambda(\text{Cu} K\alpha) = 1\cdot5418$ Å, $\mu = 6\cdot63$ cm^{-1}, $F(000) = 728$, room temperature, $R = 0\cdot063$ for 1301 observed reflections. The molecule contains five planar parts: the three aromatic rings and the two carboxylic groups. These last two planar fragments are tilted by $57\cdot7$ (2) ,and $115\cdot4$ (2)° with respect to the central aromatic ring respectively and form dihedral angles of $108\cdot1$ (3) and $85\cdot0$ (2)° with respect to their respective terminal rings. In their turn, the planes of these last

* Part XVI: Bocelli & Grenier-Loustalot (1986).