between the centres of the rings) which is 15·719 Å in the unchlorinated derivative and 15·790, 15·633 and 15·717 Å in HDDO, HDDM and HDDP, respectively. The steric hindrance between the chlorines and the carboxylic groups, particularly marked in HDDO, causes a rotation of the carboxylic group with respect to the ring with consequent significant shortening of the length of the molecule. The tilt of the carboxylic moieties with respect to their rings, range 0·2 (2)–4·5 (1)° in HDDM and HDDP, increases to 36·0 (1) and 33·8 (1)° in HDDO.

The phenyl rings are parallel to each other for symmetry requirements in HDDM, quasi-parallel [1·0 (1)°] in HDDP, whilst their least-squares planes subtend a dihedral angle of 13·5 (1)° in HDDO.

The packing of the molecules in the crystals is mainly determined by van der Waals interactions.

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Stereochemical Studies of Oligomers. XI.* The Structure of 1,2-Propanediyl Bis(*p*-chlorobenzoate) (PDP), $C_{17}H_{14}Cl_2O_4$, and 2,3-Butanediyl Bis(*p*-chlorobenzoate) (BDP), $C_{18}H_{16}Cl_2O_4$

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Abstract. Ni-filtered Cu $K\alpha$ radiation, $\bar{\lambda} = 1{\cdot}5418$ Å, room temperature. PDP: $M_r = 353{\cdot}2$, monoclinic, $C2/c$, $a = 19{\cdot}859$ (3), $b = 8{\cdot}837$ (2), $c = 19{\cdot}426$ (2) Å, $\beta = 103{\cdot}15$ (4)°, $V = 3319{\cdot}8$ (11) Å^3, $Z = 8$, $D_x = 1{\cdot}41$ g cm^{-3}, $\mu = 37{\cdot}28$ cm^{-1}, $F(000) = 1456$, final $R = 0{\cdot}041$ for 1295 observed reflections. BDP: $M_r = 367{\cdot}2$, monoclinic, $P2_1/c$, $a = 14{\cdot}679$ (2), $b = 6{\cdot}284$ (3), $c = 19{\cdot}638$ (2) Å, $\beta = 93{\cdot}24$ (4)°, $V = 1808{\cdot}6$ (9) Å^3, $Z = 4$, $D_x = 1{\cdot}35$ g cm^{-3}, $\mu = 34{\cdot}40$ cm^{-1}, $F(000) = 760$, final $R = 0{\cdot}055$ for 2920 observed reflections. The conformation of the centre of the chain of BDP is *gauche*, while the presence of one methyl group in PDP shifts the aliphatic chain away from a *trans* arrangement. The two rings are tilted by 11·9 (2), 6·5 (2) and 6·7 (1), 0·5 (1)° with respect to their carboxylic groups in the two compounds, respectively. A significant shortening of one of the C_{sp^3}—C_{sp^3} bonds of the chain of PDP is observed.

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* Part X: Bocelli & Grenier-Loustalot (1984).

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Introduction. As pointed out in the preceding papers of this series the knowledge of changes in conformation of derivatives which are 'model compounds' for polymeric materials may be very useful in spectroscopic studies and in determining the structure of related polymers. Thus several derivatives have been synthetized and are under investigation in our laboratories, and the crystal structures of two of them constitute the argument of this paper.

Experimental. For both compounds: Siemens AED single-crystal diffractometer, General Automation Jumbo 220 computer, 1 check reflection every 50 counts, profile analysis following a modified version (Belletti, Ugozzoli, Cantoni & Pasquinelli, 1979) of the Lehmann & Larsen (1974) procedure, Lp corrections, absorption ignored.

PDP: crystals from ethanol, colourless prism, 0·3 × 0·4 × 0·7 mm, cell parameters from 24 reflections ($14 \leq \theta \leq 48°$), standard reflection without significant variations, 3279 unique reflections ($R_{\rm int} = 0{\cdot}013$), 1295 observed [$I \geq 2\sigma(I)$], $2 \leq \theta \leq 70°$, $-22 \leq h \leq 22$, $0 \leq k \leq 10$, $0 \leq l \leq 22$, direct methods with *SHELX* (Sheldrick, 1976), $\sum w(\Delta F)^2$ minimized, anisotropic full matrix, H (from ΔF map) isotropic, final $R = 0{\cdot}041$, $R_w = 0{\cdot}047$ [$w = 0{\cdot}18/(\sigma^2F + 0{\cdot}01133F^2)$], no peaks $>0{\cdot}26$ e Å^{-3} in final ΔF map, $(\Delta/\sigma)_{\max} = 0{\cdot}76$, 264 parameters refined.

BDP: crystals from acetone, colourless prisms, 0·3 × 0·5 × 0·11 mm, cell parameters from 23 reflections ($14 \leq \theta \leq 22°$), only statistical variations of check reflection, 3680 unique reflections ($R_{\rm int} = 0{\cdot}023$), 2932 observed [$I \geq 3\sigma(I)$], $2 \leq \theta \leq 70°$, $-17 \leq h \leq 17$, $0 \leq k \leq 7$, $0 \leq l \leq 23$, direct methods with *SHELX*, anisotropic block matrix, H (from ΔF map) isotropic, $\sum w(\Delta F)^2$ minimized, final $R = 0{\cdot}055$, $R_w = 0{\cdot}073$ [$w = 1{\cdot}0/(\sigma^2F + 0{\cdot}0029F^2)$], $(\Delta\rho)_{\max} = 0{\cdot}30$ e Å^{-3}, $(\Delta/\sigma)_{\max} = 0{\cdot}54$, 282 parameters refined. All atomic scattering factors from *SHELX*; all calculations were performed on a Gould SEL 32/77 computer.*

Discussion. Atomic coordinates are given in Table 1, views of the molecules in Figs. 1 and 2. The mean C_{sp^2}–C_{sp^2} bond distances are 1·381 (3), 1·380 (5) and 1·384 (2), 1·384 (5) Å in PDP and BDP, respectively, while the average internal angles of the rings are 119·9 (4), 120·0 (5) and 120·1 (4), 120·0 (6)°. The C–Cl bond distances [1·735 (5), 1·736 (5) and 1·740 (3), 1·745 (4) Å] are near to the value proposed by Domenicano, Vaciago & Coulson (1975) [1·7404 (11) Å].

Table 1. *Final atomic coordinates* (×10^4) *with* B_{eq} *values* (Å^2) *for* PDP *and* BDP

PDP	x	y	z	$B_{\rm eq}$*
Cl(1)	1048 (1)	3107 (2)	7346 (1)	7·18
Cl(2)	5939 (1)	16458 (2)	12075 (1)	7·96
O(1)	1884 (2)	8879 (4)	9619 (2)	6·82
O(2)	2679 (2)	9110 (4)	8978 (2)	5·24
O(3)	4966 (2)	11382 (4)	9477 (2)	5·54
O(4)	3996 (2)	11670 (3)	9860 (2)	5·16
C(1)	1896 (2)	7103 (5)	8698 (2)	3·90
C(2)	1258 (3)	6490 (6)	8724 (3)	4·72
C(3)	1000 (3)	5263 (6)	8312 (3)	5·03
C(4)	1381 (3)	4643 (5)	7870 (2)	4·42
C(5)	2012 (3)	5244 (6)	7832 (3)	4·52
C(6)	2263 (3)	6474 (5)	8239 (2)	4·12
C(7)	2140 (2)	8426 (6)	9152 (2)	4·54
C(8)	2956 (3)	10483 (6)	9387 (3)	5·58
C(9)	2567 (4)	11897 (7)	9052 (5)	6·53
C(10)	3689 (3)	10502 (7)	9355 (3)	5·44
C(11)	4654 (3)	11964 (5)	9871 (2)	4·18
C(12)	4959 (2)	13083 (4)	10431 (2)	3·79
C(13)	4594 (3)	13607 (5)	10913 (3)	4·49
C(14)	4889 (3)	14660 (6)	11424 (3)	5·04
C(15)	5554 (3)	15162 (5)	11434 (2)	4·62
C(16)	5910 (3)	14661 (5)	10961 (3)	4·60
C(17)	5618 (3)	13616 (5)	10456 (3)	4·08
BDP				
Cl(1)	945 (1)	−3596 (2)	1228 (1)	5·76
Cl(2)	6905 (1)	−1342 (2)	3001 (1)	8·04
O(1)	1255 (2)	−1353 (3)	4581 (1)	4·48
O(2)	1749 (1)	1690 (3)	4127 (1)	3·44
O(3)	3760 (2)	5906 (4)	3771 (2)	7·09
O(4)	3440 (1)	3189 (3)	4462 (1)	3·99
C(1)	1333 (2)	−1092 (4)	3371 (1)	3·13
C(2)	1634 (2)	70 (5)	2830 (1)	4·27
C(3)	1522 (2)	−700 (6)	2169 (1)	4·86
C(4)	1108 (2)	−2645 (5)	2058 (1)	3·97
C(5)	809 (2)	−3848 (5)	2593 (1)	3·98
C(6)	923 (2)	−3051 (4)	3251 (1)	3·77
C(7)	1432 (2)	−318 (4)	4094 (1)	3·14
C(8)	1948 (2)	2577 (4)	4809 (1)	3·21
C(9)	1075 (2)	3398 (5)	5095 (1)	4·03
C(10)	2648 (2)	4296 (4)	4700 (1)	3·58
C(11)	2924 (2)	5545 (6)	5343 (2)	5·07
C(12)	3909 (2)	4140 (5)	3982 (1)	4·17
C(13)	4668 (2)	2751 (5)	3755 (1)	3·90
C(14)	4811 (2)	732 (5)	4019 (2)	5·08
C(15)	5509 (2)	−528 (6)	3797 (2)	5·98
C(16)	6052 (2)	296 (6)	3296 (2)	5·13
C(17)	5917 (2)	2274 (6)	3026 (2)	5·09
C(18)	5224 (2)	3525 (5)	3261 (2)	4·79

* According to Hamilton (1959).

The geometries of the carboxylic moieties are normal and, in accordance with the notation of Borthwick (1980), the usual narrowing of the angles opposite the C=O bonds is present.

The C_{sp^3}–C_{sp^3} bonds are generally rather shorter than the 1·537 (5) Å proposed by Sutton (1965) [but C(8)–C(9) is 1·534 (9) Å in PDP]. Moreover, one of them in PDP [C(8)–C(10) = 1·471 (9) Å] shows the very significant shortening often observed for this class of derivatives (Bocelli & Grenier-Loustalot, 1983, and papers quoted therein).

It is very interesting to compare the chain conformation of these compounds with those found in similar derivatives without or with substituents on the aliphatic chain or the rings. The torsion angles for PDP in Table 2 clearly show that the presence of one CH_3 group causes a move away from a *trans* conformation at O(4) to O(2) [174·6 (4), 169·8 (4), 152·1 (4)°]. In BDP the conformation is clearly *gauche* at the centre of the

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* Lists of structure factors, anisotropic thermal parameters and hydrogen coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39306 (28 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

	PDP	BDP
Cl(1)—C(4)	1·735 (5)	1·740 (3)
Cl(2)—C(15)	1·736 (5)	1·745 (4)
O(1)—C(7)	1·205 (6)	1·197 (3)
O(2)—C(7)	1·338 (6)	1·345 (3)
O(2)—C(8)	1·486 (6)	1·465 (3)
O(3)—C(11)	1·204 (7)	1·200 (4)
O(4)—C(10)	1·459 (7)	1·454 (3)
O(4)—C(11)	1·328 (7)	1·339 (3)
C(1)—C(2)	1·389 (7)	1·382 (3)
C(1)—C(6)	1·390 (7)	1·385 (4)
C(1)—C(7)	1·478 (6)	1·500 (3)
C(2)—C(3)	1·376 (8)	1·386 (3)
C(3)—C(4)	1·380 (8)	1·377 (5)
C(4) C(5)	1·378 (8)	1·386 (4)
C(5)—C(6)	1·370 (7)	1·387 (3)
C(8)—C(9)	1·534 (9)	1·518 (4)
C(8)—C(10)	1·471 (9)	1·514 (4)
C(11)—C(12)	1·493 (5)	1·503 (4)
C(12)—C(13)	1·388 (8)	1·382 (5)
C(12)—C(17)	1·381 (7)	1·390 (4)
C(13)—C(14)	1·389 (7)	1·385 (5)
C(14)—C(15)	1·389 (8)	1·400 (5)
C(15)—C(16)	1·355 (8)	1·361 (5)
C(16)—C(17)	1·376 (7)	1·385 (5)
C(10)—C(18)		1·522 (4)
C(7)—O(2)—C(8)	117·0 (4)	116·8 (2)
C(10)—O(4)—C(11)	114·1 (4)	117·7 (2)
C(6)—C(1)—C(7)	123·4 (4)	117·9 (2)
C(2)—C(1)—C(7)	117·7 (4)	122·6 (2)
C(2)—C(1)—C(6)	118·9 (4)	119·5 (2)
C(1)—C(2)—C(3)	120·6 (5)	120·6 (3)
C(2)—C(3)—C(4)	119·4 (5)	119·1 (2)
Cl(1)—C(4)—C(3)	119·1 (4)	119·3 (2)
C(3)—C(4)—C(5)	120·9 (5)	121·3 (2)
Cl(1)—C(4)—C(5)	120·0 (4)	119·4 (2)
C(4)—C(5)—C(6)	119·4 (5)	118·9 (3)
C(1)—C(6)—C(5)	120·9 (5)	120·5 (2)
O(2)—C(7)—C(1)	112·3 (4)	111·4 (2)
O(1)—C(7)—C(1)	125·1 (4)	124·5 (2)
O(1)—C(7)—O(2)	122·6 (4)	124·1 (2)
O(2)—C(8)—C(10)	103·7 (4)	104·1 (2)
C(8)—C(10)—C(18)		113·7 (2)
O(4)—C(10)—C(18)		109·5 (3)
O(2)—C(8)—C(9)	110·4 (5)	109·8 (2)
C(9)—C(8)—C(10)	112·4 (5)	113·8 (2)
O(4)—C(10)—C(8)	104·2 (5)	105·4 (2)
O(3)—C(11)—O(4)	123·6 (4)	124·4 (3)
O(4)—C(11)—C(12)	112·1 (4)	111·7 (2)
O(3)—C(11)—C(12)	124·3 (5)	123·9 (3)
C(11)—C(12)—C(17)	118·4 (4)	118·6 (3)
C(11)—C(12)—C(13)	121·7 (4)	121·4 (3)
C(13)—C(12)—C(17)	119·9 (4)	120·0 (3)
C(12)—C(13)—C(14)	120·4 (5)	120·4 (3)
C(13)—C(14)—C(15)	118·0 (5)	118·1 (3)
Cl(2)—C(15)—C(14)	118·9 (4)	117·6 (3)
C(14)—C(15)—C(16)	121·8 (5)	122·4 (3)
Cl(2)—C(15)—C(16)	119·3 (4)	120·0 (3)
C(15)—C(16)—C(17)	120·2 (6)	118·8 (3)
C(12)—C(17)—C(16)	119·8 (5)	120·3 (3)
C(2)—C(1)—C(7)—O(1)	11·8 (7)	−173·1 (3)
C(2)—C(1)—C(7)—O(2)	−166·8 (4)	6·7 (4)
C(6)—C(1)—C(7)—O(1)	−169·8 (5)	6·9 (4)
C(6)—C(1)—C(7)—O(2)	11·6 (6)	−173·3 (2)
C(1)—C(7)—O(2)—C(8)	178·3 (4)	−175·1 (2)
O(1)—C(7)—O(2)—C(8)	−0·3 (7)	4·6 (4)
C(7)—O(2)—C(8)—C(10)	152·1 (4)	155·6 (2)
C(7)—O(2)—C(8)—C(9)	−87·4 (6)	−82·3 (3)
O(2)—C(8)—C(10)—O(4)	−169·8 (4)	−63·4 (2)
O(2)—C(8)—C(10)—C(18)		176·8 (2)
C(9)—C(8)—C(10)—C(18)		57·2 (3)
C(18)—C(10)—O(4)—C(11)		−95·2 (3)
C(9)—C(8)—C(10)—O(4)	71·0 (6)	177·1 (2)
C(8)—C(10)—O(4)—C(11)	−174·6 (4)	142·2 (2)
C(10)—O(4)—C(11)—O(3)	3·6 (7)	5·6 (4)
C(10)—O(4)—C(11)—C(12)	−175·9 (4)	−173·6 (2)
O(4)—C(11)—C(12)—C(13)	5·7 (6)	179·6 (3)
O(4)—C(11)—C(12)—C(17)	−173·3 (4)	−179·5 (3)
O(3)—C(11)—C(12)—C(13)	−173·8 (5)	179·6 (3)
O(3)—C(11)—C(12)—C(17)	7·2 (7)	−1·4 (5)

chain [O(2)—C(8)—C(10)—O(4) = 63·4 (2)°] whilst the remaining two torsion angles [C(7)—O(2)—C(8)—C(10) = 155·6 (2), C(8)—C(10)—O(4)—C(11) = 142·2 (2)°] are both far from a *trans* conformation. In contrast, in the derivative with two methyls and without chlorines (Bocelli & Grenier-Loustalot, 1983), both the C(7)—O(2)—C(8)—C(10) and C(11)—O(4)—C(10)—C(8) torsion angles are far from a *trans* arrangement [156·6 (2), 146·4 (2)°] but the conformation of the centre of the chain is *trans* [O(2)—C(8)—C(10)—O(4) = −179·0 (2)°]. Finally, an all-*trans* arrangement was found in the analogous derivative without any substituents (Pérez & Brisse, 1976). From these data it seems that the presence of one methyl moves the involved part of the aliphatic chain away from a perfect *trans* arrangement, while the conformation of the chain with two pendant methyl groups may also be influenced by the presence of chlorine on the rings. The length of the molecules (distance between the centres of the rings) which is 10·75 Å in the unsubstituted derivative, 10·77 (2) Å in the compounds with two chlorines and two methyls and 10·71 (2), 6·55 (1) Å in PDP and in BDP, respectively, is clearly dependent on the different conformations.

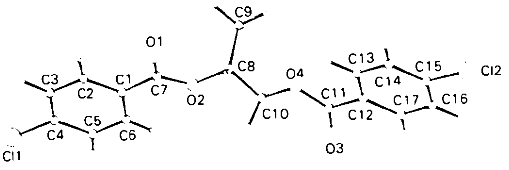

Fig. 1. Projection of PDP on (001).

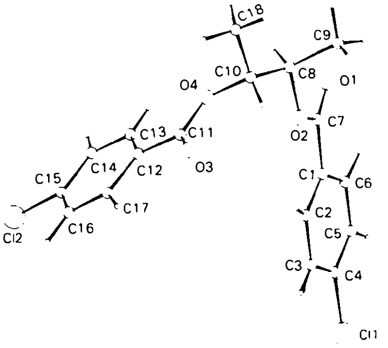

Fig. 2. Projection of BDP on (010).

The aromatic rings are tilted by 11·9 (2), 6·5 (2)° in PDP and by 6·7 (1), 0·5 (1)° in BDP with respect to their carboxylic mean planes and subtend dihedral angles of 10·0 (1) and 65·4 (1)° to each other.

The O(1) and O(3) atoms are on opposite sides with respect to the O(2)—C(8)—C(10)—O(4) sequence [out of plane −1·07 (1), 0·32 (1) and −1·70 (1), 1·88 (1) Å in PDP and BDP, respectively].

The packing of the molecules in the unit cell is mainly determined by van der Waals interactions.

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Stereochemical Studies of Oligomers. XII.* The Structure of 1,10-Decanediyl Bis(*o*-chlorobenzoate), $C_{24}H_{28}Cl_2O_4$

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Abstract. $M_r = 451 \cdot 4$, triclinic, $P\bar{1}$, $a = 13 \cdot 665$ (4), $b = 13 \cdot 114$ (3), $c = 7 \cdot 213$ (2) Å, $\alpha = 103 \cdot 53$ (4), $\beta = 74 \cdot 92$ (6), $\gamma = 110 \cdot 02$ (5)°, $V = 1157 \cdot 6$ (7) Å^3, $Z = 2$, $D_x = 1 \cdot 295$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1 \cdot 5418$ Å, $\mu = 27 \cdot 76$ cm^{-1}, $F(000) = 476$, room temperature, $R = 0 \cdot 074$ for 3116 observed reflections. The carboxylic moieties of the two independent molecules are tilted by 16·6 (2) and 24·0 (2)° with respect to their phenyl rings. The chain shows an all-*trans* conformation. Some of the C—C bonds in the chain are slightly shorter than the ideal value; the aromatic rings have normal bond lengths and angles.

Introduction. The present paper continues investigations on the structures of oligomers which seem greatly but not uniformly influenced by substituents on the phenyl rings or the aliphatic chain. In preceding papers (Bocelli & Grenier-Loustalot, 1983, 1984*a,b,c*), we have examined oligomers with ethylene, butanediyl, pentanediyl and hexanediyl chains deformed by chlorine atoms or by methyls, while the title compound shows a ten-membered chain with chlorines on the aromatic rings.

Experimental. Colourless crystals obtained after innumerable attempts by slow evaporation of a solution of the compound in methanol, pyramid-shaped single crystal, 0·09 × 0·14 × 0·23 mm, obtained with a series of cuts; data collection revealed that a small geminate (about 1/14 in volume) remained absorbed in the specimen; Siemens AED single-crystal diffractometer, General Automation Jumbo 220 computer, nickel-filtered Cu $K\alpha$ radiation, cell parameters from least squares of $(\theta, \chi, \varphi)_{hkl}$ angles of 26 reflections (16·9 <

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* Part XI: Bocelli & Grenier-Loustalot (1984*c*).

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