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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Table 1. *Fractional atomic coordinates* (×10⁴) *and* B_{eq} *values* (Å²)

	x	y	z	B_{eq}*
Molecule 1				
Cl	3012 (1)	5366 (1)	2846 (1)	5·67
O(1)	2512 (2)	3805 (2)	−3136 (3)	4·39
O(2)	1742 (3)	4156 (3)	−65 (4)	9·00
C(1)	3538 (2)	5207 (2)	−1145 (4)	3·57
C(2)	3820 (2)	5711 (2)	650 (4)	3·81
C(3)	4787 (3)	6508 (3)	768 (5)	4·81
C(4)	5485 (3)	6834 (3)	−914 (6)	5·30
C(5)	5207 (3)	6355 (3)	−2689 (5)	5·04
C(6)	4253 (3)	5560 (3)	−2805 (4)	4·19
C(7)	2502 (2)	4339 (3)	−1321 (4)	3·90
C(8)	1523 (3)	2979 (3)	−3510 (5)	4·24
C(9)	1708 (3)	2485 (3)	−5635 (4)	3·88
C(10)	718 (3)	1600 (3)	−6179 (4)	4·20
C(11)	887 (3)	1134 (3)	−8333 (5)	4·28
C(12)	−95 (3)	245 (3)	−8917 (5)	4·28
Molecule 2				
Cl	3193 (1)	11381 (1)	6724 (1)	4·39
O(1)	2152 (2)	8346 (2)	2676 (4)	9·00
O(2)	2740 (4)	10156 (3)	2890 (6)	3·57
C(1)	3176 (3)	9275 (3)	5003 (5)	3·81
C(2)	3479 (3)	10158 (3)	6458 (5)	4·81
C(3)	4014 (3)	10077 (3)	7773 (6)	5·30
C(4)	4251 (4)	9132 (4)	7633 (7)	5·04
C(5)	3943 (4)	8264 (4)	6271 (7)	4·19
C(6)	3408 (3)	8313 (3)	4949 (6)	3·90
C(7)	2638 (3)	9324 (3)	3480 (5)	4·24
C(8)	1628 (3)	8258 (3)	1107 (5)	3·88
C(9)	1477 (3)	7106 (3)	−9 (5)	4·20
C(10)	898 (3)	6923 (3)	−1661 (5)	4·28
C(11)	715 (3)	5768 (3)	−2813 (5)	4·28
C(12)	123 (3)	5583 (3)	−4462 (5)	4·27

* According to Hamilton (1959).

$\theta < 68{\cdot}9°$) automatically centred with program written by Belletti, Ugozzoli, Cantoni & Pasquinelli (1979), 4293 reflections collected ($2 < \theta < 70°$, $-15 \le h \le 15$, $-14 \le k \le 15$, $0 < l < 8$), scan range 0·55° below θ to $\{0{\cdot}55 + [(\lambda_{\alpha_1}-\lambda_{\alpha_2})/\bar{\lambda}]\tan\theta\}°$ above, intensities evaluated from a modified version of profile analysis method (Lehmann & Larsen, 1974), 1 check reflection monitored every 50 counts: only statistical variation in intensity, 3132 observed reflections with $I > 2\sigma(I)$, Lp corrections, absorption ignored, structure solved using *SHELX* (Sheldrick, 1976), block-matrix least squares of positional and anisotropic thermal parameters minimizing $\sum w(F_o - F_c)^2$, H (from ΔF map) isotropic, 26 more reflections with low *hkl* values having large ΔF excluded from last cycle of refinement because of probable effects of the presence of geminate in specimen or of extinction, final ΔF map with no significant density, final $R = 0{\cdot}074$, unit weights, scattering factors from *SHELX*, Gould-SEL 32/77 computer.*

Discussion. Table 1 gives the atomic coordinates and Table 2 bond lengths and angles and selected torsion angles. A view of the two independent molecules is shown in Fig. 1.

Bond lengths and angles in the two independent molecules are in general comparable to one another with no significant differences. The aromatic rings are planar [maximum deviations 0·008 (3) and 0·013 (4) Å in the two molecules] and the mean bond lengths and internal angles [1·387 (4), 1·376 (9) Å; 120·3 (6), 119·8 (5)°] are normal. It has been pointed out (Domenicano, Vaciago & Coulson, 1975; Domenicano, Mazzeo & Vaciago, 1976; Domenicano & Murray-Rust, 1979) that the presence of chlorine atoms in benzene rings causes a deformation in the ring skeleton due to inductive and resonance effects of the substituents. In particular, larger deviations from the ideal D_{6h} geometry involve the C(1)—C(2)—C(3) angles [121·1 (3), 120·5 (4)°]. As previously observed in all the derivatives of this series and in accordance with the notation of Borthwick (1980), the angles opposite the C=O bonds [111·3 (3), 111·5 (4)°] are significantly narrower than the adjacent ones [126·1 (3), 122·6 (4) and 124·8 (5), 123·1 (4)°]. The carbon–oxygen distances of the molecules fall within the expected range. Some of the C—C distances of the chain are slightly shorter than the ideal value [1·537 (5) Å, Sutton, 1965] for sp^3–sp^3 C—C bonds, but this behaviour has already been seen in this type of derivative. The two carboxylic groups are tilted by 16·6 (2) and 24·0 (2)° with respect to the mean aromatic ring planes. These values, particularly the first, are noticeably lower than those found in 1,4-butanediyl bis(*o*-chlorobenzoate) [31·2 (2)°; Bocelli & Grenier-Loustalot, 1984*a*] or in 1,6-hexanediyl bis(*o*-chlorobenzoate) [36·0 (1), 33·8 (1)°; Bocelli & Grenier-Loustalot, 1984*b*]. Consequently, in the present case the steric hindrance between the *ortho* chlorines and the carboxylic moieties is attenuated by factors probably connected with the presence of two molecules in the unit cell. It may be interesting to note that the coplanarity between the

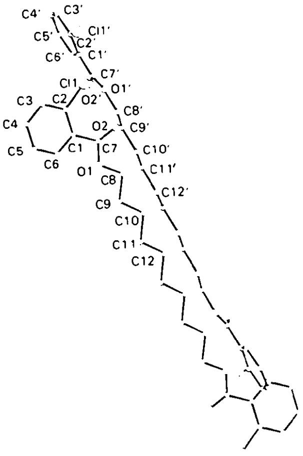

Fig. 1. Projection of the title compound showing the reciprocal orientation of the two independent molecules. Hydrogens are omitted.

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* Lists of structure factors, of anisotropic thermal parameters and of H coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39307 (21 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), *valence angles* (°) *and selected torsion angles* (°)

	Molecule 1	Molecule 2		Molecule 1	Molecule 2
Cl–C(2)	1·737 (3)	1·734 (5)	C(3)–C(4)	1·388 (5)	1·360 (8)
O(1)–C(7)	1·331 (4)	1·301 (4)	C(4)–C(5)	1·375 (6)	1·342 (6)
O(1)–C(8)	1·457 (4)	1·453 (6)	C(5)–C(6)	1·371 (5)	1·368 (8)
O(2)–C(7)	1·182 (4)	1·214 (6)	C(8)–C(9)	1·510 (4)	1·509 (5)
C(1)–C(2)	1·395 (4)	1·395 (5)	C(9)–C(10)	1·523 (5)	1·527 (6)
C(1)–C(6)	1·394 (4)	1·395 (6)	C(10)–C(11)	1·519 (4)	1·519 (5)
C(1)–C(7)	1·496 (4)	1·492 (6)	C(11)–C(12)	1·527 (5)	1·536 (6)
C(2)–C(3)	1·385 (4)	1·381 (7)	C(12)–C(12*)	1·535 (5)	1·510 (5)
C(7)–O(1)–C(8)	116·2 (3)	118·0 (4)	C(4)–C(5)–C(6)	120·6 (4)	121·1 (5)
C(6)–C(1)–C(7)	120·2 (3)	118·9 (4)	C(1)–C(6)–C(5)	121·5 (3)	120·1 (4)
C(2)–C(1)–C(7)	122·4 (3)	123·3 (4)	O(2)–C(7)–C(1)	126·1 (3)	124·8 (5)
C(2)–C(1)–C(6)	117·4 (4)	117·8 (4)	O(1)–C(7)–C(1)	111·3 (3)	111·5 (4)
Cl–C(2)–C(1)	122·9 (3)	122·2 (4)	O(1)–C(7)–O(2)	122·6 (4)	123·1 (4)
C(1)–C(2)–C(3)	121·1 (3)	120·5 (4)	O(1)–C(8)–C(9)	107·5 (4)	107·1 (4)
Cl–C(2)–C(3)	116·0 (3)	117·4 (3)	C(8)–C(9)–C(10)	111·7 (3)	110·9 (4)
C(2)–C(3)–C(4)	120·0 (4)	119·6 (4)	C(9)–C(10)–C(11)	111·8 (4)	112·9 (4)
C(3)–C(4)–C(5)	119·3 (5)	120·9 (6)	C(10)–C(11)–C(12)	112·9 (4)	112·7 (4)
			C(11)–C(12)–C(12*)	112·5 (4)	113·2 (4)
C(2)–C(1)–C(7)–O(1)	−165·4 (4)	−160·7 (5)	C(7)–O(1)–C(8)–C(9)	179·7 (4)	160·4 (4)
C(2)–C(1)–C(7)–O(2)	17·5 (7)	27·4 (8)	O(1)–C(8)–C(9)–C(10)	179·6 (4)	178·3 (4)
C(6)–C(1)–C(7)–O(1)	16·2 (6)	21·2 (6)	C(8)–C(9)–C(10)–C(11)	177·7 (4)	- 179·3 (4)
C(6)–C(1)–C(7)–O(2)	−161·0 (5)	−150·7 (6)	C(9)–C(10)–C(11)–C(12)	180·0 (4)	179·5 (4)
C(1)–C(7)–O(1)–C(8)	−176·7 (4)	−177·6 (4)	C(10)–C(11)–C(12)–C(12*)	−178·2 (4)	176·5 (4)
O(2)–C(7)–O(1)–C(8)	0·6 (7)	−5·6 (8)	C(11)–C(12)–C(12*)–C(11*)	180·0 (4)	180·0 (4)

* Symmetry-related atom.

chlorine atom and the phenyl ring found in molecule 1 is rarely observed in this type of molecular fragment. All the torsion angles of the decane chain are near to 180° and the conformation is all-*trans*. The torsion angle C(7)—O(1)—C(8)—C(9) of the second molecule is 160·4 (4)° and, consequently, the departure of this portion from the *trans* conformation is significant. The two independent molecules are quasi-perpendicular to one another, the dihedral angle between the mean planes formed by all the heavy atoms of the molecules except Cl and O(2) being 98·1 (1)° (see Fig. 1).

None of the intermolecular distances is less than a normal van der Waals contact.

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