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Stereochemical Studies of Oligomers. XXI.* 1,12-Dodecanediyl Bis(*m*-chlorobenzoate)

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Abstract. $C_{26}H_{32}Cl_2O_4$, $M_r = 479{\cdot}4$, monoclinic, $P2_1/a$, $a = 13{\cdot}239$ (2), $b = 4{\cdot}070$ (3), $c = 23{\cdot}474$ (3) Å, $\beta = 100{\cdot}91$ (3)°, $V = 1242{\cdot}0$ (9) Å^3, $Z = 2$, $D_x = 1{\cdot}28$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 26{\cdot}15$ cm^{-1}, $F(000) = 508$, room temperature, $R = 0{\cdot}060$ for 1105 unique observed reflections. The conformation of the molecule is all-*trans*. The carboxylate groups are tilted by 6·4 (2)° with respect to the aromatic rings.

Experimental. Intensities measured on a Siemens AED single-crystal diffractometer equipped with a General Automation Jumbo 220 computer employing Ni-filtered Cu $K\alpha$ radiation and a prismatic specimen of about 0·35 × 0·40 × 0·55 mm. Lattice parameters from least-squares fit of (θ,χ,φ) angles of 24 reflections automatically centered on the diffractometer. Intensities evaluated from a modified version (Belletti, Ugozzoli, Cantoni & Pasquinelli, 1979) of the Lehmann & Larsen (1974) method. The check reflection, monitored every 50 counts, did not vary significantly. Lp correction, absorption ignored.

2734 reflections measured, 2579 unique ($R_{int} = 0{\cdot}18$), 1105 with $I \geq 2\sigma(I)$ considered observed, $3 \leq \theta \leq 70°$, $-16 \leq h \leq 15$, $0 \leq k \leq 4$, $0 \leq l \leq 28$. Structure solved by direct methods with *MULTAN*80 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Refinement by full-matrix least squares using *SHELX*76 (Sheldrick, 1976), $\sum w(\Delta F)^2$ minimized, H atoms found from a ΔF map and refined isotropically, other atoms refined anisotropically, 209 variables in total, final $R = 0{\cdot}060$ and $wR = 0{\cdot}068$, $w = 1{\cdot}7379/(\sigma^2F + 0{\cdot}0243F^2)$. In the last cycle of the refinement $(\Delta/\sigma)_{max}$ was 0·26 for all atoms and $\Delta\rho = 0{\cdot}29$ e Å^{-3}.

Table 1. *Atomic fractional coordinates* (×10^4) *and equivalent isotropic temperature factors* (Å^2 × 10^4)

	x	y	z	U_{eq}*
Cl	720 (1)	1495 (6)	9488 (1)	1007 (9)
O(1)	250 (2)	−3765 (11)	7431 (1)	676 (14)
O(2)	1781 (3)	−5463 (13)	7277 (2)	846 (16)
C(1)	1701 (3)	−2550 (15)	8147 (2)	593 (20)
C(2)	1066 (4)	−1345 (16)	8502 (2)	654 (23)
C(3)	1506 (4)	40 (16)	9032 (2)	705 (24)
C(4)	2563 (4)	110 (21)	9213 (2)	869 (28)
C(5)	3172 (4)	−1076 (21)	8852 (3)	937 (31)
C(6)	2752 (4)	−2508 (18)	8325 (2)	762 (27)
C(7)	1272 (3)	−4098 (16)	7575 (2)	621 (23)
C(8)	−222 (4)	−5083 (25)	6864 (2)	678 (27)
C(9)	−1360 (3)	−4384 (24)	6774 (2)	639 (26)
C(10)	−1895 (4)	−5239 (24)	6153 (2)	622 (27)
C(11)	−3045 (3)	−4577 (22)	6044 (2)	591 (24)
C(12)	−3579 (3)	−5314 (24)	5422 (2)	593 (26)
C(13)	−4731 (3)	−4617 (23)	5314 (2)	595 (27)

* Hamilton (1959).

All the calculations were performed on an AT IBM personal computer using the *CRYSRULER* package (Rizzoli, Sangermano, Calestani & Andreetti, 1987). Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Table 1 reports the positional parameters of the heavy atoms, Table 2 gives bond distances and angles, and the molecule is illustrated in Fig. 1.†

* Part XX: Bocelli & Grenier-Loustalot (1987).

† Lists of structure factors, H-atom coordinates, anisotropic thermal parameters and selected torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43757 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/87/061223-02$01.50

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

Cl–C(3)	1·732 (6)	C(4)–C(5)	1·364 (9)
O(1)–C(7)	1·338 (5)	C(5)–C(6)	1·385 (9)
O(1)–C(8)	1·461 (6)	C(8)–C(9)	1·508 (7)
O(2)–C(7)	1·196 (7)	C(9)–C(10)	1·535 (7)
C(1)–C(2)	1·381 (8)	C(10)–C(11)	1·519 (7)
C(1)–C(6)	1·375 (6)	C(11)–C(12)	1·527 (7)
C(1)–C(7)	1·495 (7)	C(12)–C(13)	1·525 (6)
C(2)–C(3)	1·389 (7)	C(13)–C(13′)	1·543 (7)
C(3)–C(4)	1·384 (7)		

C(7)–O(1)–C(8)	115·5 (4)	O(2)–C(7)–C(1)	124·1 (4)
C(6)–C(1)–C(7)	118·0 (4)	O(1)–C(7)–C(1)	112·2 (4)
C(2)–C(1)–C(7)	121·4 (4)	O(1)–C(5)–O(2)	123·6 (4)
C(2)–C(1)–C(6)	120·6 (4)	O(1)–C(8)–C(9)	107·6 (4)
C(1)–C(2)–C(3)	119·0 (5)	C(8)–C(9)–C(10)	111·1 (4)
Cl–C(3)–C(2)	119·5 (4)	C(9)–C(10)–C(11)	112·8 (4)
C(2)–C(3)–C(4)	120·8 (5)	C(10)–C(11)–C(12)	113·2 (4)
Cl–C(3)–C(4)	119·6 (3)	C(11)–C(12)–C(13)	113·0 (4)
C(3)–C(4)–C(5)	119·0 (5)	C(12)–C(13)–C(13′)	112·8 (4)
C(4)–C(5)–C(6)	121·3 (5)	C(13)–C(13′)–C(12′)	112·8 (4)
C(1)–C(6)–C(5)	119·2 (5)		

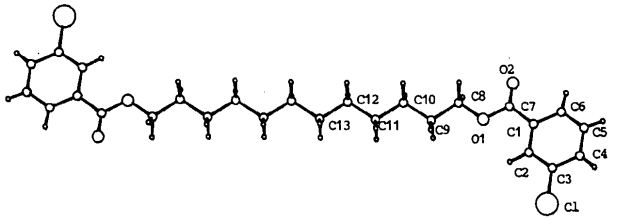

Fig. 1. Drawing of the molecule showing the atom-numbering scheme.

Related literature. The all-*trans* conformation of the chain has been widely observed in this series of derivatives (Bocelli & Grenier-Loustalot, 1986, and papers cited therein).

This work was supported by CNR and CNRS through an International Scientific Project.

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Stereochemical Studies of Oligomers. XXII.* 1,8-Octanediyl Bis(*p*-chlorobenzoate)

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Abstract. $C_{22}H_{24}Cl_2O_4$, $M_r = 423{\cdot}3$, triclinic, $P\bar{1}$, $a = 12{\cdot}264$ (2), $b = 11{\cdot}113$ (2), $c = 8{\cdot}113$ (3) Å, $\alpha = 78{\cdot}58$ (2), $\beta = 82{\cdot}29$ (2), $\gamma = 98{\cdot}40$ (3)°, $V = 1056{\cdot}9$ (4) Å^3, $Z = 2$, $D_x = 1{\cdot}33$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 30{\cdot}08$ cm^{-1}, $F(000) = 444$, room temperature, $R = 0{\cdot}039$ for 2763 unique observed reflections. The conformation of the molecule is all-*trans*. The carboxylate groups are tilted by 2·3 (1) and 3·7 (1)° with respect to the phenyl ring planes, which form a dihedral angle of 13·1 (1)° with each other.

Experimental. Intensity data collected on a Siemens AED single-crystal diffractometer equipped with a General Automation Jumbo 220 computer employing Ni-filtered Cu $K\alpha$ radiation and a specimen of about 0·2 × 0·2 × 0·6 mm. Lattice parameters from least-squares fit of (θ,χ,φ) angles of 23 reflections automatically centered on the diffractometer. Intensities

* Part XXI: Bocelli & Grenier-Loustalot (1987).

0108-2701/87/061224-03$01.50

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