given in Table 1, bond lengths and angles in Table 2, and a view of the molecule is shown in Fig. 1.*

Related literature. This work is part of a photochemical study of dibenzobarrelene diesters (Garcia-Garibay, Scheffer, Trotter & Wireko, 1990).

We thank Professor J. R. Scheffer and Dr M. Garcia-Garibay for collaborative photochemical studies, the Natural Sciences and Engineering Research Council of Canada for financial support, and the University of British Columbia Computing Centre for assistance.

Reference

Garcia-Garibay, M., Scheffer, J. R., Trotter, J. & Wireko, F. C. (1990). *Acta Cryst.* **B46**, 431–440.

---

* Lists of anisotropic thermal parameters, hydrogen positions, torsion angles and structure factors, and a packing diagram have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53756 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1991). C**47**, 1319–1320

Structure of Di-*n*-propyl Dibenzobarrelene-11,12-dicarboxylate*

By James Trotter and Fred C. Wireko

Department of Chemistry, University of British Columbia, Vancouver, BC, Canada V6T 1Y6

(*Received* 16 *July* 1990; *accepted* 13 *November* 1990)

Abstract. $C_{24}H_{24}O_4$, $M_r = 376·45$, triclinic, $P\bar{1}$, $a = 9·6978\,(4)$, $b = 10·2945\,(5)$, $c = 10·3828\,(3)$ Å, $\alpha = 82·414\,(3)$, $\beta = 81·671\,(3)$, $\gamma = 85·817\,(3)°$, $V = 1015·1\,(1)$ Å^3, $Z = 2$, $D_x = 1·232$ g cm^{-3}, Cu $K\alpha_1$, $\lambda = 1·54056$ Å, $\mu = 6·3$ cm^{-1}, $F(000) = 400$, $T = 295$ K, $R = 0·067$ for 2597 reflections. The two carboxyl groups have different orientations with respect to the C11=C12 bond; torsion angles C=C—C=O are −107·3 (5)° at C11 [anticlinal, cos^2(angle) = 0·09, not conjugated, C11—CO = 1·487 (5) Å] and −175·1 (4)° at C12 [antiperiplanar, cos^2(angle) = 0·99, fully conjugated, C12—CO = 1·475 (5) Å].

Experimental. Crystal dimensions 0·3 × 0·3 × 0·4 mm. Nonius CAD-4F diffractometer, monochromatized Cu $K\alpha$ radiation, lattice parameters from 25 reflections with $\theta = 35$–$44°$. Intensities for $\theta < 75°$, hkl: −12 to 12, −12 to 0, −13 to 13 ($\bar{h}0l$ removed from data set), ω–2θ scan, ω-scan width $(0·75 + 0·14\tan\theta)°$ at 1·3–10° min^{-1}, extended 25% on each side for background measurement; three standard reflections showed no significant variation. Lp but no absorption corrections. 4169 unique reflections, 2597 (62·3%) with $I \geq 3\sigma(I)$. Structure solved by direct methods, refined by full-matrix least-squares procedures, H atoms placed in calculated positions and not refined. Refinements on F, with $w = 1/\sigma^2(F)$, where $\sigma^2(I) = S + 4(B_1 + B_2) + (0·04I)^2$, S = scan, B_1 and B_2 = background counts. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 99–102). Locally written or locally modified versions of standard computer programs were used.† Final $R = 0·067$, $wR = 0·086$ for 254 parameters, 2597 reflections with $I \geq 3\sigma(I)$, $R = 0·10$ for all 4169 reflections, extinction correction, $g = 3·0\,(4) \times 10^4$, $S = 3·4$, $\Delta/\sigma = 0·002$ (mean), 0·028 (maximum), $\Delta\rho = -0·50$ to $+0·20$ e Å^{-3}. Positional parameters are given in Table 1, bond lengths and angles in Table 2 and a view of the molecule is shown in Fig. 1.‡

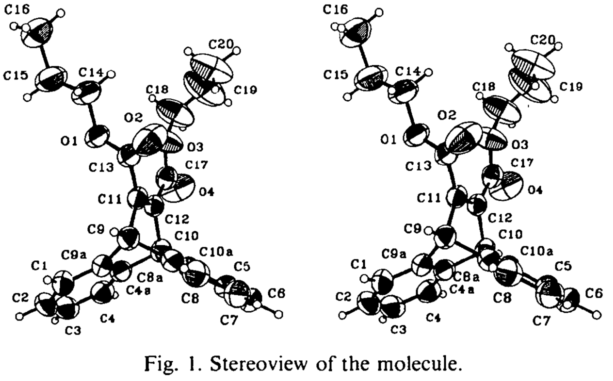

Fig. 1. Stereoview of the molecule.

---

* Dipropyl 9,10-dihydro-9,10-ethenoanthracene-11,12-dicarboxylate.

† *MULTAN*, *ORFLS*, *ORFFE* and *ORTEP*II; references given in Garcia-Garibay, Scheffer, Trotter & Wireko (1990).

‡ Lists of anisotropic thermal parameters, hydrogen positions, torsion angles and structure factors, and a packing diagram have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53757 (32 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/91/061319-02$03.00

Table 1. *Positional (fractional* × 10^4*) and equivalent isotropic* ($U \times 10^3$ Å^2) *thermal parameters, with e.s.d.'s in parentheses*

$U_{eq} = \frac{1}{3}$(trace of diagonalized *U* tensor).

	x	*y*	*z*	U_{eq}
C1	6829 (4)	305 (3)	3738 (4)	68
C2	5566 (5)	369 (5)	3228 (4)	80
C3	4655 (5)	1440 (5)	3302 (4)	80
C4	4974 (4)	2495 (4)	3866 (4)	69
C4a	6213 (3)	2455 (3)	4377 (3)	56
C5	8601 (4)	5039 (3)	3726 (4)	69
C6	9977 (6)	5141 (5)	3125 (4)	86
C7	10893 (4)	4062 (5)	3114 (4)	83
C8	10455 (4)	2852 (4)	3682 (4)	69
C8a	9100 (3)	2738 (3)	4271 (3)	55
C9	8424 (3)	1487 (3)	4960 (3)	53
C9a	7137 (3)	1357 (3)	4317 (3)	55
C10	6739 (3)	3508 (3)	5053 (3)	56
C10a	8172 (3)	3835 (3)	4310 (3)	55
C11	7892 (3)	1790 (3)	6355 (3)	50
C12	7014 (3)	2841 (3)	6404 (3)	50
C13	8507 (4)	982 (3)	7448 (4)	60
C14	8166 (5)	−631 (4)	9285 (5)	96
C15	7077 (6)	−1453 (6)	9985 (5)	118
C16	7511 (6)	−2327 (5)	11126 (5)	110
C17	6370 (4)	3434 (4)	7581 (4)	61
C18	6269 (6)	3373 (7)	9880 (5)	120
C19	7256 (8)	3813 (9)	10515 (7)	162
C20	8588 (7)	3225 (8)	10618 (6)	142
O1	7633 (3)	190 (3)	8185 (3)	79
O2	9704 (3)	1017 (3)	7589 (4)	109
O3	6847 (3)	2908 (3)	8657 (3)	95
O4	5516 (4)	4336 (3)	7548 (3)	108

Table 2. *Bond lengths* (Å) *and angles* (°), *with e.s.d's in parentheses*

C1—C2	1·397 (6)	C10—C10a	1·526 (5)
C1—C9a	1·376 (5)	C10—C12	1·530 (5)
C2—C3	1·365 (6)	C11—C12	1·329 (4)
C3—C4	1·374 (6)	C11—C13	1·487 (5)
C4—C4a	1·378 (5)	C12—C17	1·475 (5)
C4a—C9a	1·392 (4)	C13—O1	1·310 (4)
C4a—C10	1·521 (5)	C13—O2	1·194 (4)
C5—C6	1·394 (6)	C14—C15	1·450 (7)
C5—C10a	1·372 (4)	C14—O1	1·462 (5)
C6—C7	1·372 (6)	C15—C16	1·483 (6)
C7—C8	1·375 (6)	C17—O3	1·307 (4)
C8—C8a	1·373 (5)	C17—O4	1·200 (4)
C8a—C9	1·531 (4)	C18—C19	1·371 (8)
C8a—C10a	1·393 (5)	C18—O3	1·439 (5)
C9—C9a	1·520 (4)	C19—C20	1·399 (9)
C9—C11	1·530 (5)		

C2—C1—C9a	118·1 (4)	C10a—C10—C12	105·4 (3)
C1—C2—C3	121·3 (4)	C5—C10a—C8a	119·9 (3)
C2—C3—C4	120·4 (4)	C5—C10a—C10	127·6 (3)
C3—C4—C4a	119·4 (4)	C8a—C10a—C10	112·5 (3)
C4—C4a—C9a	120·3 (3)	C9—C11—C12	113·7 (3)
C4—C4a—C10	127·2 (3)	C9—C11—C13	117·5 (3)
C9a—C4a—C10	112·6 (3)	C12—C11—C13	128·5 (3)
C6—C5—C10a	118·8 (4)	C10—C12—C11	113·5 (3)
C5—C6—C7	121·0 (4)	C10—C12—C17	119·0 (3)
C6—C7—C8	120·1 (4)	C11—C12—C17	127·4 (3)
C7—C8—C8a	119·5 (4)	C11—C13—O1	113·5 (3)
C8—C8a—C9	127·2 (3)	C11—C13—O2	122·4 (3)
C8—C8a—C10a	120·7 (3)	O1—C13—O2	124·0 (3)
C9—C8a—C10a	112·1 (3)	C15—C14—O1	109·4 (4)
C8a—C9—C9a	106·8 (2)	C14—C15—C16	113·8 (4)
C8a—C9—C11	104·8 (2)	C12—C17—O3	113·7 (3)
C9a—C9—C11	106·3 (3)	C12—C17—O4	123·1 (4)
C1—C9a—C4a	120·5 (3)	O3—C17—O4	123·2 (4)
C1—C9a—C9	127·2 (3)	C19—C18—O3	113·0 (5)
C4a—C9a—C9	112·3 (3)	C18—C19—C20	126·0 (7)
C4a—C10—C10a	106·5 (3)	C13—O1—C14	116·5 (3)
C4a—C10—C12	105·9 (2)	C17—O3—C18	119·0 (3)

Related literature. This work is part of a photochemical study of dibenzobarrelene diesters (Garcia-Garibay, Scheffer, Trotter & Wireko, 1990).

We thank Professor J. R. Scheffer and Dr M. Garcia-Garibay for collaborative photochemical studies, the Natural Sciences and Engineering Research Council of Canada for financial support, and the University of British Columbia Computing Centre for assistance.

References

Garcia-Garibay, M., Scheffer, J. R., Trotter, J. & Wireko, F. C. (1990). *Acta Cryst.* B46, 431–440.

Acta Cryst. (1991). C47, 1320–1322

Structure of the Hexagonal Modification of 3′-*O*-Acetylthymidine

By A. Schouten* and J. A. Kanters

Laboratorium voor Kristal- en Structuurchemie, Rijksuniversiteit Utrecht, Transitorium 3, *Padualaan* 8,
3584 *CH Utrecht, The Netherlands*

(*Received* 13 *July* 1990; *accepted* 25 *October* 1990)

Abstract. $C_{12}H_{16}N_2O_6$, $M_r = 284{\cdot}27$, hexagonal, $P6_3$, $a = 22{\cdot}120$ (2), $c = 4{\cdot}960$ (5) Å, $V = 2102$ (2) Å^3, $Z = 6$, $D_x = 1{\cdot}347$ g cm^{-3}, $\lambda(\text{Cu }K\alpha) = 1{\cdot}54184$ Å, $\mu = 9{\cdot}4$ cm^{-1}, $F(000) = 900$, $T = 293$ K, $R = 0{\cdot}050$ for 1163 unique observed reflections with $I > 2{\cdot}5\sigma(I)$. The molecule has an *anti* conformation about the N-glycosidic bond with χ[C(2)—N(1)—C(1′)—O(4′)] = −116·8 (5)° and the sugar ring is in a half-chair conformation with pseudorotation parameters $P = 169{\cdot}3$ (6)° and $\psi = 34{\cdot}9$ (4)°. The C(4′)—C(5′) conformation is *gauche–gauche*. The structure does not exhibit base pairing; there is only one intermolecular head-to-head hydrogen bond between the bases [N(3)—H···O(4) $(-x, 1-y, \frac{1}{2}+z)$, N···O 2·876 (7) Å

---

* Author to whom correspondence should be addressed.

0108-2701/91/061320-03$03.00