

Table 3. Torsion angles (°)

C(2)—C(1)—O(1)—C(12')	176.0
C(9)—C(1)—O(1)—C(12')	-2.4
C(1')—O(1')—C(12)—C(11)	165.5
O(1')—C(12)—C(11)—C(10)	-61.0
C(12)—C(11)—C(10)—C(6)	-48.3
C(11)—C(10)—C(6)—C(5)	-34.9
C(11)—C(10)—C(6)—C(7)	83.6

The compound described in this paper was isolated from the reaction mixture after dimerization of (I). It is shown to be (IIb), *i.e.* the *meso* isomer, where the two quaternary C atoms have opposite chiralities. The conformation is centrosymmetric, and similar to *ansa* molecules since the anisolic group O(1)—C(12) is essentially planar with the benzene ring (Fig. 1). The

C(1)—O(1)—C(12)—C(11) torsion angle (Table 3) is nearly *trans*, so that the *ansa* bridging is effectively a three-carbon system C(6)—C(10)—C(11).

We thank Dr S. Chatterjee for crystals, and Dr C. I. F. Watt for helpful discussions.

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The Racemic Condensation Dimer from 2-(3-Bromopropyl)-6-hydroxy-2-methyl-1-indanone

BY PETER MURRAY-RUST AND JUDITH MURRAY-RUST

Department of Chemistry, University of Stirling, Stirling FK9 4LA, Scotland

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Abstract. C₂₆H₂₈O₄, *M_r* = 404.5, monoclinic, *P*2₁/*c*, *a* = 7.93 (2), *b* = 19.47 (6), *c* = 13.98 (5) Å, β = 101.55 (3)° from diffractometer measurements (Mo *K*α radiation). *V* = 2115 Å³, *Z* = 4, *D_c* = 1.279 Mg m⁻³, *F*(000) = 864, μ = 0.048 mm⁻¹. The substance was shown to be the racemic diastereoisomer.

Introduction. Systematic absences (from precession photographs) *h*0*l*, *l* odd and 0*k*0, *k* odd indicated space group *P*2₁/*c*. Data were collected for 0–6*kl* with θ_{max} = 22.5° on a Stoe STADI-2 diffractometer (graphite-monochromated Mo *K*α radiation). This gave 2425 data of which 1493 unique reflexions with *I* > 3σ(*I*) were used in subsequent calculations. Lorentz and polarization corrections (but none for extinction or absorption) were applied, and the data were scaled by a Wilson plot. The structure was solved by direct methods with *SHELX 76* (Sheldrick, 1976), which was used for all calculations. Complex neutral-atom scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Weighted full-matrix least-squares refinement (including isotropic H atoms) converged at *R* = 0.048 for 1493 observed reflexions (*R* = ∑||*F_o*| – |*F_c*||/∑|*F_o*|); *R_w* = 0.044 {*R_w* = ∑ (||*F_o*| – |*F_c*|| *w*^{1/2})/∑ (|*F_o*| *w*^{1/2}), *w* = 3.7157/[σ²(*F_o*) + 0.0002*F_o*²]}.

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were less than their e.s.d.'s. Positional parameters are given in Table 1, bond distances and angles in Table 2.*

* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34042 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

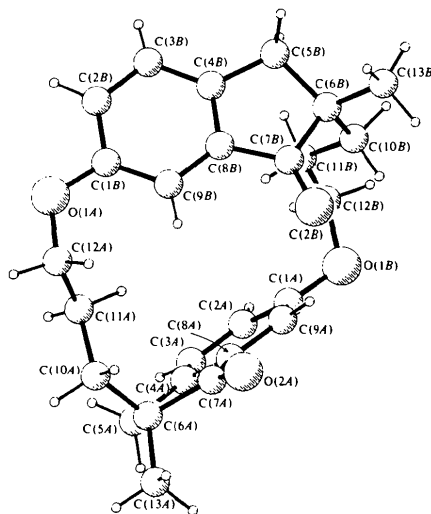


Fig. 1. General view of the molecule.

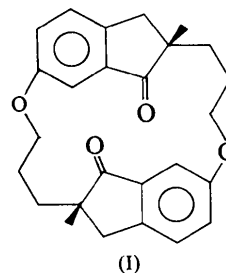
Table 1. Fractional atomic coordinates $\times 10^4$ with *e.s.d.*'s in parentheses

	x	y	z
C(1A)	3608 (5)	3204 (2)	2248 (3)
C(1B)	7948 (5)	4691 (3)	5417 (3)
C(2A)	2407 (4)	2980 (2)	2790 (3)
C(2B)	7257 (6)	5345 (3)	5467 (3)
C(3A)	2918 (5)	2585 (2)	3616 (3)
C(3B)	6774 (5)	5755 (2)	4652 (3)
C(4A)	4641 (5)	2396 (2)	3910 (3)
C(4B)	6992 (5)	5506 (2)	3752 (3)
C(5A)	5488 (5)	1967 (2)	4769 (3)
C(5B)	6547 (5)	5831 (2)	2759 (3)
C(6A)	7440 (5)	2019 (2)	4780 (3)
C(6B)	6891 (5)	5265 (2)	2041 (3)
C(7A)	7539 (6)	2397 (2)	3834 (3)
C(7B)	7844 (5)	4707 (2)	2707 (3)
C(8A)	5806 (5)	2623 (2)	3364 (3)
C(8B)	7744 (5)	4869 (2)	3715 (3)
C(9A)	5316 (5)	3024 (2)	2537 (3)
C(9B)	8234 (5)	4457 (2)	4529 (3)
C(10A)	8404 (5)	2447 (3)	5651 (3)
C(10B)	5221 (5)	4931 (2)	1457 (3)
C(11A)	7610 (5)	3150 (2)	5794 (3)
C(11B)	3893 (5)	4733 (2)	2072 (3)
C(12A)	8968 (5)	3657 (3)	6261 (3)
C(12B)	2478 (5)	4272 (3)	1560 (3)
C(13A)	8309 (5)	1320 (3)	4782 (4)
C(13B)	8013 (5)	5513 (2)	1332 (3)
O(1A)	8329 (4)	4341 (2)	6288 (2)
O(1B)	3107 (3)	3588 (2)	1405 (2)
O(2A)	8852 (4)	2479 (2)	3522 (2)
O(2B)	8528 (3)	4206 (2)	2422 (2)
H(2A)	1193 (34)	3155 (15)	2562 (20)
H(2B)	7116 (39)	5542 (17)	6059 (23)
H(3A)	2098 (39)	2432 (18)	3967 (23)
H(3B)	6262 (39)	6160 (17)	4725 (24)
H(9A)	6181 (35)	3214 (16)	2239 (21)
H(9B)	8725 (33)	4037 (15)	4459 (20)
H(10A)	9627 (36)	2505 (16)	5527 (22)
H(10B)	5578 (34)	4535 (16)	1131 (21)
H(10C)	8468 (38)	2170 (17)	6270 (22)
H(10D)	4587 (34)	5267 (15)	909 (20)
H(11A)	7025 (36)	3335 (16)	5101 (23)
H(11B)	4504 (37)	4505 (17)	2661 (22)
H(11C)	6808 (37)	3073 (17)	6143 (23)
H(11D)	3303 (38)	5176 (17)	2261 (22)
H(12A)	10009 (42)	3629 (19)	5916 (26)
H(12B)	1439 (37)	4202 (17)	1918 (22)
H(12C)	9500 (37)	3519 (17)	6971 (24)
H(12D)	1951 (32)	4435 (15)	862 (21)
H(13A)	8084 (56)	1058 (23)	5328 (37)
H(13B)	9137 (43)	5661 (19)	1699 (26)
H(13C)	9507 (40)	1393 (18)	4784 (24)
H(13D)	7433 (43)	5892 (19)	935 (26)
H(13E)	7607 (58)	1015 (23)	4160 (36)
H(13F)	8249 (39)	5112 (18)	899 (24)
H(51A)	5110 (34)	2162 (15)	5329 (21)
H(51B)	7336 (39)	6249 (18)	2755 (24)
H(52A)	5063 (35)	1472 (17)	4637 (22)
H(52B)	5449 (35)	5992 (15)	2570 (21)

Table 2. Bond distances (\AA) and angles ($^\circ$) with *e.s.d.*'s in parentheses

C(1A)—C(2A)	1.400 (6)	C(6A)—C(10A)	1.546 (6)
C(1A)—C(9A)	1.379 (5)	C(6A)—C(13A)	1.527 (6)
C(1A)—O(1B)	1.384 (5)	C(6B)—C(7B)	1.528 (6)
C(1B)—C(2B)	1.393 (7)	C(6B)—C(10B)	1.552 (5)
C(1B)—C(9B)	1.383 (6)	C(6B)—C(13B)	1.537 (6)
C(1B)—O(1A)	1.376 (5)	C(7A)—C(8A)	1.468 (6)
C(2A)—C(3A)	1.379 (6)	C(7A)—O(2A)	1.217 (6)
C(2B)—C(3B)	1.381 (7)	C(7B)—C(8B)	1.462 (6)
C(3A)—C(4A)	1.395 (5)	C(7B)—O(2B)	1.222 (5)
C(3B)—C(4B)	1.391 (7)	C(8A)—C(9A)	1.384 (5)
C(4A)—C(5A)	1.506 (5)	C(8B)—C(9B)	1.384 (6)
C(4A)—C(8A)	1.384 (6)	C(10A)—C(11A)	1.536 (7)
C(4B)—C(5B)	1.502 (6)	C(10B)—C(11B)	1.536 (6)
C(4B)—C(8B)	1.381 (6)	C(11A)—C(12A)	1.510 (6)
C(5A)—C(6A)	1.548 (5)	C(11B)—C(12B)	1.503 (6)
C(5B)—C(6B)	1.552 (6)	C(12A)—O(1A)	1.428 (6)
C(6A)—C(7A)	1.530 (6)	C(12B)—O(1B)	1.454 (6)
C(9A)—C(1A)—C(2A)	119.8 (4)	C(10B)—C(6B)—C(7B)	106.8 (3)
O(1B)—C(1A)—C(2A)	121.2 (3)	C(13B)—C(6B)—C(5B)	113.2 (3)
O(1B)—C(1A)—C(9A)	119.0 (4)	C(13B)—C(6B)—C(7B)	109.7 (3)
C(9B)—C(1B)—C(2B)	118.9 (4)	C(13B)—C(6B)—C(10B)	109.6 (3)
O(1A)—C(1B)—C(2B)	115.3 (4)	C(8A)—C(7A)—C(6A)	109.0 (4)
O(1A)—C(1B)—C(9B)	125.8 (4)	O(2A)—C(7A)—C(6A)	124.7 (4)
C(3A)—C(2A)—C(1A)	120.6 (3)	O(2A)—C(7A)—C(8A)	126.3 (4)
C(3B)—C(2B)—C(1B)	122.2 (4)	C(8B)—C(7B)—C(6B)	108.6 (4)
C(4A)—C(3A)—C(2A)	120.0 (4)	O(2B)—C(7B)—C(6B)	124.5 (4)
C(4B)—C(3B)—C(2B)	118.7 (4)	O(2B)—C(7B)—C(8B)	126.9 (4)
C(5A)—C(4A)—C(3A)	129.5 (4)	C(7A)—C(8A)—C(4A)	109.0 (3)
C(8A)—C(4A)—C(3A)	118.4 (4)	C(9A)—C(8A)—C(4A)	122.3 (3)
C(8A)—C(4A)—C(5A)	112.2 (3)	C(9A)—C(8A)—C(7A)	128.6 (4)
C(5B)—C(4B)—C(3B)	129.7 (4)	C(7B)—C(8B)—C(4B)	109.7 (4)
C(8B)—C(4B)—C(3B)	118.7 (4)	C(9B)—C(8B)—C(4B)	122.9 (4)
C(8B)—C(4B)—C(5B)	111.6 (4)	C(9B)—C(8B)—C(7B)	127.4 (4)
C(6A)—C(5A)—C(4A)	104.9 (3)	C(8A)—C(9A)—C(1A)	118.9 (4)
C(6B)—C(5B)—C(4B)	105.0 (3)	C(8B)—C(9B)—C(1B)	118.5 (4)
C(7A)—C(6A)—C(5A)	104.3 (3)	C(11A)—C(10A)—C(6A)	115.6 (3)
C(10A)—C(6A)—C(5A)	112.3 (3)	C(11B)—C(10B)—C(6B)	114.8 (3)
C(10A)—C(6A)—C(7A)	108.6 (4)	C(12A)—C(11A)—C(10A)	111.3 (3)
C(13A)—C(6A)—C(5A)	113.0 (4)	C(12B)—C(11B)—C(10B)	114.4 (3)
C(13A)—C(6A)—C(7A)	109.2 (4)	O(1A)—C(12A)—C(11A)	113.3 (3)
C(13A)—C(6A)—C(10A)	109.1 (3)	O(1B)—C(12B)—C(11B)	111.9 (3)
C(7B)—C(6B)—C(5B)	103.9 (3)	C(12A)—O(1A)—C(1B)	117.0 (3)
C(10B)—C(6B)—C(5B)	113.3 (3)	C(12B)—O(1B)—C(1A)	114.5 (3)

diastereoisomer of compound (II) in the preceding paper. It was isolated from work-up after treatment of the centrosymmetric dimer with Zn and ethanol and thus apparently involves racemization of a quaternary C atom. However, it is also possible that both diastereoisomers were formed in the cyclization and that they crystallized out at different stages in the reaction.



The conformation of (I) is unusual (Fig. 1), in that one of the anisolic groupings is no longer planar

Discussion. The compound was produced by Chatterjee, Misra, Mukherjee & Dutta (1975) as described in the preceding paper (Murray-Rust & Murray-Rust, 1979). It is here shown to be (I), *i.e.* the racemic

Table 3. *Torsion angles* (°)

C(2A)—C(1A)—O(1B)—C(12B)	67.1	C(11B)—C(10B)—C(6B)—C(5B)	-46.0	O(1A)—C(12A)—C(11A)—C(10A)	172.0
C(9A)—C(1A)—O(1B)—C(12B)	-114.7	C(11B)—C(10B)—C(6B)—C(7B)	67.6	C(12A)—C(11A)—C(10A)—C(6A)	-150.9
C(1A)—O(1B)—C(12B)—C(11B)	69.2	C(2B)—C(1B)—O(1A)—C(12A)	177.3	C(11A)—C(10A)—C(6A)—C(5A)	-49.7
O(1B)—C(12B)—C(11B)—C(10B)	69.1	C(9B)—C(1B)—O(1A)—C(12A)	-4.4	C(11A)—C(10A)—C(6A)—C(7A)	64.9
C(12B)—C(11B)—C(10B)—C(6B)	-166.8	C(1B)—O(1A)—C(12A)—C(11A)	-72.2		

(torsion angles are given in Table 3). The molecule does not have the compact *ansa* shape of the centrosymmetric dimer, nor does it have twofold symmetry (which would be possible since both quaternary C atoms have the same chirality). It is possible to build models with planar anisolic groups and no unfavourable intramolecular contacts, so it is unclear why the conformation is so irregular.

We thank Dr S. Chatterjee for crystals, and Dr C. I. F. Watt for helpful discussions.

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N,N'-Diphenylterephthalamide (DPTP)*

BY S. HARKEMA,† R. J. GAYMANS, G. J. VAN HUMMEL AND D. ZYLBERLICHT‡

Chemical Physics Laboratory, Twente University of Technology, PO Box 217, 7500 AE Enschede, The Netherlands

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Abstract. C₂₀H₁₆N₂O₂, monoclinic, *P*2₁/*n*, *a* = 6.912 (3), *b* = 21.462 (5), *c* = 5.323 (3) Å, β = 107.20 (5)°, *Z* = 2. The crystal structure was solved by direct methods and all H atoms were located: *R*_w = 4.9%. The structure contains planar phenyl rings which are rotated with respect to the plane of the amide group due to steric hindrance. The molecules are connected by hydrogen bonds.

Introduction. The present investigation is part of a series on the structures of model compounds of aromatic and aliphatic–aromatic polyamides (Harkema & Gaymans, 1977). In this paper the crystal structure of DPTP (Fig. 1) is reported.

DPTP was prepared as described by Gaymans & Harkema (1977). Recrystallization from dimethyl-

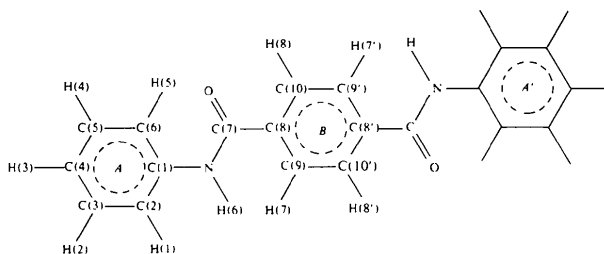


Fig. 1. Atomic arrangement of DPTP.

acetamide yielded suitable crystals. Intensities were collected at 293 K on a Philips PW 1100 diffractometer with graphite-monochromated Mo *K*α radiation (λ = 0.7107 Å). Reflexions up to θ = 30° were measured with the ω–2θ scan mode. The number of reflexions measured was 1912 and all were used in the refinement. No absorption correction was applied. The structure was solved by direct methods with *MAGIC* (Dewar, 1970). Details of the weighting scheme, scattering factors and the refinement procedure are given in Harkema & Gaymans (1977). The final value

* The Crystal and Molecular Structure of Model Compounds of Aromatic and Aromatic–Aliphatic Polyamides. II. Part I: Harkema & Gaymans (1977).

† To whom correspondence should be addressed.

‡ Present address: 7/7 Haim Haviv Street, Kiryat Yorel, Jerusalem, Israel.