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Structure of α-(Diphenylmethyleneamino)-α-phenyldeoxybenzoin, $C_{33}H_{25}NO$

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Abstract. $M_r = 451{\cdot}6$, monoclinic, $P2_1/n$, $a = 12{\cdot}936$ (5), $b = 14{\cdot}077$ (4), $c = 13{\cdot}754$ (5) Å, $\beta = 97{\cdot}97$ (3)°, $V = 2480$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}21$ Mg m^{-3}, μ(Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å) = 0·067 mm^{-1}, $F(000) = 952$, $T = 295$ K, $R = 0{\cdot}049$ for 2088 observed reflexions. The structure of the title compound has been established; bond lengths and angles are normal.

Introduction. Armesto, Ortiz & Perez-Ossorio (1981) have studied the photochemical reactions of some *N*-(diphenylmethylene)(acyl) diarylmethylamines. In one of these reactions, the compound yields an isomeric product. In order to postulate a mechanism for this reaction it is necessary to know the structure of both the starting material (I) and the photoproduct (II). It is also important to know the conformational aspects.

We now report the crystal structure of the starting material (I).

Experimental. A clear colourless, prismatic crystal prepared by Armesto *et al.* (1981); a computer-controlled four-circle CAD-4 diffractometer; cell dimensions refined by least-squares fit to the θ values of 25 reflexions; intensities of 6295 reflexions within $1 < \theta < 28°$ collected with $\omega/2\,\theta$ scans; three reflexions monitored periodically showed no crystal decomposition; intensities corrected for Lorentz and polarization effects; 2088 unique reflexions considered observed [$I > 2\sigma(I)$]; scattering factors for neutral atoms from *International Tables for X-ray Crystallography* (1974). Structure solved with *MULTAN* (Main, Lessinger, Woolfson, Germain & Declercq, 1977); following anisotropic full-matrix least-squares refinement with unit weights, a difference synthesis calculated with reflexions having $\sin\theta/\lambda < 0{\cdot}5$ Å^{-1} showed all H atoms as highest peaks; after refinement with fixed isotropic temperature factors for H atoms, the final $R = 0{\cdot}049$ and $R_w = 0{\cdot}057$; $w = 1/(a + b|F_o|)^2$ with coefficients shown in Table 1;† a final difference synthesis had no electron density >0·34 e Å^{-3}; most of the calculations carried out with XRAY70 (Stewart, Kundell & Baldwin, 1970); least-squares weights calculated with *PESOS* (Martínez-Ripoll & Cano, 1975).

Discussion. The final positional parameters are listed in Table 2. Fig. 1 (Johnson, 1965) shows the geometry of the molecule and the atom labelling. Table 3 lists bond lengths and angles. Table 4† shows the angles between the best least-squares planes for various portions of the molecule, and principal torsion angles, computed by *PARST* 5 (Nardelli, Musatti, Domiano & Andreetti, 1965).

The bond lengths are as expected. The packing in the crystal is determined only by van der Waals interactions.

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† See deposition footnote.

Table 2. *Atomic coordinates and thermal parameters*

For non-hydrogen atoms $U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}\,a_i^*\,a_j^*\,\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}/U_{iso} (Å^2 × 10^3)
N	0·0671 (2)	0·0916 (2)	0·1783 (2)	41 (1)
C(1)	0·1020 (2)	0·1767 (2)	0·1743 (2)	38 (1)
C(3)	0·0106 (2)	0·0525 (2)	0·2550 (2)	40 (1)
C(4)	0·0519 (2)	0·0897 (2)	0·3597 (2)	44 (1)
O	−0·0083 (2)	0·1183 (2)	0·4136 (2)	61 (1)
C(6)	0·1677 (3)	0·0859 (2)	0·3958 (2)	45 (1)
C(7)	0·2010 (3)	0·1275 (3)	0·4868 (3)	60 (1)
C(8)	0·3057 (4)	0·1283 (3)	0·5250 (3)	77 (2)
C(9)	0·3780 (3)	0·0869 (3)	0·4729 (4)	79 (2)
C(10)	0·3464 (3)	0·0445 (3)	0·3827 (3)	64 (2)
C(11)	0·2408 (3)	0·0436 (2)	0·3449 (3)	50 (1)
C(12)	0·0260 (2)	−0·0574 (2)	0·2550 (2)	40 (1)
C(13)	0·0239 (3)	−0·1040 (2)	0·1653 (3)	50 (1)
C(14)	0·0280 (3)	−0·2025 (3)	0·1617 (3)	58 (1)
C(15)	0·0354 (3)	−0·2555 (3)	0·2477 (3)	64 (2)
C(16)	0·0392 (3)	−0·2113 (3)	0·3382 (3)	63 (2)
C(17)	0·0337 (3)	−0·1116 (2)	0·3400 (3)	54 (1)
C(12′)	−0·1078 (2)	0·0691 (2)	0·2278 (2)	41 (1)
C(13′)	−0·1778 (3)	0·0319 (3)	0·2863 (2)	54 (1)
C(14′)	−0·2842 (3)	0·0442 (3)	0·2609 (3)	61 (1)
C(15′)	−0·3237 (3)	0·0924 (3)	0·1776 (3)	64 (1)
C(16′)	−0·2556 (3)	0·1268 (3)	0·1165 (3)	65 (1)
C(17′)	−0·1473 (3)	0·1153 (2)	0·1412 (2)	50 (1)
C(18)	0·1573 (2)	0·1986 (2)	0·0881 (2)	37 (1)
C(19)	0·1733 (3)	0·2926 (2)	0·0608 (2)	52 (1)
C(20)	0·2241 (3)	0·3113 (3)	−0·0200 (3)	64 (1)
C(21)	0·2569 (3)	0·2386 (3)	−0·0734 (3)	67 (2)

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† Lists of structure factors, anisotropic thermal parameters, bond lengths and angles involving H atoms and Tables 1 and 4 have been deposited with the British Library Lending Division as Supplemenatry Publication No. SUP 38418 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 2 (*cont.*)

	x	y	z	U_{eq}/U_{iso} ($Å^2 \times 10^3$)
C(22)	0·2409 (3)	0·1448 (3)	−0·0483 (3)	68 (2)
C(23)	0·1918 (3)	0·1254 (2)	0·0325 (2)	52 (1)
C(18′)	0·0957 (2)	0·2576 (2)	0·2455 (2)	38 (1)
C(19′)	0·0012 (3)	0·2939 (2)	0·2654 (3)	51 (1)
C(20′)	0·0004 (3)	0·3715 (3)	0·3280 (3)	66 (2)
C(21′)	0·0928 (3)	0·4135 (3)	0·3705 (3)	65 (2)
C(22′)	0·1857 (3)	0·3773 (3)	0·3514 (3)	61 (1)
C(23′)	0·1887 (3)	0·3001 (2)	0·2885 (2)	49 (1)
H(16′)	−0·278	0·159	0·052	48
H(8)	0·331 (3)	0·156 (3)	0·588 (3)	48
H(9)	0·462 (3)	0·093 (3)	0·498 (3)	48
H(11)	0·217 (3)	0·012 (3)	0·278 (3)	48
H(13)	0·017 (2)	−0·063 (2)	0·099 (2)	48
H(14)	0·029 (3)	−0·236 (3)	0·094 (3)	48
H(15)	0·036 (3)	−0·328 (3)	0·246 (3)	48
H(16)	0·046 (9)	−0·250 (8)	0·400 (8)	48
H(13′)	−0·146 (3)	−0·003 (3)	0·352 (3)	48
H(14′)	−0·335 (3)	0·021 (2)	0·310 (2)	48
H(15′)	−0·403 (3)	0·106 (3)	0·158 (3)	48
H(17′)	−0·094 (3)	0·141 (2)	0·096 (2)	48
H(20)	0·235 (3)	0·384 (2)	−0·033 (2)	48
H(22)	0·265 (3)	0·095 (3)	−0·087 (3)	48
H(20′)	−0·071 (3)	0·398 (3)	0·343 (3)	48
H(21′)	0·094 (3)	0·475 (3)	0·418 (3)	48
H(22′)	0·262 (3)	0·408 (3)	0·382 (3)	48
H(23′)	0·255 (3)	0·273 (3)	0·270 (3)	48
H(7)	0·145 (3)	0·157 (2)	0·526 (2)	67
H(10)	0·398 (3)	0·014 (2)	0·342 (2)	58
H(17)	0·037 (2)	−0·080 (2)	0·409 (2)	45
H(19)	0·140 (3)	0·349 (3)	0·095 (3)	27
H(21)	0·292 (2)	0·250 (2)	−0·133 (2)	32
H(23)	0·180 (2)	0·056 (2)	0·055 (2)	41
H(19′)	−0·068 (2)	0·260 (2)	0·238 (2)	33

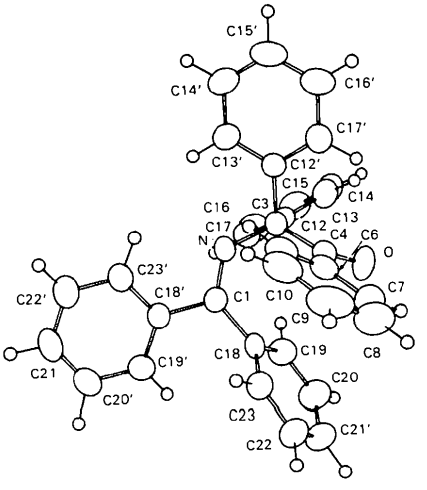

Fig. 1. *ORTEP* (Johnson, 1965) drawing of the molecule, showing the atom numbering.

Table 3. *Bond lengths* (Å) *and angles* (°) (*e.s.d.'s average* 0·005 Å *for lengths and* 0·3° *for angles*)

C(1)–N	1·284	C(16)–C(17)	1·405
C(1)–C(18)	1·500	C(12′)–C(13′)	1·394
C(1)–C(18′)	1·511	C(12′)–C(17′)	1·392
C(3)–N	1·470	C(13′)–C(14′)	1·382
C(3)–C(4)	1·555	C(14′)–C(15′)	1·369
C(3)–C(12)	1·559	C(15′)–C(16′)	1·386
C(3)–C(12′)	1·543	C(16′)–C(17′)	1·405
C(4)–O	1·216	C(18)–C(19)	1·400
C(4)–C(6)	1·513	C(18)–C(23)	1·393
C(6)–C(7)	1·395	C(19)–C(20)	1·393
C(6)–C(11)	1·386	C(20)–C(21)	1·361
C(7)–C(8)	1·383	C(21)–C(22)	1·388
C(8)–C(9)	1·384	C(22)–C(23)	1·382
C(9)–C(10)	1·386	C(18′)–C(19′)	1·388
C(10)–C(11)	1·393	C(18′)–C(23′)	1·400
C(12)–C(13)	1·395	C(19′)–C(20′)	1·392
C(12)–C(17)	1·388	C(20′)–C(21′)	1·388
C(13)–C(14)	1·387	C(21′)–C(22′)	1·364
C(14)–C(15)	1·390	C(22′)–C(23′)	1·393
C(15)–C(16)	1·386		
C(1)–N–C(3)	126·3	C(14)–C(15)–C(16)	120·8
N–C(1)–C(18′)	128·6	C(15)–C(16)–C(17)	117·9
N–C(1)–C(18)	115·8	C(12)–C(17)–C(16)	122·1
C(18)–C(1)–C(18′)	115·6	C(3)–C(12′)–C(17′)	120·8
N–C(3)–C(12′)	110·2	C(3)–C(12′)–C(13′)	120·5
N–C(3)–C(12)	107·2	C(13′)–C(12′)–C(17′)	118·6
N–C(3)–C(4)	113·4	C(12′)–C(13′)–C(14′)	120·8
C(12)–C(3)–C(12′)	105·8	C(13′)–C(14′)–C(15′)	121·1
C(4)–C(3)–C(12′)	112·0	C(14′)–C(15′)–C(16′)	119·1
C(4)–C(3)–C(12)	107·8	C(15′)–C(16′)–C(17′)	120·7
C(3)–C(4)–C(6)	119·3	C(12′)–C(17′)–C(16′)	119·8
C(3)–C(4)–O	120·7	C(1)–C(18)–C(23)	120·4
O–C(4)–C(6)	120·0	C(1)–C(18)–C(19)	120·7
C(4)–C(6)–C(11)	124·3	C(19)–C(18)–C(23)	118·9
C(4)–C(6)–C(7)	116·7	C(18)–C(19)–C(20)	119·8
C(7)–C(6)–C(11)	119·1	C(19)–C(20)–C(21)	120·4
C(6)–C(7)–C(8)	120·6	C(20)–C(21)–C(22)	120·8
C(7)–C(8)–C(9)	119·7	C(21)–C(22)–C(23)	119·4
C(8)–C(9)–C(10)	120·6	C(18)–C(23)–C(22)	120·8
C(9)–C(10)–C(11)	119·3	C(1)–C(18′)–C(23′)	118·5
C(6)–C(11)–C(10)	120·7	C(1)–C(18′)–C(19′)	122·3
C(3)–C(12)–C(17)	122·7	C(19′)–C(18′)–C(23′)	119·2
C(3)–C(12)–C(13)	118·7	C(18′)–C(19′)–C(20′)	119·6
C(13)–C(12)–C(17)	118·5	C(19′)–C(20′)–C(21′)	121
C(12)–C(13)–C(14)	120·4	C(20′)–C(21′)–C(22′)	119·3
C(13)–C(14)–C(15)	120·3	C(21′)–C(22′)–C(23′)	120·8
		C(18′)–C(23′)–C(22′)	120·1

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