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Structure of 2-[α-(Diphenylmethylimino)benzyl]benzophenone, $C_{33}H_{25}NO$

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Abstract. $M_r = 451{\cdot}6$, monoclinic, $P2_1/c$, $a = 18{\cdot}745\ (5)$, $b = 9{\cdot}257\ (4)$, $c = 14{\cdot}261\ (5)$ Å, $\beta = 91{\cdot}64\ (2)°$, $V = 2473\ (8)$ Å^3, $Z = 4$, $D_x = 1{\cdot}21$ Mg m^{-3}, μ(Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å) $= 0{\cdot}067$ mm^{-1}, $F(000) = 952$, $T = 295$ K, final $R = 0{\cdot}043$ and $R_w = 0{\cdot}047$ for 2132 observed reflexions. Bond lengths and angles are normal.

Introduction. Armesto & Gomez-Gallego (1982) have prepared and studied spectroscopically the title compound (II). This compound is the main product in the photochemical reaction of (I), whose structural formula is Ph–CO–C(Ph)$_2$–N=C(Ph)$_2$. The crystal structure of (I) has been determined by Ruiz-Valero, Gutiérrez-Puebla & Monge (1983).

In order to postulate a mechanism for this reaction, it is necessary to know the structure of the photoproduct (II). A spectroscopic study of (II) does not provide enough information about its molecular structure. Therefore it was necessary to solve its crystal structure.

Experimental. A clear colourless, prismatic crystal; Enraf–Nonius CAD-4 diffractometer; intensities of 6321 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; 2132 considered observed [$I > 2\sigma(I)$]; no absorption correction; scattering factors for neutral atoms from *International Tables for X-ray Crystallography* (1974). Structure was solved by *MULTAN* (Main, Lessinger, Woolfson, Germain & Declercq, 1977); the best E map revealed all the non-hydrogen atoms; after anisotropic full-matrix least-squares refinement, a difference synthesis calculated for reflexions with $\sin\theta/\lambda < 0{\cdot}5$ Å^{-1} showed all H atoms as the highest peaks of the map; $w = 1/(a + b|F_o|)^2$, with coefficients† calculated by the program *PESOS* (Martínez-Ripoll & Cano, 1975); after refinement with isotropic temperature factors for H atoms, final $R = 0{\cdot}043$ and $R_w = 0{\cdot}047$; a final difference synthesis showed no significant electron density.

Table 1. *Atomic coordinates and thermal parameters for* (II)

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}/U_{iso} (Å^2 × 10^3)
N	0·2197 (1)	0·1832 (3)	0·9396 (2)	43 (1)
O	0·4720 (1)	0·3230 (3)	0·8249 (2)	73 (1)
C(1)	0·2873 (1)	0·1957 (3)	0·9523 (2)	38 (1)
C(3)	0·1890 (1)	0·0724 (3)	0·8767 (2)	44 (1)
C(4)	0·3421 (1)	0·0903 (3)	0·9184 (2)	39 (1)
C(5)	0·3983 (1)	0·1273 (3)	0·8600 (2)	41 (1)
C(6)	0·4501 (2)	0·0240 (4)	0·8403 (2)	54 (1)
C(7)	0·4458 (2)	−0·1139 (4)	0·8758 (2)	63 (1)
C(8)	0·3920 (2)	−0·1498 (4)	0·9347 (3)	63 (1)
C(9)	0·3401 (2)	−0·0489 (3)	0·9561 (2)	50 (1)
C(10)	0·4108 (1)	0·2772 (3)	0·8237 (2)	46 (1)
C(4′)	0·3142 (1)	0·3211 (3)	1·0092 (2)	38 (1)
C(5′)	0·2692 (2)	0·4349 (3)	1·0290 (2)	55 (1)
C(6′)	0·2941 (2)	0·5526 (4)	1·0801 (3)	67 (1)
C(7′)	0·3645 (2)	0·5586 (4)	1·1115 (2)	63 (1)
C(8′)	0·4089 (2)	0·4458 (4)	1·0928 (2)	59 (1)
C(9′)	0·3849 (2)	0·3266 (4)	1·0423 (2)	49 (1)
C(12)	0·3516 (1)	0·3689 (3)	0·7854 (2)	43 (1)
C(13)	0·2931 (2)	0·3099 (3)	0·7375 (2)	48 (1)
C(14)	0·2411 (2)	0·3991 (4)	0·6972 (2)	59 (1)
C(15)	0·2469 (2)	0·5476 (4)	0·7071 (3)	65 (1)
C(16)	0·3048 (2)	0·6059 (4)	0·7557 (3)	69 (1)
C(17)	0·3573 (2)	0·5183 (3)	0·7935 (2)	57 (1)
C(18)	0·1348 (1)	0·1450 (3)	0·8100 (2)	46 (1)
C(19)	0·1221 (2)	0·0892 (4)	0·7214 (2)	66 (1)
C(20)	0·0726 (2)	0·1543 (4)	0·6599 (3)	80 (2)
C(21)	0·0355 (2)	0·2748 (5)	0·6863 (3)	76 (2)
C(22)	0·0481 (2)	0·3313 (4)	0·7742 (3)	78 (2)
C(23)	0·0976 (2)	0·2666 (4)	0·8360 (2)	65 (1)
C(18′)	0·1534 (1)	−0·0460 (3)	0·9323 (2)	47 (1)
C(19′)	0·1103 (2)	−0·0145 (4)	1·0067 (2)	60 (1)
C(20′)	0·0764 (2)	−0·1241 (5)	1·0553 (3)	75 (2)
C(21′)	0·0853 (2)	0·2646 (5)	1·0293 (4)	86 (2)
C(22′)	0·1267 (2)	0·2988 (4)	0·9563 (4)	93 (2)
C(23′)	0·1619 (2)	−0·1900 (4)	0·9070 (3)	70 (1)
H(3)	0·226 (1)	0·031 (3)	0·836 (2)	17 (7)
H(6)	0·489 (2)	0·059 (3)	0·796 (2)	42 (9)
H(7)	0·482 (2)	−0·182 (4)	0·855 (2)	52 (11)
H(8)	0·388 (2)	0·249 (3)	0·961 (2)	42 (9)
H(9)	0·303 (1)	0·071 (3)	1·003 (2)	13 (7)
H(5′)	0·222 (1)	0·427 (3)	1·004 (2)	14 (8)
H(6′)	0·261 (2)	0·630 (3)	1·090 (2)	40 (9)
H(7′)	0·381 (2)	0·642 (3)	1·146 (2)	31 (9)
H(8′)	0·457 (2)	0·449 (3)	1·116 (2)	43 (9)
H(9′)	0·417 (2)	0·236 (3)	1·032 (2)	36 (9)
H(13)	0·290 (1)	0·206 (3)	0·730 (2)	24 (9)
H(14)	0·198 (2)	0·354 (3)	0·659 (2)	40 (10)
H(15)	0·208 (2)	0·614 (3)	0·674 (2)	38 (10)
H(16)	0·308 (2)	0·708 (3)	0·764 (2)	46 (10)
H(17)	0·402 (2)	0·559 (3)	0·827 (2)	39 (9)
H(19)	0·149 (2)	−0·001 (4)	0·705 (2)	51 (11)
H(20)	0·064 (2)	0·107 (4)	0·601 (3)	71 (13)
H(21)	−0·001 (2)	0·321 (4)	0·641 (3)	69 (12)
H(22)	0·021 (2)	0·424 (4)	0·799 (3)	77 (13)
H(23)	0·107 (2)	0·315 (4)	0·898 (2)	48 (10)
H(19′)	0·104 (2)	0·093 (4)	1·028 (2)	50 (10)
H(20′)	0·043 (2)	−0·095 (4)	1·110 (3)	90 (13)
H(21′)	0·062 (2)	−0·346 (4)	1·065 (3)	79 (13)
H(22′)	0·135 (2)	−0·397 (4)	0·930 (3)	93 (13)
H(23′)	0·194 (2)	−0·207 (3)	0·850 (2)	43 (10)

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† Lists of structure factors, anisotropic thermal parameters, bond lengths and angles involving H atoms, Table 3 and the coefficients of the weighting scheme have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38417 (29 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. *Bond lengths* (Å) *and angles* (°) (*e.s.d.'s are* 0·005 Å *and* 0·4°, *respectively*)

N–C(1)	1·282	C(8')–C(9')	1·386
N–C(3)	1·469	C(12)–C(13)	1·388
O–C(10)	1·224	C(12)–C(17)	1·391
C(1)–C(4)	1·506	C(13)–C(14)	1·390
C(1)–C(4')	1·496	C(14)–C(15)	1·386
C(3)–C(18)	1·528	C(15)–C(16)	1·382
C(3)–C(18')	1·518	C(16)–C(17)	1·374
C(4)–C(5)	1·404	C(18)–C(19)	1·380
C(4)–C(9)	1·397	C(18)–C(23)	1·380
C(5)–C(6)	1·398	C(19)–C(20)	1·395
C(5)–C(10)	1·502	C(20)–C(21)	1·372
C(6)–C(7)	1·376	C(21)–C(22)	1·373
C(7)–C(8)	1·372	C(22)–C(23)	1·400
C(8)–C(9)	1·388	C(18')–C(19')	1·383
C(10)–C(12)	1·489	C(18')–C(23')	1·392
C(4')–C(5')	1·384	C(19')–C(20')	1·391
C(4')–C(9')	1·394	C(20')–C(21')	1·364
C(5')–C(6')	1·384	C(21')–C(22')	1·353
C(6')–C(7')	1·383	C(22')–C(23')	1·404
C(7')–C(8')	1·366		

C(1)–N–C(3)	121·1	C(7')–C(8')–C(9')	121·3
N–C(1)–C(4')	117·6	C(4')–C(9')–C(8')	119·8
N–C(1)–C(4)	125·3	C(10)–C(12)–C(17)	118·8
C(4)–C(1)–C(4')	117·1	C(10)–C(12)–C(13)	121·7
N–C(3)–C(18')	110·8	C(13)–C(12)–C(17)	119·4
N–C(3)–C(18)	108·3	C(12)–C(13)–C(14)	120·3
C(18)–C(3)–C(18')	110·4	C(13)–C(14)–C(15)	119·7
C(1)–C(4)–C(9)	116·7	C(14)–C(15)–C(16)	119·8
C(1)–C(4)–C(5)	124·2	C(15)–C(16)–C(17)	120·7
C(5)–C(4)–C(9)	118·8	C(12)–C(17)–C(16)	120·1
C(4)–C(5)–C(10)	123·9	C(3)–C(18)–C(23)	121·6
C(4)–C(5)–C(6)	119·4	C(3)–C(18)–C(19)	120·0
C(6)–C(5)–C(10)	116·5	C(19)–C(18)–C(23)	118·5
C(5)–C(6)–C(7)	120·8	C(18)–C(19)–C(20)	120·5
C(6)–C(7)–C(8)	120·1	C(19)–C(20)–C(21)	120·8
C(7)–C(8)–C(9)	120·2	C(20)–C(21)–C(22)	119·0
C(4)–C(9)–C(8)	120·6	C(21)–C(22)–C(23)	120·4
O–C(10)–C(5)	118·1	C(18)–C(23)–C(22)	120·8
C(5)–C(10)–C(12)	122·1	C(3)–C(18')–C(23')	120·0
O–C(10)–C(12)	119·8	C(3)–C(18')–C(19')	121·6
C(1)–C(4')–C(9')	120·9	C(19')–C(18')–C(23')	118·4
C(1)–C(4')–C(5')	120·3	C(18')–C(19')–C(20')	120·8
C(5')–C(4')–C(9')	118·8	C(19')–C(20')–C(21')	120·0
C(4')–C(5')–C(6')	120·6	C(20')–C(21')–C(22')	120·6
C(5')–C(6')–C(7')	120·4	C(21')–C(22')–C(23')	120·4
C(6')–C(7')–C(8')	119·2	C(18')–C(23')–C(22')	119·8

Discussion. The final positional parameters are listed in Table 1. Fig. 1 is a computer-generated perspective drawing of the molecule. Table 2 shows bond lengths and angles; these are normal. Table 3* shows the angles between least-squares planes for various portions of the molecule and principal torsion angles, computed by *PARST* 5 (Nardelli, Musatti, Domiano & Andreetti, 1965).

* See deposition footnote.

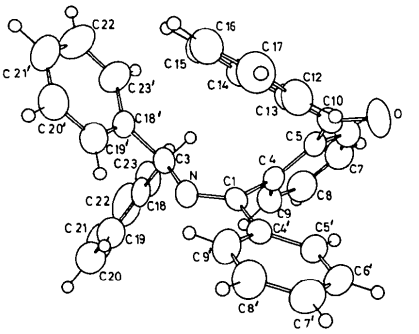

Fig. 1. *ORTEP* (Johnson, 1965) drawing of the molecule, showing the atom numbering.

The photochemical transformation of (I) into (II) can be interpreted as a 1,5 acyl migration.

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Structure of 3',5'-Di-*O*-acetyl-5-bromo-2'-deoxyuridine, $C_{13}H_{15}BrN_2O_7$

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Abstract. $M_r = 391{\cdot}2$, monoclinic, $C2$, $a = 16{\cdot}444$ (10), $b = 6{\cdot}651$ (6), $c = 17{\cdot}246$ (10) Å, $\beta = 56{\cdot}9$ (1)°, $U = 1580$ Å^3, $Z = 4$, $D_x = 1{\cdot}64$ Mg m^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, $\mu = 2{\cdot}552$ mm^{-1}, $T = 293$ K, $F(000) = 792$, $R = 0{\cdot}077$ for 1185 observed reflexions (Friedel pairs not merged). The sugar-ring pucker in

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