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[1]Benzoxepino[2,3-b]quinoxaline and [3]Benzoxepino[1,2-b]quinoxaline: Two Previously Unknown Photoproducts from Benzo[a]phenazine 7-Oxide

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AND LUCIA INCOCCIA AND FABIO COMIN

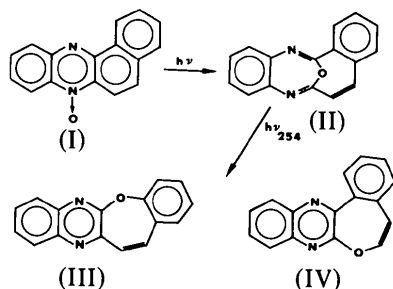*Istituto di Cristallografia dell'Università di Pavia, Via Bassi 4, 27100 Pavia, Italy*

Two new products from the photoisomerization of benzo[a]phenazine 7-oxide have been isolated and crystallized: $C_{16}H_{10}N_2O$, m.p. 145–147°C, orthorhombic, *Fdd*2, $a = 39.931$ (3), $b = 26.864$ (2), $c = 4.471$ (2) Å, $Z = 16$; and $C_{16}H_{10}N_2O$, m.p. 129–130°C, orthorhombic, *Pna*2_1, $a = 12.201$ (3), $b = 7.443$ (2), $c = 13.328$ (3) Å, $Z = 4$. Intensity data were collected at room temperature on a Philips PW 1100 computer-controlled diffractometer (Cu $K\alpha$ graphite-monochromatized radiation). Both crystal structures were solved by direct methods and refined anisotropically to final conventional unweighted R indices of 0·042 and 0·052 respectively for the reflections with $I > 2\sigma(I)$. The molecular conformations of both compounds are discussed.

Introduction

Irradiation of benzo[a]phenazine 7-oxide (I) yields the annulene (II) *via* an oxaziridine or 'quasi-oxaziridine' intermediate (Albini, Barinotti, Bettinetti & Pietra, 1976).

Compound (II) is photostable under irradiation at 366 nm (maximum of the first absorption band: 364 nm), while irradiation at 254 nm (maximum of the second absorption band: 261 nm) leads to isomerization, although with a low quantum yield.

The structures of the two principal products obtained

(I)

(II)

(III)   (IV)

could not be unequivocally proved by UV or NMR spectra. X-ray analysis revealed that (III) is [1]benz-oxepino[2,3-*b*]quinoxaline and (IV) is [3]benz-oxepino[1,2-*b*]quinoxaline. This reaction is, therefore, the first photochemical sigmatropic rearrangement of a 1,3-oxazepine, as the only reactions previously reported are electrocyclic rearrangements, which are obviously sterically hindered in the present case.

It is noteworthy that widespread attention has recently been focused (Ishikawa & Griffin, 1977) on arene oxides and dioxides and their derivatives because of their mutagenic and/or carcinogenic activity.

Structure of [1]benzoxepino[2,3-*b*]quinoxaline

Experimental

Yellow needles of compound (III) were obtained from a warm saturated solution in *n*-heptane. Elemental chemical analysis gave the formula $C_{16}H_{10}N_2O$ (m.p. 145–147°C). Unit-cell dimensions were obtained at room temperature with a Philips PW 1100 computer-controlled diffractometer; systematic absences were those characteristic of space group *Fdd*2. [a = 39·931 (3), b = 26·864 (2), c = 4·471 (2) Å, Z = 16.]

Intensity data for 723 independent reflections were collected up to $\theta = 50°$ with an $\omega/2\theta$ scan mode using
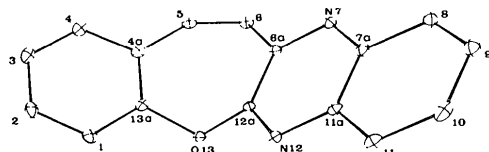

Fig. 1. *ORTEP* plot showing the atomic numbering used for compound (III). Thermal ellipsoids are drawn at 5% probability.
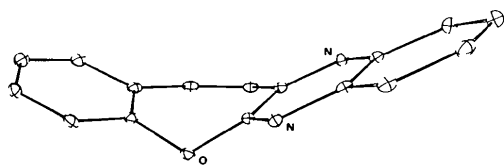

Fig. 2. *ORTEP* perspective view showing the molecular folding in compound (III). Thermal ellipsoids are drawn at 5% probability.

Table 1. *Compound* (III): *final fractional coordinates, with estimated standard deviations in parentheses, and equivalent* (*Hamilton*, 1959) *thermal parameters* ($Å^2$) *of all non-hydrogen atoms*

	x	y	z	B_{H}
C(1)	0·2633 (2)	−0·1728 (2)	0·483 (2)	4·8 (2)
C(2)	0·2304 (2)	−0·1829 (2)	0·556 (3)	5·7 (2)
C(3)	0·2045 (2)	−0·1547 (3)	0·441 (3)	5·7 (2)
C(4)	0·2113 (2)	−0·1167 (3)	0·240 (3)	5·1 (2)
C(4a)	0·2443 (2)	−0·1052 (2)	0·154 (2)	4·1 (2)
C(5)	0·2507 (2)	−0·0651 (2)	−0·056 (2)	4·5 (2)
C(6)	0·2777 (2)	−0·0369 (2)	−0·075 (2)	4·2 (2)
C(6a)	0·3069 (1)	−0·0387 (2)	0·120 (2)	3·3 (2)
N(7)	0·3234 (1)	0·0029 (2)	0·158 (2)	3·8 (2)
C(7a)	0·3501 (1)	0·0019 (2)	0·342 (2)	3·6 (2)
C(8)	0·3692 (2)	0·0461 (2)	0·387 (3)	4·9 (2)
C(9)	0·3960 (2)	0·0461 (3)	0·574 (3)	5·7 (2)
C(10)	0·4057 (1)	0·0023 (3)	0·724 (2)	5·8 (3)
C(11)	0·3882 (2)	−0·0415 (2)	0·681 (3)	5·0 (2)
C(11a)	0·3604 (1)	−0·0423 (2)	0·487 (2)	3·8 (2)
N(12)	0·3434 (1)	−0·0858 (2)	0·441 (2)	3·9 (2)
C(12a)	0·3180 (2)	−0·0835 (2)	0·266 (2)	3·5 (2)
O(13)	0·3030 (1)	−0·1282 (1)	0·199 (2)	4·3 (2)
C(13a)	0·2693 (1)	−0·1342 (2)	0·283 (2)	3·7 (1)

Cu $K\alpha$ graphite-monochromatized radiation (λ = 1·5418 Å). Intensities were processed according to Davies & Gatehouse (1973) to give values of F_o and $\sigma(F_o)$; no corrections were made for absorption.

The structure was solved by direct methods (*MULTAN*, Germain, Main & Woolfson, 1971) and refined by full-matrix least-squares methods with anisotropic temperature factors for all non-hydrogen atoms.

Coordinates of the ten H atoms were calculated on the basis of geometrical considerations and most of them were confirmed by a difference Fourier synthesis map; they were inserted in the structure factor calculations but not refined.

The final conventional unweighted R index was 0·042 for the 623 reflections with $I > 2\sigma(I)$. Scattering factors were those listed for neutral atoms by Doyle & Turner (1968), and for H those of Stewart, Davidson & Simpson (1965).

Atomic numbering, perspective views and geometric and isotropic thermal parameters are in Figs. 1 and 2, and Table 1.*

Structure of [3]benzoxepino[1,2-*b*]quinoxaline

Experimental

White needles of compound (IV) were obtained from a warm saturated *n*-heptane solution. Chemical

* Lists of structure factors and anisotropic thermal parameters for both compounds have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33240 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.
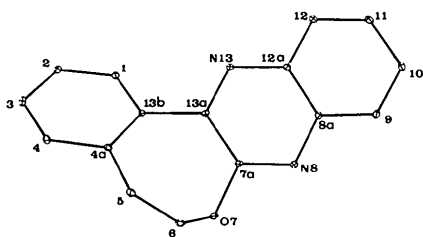
Fig. 3. *ORTEP* plot showing the atomic numbering used for compound (IV). Thermal ellipsoids are drawn at 5% probability.
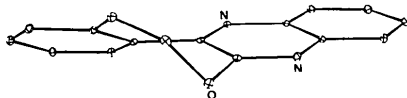

Fig. 4. *ORTEP* perspective view of compound (IV). Thermal ellipsoids are drawn at 5% probability.

Table 2. Compound (IV): final fractional coordinates, with estimated standard deviations in parentheses, and equivalent (Hamilton, 1959) thermal parameters ($Å^2$) of all non-hydrogen atoms

	x	y	z	B_{ii}
C(1)	−0·0079 (4)	0·6942 (7)	1·0194 (6)	4·0 (1)
C(2)	−0·1026 (5)	0·6705 (8)	1·0776 (6)	4·4 (1)
C(3)	−0·1782 (5)	0·8099 (8)	1·0857 (6)	5·0 (1)
C(4)	−0·1587 (4)	0·9682 (8)	1·0357 (6)	4·6 (2)
C(4a)	−0·0625 (4)	0·9969 (6)	0·9786 (5)	3·5 (1)
C(5)	−0·0502 (5)	1·1709 (7)	0·9309 (6)	4·2 (2)
C(6)	0·0444 (6)	1·2511 (7)	0·9112 (6)	4·7 (2)
O(7)	0·1478 (3)	1·1828 (4)	0·9344 (5)	4·7 (1)
C(7a)	0·1749 (4)	1·0250 (6)	0·8868 (6)	3·6 (1)
N(8)	0·2625 (3)	1·0336 (5)	0·8309 (5)	4·0 (1)
C(8a)	0·2978 (4)	0·8758 (7)	0·7904 (5)	3·5 (1)
C(9)	0·3936 (5)	0·8747 (9)	0·7315 (6)	4·9 (1)
C(10)	0·4304 (5)	0·7191 (9)	0·6888 (6)	5·2 (2)
C(11)	0·3743 (5)	0·5576 (9)	0·7090 (7)	5·1 (1)
C(12)	0·2796 (5)	0·5542 (8)	0·7659 (6)	4·3 (1)
C(12a)	0·2400 (4)	0·7152 (7)	0·8070 (5)	3·4 (1)
N(13)	0·1467 (3)	0·7122 (5)	0·8653 (5)	3·2 (1)
C(13a)	0·1130 (4)	0·8627 (6)	0·9048 (6)	3·1 (1)
C(13b)	0·0130 (3)	0·8558 (6)	0·9696 (5)	2·9 (1)

analysis gave the formula $C_{16}H_{10}N_2O$ (m.p. 129–130°C).

Intensity data collection was carried out with the same conditions as for (III) up to $\theta = 70°$. From systematic absences and from the statistical distribution of the normalized structure factors, space group $Pna2_1$ was deduced. [$a = 12\cdot201$ (3), $b = 7\cdot443$ (2), $c = 13\cdot328$ (3) Å, $Z = 4$.]

Table 3. Compound (III): bond distances (Å) for non-hydrogen atoms with standard deviations in parentheses

C(1)—C(2)	1·380 (9)	C(9)—C(10)	1·409 (10)
C(2)—C(3)	1·381 (10)	C(10)—C(11)	1·378 (9)
C(3)—C(4)	1·385 (10)	C(11)—C(11a)	1·411 (9)
C(4)—C(4a)	1·407 (9)	C(11a)—N(12)	1·366 (7)
C(4a)—C(5)	1·453 (9)	N(12)—C(12a)	1·278 (7)
C(5)—C(6)	1·317 (8)	C(12a)—O(13)	1·376 (6)
C(6)—C(6a)	1·458 (8)	O(13)—C(13a)	1·406 (6)
C(6a)—N(7)	1·309 (6)	C(4a)—C(13a)	1·391 (8)
N(7)—C(7a)	1·350 (7)	C(6a)—C(12a)	1·439 (8)
C(7a)—C(8)	1·424 (8)	C(7a)—C(11a)	1·414 (8)
C(8)—C(9)	1·357 (10)	C(1)—C(13a)	1·391 (9)

Table 4. Compound (III): bond angles (°) for non-hydrogen atoms with standard deviations in parentheses

C(1)—C(2)—C(3)	121·0 (7)	C(8)—C(7a)—C(11a)	118·7 (6)
C(2)—C(3)—C(4)	120·0 (7)	C(8)—C(9)—C(10)	120·6 (6)
C(3)—C(4)—C(4a)	121·3 (7)	C(9)—C(10)—C(11)	120·5 (7)
C(4)—C(4a)—C(13a)	116·1 (7)	C(10)—C(11)—C(11a)	119·8 (7)
C(4a)—C(5)—C(6)	127·7 (6)	C(11)—C(11a)—C(7a)	119·8 (6)
C(5)—C(6)—C(6a)	126·7 (6)	C(11)—C(11a)—N(12)	119·9 (6)
C(6)—C(6a)—C(12a)	123·2 (6)	N(12)—C(11a)—C(7a)	120·3 (6)
C(6a)—N(7)—C(7a)	117·3 (5)	C(11a)—N(12)—C(12a)	116·3 (5)
N(7)—C(6a)—C(12a)	120·0 (5)	N(12)—C(12a)—C(6a)	124·2 (6)
C(4)—C(4a)—C(5)	123·3 (7)	N(12)—C(12a)—O(13)	115·8 (5)
C(5)—C(4a)—C(13a)	123·7 (6)	O(13)—C(12a)—C(6a)	119·6 (6)
C(6)—C(6a)—N(7)	116·7 (5)	C(12a)—O(13)—C(13a)	117·3 (4)
N(7)—C(7a)—C(8)	119·6 (6)	O(13)—C(13a)—C(4a)	121·0 (6)
N(7)—C(7a)—C(11a)	121·7 (5)	O(13)—C(13a)—C(1)	115·0 (6)
C(7a)—C(8)—C(9)	120·5 (7)	C(13a)—C(1)—C(2)	117·7 (6)
		C(1)—C(13a)—C(4a)	123·8 (6)

Table 5. Compound (III): relevant torsion angles (°)

The mean standard deviation is 1·0°.

C(3)—C(4)—C(4a)—C(5)	−1	C(4)—C(4a)—C(5)—C(6)	−29
C(2)—C(1)—C(13a)—O(13)	4	C(4)—C(4a)—C(13a)—O(13)	−4
C(4a)—C(5)—C(6)—C(6a)	179	C(1)—C(13a)—C(4a)—C(5)	2
C(5)—C(6)—C(6a)—C(12a)	−150	C(1)—C(13a)—O(13)—C(12a)	61
C(6)—C(6a)—C(12a)—O(13)	−174	C(13a)—C(4a)—C(5)—C(6)	149
C(6a)—C(12a)—O(13)—C(13a)	113	C(7a)—N(7)—C(6a)—C(6)	0
C(12a)—O(13)—C(13a)—C(4a)	−115	N(7)—C(6a)—C(12a)—O(13)	7
O(13)—C(13a)—C(4a)—C(5)	178	C(11a)—N(12)—C(12a)—O(13)	−6
C(5)—C(6)—C(6a)—N(7)	28	N(12)—C(12a)—C(6a)—C(6)	1
N(12)—C(12a)—O(13)—C(13a)	−62		

The structure was solved by direct methods (*MULTAN*, Germain, Main & Woolfson, 1971); 876 reflections with $I > 2\sigma(I)$ were regarded as observed in the following calculations.

A difference Fourier synthesis led to the determination of the positional parameters for the ten H atoms in the asymmetric unit.

The refinement of the structure was performed using a full-matrix least-squares method with anisotropic temperature factors for the non-hydrogen atoms; the final unweighted R index was 0·052 for the observed reflections.

Scattering factors were those listed by Doyle & Turner (1968) and by Stewart *et al.* (1965) for H. The results are reported in Figs. 3 and 4, and Table 2.*

Discussion

Bond distances, bond angles and torsion angles for the two structures are listed in Tables 3–8.

The phenyl and quinoxaline rings are planar (Table 9). It is noteworthy that in compound (III) the dihedral angle between these two planes is 46°. Tôth & Klasine (1974) have reported a theoretical study on the likely boat conformation of similar molecules; although they

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* See previous footnote.

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pointed out the lack of crystallographic evidence, they defined a semi-empirical parameter θ, which is a function of the internal angles of the heterosubstituted ideal seven-membered ring, related to the folding of the molecule and to its electronic transition energies. From crystal structure results we estimated a θ value ≃30°, in good agreement with those suggested by Tôth & Klasine on the basis of UV spectral data.

Calculation of the exact θ value cannot be performed because of the strain of the real structure compared with the theoretical model: in fact, the directions used to define θ are not coplanar in this case.

As can be easily inferred from Figs. 2 and 4, the molecular folding is quite different for the two compounds. This is, of course, a consequence of the bond pattern: the butterfly-like conformation of compound (III) is not achievable by compound (IV), in which there is a direct link between the benzene and the quinoxaline rings. On the other hand, the greater flexibility of the C(5), C(6), O(7) chain, compared with the stiffness of the former structure, allows a twisting of the two above-mentioned planes (the dihedral angle is 30° in the present case).

Geometrical parameters for the two quinoxaline

Table 6. *Compound* (IV): *bond distances* (Å) *for non-hydrogen atoms with standard deviations in parentheses*

C(1)–C(2)	1·394 (8)	C(8a)–C(9)	1·400 (9)
C(2)–C(3)	1·388 (8)	C(8a)–C(12a)	1·402 (7)
C(3)–C(4)	1·374 (9)	C(7a)–C(13a)	1·442 (7)
C(4)–C(4a)	1·407 (9)	C(9)–C(10)	1·365 (10)
C(4a)–C(13b)	1·397 (6)	C(10)–C(11)	1·406 (9)
C(4a)–C(5)	1·450 (8)	C(11)–C(12)	1·375 (10)
C(5)–C(6)	1·318 (9)	C(12)–C(12a)	1·403 (8)
C(6)–O(7)	1·385 (8)	C(12a)–N(13)	1·370 (7)
O(7)–C(7a)	1·374 (7)	N(13)–C(13a)	1·304 (7)
C(7a)–N(8)	1·297 (8)	C(13a)–C(13b)	1·487 (8)
N(8)–C(8a)	1·361 (7)	C(13b)–C(1)	1·397 (7)

Table 7. *Compound* (IV): *bond angles* (°) *for non-hydrogen atoms with standard deviations in parentheses*

C(1)–C(2)–C(3)	119·3 (6)	N(13)–C(13a)–C(13b)	117·4 (4)
C(2)–C(3)–C(4)	119·4 (6)	C(13a)–C(13b)–C(1)	116·9 (4)
C(3)–C(4)–C(4a)	122·3 (5)	C(13b)–C(1)–C(2)	121·5 (5)
C(4)–C(4a)–C(5)	117·2 (5)	C(4a)–C(13b)–C(1)	119·2 (5)
C(4a)–C(5)–C(6)	125·5 (5)	C(4)–C(4a)–C(13b)	118·2 (5)
C(5)–C(6)–O(7)	125·1 (5)	C(13b)–C(4a)–C(5)	124·5 (5)
C(6)–O(7)–C(7a)	115·2 (5)	C(13a)–C(13b)–C(4a)	123·8 (5)
O(7)–C(7a)–N(8)	114·7 (4)	O(7) C(7a)–C(13a)	121·0 (5)
C(7a)–N(8)–C(8a)	116·2 (4)	C(7a)–C(13a)–C(13b)	123·3 (5)
N(8)–C(8a)–C(9)	119·2 (5)	C(7a)–C(13a)–N(13)	119·3 (5)
C(8a)–C(9)–C(10)	120·6 (6)	N(8)–C(7a)–C(13a)	124·2 (5)
C(9)–C(10)–C(11)	119·2 (6)	N(8)–C(8a)–C(12a)	121·0 (5)
C(10)–C(11)–C(12)	121·5 (6)	C(8a)–C(12a)–N(13)	121·0 (5)
C(11)–C(12)–C(12a)	119·0 (5)	C(8a)–C(12a)–C(12)	119·7 (5)
C(12)–C(12a)–N(13)	119·3 (5)	C(9)–C(8a)–C(12a)	119·8 (5)
C(12a)–N(13)–C(13a)	118·2 (4)		

Table 8. *Compound* (IV): *relevant torsion angles* (°) *with standard deviations in parentheses*

C(2)–C(1)–C(13b)–C(13a)	−3·5 (5)	O(7)–C(7a)–N(8)–C(8a)	−6·1 (5)
C(3)–C(4)–C(4a)–C(5)	1·1 (6)	C(13a)–C(7a)–O(7)–C(6)	−116·4 (9)
C(4)–C(4a)–C(5)–C(6)	−29·5 (8)	O(7)–C(7a)–C(13a)–C(13b)	−176·0 (7)
C(13b)–C(4a)–C(5)–C(6)	148·8 (9)	O(7)–C(7a)–C(13a)–N(13)	5·9 (7)
C(5)–C(4a)–C(13b)–C(1)	0·0 (7)	N(8)–C(7a)–C(13a)–C(13b)	−0·3 (6)
C(4)–C(4a)–C(13b)–C(13a)	5·3 (6)	N(13)–C(13a)–C(13b)–C(1)	−152·0 (6)
C(5)–C(4a)–C(13b)–C(13a)	−176·4 (9)	N(13)–C(13a)–C(13b)–C(4a)	31·4 (7)
C(4a)–C(5)–C(6)–O(7)	178·9 (10)	C(7a)–C(13a)–C(13b)–C(4a)	−146·7 (8)
C(5)–C(6)–O(7)–C(7a)	−116·6 (8)	C(7a)–C(13a)–C(13b)–C(1)	29·9 (5)
C(6)–O(7)–C(7a)–N(8)	−59·8 (6)		

Table 9. *Least-squares planes and interplanar angles*

The general equation is $lx + my + nz + d = 0$; $D = (l^2 + m^2 + n^2)^{1/2}$, $\cos \alpha = -l/D$, $\cos \beta = -m/D$, $\cos \gamma = -n/D$.

Compound (III)
Plane 1: C(1), C(2), C(3), C(4), C(4a), C(13a) [mean deviation = 0·004 (4) Å]

l	m	n	d	$\cos \alpha$	$\cos \beta$	$\cos \gamma$
−2·9581	−17·1063	−3·4314	−0·5432	−0·0741	−0·6368	−0·7675

Plane 2: C(6a), N(7), C(7a), C(8), C(9), C(10), C(11), C(11a), N(12), C(12a) [mean deviation = 0·012 (3) Å]

l	m	n	d	$\cos \alpha$	$\cos \beta$	$\cos \gamma$
23·6563	−5·9264	−3·4642	−7·0890	0·5924	−0·2206	−0·7748

Interplanar angle: 46°.

Compound (IV)
Plane 1: C(1), C(2), C(3), C(4), C(4a), C(13b) [mean deviation = 0·007 (3) Å]

l	m	n	d	$\cos \alpha$	$\cos \beta$	$\cos \gamma$
5·8600	2·5504	10·7298	12·6661	0·4842	0·3426	0·8051

Plane 2: C(7a), N(8), C(8a), C(9), C(10), C(11), C(12), C(12a), N(13), C(13a) [mean deviation = 0·011 (2) Å]

l	m	n	d	$\cos \alpha$	$\cos \beta$	$\cos \gamma$
6·7479	−1·2576	10·8322	−9·4766	0·5576	−0·1690	0·8127

Interplanar angle: 30°.

rings are in the range usually accepted (Visser & Vos, 1971). In this case a deformation pattern due to a strained substitution is also observed: C(6a)—C(12a) [compound (III)] and C(7a)—C(13a) [compound (IV)] are lengthened [1·44 (1) Å] and quinoxaline internal angles next to the oxepine ring are widened (about 124° for both molecules).

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