The Photoisomerization of 2-Phenyl-3*H*-indol-3-one *N*-Oxide (2-Phenylisatogen) to 2-Phenyl-4*H*-3,1-benzoxazin-4-one

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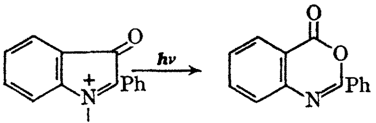
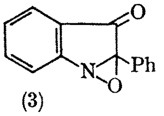
Summary 2-Phenyl-3*H*-indol-3-one *N*-oxide is easily photoisomerized to 2-phenyl-4*H*-3,1-benzoxazin-4-one.

It has been shown[1] that 2-substituted quinoline *N*-oxides undergo light-induced rearrangements to 2-substituted 3,1-benzoxazepines. No structurally related five-membered heterocycle has yet been shown to undergo an analogous photolytic rearrangement.[2] We describe the photoisomerization of 2-phenyl-3*H*-indol-3-one *N*-oxide,[3] (1), to 2-phenyl-4*H*-3,1-benzoxazin-4-one,[4] (2).



(1) (2)



(3)

We examined the light-induced reaction(s) of (1) in several frequency ranges.† Irradiation of (1) (1 g.) in various solvents (800 ml.) with a Hanovia 450 w high-pressure immersion lamp (no filter) for 1—2 hr. gave (2) in the following yields:‡ in ethanol, 53%; in benzene, 60%; in cyclohexane, 85%; and in cyclohexane, 93%. Recovery of unchanged (1) in every case accounted for virtually all of the starting material. A tentative sequence leading to (2) is by way of the oxaziridine, (3), a transformation characteristic of nitrones.[7]

The reaction proceeds in better yield with nonpolar solvents which suggests that a polar mechanism is not operative. A diradical mechanism probably occurs and its existence is being investigated by sensitization and quenching studies.

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† Irradiation of (1) has been studied with Rayonet 2537 and 3500 Å lamps and with a total-immersion lamp.

‡ Yields are considerably less with a Pyrex filter or with Rayonet 3500 Å lamps. Yields are approximately identical with or without O_2 degassing.

[1] O. Buchardt, B. Jensen, and I. K. Larsen, *Acta Chem. Scand.*, 1967, **21**, 1841; C. Kaneko, S. Yamada, I. Yokoe, and M. Ishikawa, *Tetrahedron Letters*, 1967, 1873.

[2] (1) can be converted into (2) by acid hydrolysis; see R. J. Richman and A. Hassner, *J. Org. Chem.*, 1968, **33**, 2548. M. Hooper and D. G. Wibberley, *J. Chem. Soc.* (*C*), 1966, 1596, report conversions of 2-substituted 3*H*-indol-3-one *N*-oxides into 2-substituted benzoxazinones by alkaline hydrolysis.

[3] D. A. Jones, Ph.D. Dissertation, University of Minnesota, 1961.

[4] Compound (2) was synthesized independently according to the procedure described by M. T. Bogert, R. A. Gortner, and C. G. Amend, *J. Amer. Chem. Soc.*, 1911, **33**, 949; m.p., mixed m.p., and i.r. and u.v. spectra are identical.

[5] (a) M. J. Kamlet and L. A. Kaplan, *J. Org. Chem.*, 1957, **22**, 576; (*b*) J. S. Splitter and M. Calvin, *ibid.*, 1958, **23**, 651; 1965, **30**, 3427; (c) R. Bonnett, V. M. Clark, and A. R. Todd, *J. Chem. Soc.*, 1959, 2102; (d) E. C. Taylor and G. G. Spence, *Chem. Comm.*, 1966, 767; 1968, 1037; (e) L. S. Kaminsky and M. Lamchen, *J. Chem. Soc.* (*C*), 1966, 2295.