The Reactivity of Isobenzofuran

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Summary The reactivity of isobenzofuran with singlet oxygen was found to be between that of furan and 1,3-diphenylisobenzofuran as predicted from their ionization potentials.

THE synthesis of isobenzofuran (**1**) by a variety of methods has recently been reported.[1] It was shown that (**1**) undergoes polymerization at and below room temperature. Wiersum[1c] also reported that (**1**) reacts with typical dienophiles, such as maleic anhydride, *N*-phenylmaleimide, and methyl vinyl ketone.

We now report on the rate of reaction of isobenzofuran (**1**) with singlet oxygen, produced under dye-sensitized (methylene blue) conditions in methanol, and compare the results with the other singlet oxygen reactions of furans. This is the first quantitative experimental result on the relative reactivity of (**1**) in a chemical reaction.

Isobenzofuran was prepared according to the method outlined by Warrener,[1a] and its u.v. absorption, fluorescence emission, and n.m.r. spectra were shown to be identical to those reported.[1] The ratio of the rate constant of decay (k_d) of singlet oxygen (methanol) to the rate constant for the reaction (k_{rx}) of (**1**) with singlet oxygen (β value, k_d/k_{rx}) was determined by a previously published method.[2] The β value for the reaction of (**1**) with singlet oxygen is given in the Table, together with the β values for other furans.[2] The rate constant of reaction of these compounds with singlet oxygen were calculated using the equation:

$$k_{rx} = k_d/\beta$$

where $k_d = 9{\cdot}0\ (\pm 0{\cdot}6) \times 10^4\ s^{-1}$.[3]

Rate constants for the photo-oxidation of furans in methano

Compound	β(M) $\times 10^3$	k_{rx} (s^{-1} M^{-1})	I.P.
Furan	2·62[a]	$3{\cdot}43 \times 10^7$	8·89[c]
Isobenzofuran (**1**) ..	0·983	$9{\cdot}15 \times 10^7$	7·91[d]
2,5-Diphenylfuran ..	0·953[a]	$9{\cdot}45 \times 10^7$	—
1,3-Diphenylisobenzofuran (**2**)	0·073[b]	$1{\cdot}23 \times 10^9$	7·09[d]

[a] From ref. 2; [b] from ref. 5; [c] from ref. 6; [d] from ref. 7.

It has recently been shown that the rate constants of photo-oxidation reactions can be related to the ionization

potential of the acceptor.[4] On this basis, it is not surprising that the rate constant for the reaction of (**1**) with singlet oxygen is intermediate between that for furan and 1,3-diphenylisobenzofuran (**2**) (see Table).

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