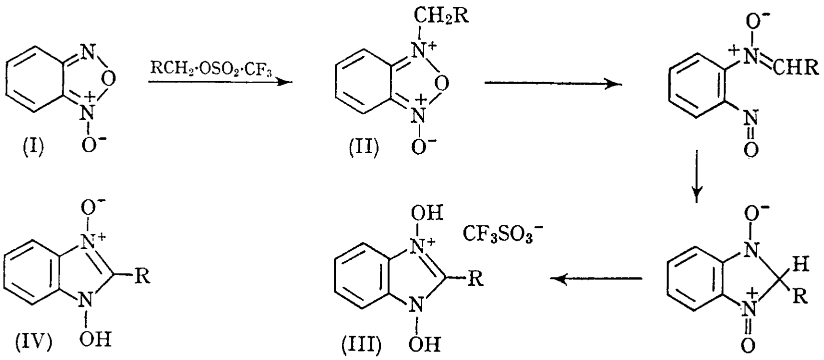
Alkylations of Benzofuroxan with Concurrent Rearrangements to 1-Hydroxybenzimidazole 3-Oxides

By A. J. BOULTON, A. C. GRIPPER GRAY, and A. R. KATRITZKY
(*The School of Chemical Sciences, University of East Anglia, Norwich*)

WE report novel rearrangements which occur subsequent to alkylation of benzofuroxan. Although inert to most alkylating agents, including trialkyloxonium salts, benzofuroxan (I) reacts with methyl and benzyl trifluoromethanesulphonate (the latter prepared *in situ*) to yield products of the analytical composition of one molecule of benzofuroxan and one molecule of alkylating agent. Spectral properties, and in particular, the n.m.r. spectra of the products, indicated the formation of 1-hydroxybenzimidazole 3-oxide salts of type (III), rather than simple quaternary salts. We consider the rearrangement to have taken place by the route indicated (I → II → III). The salts were readily converted into the free 1-hydroxybenzimidazole 3-oxides (IV). The structures of the



products were proved by the identity of the 2-phenyl derivative (IV; R = Ph) with an authentic specimen prepared by Quilico's method,[1] and by the ultraviolet-spectral comparison of (IV; R = H) with the methyl derivative (IV; R = Me), prepared from *o*-benzoquinone dioxime and acetaldehyde, a new preparative route modelled on the synthesis of monocyclic 1-hydroxybenzimidazole 3-oxides by La Parola.[2]

(*Received, September 8th*, **1966**; *Com.* 673.)

---

[1] F. Minisci, R. Galli, and A. Quilico, *Tetrahedron Letters*, **1963**, 785.

[2] G. La Parola, *Gazzetta*, **1945**, **75**, 216; *cf.*, L. B. Volodarsky, A. N. Lisak, and V. A. Koptyug, *Tetrahedron Letters*, **1965**, 1565.