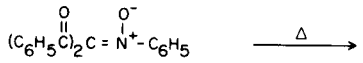
Thermal Isomerization of *N*-Phenyldibenzoylnitrone

Harold O. Larson, Karen Y. W. Ing, and Danny L. Adams

Department of Chemistry, University of Hawaii

Sir:

Although the photolysis of nitrones to oxaziridines is a well known reaction (1), the thermal conversion of nitrones to oxaziridines apparently has not been observed (2-5). We wish to report the isomerization of the nitrone **1** to the oxaziridine **2** at the reflux temperature of a *p*-xylene solution for eight hours. *N*-Phenyldibenzoyloxaziridine was obtained in a yield of 70%; m.p. 130-131° (lit., 131° (6)); *Anal.* Calcd. for $C_{21}H_{15}NO_3$: C, 76.58; H, 4.59; N, 4.25. Found: C, 76.67; H, 4.59; N, 4.40. A mixture melting point determination involving oxaziridine prepared by photolysis (7) showed no depression in melting point. The infrared spectra of the oxaziridine prepared by photolytic and thermal reactions were identical. The lowest temperature limit for the thermal isomerization was not established, and the isomerization does occur at 230° (10 minutes) in light paraffin oil under nitrogen.



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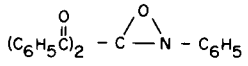

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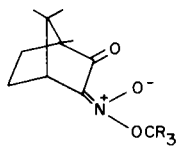
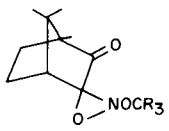


3 R = Ph



4 R = Ph

Nitrones are known to rearrange to amides with a variety of reagents (8), and several mechanisms have been proposed including the route of thermal isomerization to an oxaziridine, which then may rearrange to an amide (9). The isolation of **2** is due to its remarkable thermal stability (7) and constitutes evidence for the mechanism by which nitrones rearrange.

Our conversion (10) of the stable nitronic ester **3** to the heterocycle **4** elicited some doubts inasmuch as the synthesis of an oxaziridine by a thermal process was not known at that time. The isomerization, **1** → **2**, provides a crucial example for the synthesis of the oxaziridine ring system by a thermal process. The method is limited, of course, to thermally stable oxaziridines.

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(8) These rearrangements are summarized in reference 3, pp. 345-346, and reference 5, pp. 36-49.

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Received July 16, 1970 Honolulu, Hawaii 96822