THERMOCATALYTIC CONVERSION OF METHYL 3-PHENYL-2H-AZIRINE-2-CARBOXYLATE

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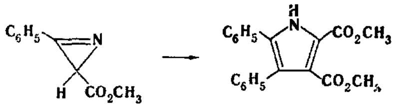
It is known that 3-phenyl-2H-azirines are converted at 200-250 deg C to pyrrole derivatives [1, 2]. Similar transformations have been described for the catalytic process that occurs in the presence of iron carbonyls [3]. For the first time we have accomplished the thermocatalytic conversion of a functionally substituted 2H-azirine – methyl 3-phenyl-2H-azirine-2-carboxylate (I) – to dimethyl 4,5-diphenylpyrrole-2,3-dicarboxylate (II) at 80 deg C in the presence of cuprous stearate.



I II

A mixture consisting of a solution of 0.5 g (0.03 mole) of azirine I [4] in 25 ml of cyclohexane and 0.25 g (0.007 mole) of cuprous stearate was heated in an argon atmosphere for 2 h, after which the solvent was removed, and the residue was recrystallized from methanol to give 0.4 g (83%) of pyrrole II with mp 192 deg C [5]. The spectral characteristics of the pyrrole were in agreement with the assigned structure. PMR spectrum (in $CHCl_3$), δ: 3.57 and 3.45 ppm (s, OCH_3). IR spectrum (in $CHCl_3$): 3438 (NH); 1720 and 1696 cm^{-1} ($C=O$). UV spectrum (in ethanol), λ_{max} ($\log \varepsilon$): 239 (4.08) and 279 nm (4.10). Mass spectrum (m/e): 335, 303, 272, 244, 216, 189, and 141. Found: C 71.4; H 5.1; N 4.0%. $C_{20}H_{17}NO_4$. Calculated: C 71.3; H 5.1; N 4.2%.

In contrast to the formation of pyrroles as a result of intramolecular cyclization of vinyl-substituted azirines [2], the formation of pyrrole II in the investigated reaction proceeds with the participation of two molecules of the azirine. The azirine ring evidently undergoes heterolytic cleavage in this case [1].

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