Comparison of kinetic and thermodynamic parameters of reaction of individual conformers of α-substituted β-ethoxyvinyl trifluoromethyl ketones with secondary amines

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2024

Czasopismo

Reaction Kinetics, Mechanisms and Catalysis

Numer woluminu

137

Strony

719-736

DOI

10.1007/s11144-024-02578-1

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The kinetic and thermodynamic parameters of the reaction of three most possible
conformers (viz. E-s-E-s-E-trans, E-s-Z-s-E-trans, and E-s-Z-s-E-gosh) of
α-substituted β-ethoxyvinyl trifluoromethyl ketones C2H5O–CH=CR-COCF3 (I–III)(I: R = H; II: R = F; III: R2= CH3)
with two secondary amines, namely diethyl amine(2a) and bis-(methoxyethyl) amine (2b), was studied in carbon tetrachloride as solvent.The details of appropriate enaminoketone formation are discussed in terms ofan addition–elimination substitution. It is shown the limiting step of the reaction of all conformers presented in significant quantities, to be the formation of zwitterion intermediate. At high amine concentrations the third-order rate coefficient appears in reaction rate equation as a consequence of catalyzed route of the intermediate decomposition. The reaction of all three conformers has low ΔH≠ and high negative ΔS≠ values owing to highly polar zwitterion formation as the intermediate.

Słowa kluczowe

Nucleophilic (Adn-E) substitution, Ethoxyvinyl trifluoromethyl ketones, Conformers, Secondary amines

Adres publiczny

http://dx.doi.org/10.1007/s11144-024-02578-1

Strona internetowa wydawcy

http://link.springer.com