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Influence of the features of the spatial and electronic structure of *α*-substituted *β*-ethoxyvinyl trifluoromethyl ketones and secondary amines on their reactivity.

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Streszczenie

Spatial and electronic structure of possible isomers/conformers of three α-substituted β-ethoxyvinyl trifluoromethyl ketones with general formula $F_3CCO–CR=CH–OC_2H_5$, where R = H (**I**), R=F (**II**), and R = CH_3, (**III**), their ability to form H-bonds with two secondary amines, namely, diethyl amine (**1**) and *bis*(methoxyethyl)amine (**2**) have been studied. It was shown that all studied α-substituted enones are *E*-isomers forming predominantly three conformers, *viz E-s-E-s-E*-trans, *E-s-Z-s-E*-trans, and *E-s-Z-s-E*-gosh, percentage of separate conformer depending not only on environment but also on steric and/or special (repulsion) interaction between α-substituent and trifluorocarbonyl group. Hydrogen bonding ability evaluated in thermodynamic scale of hydrogen bond basicity revealed that pK_{HB} values of each conformer strongly depends on steric and/or effective charge change on carbonyl oxygen due to influence of α-substituent. Formation of H-bonded ternary complex between enone conformer and secondary amine changes electron density distribution in conformer conjugated chain, reducing positive charge on C_β and thus changing conformer electrophilicity. On the other hand cooperativity effect in amine dimer increases net charge on amine nitrogen thus enhancing amine nucleophilicity.

Słowa kluczowe

Conformers, α-substituted β-ethoxyvinyl trifluoromethyl ketones, Secondary amines, Hydrogen bond, Cooperativity effect, Electrophilicity, Nucleophilicity

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