

Thematic course: Theoretical study of aromatic nitroso oxide isomerization. Part II.

The correlation analysis of the experimental reaction rate constants of arylnitroso oxides and global reactivity indices

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Abstract

The correlation dependencies of global reactivity indices and experimental decay constants of *cis* and *trans* isomers of *para*-substituted phenylnitroso oxides have been studied. The contribution of the resonance forms to general electronic structure of arylnitroso oxides and its effect on the decay processes of isomeric arylnitroso oxides was analyzed using characteristic atomic charges of NOO group. The effect of solvation on the phenylnitroso oxide resonance forms has been investigated.