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Reactivity indexes of alkenes aminomethylation

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Abstract

Aminomethylation of alkenes is one of the simple and convenient method for obtaining various types of amines. The reaction proceeds under mild conditions and allows to introduce in one step $-CH_2-NH_2$ fragment, which suitable for subsequent transformations. Despite the similarity of the mechanisms of the reactions of Mannich and Prinse, the possibility of involving alkenes in the aminomethylation reaction is still insufficiently studied. So far, the range of alkenes involved in this reaction is very limited, and the prospects for its expansion have not been theoretically worked out. We believe that an important tool in assessing the reactivity of alkenes and, consequently, determining their activity in the reaction of aminomethylation are indexes of reactivity. Therefore, the search for correct reactivity indexes of alkenes in the aminomethylation reaction is an actual problem.

Consideration of the generally accepted indexes of reactivity such as partial charge on the atom, the occupancy of the orbitals, the bond orders makes it impossible to form an adequate model describing the reactivity of alkenes in the aminomethylation reaction.

It was shown that only NBO analysis of the electronic structure of alkenes the results of the calculations in the approximation B3LYP/6-31G(d,p) and MP2/6-31G(d,p) can be obtained in the correct model of the activity of alkenes. Correct indexes of reactivity, correctly taking into account the features of the reaction mechanism and the structure of alkenes with double bonds, are obtained by consideration of the uneven distribution of the electron density of π-bond of the double bond alkenes. The proposed indexes are in good agreement with the literature data on reactivity of alkenes in the aminomethylation reaction and can be used to predict their reactivity.

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