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Selectivity of electrophilic substitution reaction in alkylbenzenes

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Abstracs

The electrophilic substitution reactions (nitration and bromination) in benzene and its some mono- and dialkylsubstituted derivatives with alkyl groups C1-C4 are explored. New reagents (*N*-bromosuccinimide, urea nitrate) in ambience acetic and trifluoracetic acids are used, as well as ion liquid BMIMBr and $BMIMBr_3$. Substrat and positional selectivities of that reactions and conditions of the syntheses some isomers, being of interest for pharmaceutical chemistry, are determined. Theoretical analysis of nitration reactions selectivity with use the theories to functions Fukui are carry out. Linear correlations of selectivity that reaction and this parameter are found. It is shown fruitfulnes of theoretical description of aromatic substitution reactions on the base of dynamic quantum chemical reactionary abilities indexes.