ELECTRONIC EFFECTS OF CONJUGATED ENONES ON THEIR REACTIVITY IN TRANSFORMATIONS OF ADD_N TYPE

É. R. Latypova,[1] R. Ya. Kharisov,[2] I. V. Vakulin,[1] R. F. Talipov,[1] and G. Yu. Ishmuratov[2]

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Using RHF/3-21G, RHF/6-31G(*d*, *p*), MP2/6-31G(*d*, *p*), B3LYP/6-31G(*fd*, *p*) approximations the structure and ^{13}C NMR spectra of 2-alkylsubstituted cyclohexene-2-ones and 2-alkylacroleins are studied and calculated. In the series of 2-alkylcyclohexene-2-ones the effect of the substituent on a deviation from coplanarity of the C=C–C=O fragment is more expressed in comparison with 2-alkylacroleins. This deviation (5°) is not enough to explain the observed properties of 2-alkylcyclohexene-2-ones due to disturbed conjugation. The particular behavior of (R)-4-mentenone in reactions of 1,4-addition and ozonolysis is explained by a more expressed +*I*-effect of the alkyl substituent in α-position.

Keywords: (R)-4-mentenone, 2-alkylsubstituted cyclohexene-2-ones and alkylacroleins, conformation analysis, *ab initio* calculations.