Ab initio Vibrational Analysis of Cyclopropene and Its 1-Methyl and 1,2-Dimethyl Derivatives

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Abstract - Analysis of experimental vibrational spectra of cyclopropene and its 1-methyl and 1,2-dimethyl derivatives is performed in HF/6-31G approximation using the scaling technique. Scale factors for the cyclopropene force field are determined using only the experimental frequencies of the light (h_4) isotopomer. The scaled quantum mechanical force field is used to predict the vibrational spectra of all the deuterated isotopomers of cyclopropene. Some reassignments of the experimental bands are suggested. The set of scale factors was supplemented by five scale factors (starting value = 0.8) for the coordinates responsible for the vibrations of the methyl moiety in 1-methylcyclopropene. Solution of the vibrational problem with this empirically corrected force field allowed us to reassign some of the experimental bands of 1-methylcyclopropene. These five scale factors were optimized using the experimental frequencies of 1-methylcyclopropene. The final set of scale factors was used for empirical correction of the quantum mechanical force field of 1,2-dimethylcyclopropene. The vibrational analysis of the latter compound was carried out for the first time. Some tendencies regularities in the vibrational spectra of this molecular series are revealed and discussed.