QUANTUM CHEMICAL ANALYSIS OF THE STRUCTURE AND SPECTROSCOPIC PROPERTIES OF ARYL VINYL ETHERS

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A series of aromatic vinyl ethers and some compounds close to them in structure are studied by DFT (B3LYP/6-311+G(2*d*,*p*)) and MP2(full)/6-311+G(2*d*,*p*) methods. Measurements of Raman spectra are also used. The calculation of vibrational spectra of aryl vinyl ether (AVE) isomers shows that stretching vibrations ν(C=C) are most conformation sensitive. The calculated value of *I*(C=C) for vinyl phenyl ether more than twice exceeds the corresponding value for vinyl methyl ether. The calculated and experimental values of *I*(C=C) are consistent with the hypothesis about the presence of a common conjugated π-system in the molecules of substituted AVEs. Here the bridging oxygen atom provides the π,*p*,π-interaction.

Keywords: DFT calculations, IR spectroscopy, Raman spectroscopy, aryl vinyl ethers, double bond vibration.