VIBRATIONAL OVERTONE SPECTROSCOPY OF CYCLOHEXADIENE IRON TRICARBONYL AND 1,3-CYCLOHEXADIENE

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Vibrational overone spectra of cyclohexadiene iron tricarbonyl and 1,3-cyclohexadiene for both gas and liquid phases have been recorded and compared for the first, second, third and fourth overtone regions. The cyclohexadiene iron tricarbonyl spectrum exhibits significant changes compared to the spectrum of unbound ligand indicating that complexation with iron tricarbonyl strongly affects the structure and properties of 1,3-cyclohexadiene. The assignments have been made for the uncomplexed ligand based on the Harmonically Coupled Anharmonic Oscillators (HCAO) model. Preliminary assignments have been suggested for the complex. The proposed assignments are suported by the results of ab initio Hartree-Fock calculations.