IR SPECTRUM AND INTERMOLECULAR INTERACTIONS IN THE CO2 - HF AND CO2 - HCl COMPLEXES

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Frequencies, widths and absolute intensities of the bands of simultaneous vibrational transitions were calculated and measured in spectra of absorption for gaseous and liquid mixtures of carbon dioxide with hydrogen chloride and hydrogen fluoride. Side by side with the simulation calculations of the intensities of investigated spectra, for the first time non-empirical quantum chemical calculations were used. There was demonstrated a necessity of an additional taking into account the contribution of the absorption of complexes with weak hydrogen bond in a system CO2... HCl in order to explain a significant intensity of the bands of simultaneous transitions ((HCl) + (1(CO2) and ((HCl) + 2(2(CO2). There was demonstrated, using as an example CO2...HCl system, an insignificant role of multiparticle interactions in the formation of the intensity of bands of simultaneous transitions in IR absorption spectra of condensed phase.