Contribution ID: **80** Type: **Poster**

Intermolecular interaction of (CH3)2CO•••HCl complex: IR spectra, DFT method, QTAIM, NCI, RDG, ELF, LOL, FMO analyses.

Friday, November 8, 2024 4:09 PM (3 minutes)

Infrared absorption spectra of free molecules (CH3)2CO/HCl and (CH3)2CO•••HCl complex are recorded in the 4000-400 cm−1 region with a Bruker IFS-125 Fourier spectrometer in gas state and with Kr, Xe solutions at different temperatures. In the free acetone and its complex with HCl, the spectral characteristics of the fundamental ranges Q(C=O),
, Q-(C-C), and νHCl are measured. Particular attention is paid to determining the effect of H-Cl and C=O on the bond length, frequency, and intensity in the (CH3)2CO•••HCl complex. In the calculations, intermolecular interactions, anharmonic potential energy, and dipole moment surfaces are analysed using the DFT method based on the B3LYP/6-311++G(d,p) basis set. Topological (QTAIM, NCI, RDG, ELF, and LOL) studies are used to examine interactions (hydrogen bond and Van der Waals interactions) at the crucial locations of connections. Information on the HUMO-LUMO gap and other electronic characteristics is given. A good agreement is observed between experimental and theoretical results.

Type of presence

Presence online

Primary author: Ms NURMURODOVA, Gulshan (Samarkand State University)

Co-authors: Mr KHUJAMOV, Utkir (Samarkand State University); Dr MURODOV, Gulamkhon (Samarkand State University)

Presenter: Ms NURMURODOVA, Gulshan (Samarkand State University)

Session Classification: Poster Session