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Isotope effects on the IR spectrum of the CX3Y•••HCl complex in liquefied argon: DFT calculations, topological analyses, and electronic properties

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Infrared spectra (4000-400 cm-1) of free molecules CX3Y (X=H, D, Y=F, Cl, Br), HCl, and CX3Y•••HCl mixtures in liquefied argon (90, 100-120 K) are recorded. The intermolecular interactions of the CX3Y•••HCl complexes are studied using the DFT method based on the B3LYP/6–311++G(d,p) basis set. The effect of deuterium (D), an isotope of the hydrogen atom (H), on the vibrational spectra of hydrogen-bonded complexes is discussed. Harmonic and anharmonic vibration frequencies are determined in calculations. The intermolecular interactions in these complexes are studied for the first time using topological (AIM, NCI, RDG, ELF, and LOL) analyses. NBO analysis and Mulliken atomic charge distribution are used to study the charge transfer mechanism in intermolecular interactions. The HUMO-LUMO gap and MEP are used to determine the electronic properties. The good agreement shows between the experimental and theoretical results

Type of presence

Presence online

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