Cooperative effects in blue-shifted hydrogen bonded cluster of $CF_3H\cdots(HF)_{1\leq\eta\leq3}$ sub>from first principles simulations.

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Streszczenie

Ab initio molecular dynamics technique has been used to estimate the structural, electronic and vibrational properties of the blue-shifted hydrogen bonded $CF_3H\cdots(HF)_{1\leq\eta\leq3}$ complexes. Different reaction pathways and aggregation products have been studied as a function of temperature. The self-aggregation of HF molecules and the formation $CF_3H\cdots(HF)_{1\leq\eta\leq3}$ of and cyclic structures have been found at the temperature of 50 K. The estimated energetic cooperative effects stabilize these structures even at higher temperature which is not the case in the $CF_3H\cdots(HF)_{1\leq\eta\leq3}$ complex. The structural cooperative effects manifest in the $(HF)_{2-3}$ chain formation which size determines the binding energy. The anharmonic spectra obtained from molecular dynamics simulations show the pronounced vibrational cooperative effects and might support future low temperature experiments utilizing molecular beam, supersonic jet or ultracold Helium droplet technique.

Słowa kluczowe

Conventional and improper hydrogen bonds, Cooperative effects, Density functional calculations, Molecular dynamics

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