Intermolecular Potential Energy Surfaces for HCN-H_2 van der Waals Complex and Their Applications in the Research of HCN-(pH$_2$)$_N$ Clusters

(Jilin Univ.[a]) Yu Zhai[a], Hui Li[a]
Email:prof_huili@jlu.edu.cn

Morse/Long-Range potential energy model is a spectroscopically accurate model which has been expended to Multi-Dimension Morse/Long-Range (MD-MLR) model to describe the intermolecular interaction. In this work, we adopt the MD-MLR model to fit *ab initio* pointwise energies got from vibrationally averaging over the intramolecular vibrational coordinate, which corresponding to the ground-state HCN-H_2 and excited-state HCN-H_2 interactions, respectively. Furthermore, reduce-dimension PESs, which describe the effective interaction between HCN at different state and *para*-hydrogen (pH$_2$), are got from adiabatic 'hindered-rotor' average. The obtained 2D PESs are used in Path Integral Monte Carlo (PIMC) quantum simulation of HCN-(pH$_2$)$_N$. The band origin shifts of HCN in the quantum clusters are calculated based on these PESs. The predicted Infrared spectra of HCN-H_2 and the simulation results for HCN-(pH$_2$)$_N$ agree well with the experiments.