Local Mode-Based Infrared Probe Spectra: a Case Study of Formic Acid-Water Clusters and Solutions

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A new method based on perturbation theory and statistical method is developed to simulate the IR spectra of clusters and solutions. This approach could be used to quickly predict more accurate spectra corresponding to formic acid C=O stretching in water clusters and condensed states than traditional methods. Vibrational localization method[1] can be used to select the most related modes to the C=O stretching, which is helpful to find a more effective vibrational space in following calculations. *Ab initio* molecular dynamics simulation is used to sample intermolecular configurations of clusters, and quantum treatment based on the perturbation approximation is made following that. Fourier transformation is performed to get the spectrum with not only peak positions but also line shapes. Hence, the method could get an experiment-comparable time-dependent transition frequencies of the system. This method was firstly successfully applied in the study of HCl-water clusters[2]. In this work, we will extend this approach and applied it in studying the IR `proble` spectra of formic acid-water clusters and solutions.

[1] Christoph R. Jacob, Sandra Luber and Markus Reiher *J. Phys. Chem. B*, 113(18) 6558-6573 (2009)

[2] Rui-Jie Xue, Adam Grofe, He Yin, Zexing Qu, Jiali Gao,and Hui Li. *J. Chem. Theory. Comput.* 13, 191-201 (2017)