

Abstract Submitted
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Dynamics of N-methylacetamide in methanol via ab initio molecular dynamics VIVEK K. YADAV, MICHAEL L. KLEIN, ICMS, Temple University, Philadelphia — There has been much interest in the two-dimensional infrared (2D IR) amide I vibrational bands of proteins as well as molecules such as N-methylacetamide (NMA), which present peptide-like H-bonding possibilities to a solvent. To assist in rationalizing a large body of experimental 2D IR data on NMA in both aqueous and non-aqueous solvents, we have performed an ab initio molecular dynamics simulation of NMA in methanol. The trajectory was generated using ab initio molecular dynamics. The AIMD simulation is performed at a $\sim 30\text{K}$ elevated temperature in order to roughly account for the structural softening of hydrogen bonds that arise from nuclear quantum effects. The calculated average hydrogen bond lifetime for the amide mode I frequency is ~ 1.9 ps which are in good agreement with the classical theoretical and experimental results. Our calculated bulk methanol-methanol hydrogen bond lifetime also matched with the experimental findings. We theoretically performed 2D IR where the change in spectral shape with respect to time is directly influenced by the decay of the frequency-frequency correlations, which represents a desired experimental property.

Vivek K. Yadav
Temple Univ

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