

Chapter

Structure and Dynamics of Electronic Excited States

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Solvation of Radicals in Small Clusters

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Abstract

The spectra and solvation behavior of several radical systems, cooled in a supersonic jet expansion, are studied using laser induced fluorescence and time-of-flight mass spectroscopic techniques. The systems included in this study are small radicals, CH_3O and NCO , and larger aromatic radicals, picolyl, lutidyl, cyclopentadienyl, and its derivatives. Intensive *ab initio* and Leonard-Jones potential energy surface calculations are performed to understand the spectra, the geometries, and the van der Waals interactions of these radicals and their clusters. Inter- and intra-molecular dynamics of excited state species, possible chemical reactions, as well as substituent effects on cluster chemistry are discussed.

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