



Molecular Spectroscopy and Dynamics of Reactive Chemical Intermediates

By Lloyd Muzangwa

SPS Aug 2015, 2015. Taschenbuch. Book Condition: Neu. 220x150x13 mm. This item is printed on demand - Print on Demand Neuware - Laser Induced Fluorescence (LIF), Single Vibronic Level (SVL) emission and Resonance Enhanced Multiple Photon Ionization (REMPI) spectroscopy has been used to probe the electronic states of NiI, NiBr, NiCl, CCN and chlorobenzene clusters (ClBz)_n where n = 1-4. In this work, term energies and a complete set of vibrational parameters were derived for all the electronic states accessible for NiI, NiBr, NiCl and CCN. These vibrational parameters were compared to the recent high level ab initio calculations. REMPI spectra of chlorobenzene clusters formed in a He/Ar supersonic jet were obtained. Different types of non-covalent interactions (-stacking, CH/ interactions, and halogen bonding) were found to be in operation in the ClBz clusters. To rationalize the experimental results, the clusters were characterized computationally using Density Functional Theory (DFT) and Time-Dependent DFT methods in combination with correlation consistent basis sets. 224 pp. Englisch.



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