PFI-ZEKE PHOTOELECTRON SPECTROSCOPY OF ALKALI METAL-ETHER COMPLEXES

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This talk will present the PFI-ZEKE photoelectron spectra of two alkali metal-ether complexes: Li(DME) and Li(DXE); DME = CH_3OCH_3, DXE = $CH_3O(CH_2)_2OCH_3$. Both complexes were produced in a pulsed molecular beam and identified by time-of-flight mass spectrometry. The ZEKE spectra of these complexes show adiabatic ionization potentials and vibrational structures consisting of metal-ligand and ligand-based vibrations. The spectroscopic measurements were combined with density functional theory and Franck-Condon factor calculations to establish ground electronic states and geometries of the neutral and ionic species. For Li(DME), the neutral and ionic complexes were determined to be in C_{2v} symmetry with Li binding to oxygen. For Li(DXE), the Li atom binds to both oxygen atoms in a C_2 five-membered ring structure, with the O-C-C-O dihedral angle of $\sim 50^o$ in both the ion and neutral species. The ground electronic states of the DME complex and its ion are $^2A_1$ and $^1A_1$, whereas those of the corresponding DXE complex and its ion are ^2A and ^1A, respectively. Furthermore, the binding energies of the two neutral complexes were derived using a thermodynamic cycle. This simple calculation requires the ionization energies of the metal atom and complex as well as the dissociation energy of the cation complex.