

## 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 =  $\text{CH}_3\text{OCH}_3$ , DXE =  $\text{CH}_3\text{O}(\text{CH}_2)_2\text{OCH}_3$ . 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  $\sim 50^\circ$  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.