PULSED-FIELD IONIZATION ELECTRON SPECTROSCOPY AND AB INITIO CALCULATIONS OF METAL (Li, Ca) COMPLEXES OF PYRIDINE AND PYRIDAZINE

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1:1 Metal (M = Li, Ca) complexes of pyridine ($C_5H_5N$) and pyridazine ($1,2-C_4H_4N_2$) were produced by interactions between laser-vaporized metal atoms and vapor of the ligands in a supersonic molecular beam source. Vibrationally resolved spectra of these complexes were obtained with pulsed field ionization-zero electron kinetic energy (ZEKE) spectroscopy. The ZEKE spectra displayed strong transitions between the zero vibrational levels of the ground electronic states of the neutral molecule and ion and several metal-ligand and ligand-based vibrational excitations. The adiabatic ionization energies of Li-pyridine, Li-pyridazine, Ca-pyridine and Ca-pyridazine were measured to be 32460, 37870, 39064 and 41928 cm$^{-1}$, respectively, with an uncertainty of about 5 cm$^{-1}$. Density functional and second-order Møller-Plesset perturbation theory calculations predicted that the most stable structures of these complexes were formed by metal binding to one or two nitrogen atoms. These predictions matched with the observed ZEKE spectra for Li-pyridine, Li-pyridazine and Ca-pyridine. However, the theoretical calculations failed to reproduce the ZEKE spectrum of Ca-pyridazine.