

PFI-ZEKE SPECTROSCOPY OF COPPER-AROMATIC NITROGEN HETEROCYCLIC COMPLEXES

XU WANG, JASON F. FULLER, and DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY, 40605-0055.*

Single-photon pulsed field ionization-zero electron kinetic energy (PFI-ZEKE) photoelectron spectroscopy has been used to study the complexes of copper with pyridine (C_5H_5N), 2,2'-bipyridine ($C_{10}H_8N_2$) and 1,10-phenanthroline ($C_{12}H_8N_2$). In all cases, adiabatic ionization potentials and Cu-ring vibrational frequencies were measured from the ZEKE spectra. Additional ring-based vibrations were observed for Cu-bipyridine and -phenanthroline. All three Cu complexes were determined to be in C_{2v} symmetry with the metal atom σ bonding to the nitrogen of pyridine or two nitrogens of the polypyridines. Since the most stable conformation of the free 2,2'-bipyridine ligand is coplanar with *trans*-standing nitrogens, Cu coordination has induced a ring rotation of 180° to bring the two nitrogens in a *cis* configuration.