PFI-ZEKE SPECTROSCOPY OF COPPER-AROMATIC NITROGEN HETEROCYCLIC COMPLEXES

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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 nitrognes 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.