MONODENTATE BINDING OF ETHYLENEDIAMINE TO COPPER FROM PFI-ZEKE SPECTROSCOPY

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Ethylenediamine ($NH_2CH_2CH_2NH_2$), once described as "God's gift to the coordination chemist," is by far the most widely studied acyclic bidentate amine in coordination chemistry. Although the ligand binds to metal atoms mainly in a bidentate mode, this study has discovered that in the gas phase it prefers a monodentate binding with a copper atom. The Cu-ethylenediamine complex was produced in a laser vaporization molecular beam and investigated by pulsed field ionization-zero electron kinetic energy (PFI-ZEKE) spectroscopy and *ab initio* calculations. The adiabatic ionization potential and frequencies of Cu-N stretching and Cu-ring wagging vibrations were measured from the PFI-ZEKE spectrum. Four possible isomers of the complex were predicted to be similar in energy with the MP2 calculations. The comparison of the observed and simulated spectra identified the isomer with Cu binding to single nitrogen, where the ligand is in a staggered *gauche* configuration with an intramolecular hydrogen bond.