PREFERRED METAL BINDING SITE OF ANILINE

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Group III metal-aniline complexes, M-aniline (M = Sc, Y, and La), were produced by interactions between laser-vaporized metal atoms and aniline vapor in a pulsed molecular beam source, identified by photoionization time-of-flight mass spectrometry, and studied by pulsed-field ionization zero electron kinetic energy (ZEKE) spectroscopy and density functional theory calculations. Adiabatic ionization energies and several vibrational intervals were measured from the ZEKE spectra. Metal binding sites and electronic states were determined by combining the ZEKE measurements and theoretical calculations. Although aniline has various possible sites for metal coordination, the preferred site was determined to be phenyl ring. The metal binding with the phenyl ring yields *syn* and *anti* conformers. In these conformers, the neutral complexes are in doublet ground states and the corresponding singly charged cations in singlet states.