PULSED FIELD IONIZATION-ZERO ELECTRON KINETIC ENERGY PHOTOELECTRON SPECTROSCOPY OF LITHIUM PERYLENE AND CORONENE COMPLEXES

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Unlike the benzene molecule where all carbon atoms are equivalent, the carbon atoms and six-membered rings in polycyclic aromatic hydrocarbons (PAHs) are different. This study aimed to determine the Li binding sites in two PAH molecules: perylene ($C_{20}H_{12}$) and coronene ($C_{24}H_{12}$). The Li-PAH complexes were synthesized by reactions of the Li atoms with the vapor of the PAH ligands in supersonic molecular beams. The Li atoms and PAH molecules were produced by laser ablation of a rod made of mixed metal and ligand powders. These complexes were identified by time-of-flight mass spectrometry and characterized by pulsed field ionization-zero electron kinetic energy (PFI-ZEKE) photoelectron spectroscopy and density functional theory calculations. The PFI-ZEKE spectra of Li-perylene and -coronene exhibited strong 0-0 transitions at 37538(5) and 33468(5) cm^{-1}, respectively, and a number of vibrational intervals associated with metal-ring and ring-based vibrational excitations. The theoretical calculations predicted several low-energy structures with Li binding to different aromatic rings. By comparing the experimental spectra with the theoretical predictions, the preferred Li binding sites were determined to be the side rings with higher aromaticity.