PULSED FIELD IONIZATION ELECTRON SPECTROSCOPY OF CYCLOPENTADIENYL DIALUMINUM COMPLEX

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The cyclopentadienyl dialuminum complex, $(C_5H_5)Al_2$, is synthesized in a supersonic molecular beam, where aluminum atoms and dimers are produced by laser vaporization, and cyclopentadienyl radicals are generated from photolysis of cyclopentadiene (C_5H_6) molecules. Vibrationally resolved electronic spectra of the complex are measured using pulsed-field ionization zero electron kinetic energy spectroscopy. Three initial conformations are considered for the complex: one with an Al atom binding to each side of the C_5H_5 ring and two others with an Al_2 molecule lying vertically or horizontally on one side of the ligand ring. A structure with the Al_2 molecule lying vertically on the top of the C_5H_5 ring is identified by comparing the spectroscopic measurements to $ab\ initio$ calculations. The $(C_5H_5)Al_2$ neutral complex has a $^2A''$ ground electronic state in Jahn-Teller distorted C_s symmetry and the corresponding ion has a $^1A_1$ ground state in C_{5v} symmetry. The ionization energy of $(C_5H_5)Al_2$ is measured to be 40690(5) cm^{-1}. For the cationic $^1A_1$ state, the frequencies of the metal-ligand stretching, metal-metal stretching, and metal-ligand bending modes are 482, 175, and 50 cm^{-1}, respectively. In addition, a (C_5H_5)-Al_2 bending mode of the neutral $^2A''$ state is measured to be 26 cm^{-1}.