PULSED-FIELD IONIZATION ELECTRON SPECTROSCOPY OF ALUMINUM-URACIL

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Aluminum uracil ($Al-C_4H_4N_2O_2$) was formed by the interaction of the laser-vaporized metal and nucleobase in a pulsed nozzle cluster source. Electronic spectra of the complex were measured by using pulsed field ionization zero electron kinetic energy spectroscopy. The spectroscopic measurements determine the ionization energy of 43064(7) cm^{-1}, two Al^+-uracil stretches of 303 and 614 cm^{-1}, and Al^+/Al-uracil out-of-plane/in-plane bends of the same frequency of 51 cm^{-1}. The 303 cm^{-1} stretch is characterized largely by the Al^+ displacement, where the 614 cm^{-1} stretch is described by the ligand dislocation. The complex has a number of the low-energy conformers due to multiple binding sites of uracil. The comparison of the ZEKE spectrum and theoretical calculations establishes that the complex favors Al binding with the O4 atom under C_s symmetry.