GROUND ELECTRONIC STATES OF Ni-(2,2'-BIPYRIDINE) AND ITS MONOCATION

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Ni-(2,2'-bipyridine) was produced in a supersonic jet. The electronic spectrum of the complex was measured by using single-photon pulsed field ionization zero electron kinetic energy electron spectroscopy (PFI-ZEKE). The spectrum shows the band origin at 37919(15) cm^{-1} and vibrational intervals of 267, 1035, and 1175 cm^{-1}. With the aid of the B3LYP density functional and Franck-Condon factor calculations, the spectrum is attributed to the vibronic transitions from the $^3A_2$ ground state of the neutral complex to the $^2B_2$ ground state of the corresponding ion. The 267 cm^{-1} progression is assigned to the Ni-bipyridine symmetric stretch in the cation, whereas the 1035 and 1175 cm^{-1} intervals arise from ligand-based vibrations.