RESONANT MULTIPHOTON FRAGMENTATION SPECTROSCOPY OF NIOBIUM DIMER CATION IN A REFLECTRON TIME-OF-FLIGHT (TOF) MASS SPECTROMETER AND DENSITY FUNCTIONAL CALCULATIONS.

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Resonant multiphoton fragmentation spectra of niobium dimer cation (Nb_2^+) have been obtained by utilizing laser vaporization of an Nb metal target. Ions are mass-selected with a time-of-flight mass spectrometer followed by a mass gate, then fragmented with a pulsed dye laser, and resulting fragment ions are detected with a second time-of-flight reflectron mass spectrometer and multichannel plate. Photon resonances are detected by monitoring ion current as a function of fragmentation laser wavelength. A rich, but complex spectrum of the cation is obtained. The bands display a characteristic multiple structure, which may be interpreted as involving transitions from the $X^4\Sigma_g^-$ ground state to several excited states. The second order spin orbit splitting in the ground sate of Nb_2^+ was measured to be about $142 \pm 5\,\mathrm{cm}^{-1}$. In addition various DFT were performed to calculate the quartet- and doublet-electronic energy levels of the Nb_2^+ and the force constants (k) and inter nuclear distances (R) of the neutral and ionic dimer molecules from the first-row to third-row transitions metals at their ground states. R dependence of the logarithmic values of these calculated force constants, ln(k), provided an analogous linear equations for each set of data such as: ln(k(anion)) = 6.9223-2.8994*R, ln[k(neutral)] = 6.7887-2.7985*R, ln(k(cation)) = 5.9952-2.4163*R for the first row transitions metals; ln(k(anion)) = 7.0685-2.5864*R, ln(k(neutral)) = 7.1295-2.5990*R, ln(k(cation)) = 7.4209-2.7656*R for the second row transitions metals and ln(k(anion)) = 7.2073-2.5432*R, ln(k(neutral)) = 7.0825-2.4676*R, ln(k(cation)) = 7.4625-2.6191*R for the third row transitions metals.