A STUDY OF NbMo AND NbMo\(^-\) BY ANION PHOTOELECTRON SPECTROSCOPY

PRAVEENKUMAR BOOPALACHANDRAN, SRIJAY S. RAJAN, MELISSA A. BAUDHUIN, and DOREEN G. LEOPOLD, Department of Chemistry, University of Minnesota, Minneapolis, MN 55455.

We report the 488 and 514 nm anion photoelectron spectra of NbMo\(^-\). R2PI spectroscopic studies have established that neutral NbMo has a \(^2\Delta_{5/2}\) ground state and a short bond length \(^a\). We find that the NbMo\(^-\) anion has a \(^1\Sigma^+\) ground state in which the "extra" electron occupies the \((4d)\delta\) bonding orbital, giving a \(1\sigma^21\pi^21\delta^22\sigma^2\) valence electron configuration. Thus, NbMo\(^-\) has a formal bond order of 6, and is isoelectronic with Mo\(_2\). Low-lying excited states of NbMo \((^2\Sigma^+)\) and NbMo\(^-\) \((^4\Delta\) are also observed. The spectra provide the electron affinity of NbMo, energies of the \(^2\Sigma^+\) and \(^3\Delta\) excited states, vibrational frequencies in the anion and neutral molecule ground states and the \(^2\Sigma^+\) state, \(^2\Delta \) and \(^3\Delta\) spin-orbit splittings, and (from Franck-Condon analyses) bond length measurements for the anion ground state and the observed excited states. These results are compared with previous anion photoelectron spectroscopic data for the Group 5/6 congeners VCr and VMo, and with density functional theory predictions.