A STUDY OF NbMo AND $NbMo^-$ BY ANION PHOTOELECTRON SPECTROSCOPY

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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)δ bonding orbital, giving a $1\sigma^2 1\pi^4 1\delta^4 2\sigma^2$ 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 $NbMo^-$ ($^3\Delta$) 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.

[a] R. Nagarajan and M. D. Morse, J. Chem. Phys. 127, 164305 (2007).