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

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We report the 488 nm photoelectron spectrum of the $NbCr^-$ anion. For the $^2\Delta$ ground state of neutral NbCr, the short bond length (1.894 Å) and high bond energy (D_0 3.0263(6) eV) measured by R2PI spectroscopy[a] indicate high order multiple bonding. We find that the $NbCr^-$ 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 and a formal bond order of 6. Low-lying excited states of NbCr (assigned as two $^2\Sigma^+$ states) and $NbCr^-$ ($^3\Delta$) are also observed. The spectra provide the electron affinity of NbCr, energies of the $^2\Sigma^+$ and the $^3\Delta$ excited states, vibrational frequencies for the NbCr and $NbCr^-$ ground states and for the $^2\Sigma^+$ excited states, and (from Franck-Condon analyses) differences among the bond lengths of the observed states. These results are compared with our previous data for the Group 5/6 congeners NbMo, VCr, and VMo, and with DFT predictions. We also report results for ongoing experiments on the flow tube reactions of the Group V metals Nb and Ta with butadiene, and the vibrationally-resolved photoelectron spectra of some of the organometallic reaction product anions.

[a] S. M. Sickafoose, J. D. Langenberg, and M. D. Morse, J. Phys. Chem. A. 104, 3521-3527 (2000).