

## A STUDY OF NbCr AND NbCr<sup>-</sup> BY ANION PHOTOELECTRON SPECTROSCOPY

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

We report the 488 nm photoelectron spectrum of the NbCr<sup>-</sup> anion. For the <sup>2</sup>Δ ground state of neutral NbCr, the short bond length (1.894 Å) and high bond energy (D<sub>0</sub> 3.0263(6) eV) measured by R2PI spectroscopy<sup>a</sup> indicate high order multiple bonding. We find that the NbCr<sup>-</sup> anion has a <sup>1</sup>Σ<sup>+</sup> ground state, in which the "extra" electron occupies the (4d)δ bonding orbital, giving a 1σ<sup>2</sup>1π<sup>4</sup>1δ<sup>4</sup>2σ<sup>2</sup> valence electron configuration and a formal bond order of 6. Low-lying excited states of NbCr (assigned as two <sup>2</sup>Σ<sup>+</sup> states) and NbCr<sup>-</sup> (<sup>3</sup>Δ) are also observed. The spectra provide the electron affinity of NbCr, energies of the <sup>2</sup>Σ<sup>+</sup> and the <sup>3</sup>Δ excited states, vibrational frequencies for the NbCr and NbCr<sup>-</sup> ground states and for the <sup>2</sup>Σ<sup>+</sup> 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.

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<sup>a</sup>S. M. Sickafoose, J. D. Langenberg, and M. D. Morse, *J. Phys. Chem. A*, 104, 3521-3527 (2000).