ANION PHOTOELECTRON SPECTROSCOPY OF NbW^- and $W_2{}^-$

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The 488 nm vibrationally-resolved photoelectron spectra of NbW^- and $W_2{}^-$ are reported. The electron affinity of W_2 (${}^1\Sigma_g{}^+ \leftarrow {}^2\Sigma_u{}^+$) is found to be 1.118 ± 0.007 eV, which differs from the value reported in a previous anion photoelectron spectroscopic study of $W_2{}^-$ (1.46 eV)[a], but was accurately predicted by density functional calculations (1.12 eV)[b]. The fundamental vibrational frequency of W_2 is measured to be 345 ± 15 cm^{-1}, in agreement with the value previously reported in matrix resonance Raman studies (337 cm^{-1})[c]. The $W_2{}^-$ anion is measured to have a fundamental frequency of 320 ± 15 cm^{-1}. Several weak transitions to excited electronic states are seen and tentatively assigned based on calculated energies. NbW has an electron affinity of 0.856 ± 0.007 eV. Vibrational frequencies are found, by Franck-Condon fitting of overlapping transitions, to be 365 ± 20 cm^{-1} for NbW^- and 410 ± 20 cm^{-1} for NbW. This increase in vibrational frequency upon photodetachment suggests that the extra electron is in an antibonding orbital, leading to ground state assignments of ${}^3\Delta$ and ${}^2\Delta$ for the anion and neutral, respectively. These results are compared to those obtained for other Group V and Group VI transition metal dimers and trends are discussed.

[a] H. Weidele et al., Chem. Phys. Lett. 237 (1995) 425-431

[b] Z. J. Wu, X. F. Ma, Chem. Phys. Lett. 371 (2003) 35-39

[c] Z. Hu, J.-G. Dong, J. R. Lombardi, D. M. Lindsay, J. Chem. Phys. 97 (1992) 8811-8812