The electronic spectrum of tantalum hydride and deuteride

Thomas D. Varberg[a], Stephanie Y. Lee[a], Casey R. Christopher[a], Kara J. Manke[a], and Tyson R. Vervoort[a]

[a] Department of Chemistry, Macalester College, 1600 Grand Ave., St. Paul, MN 55105 USA,
Tel.: +011 651 696 6468 , Fax: +011 651 696 6432, E-mail: varberg@macalester.edu

We have recorded the electronic spectrum of the molecule TaH (and TaD) in the gas phase for the first time. The molecules were prepared in a hollow cathode discharge, and the spectrum was recorded by laser excitation spectroscopy. Our initial experiments were undertaken using a pulsed dye laser at a resolution of ~0.1-cm^{-1}, and we observed nine bands of TaH and four of TaD over the 610–670-nm region. All of these bands are red-degraded, and rotational analyses indicate that most of the bands originate from the same $\Omega = 2$ state, presumed to be the ground electronic state of the molecule.

This initial work was followed by high-resolution spectroscopy of two of the bands (at 633 nm for TaH and 632 nm for TaD) using a continuous-wave ring dye laser. Both of these bands are $\Omega' = 2 \leftarrow \Omega'' = 2$ in character and were rotationally analyzed using a Hund's case (c) Hamiltonian, leading to precise rotational and centrifugal distortion constants for the upper and lower states. We also observed hyperfine structure arising from the ^{181}Ta nucleus ($I = 7/2$, 100% abundant), which we have fitted using appropriate magnetic dipole and electric quadrupole interaction parameters.

The fitted value of the ground rotational constant in TaH is $B_0 = 5.4472(6)\ \text{cm}^{-1}$, which yields a bond length of $r_0 = 1.75722(9)$ Å. This value is in good agreement with the *ab initio* calculations of Casarrubios and Seijo [1] and Koseki, Matsushita, and Gordon [2]. We propose that the lower level in our transitions is the $\Omega = 2$ component of a $\sigma^2\delta\pi^3$, $^{\square}\Phi_r$ ground state.

[1] M. Casarrubios, L. Seijo, *J. Chem. Phys.* **1999**, *110*, 784.
[2] S. Koseki, T. Matsushita, M. S. Gordon, *J. Phys. Chem. A* **2006**, 110, 2560.