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BOND DISSOCIATION ENERGIES OF EARLY TRANSITION METAL-MONOBORIDES

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Transition metals are very important both scientifically, and in everyday life. They are used in an array of disciplines, from catalysis to technology, and their numerous applications make transition metals a research topic of high interest. Unfortunately, they are chemically complex and their plethora of low-lying states makes them difficult to study experimentally, leading to a lack of precise data.

This project focused on the measurement the bond dissociation energies (BDEs) of early transition metal (Sc, Ti, V, Y, Zr, Nb, La, Hf, Ta, W)-monoborides, none of which had been studied experimentally prior to this work. These were measured by the Morse Group via Resonant 2-Photon Ionization Spectroscopy (R2PI). This method utilizes the high density of bound and repulsive excited states about the ground separated atom limit by observing the onset of a predissociation threshold as soon as the BDE is reached. Transition metal-boride compounds are of particular interest due to their many interesting and useful physiochemical properties, such as their thermal stability, electrical conductivity, and hardness.

The interest in these borides makes them a prime target for computational studies, which is a great way to reduce time and chemical waste of studying complex molecules, but which has a pitfall: computational chemistry is most effective when there are experimentally-derived values to benchmark to. In his Nobel lecture, John Pople articulated the acceptable standard for "chemical accuracy" in quantum chemical calculations as being within 1kcal mol^{-1} of the experimentally measured value for molecules that contain main-group elements. For many molecules this is an attainable benchmark using current computational methods. However, for transition metals, meeting this benchmark still poses difficulty, which is exacerbated by the fact that many species have not been experimentally studied, or have large uncertainties associated with their measurements. This has led to a relaxation of the benchmark for transition metal-containing species to 3 kcal mol^{-1}. Even so, it is often extremely difficult to reach this level of accuracy, in large part due to a lack of experimental data with uncertainties that meet this standard.

The Morse Group was able to successfully measure these transition metal-boride BDEs, providing the first experimental data available, thus paving the path for future studies on these molecules. In addition, the group performed supplemental quantum calculations in order to provide further insight into the nature of these bonds, and to help determine the ground state configurations of these molecules.

Previously, the Morse Group had already measured the BDEs of the late transition metal-borides, and has now also measured the BDEs of transition metal-diborides. In future works, the group plans to rotationally resolve and measure the bond lengths of several diatomic metal-borides, including CuB, AgB, AuB, and OsB.