Core Electron Ionization and the Periodic Table
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The basis for atomic number of the elements was provided by the x-ray spectroscopy experiments of English physicist Henry Moseley in the early 20th century. Moseley measured the energy of x-rays emitted by the elements and found the following relationship: $\sqrt{\Delta E} = k_1(Z-k_2)$, where $\Delta E$ is the energy, $Z$ is the element’s atomic number, and $k_1$ and $k_2$ are constants. This relationship is known as Moseley’s Law. Moseley found that the value of $k_2$ is near 1 for the $K\alpha$ transition. His results were purely empirical, that is, with no theoretical interpretation. In our work, we seek to provide a quantum mechanical interpretation of Moseley’s Law. No such direct interpretation exists in the current literature.

We employed two theoretical models in order to interpret the empirical results of Moseley: a simple spreadsheet screening constant model and a sophisticated computational chemistry model. Both models are based upon quantum mechanics. In the screening constant model, total atomic energies were calculated by employing the concept of effective nuclear charge. Differences in these energies provide the energy of the $K\alpha$ transition. This model was first developed by Slater¹ in 1930 and later improved upon by Gould² in 1991. The results from this model are shown in Figure 1a and illustrate excellent agreement with the empirical result of Moseley; the value of $k_2$ is 1.0032, near 1 as required by the experimental data. Our second model employed the computational chemistry software GAMESS³ (General Atomic and Molecular Electronic Structure System). We used the CUHF theoretical method⁴, which was incorporated into GAMESS software in May, 2013 (Iowa State University, Dr. Michael Schmidt). Again, we calculate energy differences between the relevant ions in order to compare with Moseley’s experimental data. Our computational results are shown in Figure 1b and again show excellent agreement with the experimental data of Moseley in that we find the value of $k_2$ to be 0.9796, that is, near 1.

This research experience has been a great benefit to me. I enjoyed being able to combine chemistry with mathematics, physics, and computer science on a project that explores the foundations of the electronic structure of atoms. I also have gained valuable scientific writing and presentation experience that will benefit me in my future academic and professional work. I am very grateful for this opportunity.

References: