Atomic Screening Constants and Effective Nuclear Charge

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The Slater-Zener model[1,2] provides a simple but accurate understanding of the electronic structure of atoms. It is based upon the idea that electrons are attracted to the positively charged nucleus, but shield (screen) one another from experiencing the full nuclear attraction. This results in each electron having an "effective nuclear charge". Slater wrote a series of "rules" that provided screening constants to calculate effective nuclear charge. For example, he estimated that a 1s electron screens a 2s electron by 0.85 electron charge units. His model allows inner electrons to screen outer electrons, but not the other way around. That is, "outer screening" is not allowed. This model works well for rows 1 and 2 in the periodic table, but diverges from experiment as one moves down the periodic table. This being the case, and given what we now know about electron wave-functions and probability distributions, the claim that outer electrons do not shield inner electrons is a model we set out to test.

My research this summer was to optimize a new set of screening constants to model various sets of experimental data, e.g., atomic size and ionization energy. The hope was that we would be able to achieve good agreement with the entire periodic table simply by allowing for a small amount of outer screening. To do this, we used a computer program by Microsoft called Excel Solver, which changes a set of variables, within given constraints, in order to minimize or maximize an objective cell in Excel. In our case, this meant changing the screening constants, within the constraints of what makes chemical sense, in order to minimize the error between the results of the model and experiment.

With every possible screening combination of the 1s through 5p orbitals, we needed to optimize 121 different variables. If each was independent of the others, Solver would be able to find many different combinations that gave good results. So to constrain it, we forced some constants to be zero and some to be exactly one, as was theoretically sound. We first allowed Solver to optimize the constants through the 2p orbital, and then extended those constants out by shells through the 5p orbital, where each was related to the shell before by only two variables, one for the inner screening constants and the other for the outer screening constants. What we found was exactly as expected. The outer screening constants increased as we moved down the periodic table and the inner screening constants decreased. This new set of constants produce results that agree much better with experiment than Slater's original constants.

This project was a continuation of my work from last year, which after being written up, was rejected by the *Journal of Physical Chemistry*. While the rejection was disappointing at the time, it gave us time to see how this summer's project could fit in with, and strengthen our argument. Thus, the rejection was a blessing in disguise, as it has bettered our 2015 paper, and taught me a lot about the publication process and the general way research is conducted. Like last year, this summer gave me valuable experience in the use of computational methods and the application of theory. Aside from the chemistry that I learned, I was continually blessed by my mentors and fellow researchers. Being able to collaborate with my peers was a lot of fun, but also taught me to communicate effectively and efficiently. I am extremely grateful for Calvin College and this great opportunity.

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2. Zener, C. (1930). Analytic Atomic Wave Functions. *Physical Review*, *36*(1), 51–56. http://doi.org/10.1103/PhysRev.36.51