Estimating f-electron Shielding Constants Using Subsequent Ionization Energies

Choy, Nasya (School: Arkansas School for Mathematics, Sciences and the Arts)

Reed and Slater's rules do not accurately calculate effective nuclear charge in f-filling elements, and subsequent ionization energy values of these elements are difficult to find experimentally. Previous researchers made inaccurate estimates for f-electron shielding constants and subsequent ionization energies of f-filling elements using graphical-numerical methods, trends in s, p, and d shielding values, and educated guesses. The goal of this project is to find better f-electron shielding values using subsequent experimental ionization energies as data points. This project back-solves for shielding constants using a combination of publicly available subsequent ionization energies and GRG nonlinear and evolutionary optimization algorithms. By finding the best combination of shielding constant values, this study found estimates for shielding constants denoted "SIISF", "PIISF", and all f-electron shielding constants except those denoted "FISF". Theoretical values for subsequent ionization energies of a selection of f-filling elements were also determined. The error of Reed's Rules when calculating subsequent ionization energies is 298.8% while the error of the updated model is 17.5%, resulting in a statistically significant difference ($p < 0.00001$) of moderate size. The ability to quickly and easily estimate effective nuclear charge for f-filling elements would allow for more convenient predictions of the properties of the f-filling elements, especially the lanthanide contraction, and could be used in future projects to estimate atomic radii, and density.