Problem-Solving with Python: Modeling of Lanthanide Shift Reagent Complexes

D. Zlatković,* M. Đorđević Zlatković, N. Radulović*

Faculty of Sciences and Mathematics, University of Niš, Serbia

**DZ: dragan.zlatkovic@gmail.com, NR: nikoradulovic@yahoo.com*

Herein we describe a program written in Python programming language that employs a simple complete-search algorithm for determining the geometry of a lanthanide-substrate (LS) complex. The program can be used as a work project in an introductory programming course for chemistry students to illustrate the concepts such as decision-making, repetition, functions, lists, file reading, and data visualization. Students are presented with the problem to determine the position of a lanthanide ion in an LS complex by using the results of the NMR titration experiment of menthol with $Eu(fod)_3$. The problem is subdivided into several stages: 1) assignment of the ^1H NMR shifts in the menthol molecule; 2) determination of $\Delta\delta$ values for each proton; 3) molecular modeling of menthol; 4) writing a Python program that would calculate the Eu position which gives the best correlation with the experimental data. This project should not only improve the coding and problem-solving skills of the students but also offer them an opportunity to practice their NMR elucidation technique.

Keywords: Graduate Education, Organic Chemistry, Computer-Based Learning, Problem Solving, Computational Chemistry, NMR Spectroscopy

Acknowledgement: This work was supported by the Ministry of Science, Technological Development and Innovations of the Republic of Serbia (Contract Number451-03-47/2023-01/ 200124).