8th International Conference on Research in TEACHING and EDUCATION

RTECONF

Vienna, Austria
01 - 03 March, 2024

Web Servers to Understand Chemical Concepts

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Abstract

The project is designed to impart knowledge about ligands, substituents, and elements bonded to or surrounding a metal in a catalytic context. Leveraging successful web servers in the research field, the project enables researchers, irrespective of their computer chemistry expertise, to access pertinent information effortlessly. The methodology involves using a steric index, $\%V_{Bur}$, which gauges the occupancy in the metal's first sphere to reveal the catalytic performance of the corresponding catalyst. The web server, available at https://www.molnac.unisa.it/OMtools/sambvca.php, facilitates the calculation of steric hindrance for any ligand. For students in the Master in Advanced Catalysis and Molecular Modeling (MACMoM) program at the University of Girona, the project becomes an inspiring exercise. Through experimental and computational approaches, students correlate catalytic reaction pathway yields with the %VBur steric index. The exercise entails delving into past experimental results, manipulating xyz coordinates from X-Ray data, and employing linear and multilinear regressions. Importantly, each student in the class tackles a unique problem, fostering collaboration as solutions are shared within the group. This collaborative aspect not only aids in unraveling complex systems but also enhances the collective understanding of the intricacies involved. Emphasizing self-directed learning, the project encourages students to connect theory with results, promoting a deeper comprehension of the impact of specific groups.

Keywords: chemistry, educational exercise, ligand; steric hindrance, project-based learning