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Chemistry as a foundation for scientific endeavors

Historically, the Diels-Alder chemical reaction has been of great interest to the scientific community due to its synthetic capacity. In this reaction, two organic fragments, or compounds formed by carbon and hydrogen, react to form a six-membered cycle. How this reaction is produced remains an open question for those performing fundamental science.

Regarding this, Dr. Patricia Pérez, Professor for the Faculty of Exact Sciences at the Universidad Andrés Bello, is searching for models of chemical reactivity that could describe the formation and breaking of carbon-carbon bonds in organic reactions. For this, the theoretical framework of the project is based on the Density Functional Theory that, together with other theoretical tools, will provide insights into the processes of a chemical reaction, from the starting substances until the final product.

"Research begins with simple models that explain some of the experimental behavior of a real system. If the model conforms to the experimental behavior and anticipates other experimental factors, it is valid and can be used in systems of greater complexity," explains Dr. Pérez.

The central goals of this research project are to contribute to the development of fundamental science and increase knowledge of the world around us. Likewise, project findings could later be applied to advancements in the applied sciences and technology.

Dr. Patricia Pérez adds that, "one of the most important contributions of this research has been the construction of reactivity scales. Through this, we have quantified electrophilic and nucleophilic concepts that, 60 years ago, were purely qualitative. Within the field of organic chemistry, these scales have contributed to the quantitative classification of cycloaddition processes as polar, non-polar, or zwitterionic."