Computational Chemistry and Organic Synthesis: Let Us Build a Bridge

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Progress in quantum chemistry and computational techniques allows chemists to understand and predict the outcome of organic reactions in a very efficient fashion. Hereby we demonstrate the power of bridging experiment and theory on some recent examples from our lab.

The Claisen rearrangement is a classical textbook reaction.[1] However, it still holds the potential to provide new experimental results and a series of novel Claisen-type rearrangements have recently been developed by the Maulide group.[2] Our combined theoretical/experimental study of these transformations reveals a diversity of possible pathways and products. The calculations clarify the experimental results and predict new reactions.[3]

The Maulide Group has also discovered a new synthetic approach leading to imidazoles with concomitant observation of an unusual sulfonyl migration.[4] Our in-depth theoretical analysis of possible intermediates and transition states shed more light on this rearrangement.

Moreover, some reactions can even proceed via several different unclear mechanisms. One of those examples is our TEMPO-mediated aminoxylation of ynamides.[5] The calculations explain the experimentally observed phenomena.

References

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