How to find reaction mechanisms?

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A plethora of theoretical and computational methods on different levels of abstraction are used to interpret experimental findings in Chemistry. While this traditional role of Theoretical and Computational Chemistry is very important, e.g. to choose between equally plausible hypothesis, the potential of this discipline as a true discovery tool for fundamentally novel chemical behavior has not yet been fully taped. The specification and identification of recurrent reaction patterns and high-order reaction behavior in reactive systems or the discovery of possible elementary energetic constraints that shape the structure of reaction networks on the large scale, requires an adequate formalism allowing to first express and second study these type of phenomena. Over the past years, we have developed such a formalism, which is rooted in category theory, and models chemical transformation on an atomic level as algebraic graph rewrite. A key feature of our formalism is the possibility to construct arbitrary chemical reaction spaces in a unified manner. This characteristics paves the way for a rigorous static and dynamic analysis of reactive systems as well as to attack questions connected to the temporal ordering of reaction steps or causality. I will present deterministic and stochastic applications of our graph-grammar formalism ranging from enzyme mechanisms to polyketide biosynthesis to the design of metabolic pathways.

References

[1] J. L. Andersen, C. Flamm, D. Merkle and P. F. Stadler, An intermediate level of abstraction for computational systems chemistry, Philos. Trans. Roy. Soc. A **375**(2109) (2017), DOI 10.1098/rsta.2016.035