Exploring chemical reaction networks with KiNetX

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Abstract: A tool for automated quantum mechanical exploration of molecular reactivity previously published by our group, Chemoton [1], generates complex chemical reaction networks and associated properties such as activation energies. The size of the networks quickly becomes intractable, in particular if the involved species cause multiple side reactions. Then, the relevant kinetics of a chemical species might be hidden under a myriad of reactive conformers. For a kinetic analysis, the chemical reaction network must be converted to a set of possibly stiff ordinary differential equations (ODE). Ideally, the resulting chemical kinetics analysis is then carried out under full error control. KiNetX [2] is a C++ software aimed at the analysis of complex chemical reaction networks and their efficient exploration. Our software has been developed to possess four features. It is able to convert the graph structure of the network into a set of ODE and to identify and prune kinetically irrelevant species. Moreover, it propagates the first-principle uncertainty in activation energies estimated by Chemoton [3] as uncertainty in concentration trajectories. Most importantly, it collects the knowledge acquired through this analysis and drives the chemical reaction network exploration of Chemoton, for instance, avoiding wasting resources exploring kinetically irrelevant portions of the graph or identifying critical paths where more refined calculation methods should be employed.

References

[1] G. N. Simm and M. Reiher. *Context-driven exploration of complex chemical reaction networks*, J. Chem. Theory Comput., **13**(12):6108–6119, 2018.

[2] J. Proppe and M. Reiher. *Mechanism Deduction from Noisy Chemical Reaction Networks*, ArXiv e-prints, 2018.

[3] J. Proppe, T. Husch, G. N. Simm and M. Reiher. *Uncertainty quantification for quantum chemical models of complex reaction networks*, Faraday Discuss., **195**:497-520, 2016.