

Understanding gas-phase processes via experiments and theory: tools to add further understanding.

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Over the last 50 years direct time-resolved measurements have provided a phenomenal amount of detailed kinetic data on isolated reactions. This data is often used to test our understanding of complex systems by inputting it into atmospheric and combustion models and then compare the modelled predictions against *in situ* data measured in these environments. This is a symbiotic relationship that can highlight how good the kinetic measurement is and if there are missing reactions / processes in the model.

More recently theory has evolved sufficiently such that *ab initio* structure calculations in combination with rate theory can also provide reliable rate constant data, and thus provides an additional component in this symbiotic relationship between experiments and models that further constrains the parameters of the system.

While theory is able to look at isolated reactions this ideal situation is not always the case for experiments as important reaction intermediates are often only formed in the presence of other reacting species, e.g. the branching agent in combustion chemistry QOOH is in equilibrium with the peroxy radical, RO₂, so the **system is of increased complexity**. Under such conditions it is important to have experimental techniques that can make measurements and because the system is complex analysis of the data needs to be more sophisticated, and most likely linked to theory if the system is going to yield meaningful kinetic parameters.

In my talk I will highlight a range of experimental techniques used to determine kinetic data, with emphasis on techniques that are able to make measurements when the system is complex. I'll also highlight data analysis methods, in particular the use of Master Equation fitting to data, where the energy of a species on the potential energy surface of the reaction might be one of the adjustable parameters.