2.056 The MAGNIFY project – Updated protocols for ozonolysis and photolysis of organic compounds.

Early Career Scientist

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Abstract:

Atmospheric chemistry impacts on air quality, climate change, and a wide range of societal and economic issues such as effects on human health, including premature deaths, and reduced crop yields from air pollution. Chemical mechanisms are key to understanding the impacts of these effects and predicting future changes. However, owing to the large number of different compounds identified in the troposphere (currently $> 10^5$), it is impossible to develop the complex explicit chemical mechanisms needed

based solely on experimental information.

The MAGNIFY project (Mechanisms for Atmospheric chemistry: GeneratioN, Interpretation and FidelitY) aims to address these pressing research issues by updating and extending the Master Chemical Mechanism (MCM, http://mcm.leeds.ac.uk) using state-of-the-art methods to predict missing mechanistic and kinetic data. With currently ~7,600 species and ~17,000 reactions, this open-access mechanism is one of the most widely used and cited benchmark mechanisms for atmospheric chemistry. A major focus of the current project is a complete overhaul of its construction rules so that future generations can be auto-generated using the GECKO-A expert system (Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere, http://geckoa.lisa.u-pec.fr), opening it up more to the community via the internet and assure a sustained provision and maintenance of future MCM versions.

Here, we focus on updates to the construction protocols for ozonolysis, including the chemistry of resulting Criegee intermediates, as well as photolysis, where the scarcity of experimental data has hindered the development of robust prediction methods for cross sections and quantum yields. Special attention is given to multifunctional compounds, which are expected to be ubiquitous in the atmosphere. However, kinetic and mechanistic measurements of multifunctional species chemistry are still needed for the development and implementation of robust protocol rules.