Home of Atmospheric Computational Chemistry group

This is the home page of the Atmospheric Computational Chemistry group.

Our group studies the chemical reactions of atmospheric condensable vapors and their precursors using computational methods, with emphasis on reactive sulfur- and nitrogen-containing molecules, and on atmospheric autoxidation reactions of complex organic molecules. The foundation is provided by a large variety of quantum chemical methods, from state-of-the-art multireference configuration interaction (MRCI) and coupled cluster (CC) methods to density functional theory (DFT). Molecular-level reaction mechanisms and potential energy surfaces are then used as input for reaction dynamic calculations in order to obtain information on real reaction rates in the atmosphere.

Our main current research areas are:

-Elucidating the mechanisms involved in the formation of highly oxygenated multifunctional compounds from volatile organic compounds (mainly alkenes such as cyclohexene, isoprene or monoterpenes) in the gas-phase

-Modeling of the detection efficiencies of mass spectrometers employing different chemical ionization methods, and using computational data to aid the interpretation of mass spectrometric data from atmospheric chemistry experiments.

-Modeling key properties of polyfunctional molecules with atmospheric relevance, including saturation vapor pressures and Setschenow constants describing salting in/out behaviour.

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