

Colloquium

SFB 956

Conditions and Impact of Star Formation

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Physikalische Institute Köln

Lecture Hall III

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Recent Advances in Reactive Scattering: From Combustion Chemistry to Interstellar Chemistry

The reactions of ground state 3P oxygen atoms with unsaturated hydrocarbons have been the subject of extensive research because of their important role in combustion and atmospheric chemistry. Recently, these reactions have been recognized to have also general implications for the chemistry of interstellar medium (ISM). While efficient reactions with C-containing radicals in O-poor/C-rich environments do not destroy the C-C bond (rather elongate the C-atom skeleton), in O-rich environments of the ISM the growth of unsaturated hydrocarbons is strongly reduced, as these molecules are degraded to CO (or its precursor species HCCO and HCO) in the same way as it occurs in terrestrial environments of oxidizing (O-rich) flames.

For reliable modeling of combustion as well as of ISM oxygen chemistry, detailed knowledge is required of primary products and branching ratios for $O(^3P)$ +unsaturated hydrocarbon reactions. However, despite extensive kinetics and theoretical work over many decades, limited information exists on the nature of primary products, branching ratios, the role of intersystem crossing (ISC) from triplet to singlet potential energy surfaces (PESs) and overall reaction dynamics. The method most suitable for providing this critical information is the crossed molecular beams (CMB) scattering technique with mass spectrometric detection, empowered with "soft" ionization.

In this talk, I report on our recent investigations of the reaction dynamics of $O(^3P)$ with acetylene, ethylene, allene, methylacetylene and propene using the CMB method. By exploiting "soft" electron-ionization we have probed all energetically allowed product channels and characterized the dynamics, branching ratios and extent of ISC. The experimental results are compared with statistical calculations on *ab initio* PESs. For the benchmark multichannel non-adiabatic reaction $O+C_2H_4$, results are also compared with those of synergic quasiclassical trajectory surface-hopping computations on full-dimensional coupled *ab initio* triplet/singlet PESs. Recent upgraded chemical models for various astrochemical environments, which include a revision of $O(^3P)$ +unsaturated hydrocarbon reactions, are noted.

