Probing Molecular Growth, Interactions and Networks

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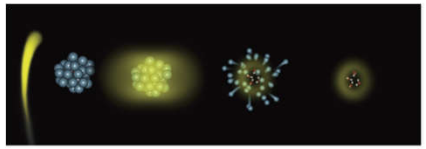
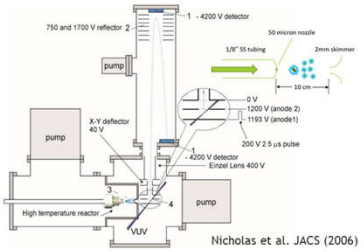
Background, Significance, and Design

- An investigation of complex multistep and multiphase chemical transformations built from isolated elementary bimolecular reactions to gas-surface reaction dynamics.

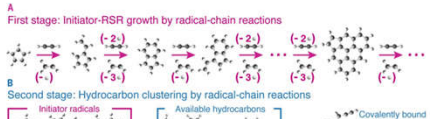
1. Molecular Cluster Chemistry and Hydrogen-Bonding Networks

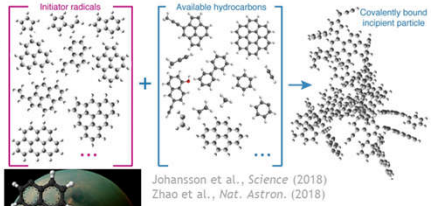


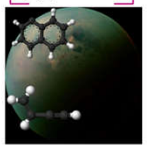


Nicholas et al. JACS (2006)

2. Molecular Chemistry of Polycyclic Aromatic Hydrocarbon Growth





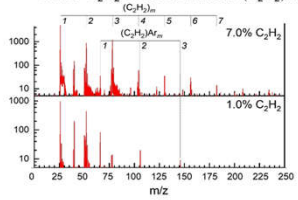


Johansson et al., *Science* (2018)
Zhao et al., *Nat. Astron.* (2018)

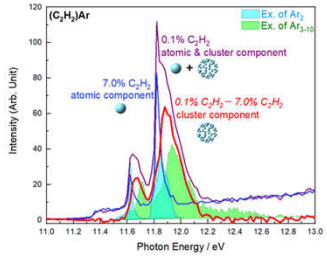
- ❑ Soot formation: air pollution
- ❑ Astrochemistry

1. *Molecular Cluster Chemistry*

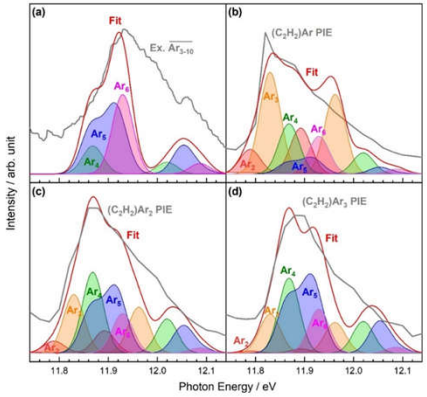
MS: Higher C_2H_2 concentration: $(C_2H_2)_m$
Lower C_2H_2 concentration: $(C_2H_2)Ar_n$



PIE scan: Two components, atomic vs cluster



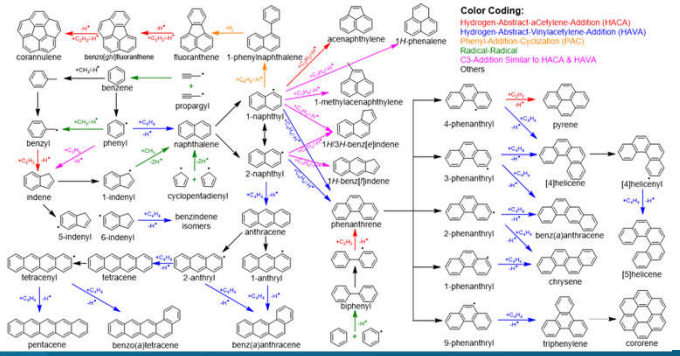
Theoretical fitting



Penning-ionization mechanism: The PIE curves of $(C_2H_2)Ar_n$ reflect the excitation spectra of Ar_n clusters with a relatively narrow size distribution and allow for a new approach to probe excited states of neutral Ar_n clusters directly.

2. *Growth of Polycyclic Aromatic Hydrocarbon Growth*

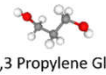
Self-reaction of propargyl-propargyl



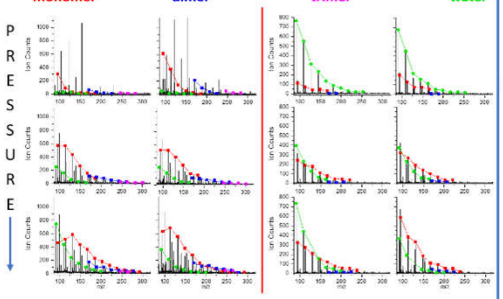
Future Directions

Photoionization Dynamics of Polyol– Water Clusters- Insight into hydrogen bond networks

1,2 Propylene Glycol

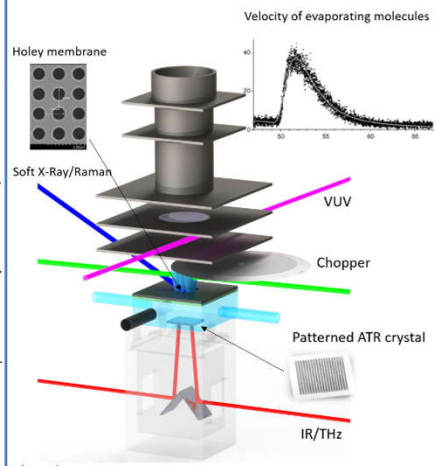


1,3 Propylene Glycol



- Variables = Temperature, Pressure, Ionization energy.
- Water-glycol cluster formation mechanism is different
- Fragmentation is different

Evaporation dynamics probed by MS and VMI



Acknowledgements: DOE-Gas Phase Chemical Physics Program