

# IR/UV Double Resonance Study of the 2-Phenylallyl Radical and its Flash Pyrolysis Products

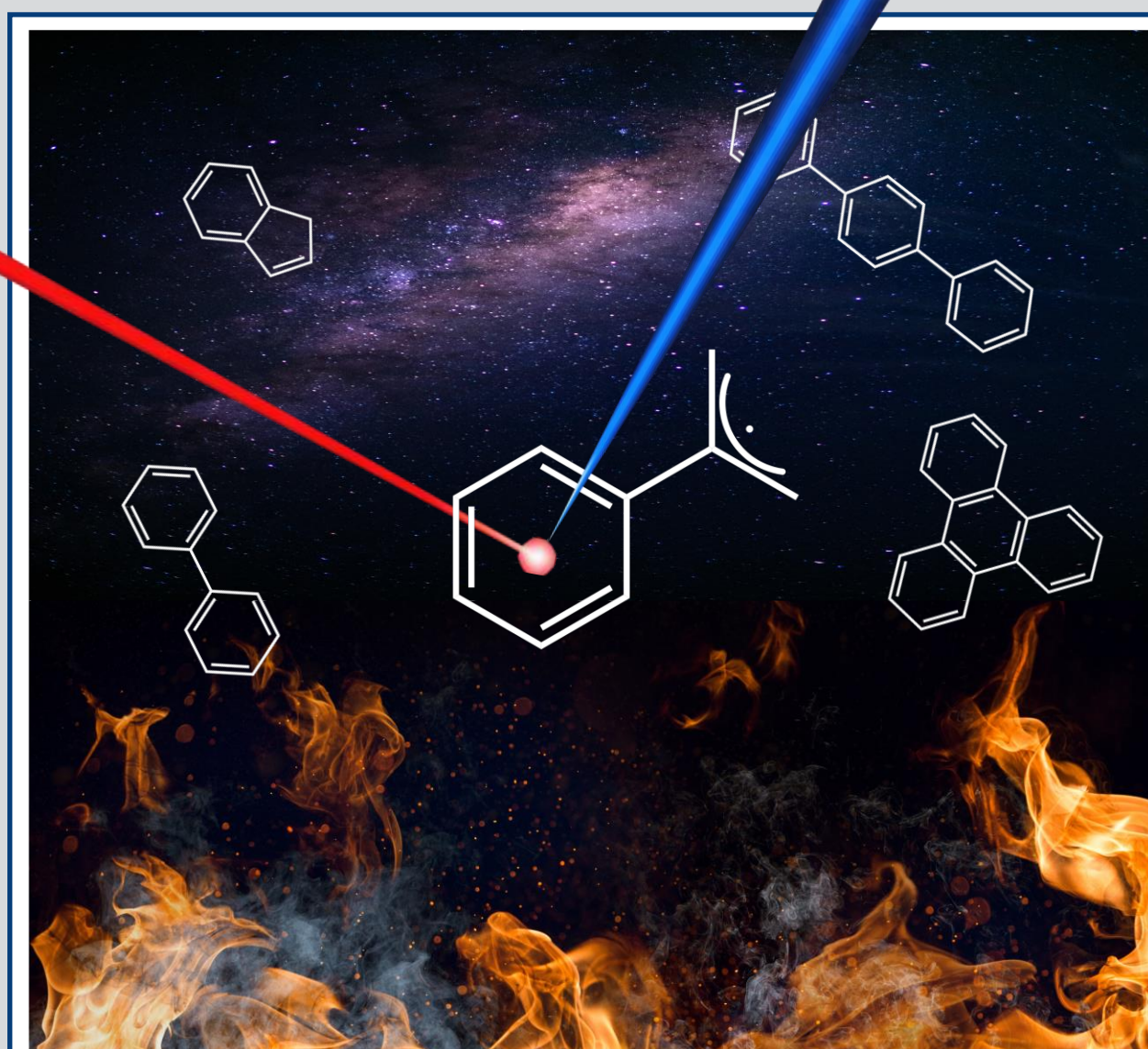
T. Preitschopf,<sup>[a]</sup> F. Sturm,<sup>[a]</sup> I. Stroganova,<sup>[b]</sup> A. Lemmens,<sup>[c]</sup> A. Rijs,<sup>\*[b]</sup> and I. Fischer<sup>\*[a]</sup>

<sup>[a]</sup> Institute of Physical and Theoretical Chemistry, University of Wuerzburg, Germany

<sup>[b]</sup> Faculty of Science, BioAnalytical Chemistry, Vrije Universiteit Amsterdam, The Netherlands


<sup>[c]</sup> FELIX Laboratory, Institute for Molecules and Materials, Radboud University, The Netherlands

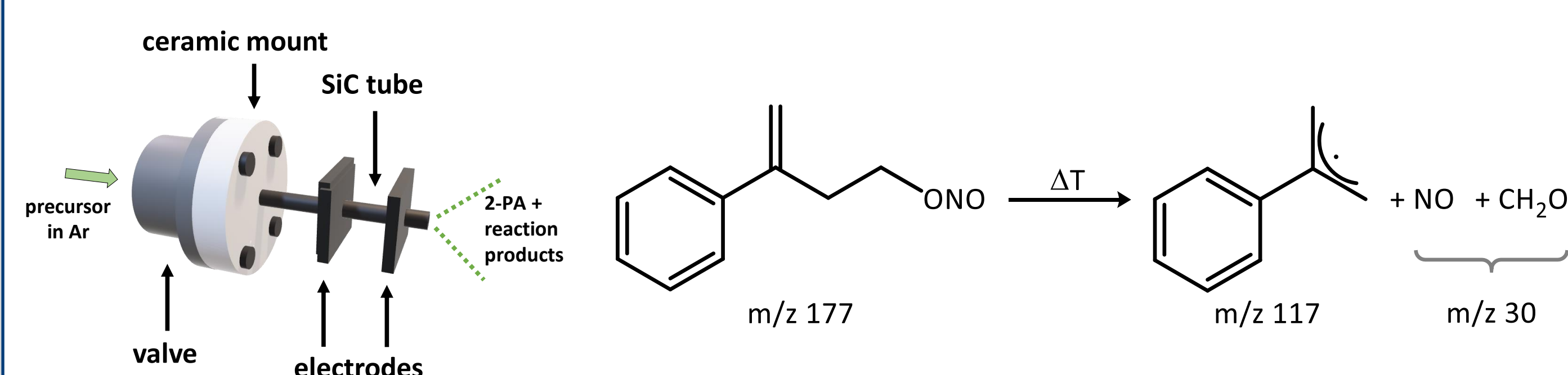
## Motivation



- resonance-stabilized radical
- no spectroscopic information available so far on 2-PA
- possible intermediate in PAH formation in combustion processes and interstellar space

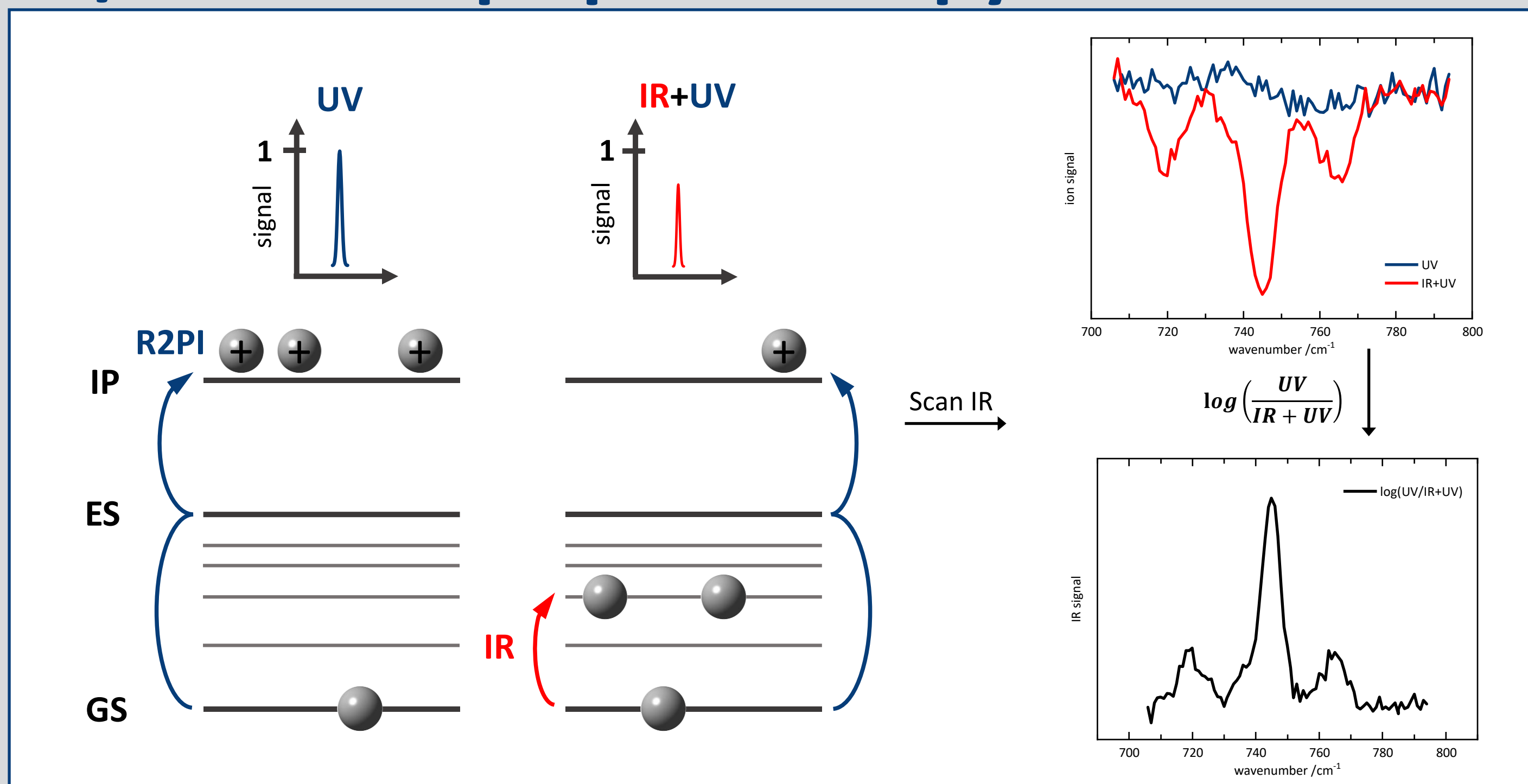
## Experimental/Theory

- UV light produced by Nd:YAG laser pumped dye laser
- mid-IR radiation provided by free electron laser 
- nitrite precursor synthesized in our group
- pyrolytic flow microreactor to generate 2-PA and promote bimolecular reactions

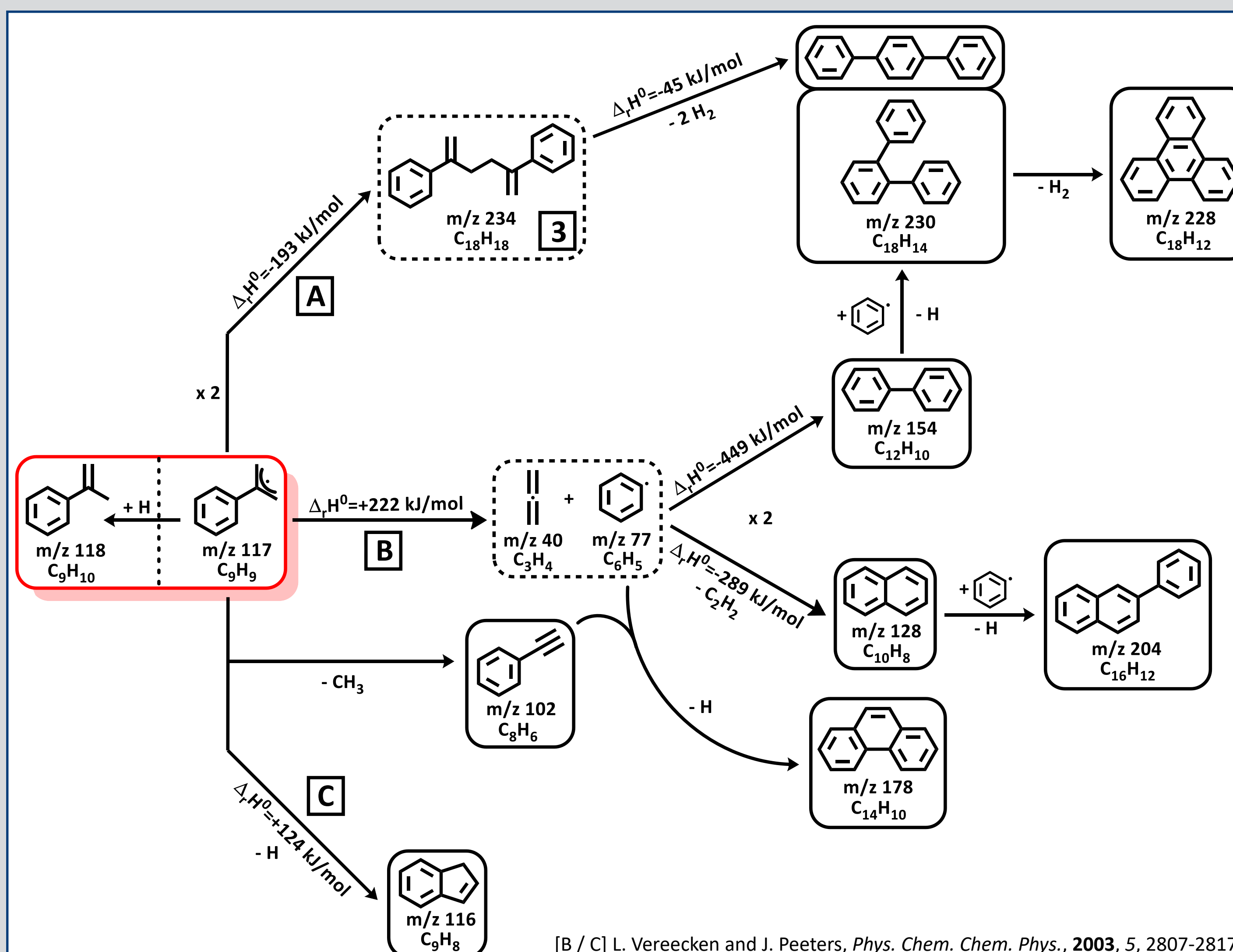


- DFT/B3LYP/6-311G++G(d,p) level of theory
- scaling factor 0.985, broadened with  $\sigma=10 \text{ cm}^{-1}$  (Gaussian)

## IR/UV Ion Dip Spectroscopy



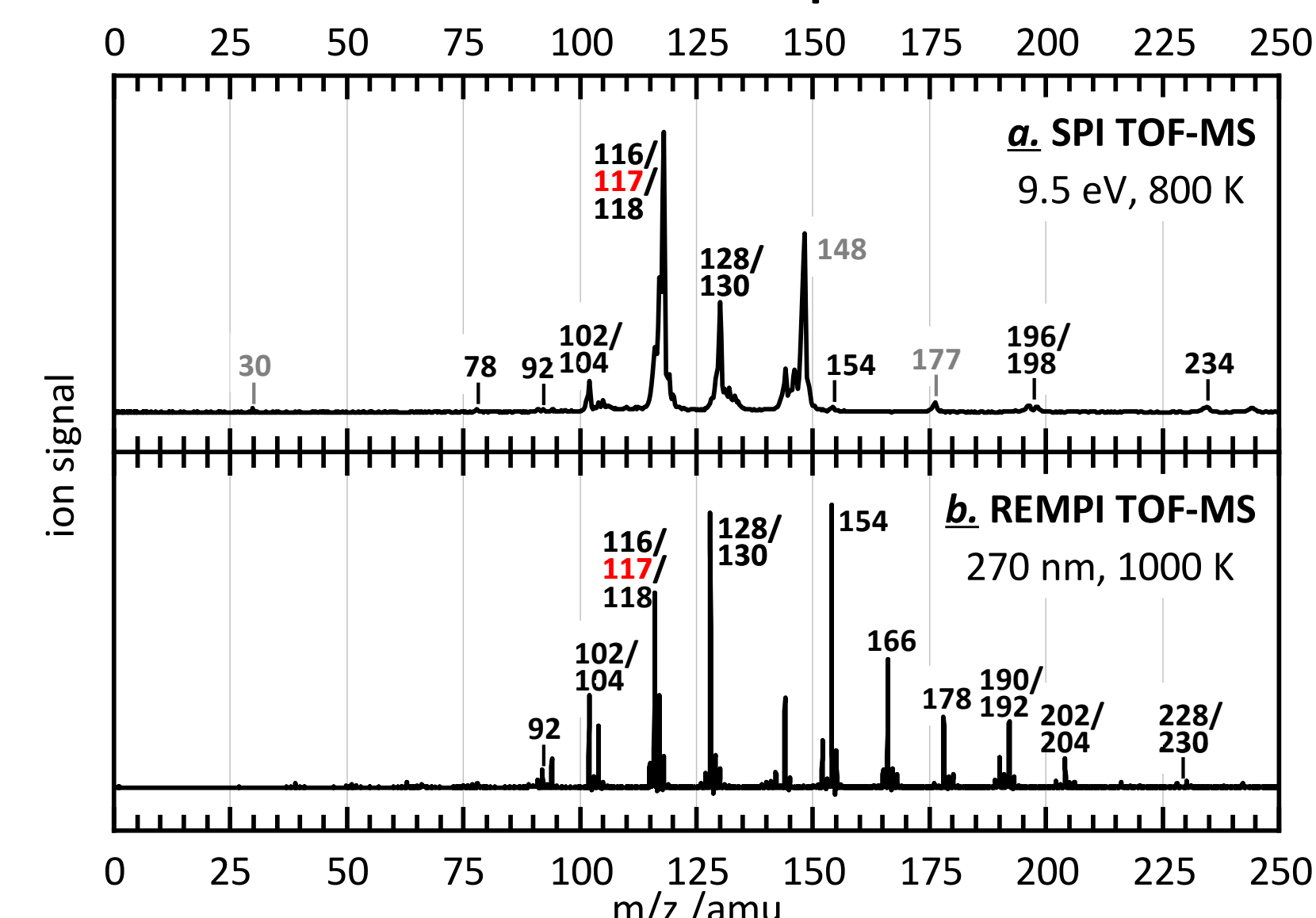
## Reaction Scheme



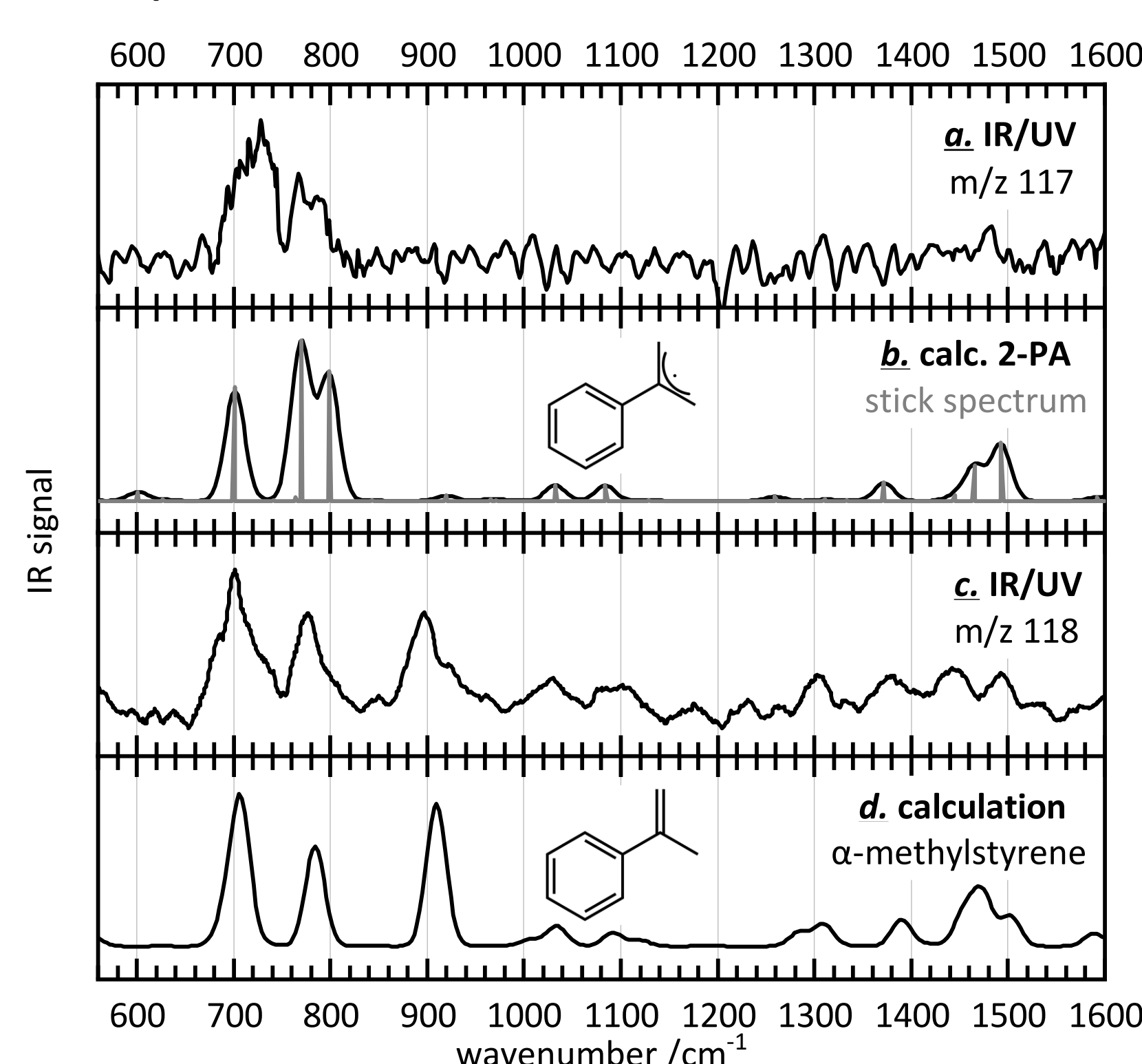
[B / C] L. Vereecken and J. Peeters, *Phys. Chem. Chem. Phys.*, **2003**, *5*, 2807-2817.

## Results

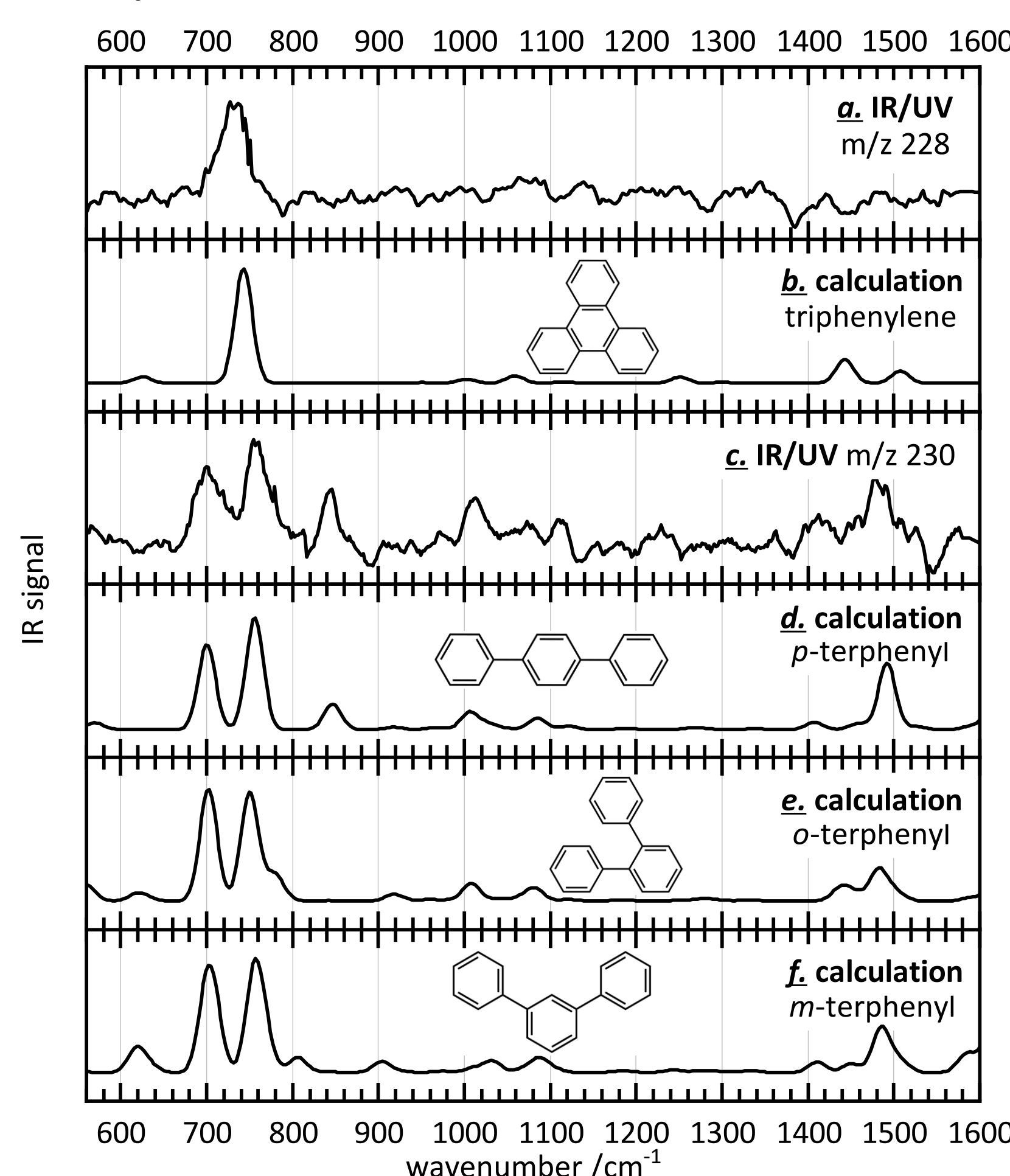
- SPI and REMPI TOF Mass Spectra



- IR/UV m/z 117 and 118



- IR/UV m/z 228 and 230



## Conclusion

- 2-PA is efficiently formed by pyrolysis from corresponding nitrite precursor
- three competing key reactions of 2-PA contribute to molecular growth via
  - radical-radical self-reaction
  - dissociation to phenyl, followed by PAC
  - isomerization and H abstraction to indene

## Fundings/Acknowledgements

