

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

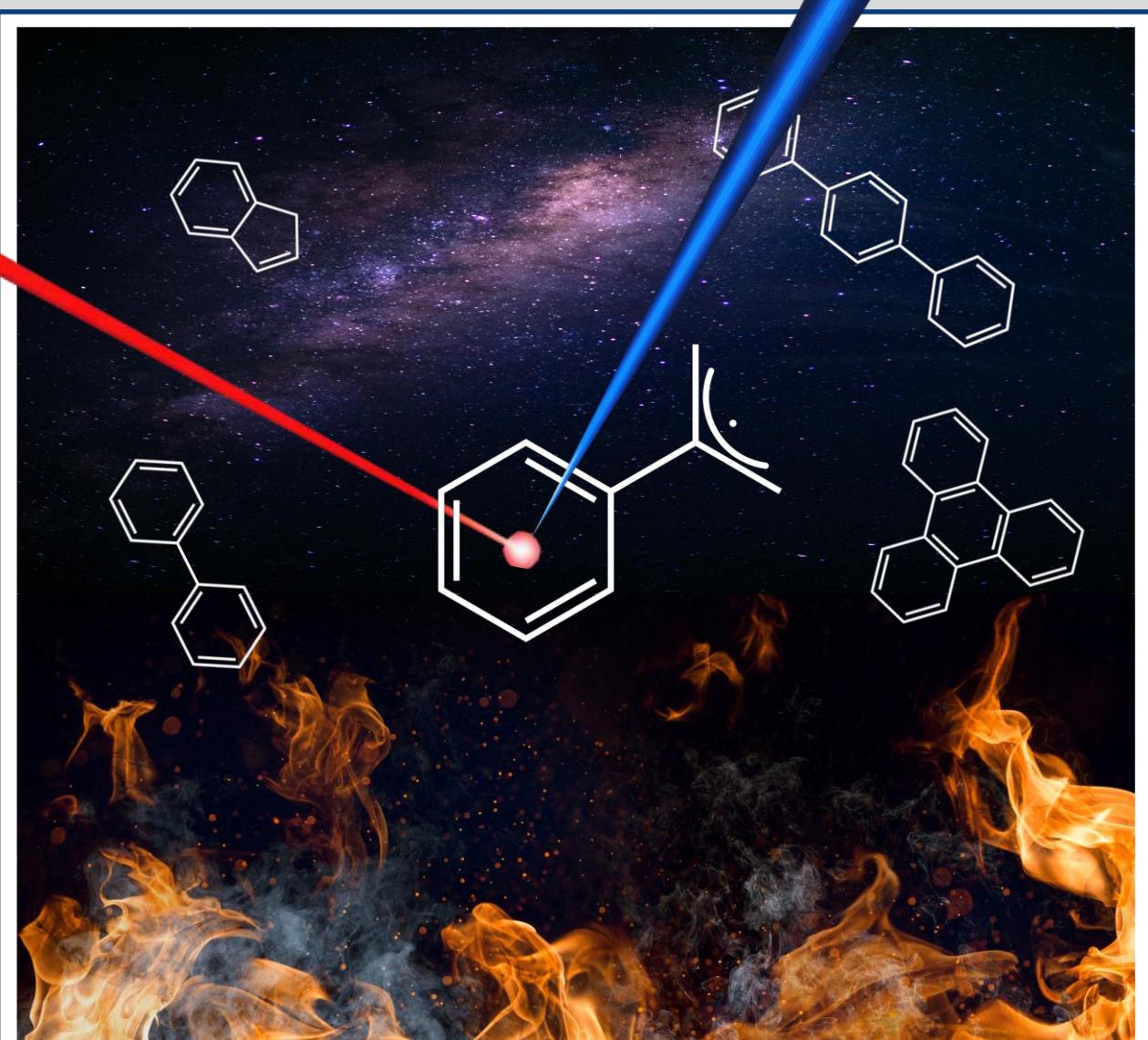
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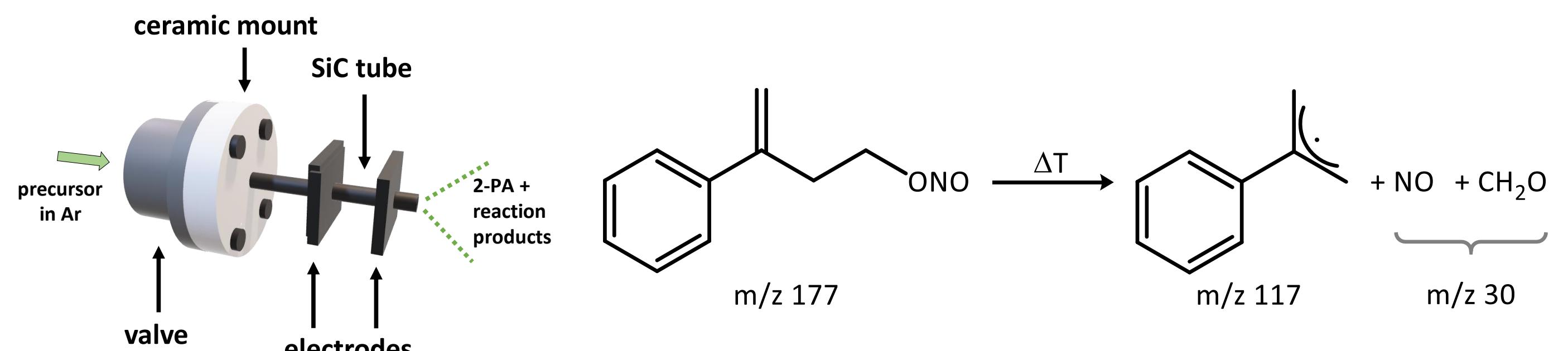
Motivation



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

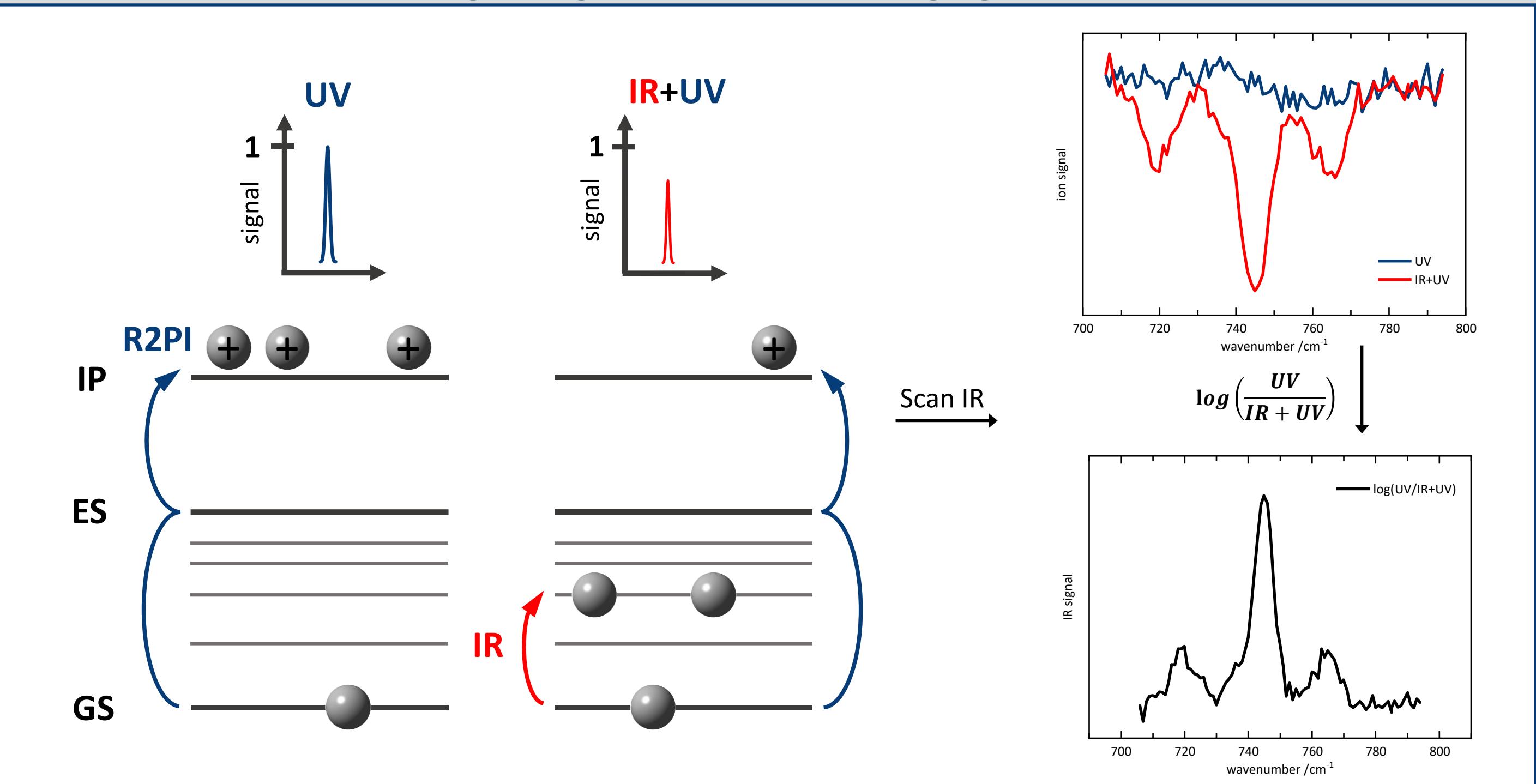
Experimental/Theory

- - 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

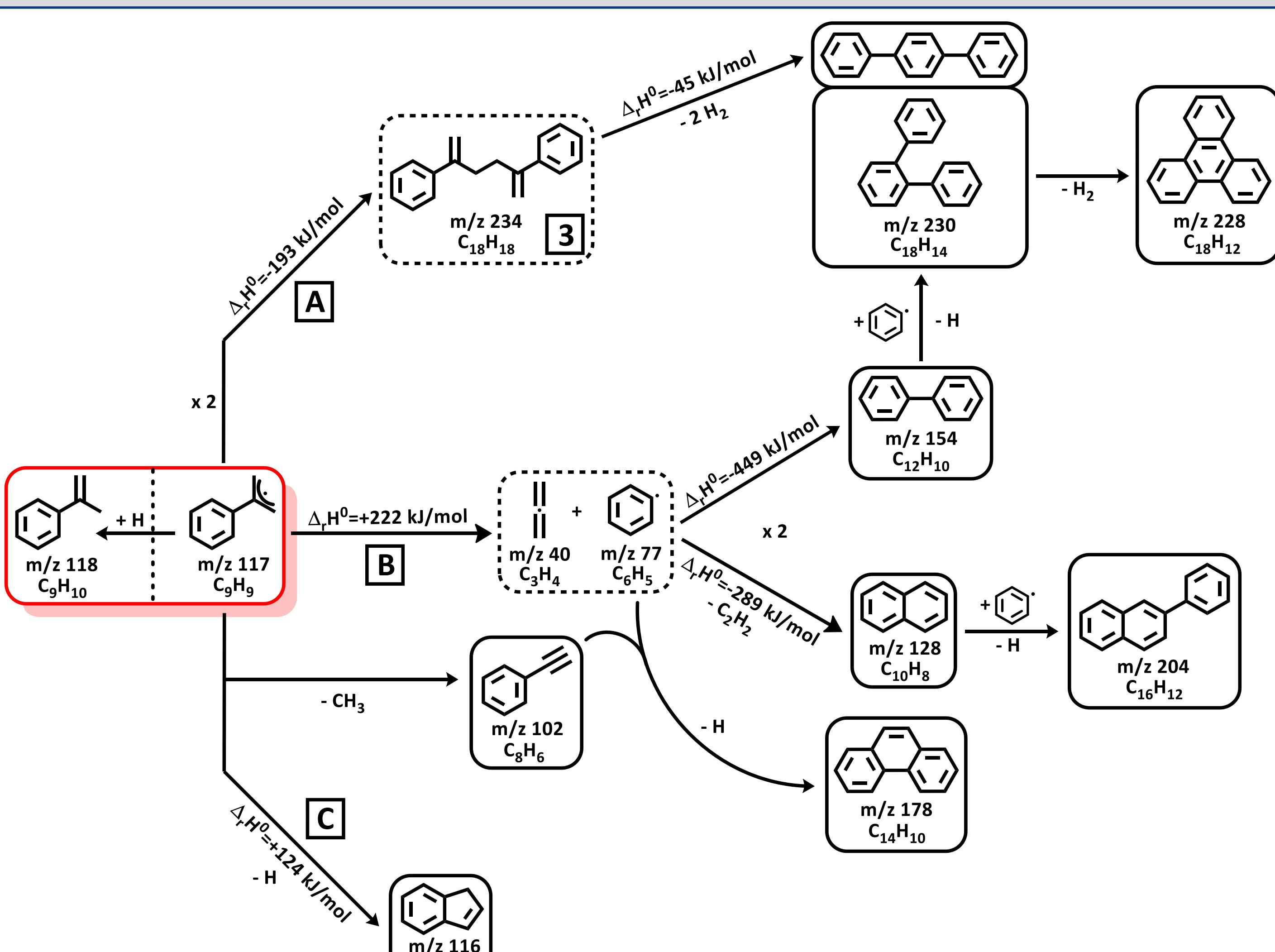


- - DFT/B3LYP/6-311G++G(d,p) level of theory
 - - scaling factor 0.985, broadened with $\sigma=10\text{ cm}^{-1}$ (Gaussian)

IR/UV Ion Dip Spectroscopy

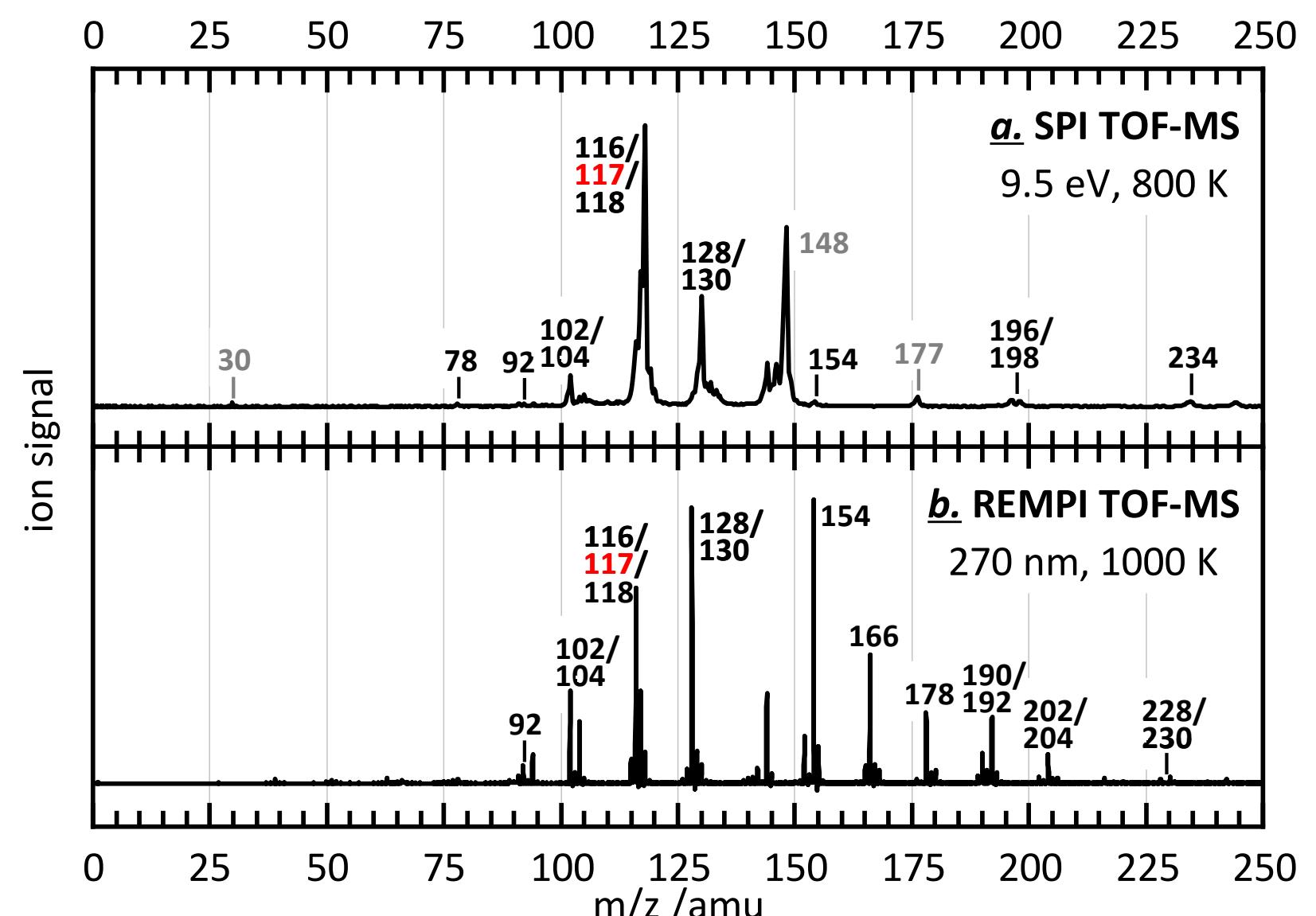


Reaction Scheme

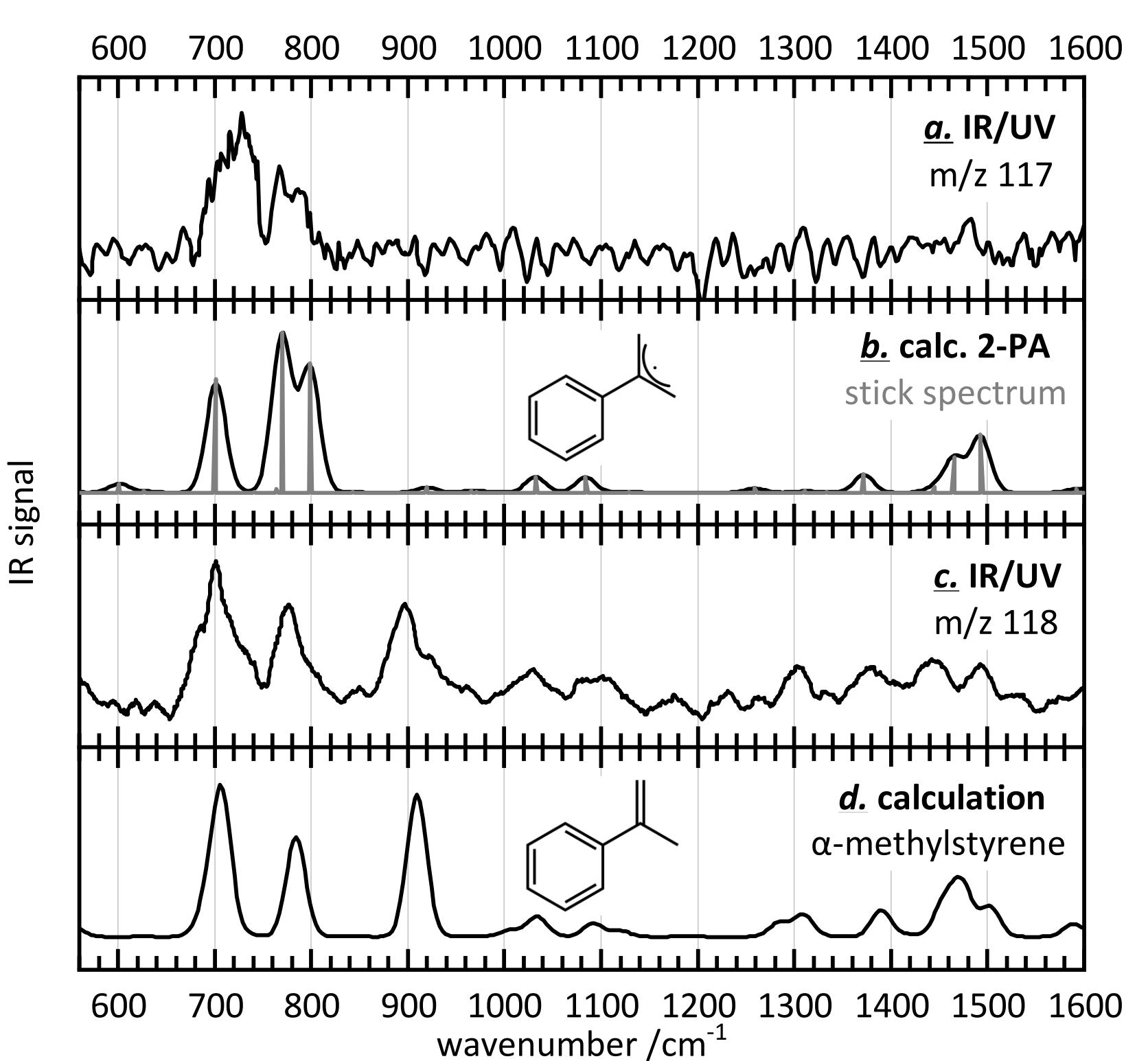


Results

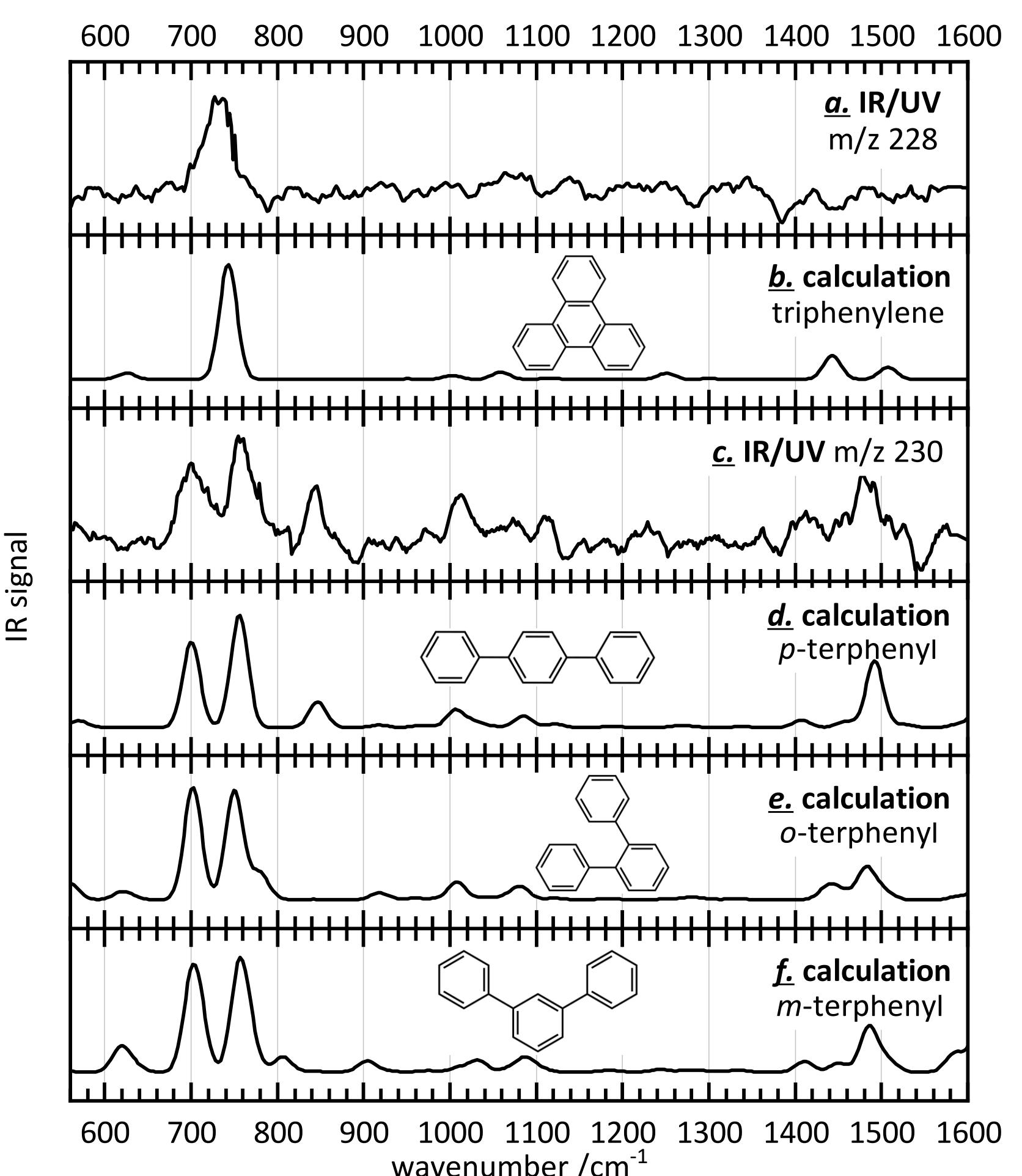
- ## ■ SPI and REMPI TOF Mass Spectra



- 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

