Spectroscopy of *m*-benzyne and its high temperature reaction products

M. Gerlach[1], T. Preitschopf[1], I. Stroganova[2], E. Karaev[1], D. Schaffner[1], F. Sturm[1], P. Hemberger[3], A. Lemmens[2], I. Fischer[1]

[1] Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Germany

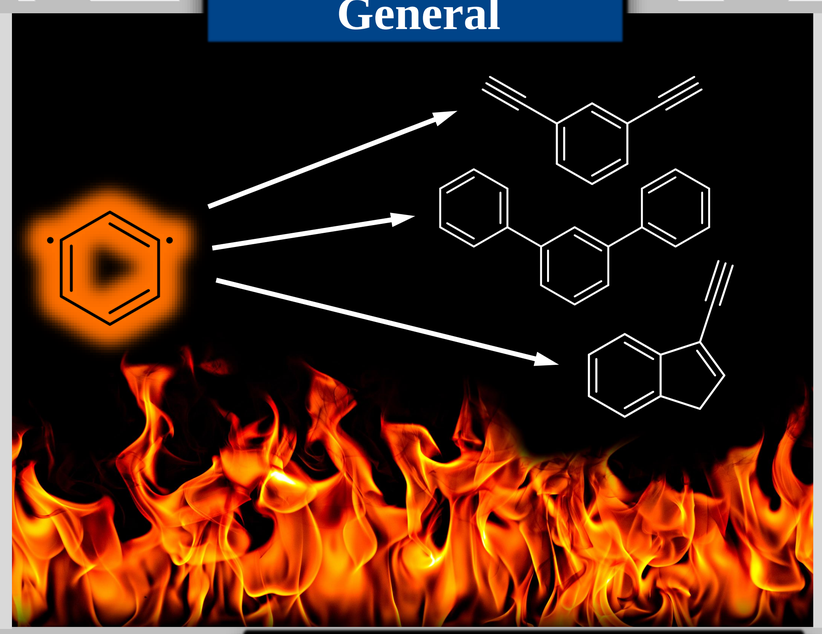
[2] FELIX Laboratory, Radboud University, The Netherlands

[3] Synchrotron SLS, Paul-Scherrer-Institut, Switzerland

Motivation & Goals

- *m*-benzyne has been investigated extensively by theoretical methods
- Experimentally only IR-spectra exist
- *m*-benzyne may also play a role in combustion chemistry as a highly reactive intermediate
- Our goal is to generate *m*-benzyne pyrolytically and investigate its properties and high temperature reactions

General

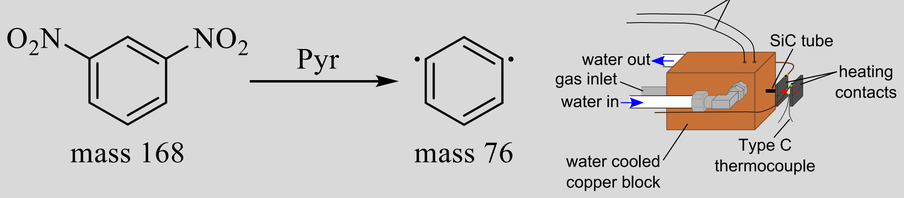


Literature

- Sander *et al.* generated *m*-benzyne using the different precursors and found a biradicaloid structure.[1]
- Theoretical calculations on the neutral species found a very flat potential energy surface along the C1C3 coordinate. The calculations predicted a distance of 2.05 Å.[2]
- Calculating the cationic structure lead to two close-lying states with highly different C1C3 distances.[3]

Experimental details

Generation of *m*-benzyne



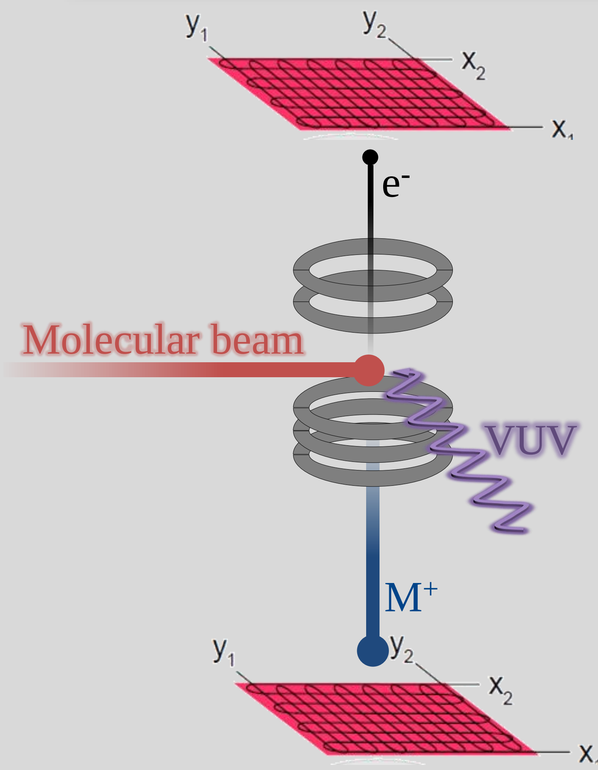
SLS Beamline

- VUV radiation produced by bending magnet
- The light is monochromatized using a 150 l/mm grating

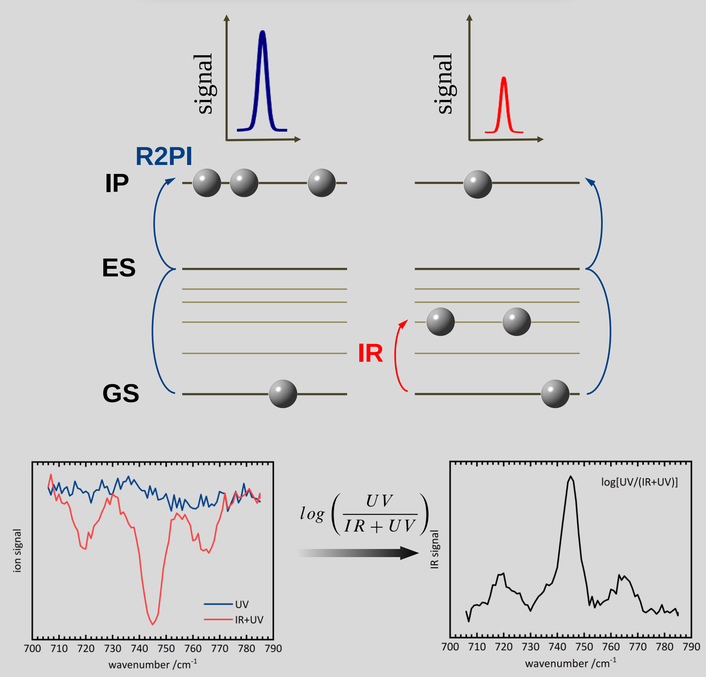
FELIX Beamline

- Pulsed UV radiation produced by dye laser pumped by Nd:YAG laser at repetition rate of 20 Hz
- Mid-IR radiation provided by free electron laser at 10 Hz

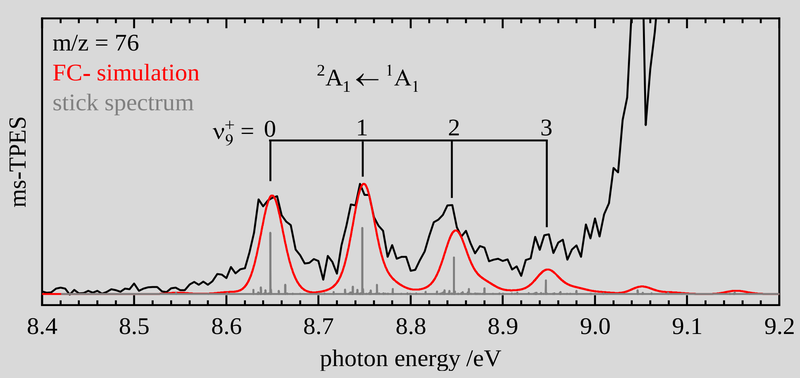
PEPICO Setup

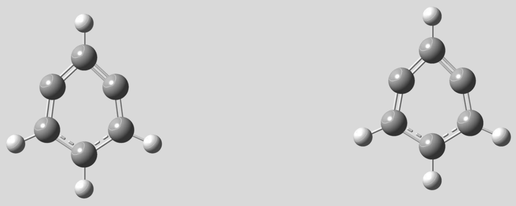


IR/UV Ion Dip



TPES



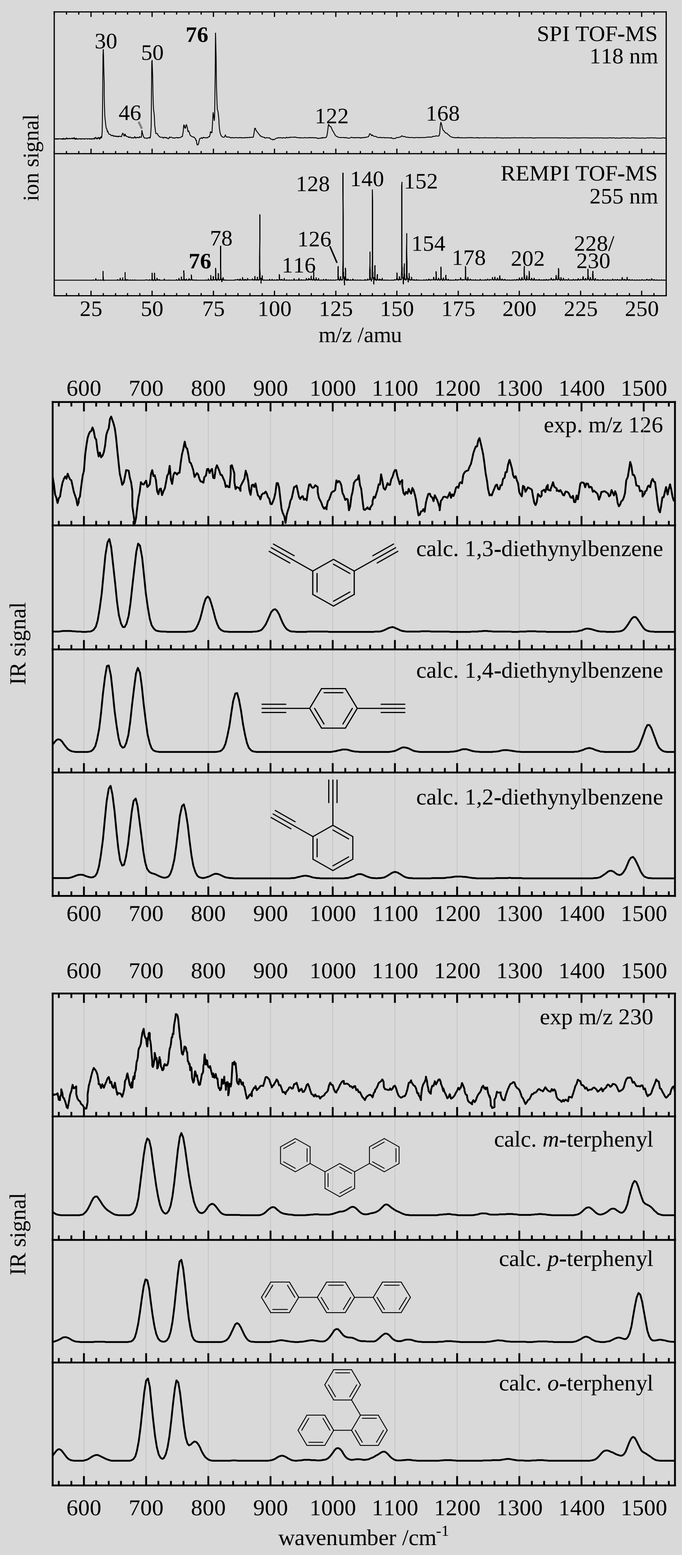


Neutral

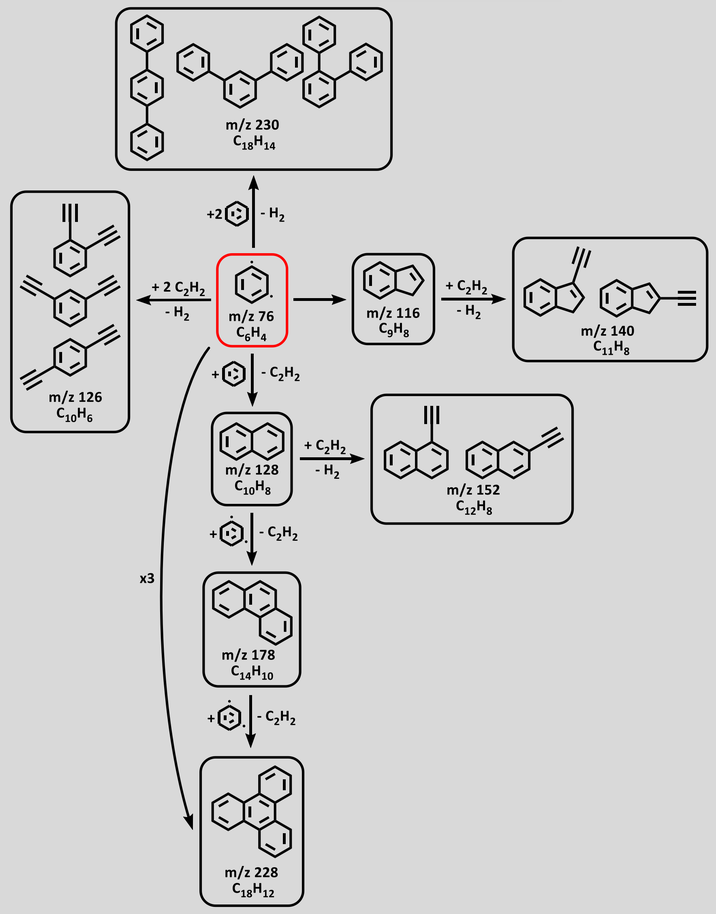
Cation

Coordinate	Neutral	Cation
C1 – C3 dist.	2.00 Å	1.99 Å
C1C2C3 angle	94.0°	93.8°
C4C5C6 angle	112.9°	117.9°

IR/UV Ion Dip



Reaction scheme



Conclusion

- We successfully recorded the ms-TPES and identified the involved structures by Franck-Condon simulations
- *m*-benzyne shows rich bimolecular chemistry forming PAHs

References

1. W. Sander, M. Exner, M. Winkler, A. Balster, A. Hjerpe, E. Kraka, D. Cremer, *J. Amer. Chem. Soc,* **2002**, *124*, 13072-13079.
2. M. Winkler, W. Sander, *J. Phys. Chem. A,* **2001**, *105*, 10422-10432.
3. H. Li, M.-B. Huang, *Phys. Chem. Chem. Phys.,* **2008**, *10*, 5381-5387.