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

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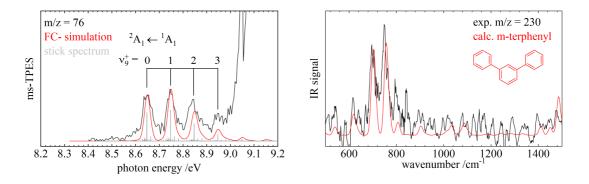
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m-benzyne and its relatives o- and p-benzyne are a fascinating class of reactive organic intermediates that are considered to play an important role in the formation of polycyclic aromatic hydrocarbons (PAH) in combustion processes. While o-benzyne has been extensively studied to understand its electronic structures and its chemical reactivity, less is known about *m*-benzyne and *p*-benzyne. Here, we present the gas phase generation and spectroscopy of the meta isomer generated by the pyrolysis of 1,3-dinitrobenzene.[1] Using this technique, we conducted two different experiments.

First, we investigated the isolated *m*-benzyne at the VUV Beamline at the Swiss Light Source (SLS) in Villigen, CH. Employing the CRF-PEPICO setup allowed us to record mass-selected threshold photoelectron spectra of *m*-benzyne. We support our observations by conducting Franck-Condon simulations of *m*-benzyne and assigning the observed signals to a vibrational progression in the cation.

Second, the high-temperature reaction products of *m*-benzyne were investigated at the free electron laser, FELIX, in Nijmegen, NL. The setup couples the IR beam of the free electron laser in the mid-IR region with a UV laser to perform mass-selective IR/UV ion dip spectroscopy. This enables the separate recording of the IR spectrum of each mass present in the gas phase. Our findings indicate strong similarities between the bimolecular products of *m*-benzyne and *o*-benzyne, which was investigated in our group previously.[2]



References

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