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Pentadiynylidene, Methylpentadiynylidene and Dimethylpentadiynylidene: Threshold Photoelectron Spectroscopy of $R^1-C_5-R^2$ Carbon Chains

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The three unsaturated and carbon-rich pentadiynylidenes of the composition $R^1-C_5-R^2$ are highly reactive biradicals or triplet carbenes in the electronic ground state of the neutral. Nevertheless, they occur as intermediates in harsh chemical environments. Particularly in the chemistry of interstellar medium [1], planetary atmospheres [2] and in combustion processes of fuel-rich hydrocarbon flames [3] these triplet carbenes are key components. They were only briefly studied by matrix isolated technique coupled with IR, EPR and UV/VIS spectroscopy [4]. Threshold Photoelectron Spectra (TPES) of $H-C_5-H$, $Me-C_5-H$ and $Me-C_5-Me$ with predominant carbene character at C3 didn't exist.

To obtain first insights we applied double imaging Photoelectron Photoion Coincidence (i^2 PEPICO) Spectroscopy in this study, which is capable to supply mass selective TPES.

1-Diazo-penta-2,4-diyne, 1-diazo-hexa-2,4-diyne and 2-diazo-hexa-3,5-diyne, synthesized by the procedure of Bowling et al. [4], were selected as precursors generating triplet pentadiynylidene, methylpentadiynylidene and dimethylpentadiynylidene. Afterwards, the corresponding carbenes were produced by flash pyrolysis, stabilized in the gas phase and photoionized by tunable vacuum ultraviolet synchrotron radiation.

This presentation will offer first results in the photoelectron spectroscopy of pentadiynylidenes, executed at the Swiss Light Source (SLS) for synchrotron radiation (Villigen, Switzerland).

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Summary

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