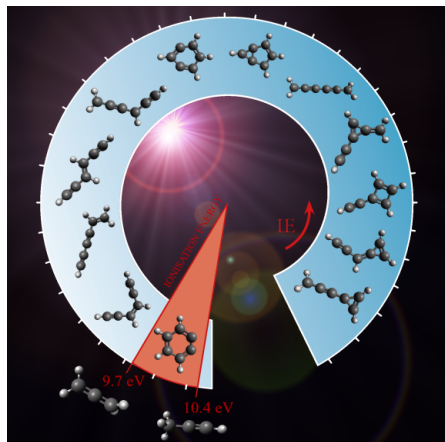


STRUCTURAL ELUCIDATION OF IONS USING CHEMICAL REACTIONS

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A general method is proposed to disentangle isomeric structures by combining mass spectrometry, tunable synchrotron light source, and quantum-chemistry calculations. Reactive chemical monitoring technique is used and consists in tracking reactivity changes as a function of photoionization energy *i.e.*, internal energy related to isomerization barriers. The capability of this technique will be illustrated with charge transfer reactions of $C_6H_4^+$ isomers with allene and propyne.^a The methodology can be generalized using neutral reaction partners with ionization energies forming a chemical ruler to elucidate the ionic structure. It can also serve as a structural probe as a function of photoionization energy, unveiling isomerization routes.

^a Jacovella *et al.* Structural elucidation of $C_6H_4^+$ using chemical reaction monitoring: Charge transfer versus bond forming reactions, *ChemPhysChem* (2021), doi: 10.1002/cphc.202100871
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