Computational modelling of the ionization of organic biradicals

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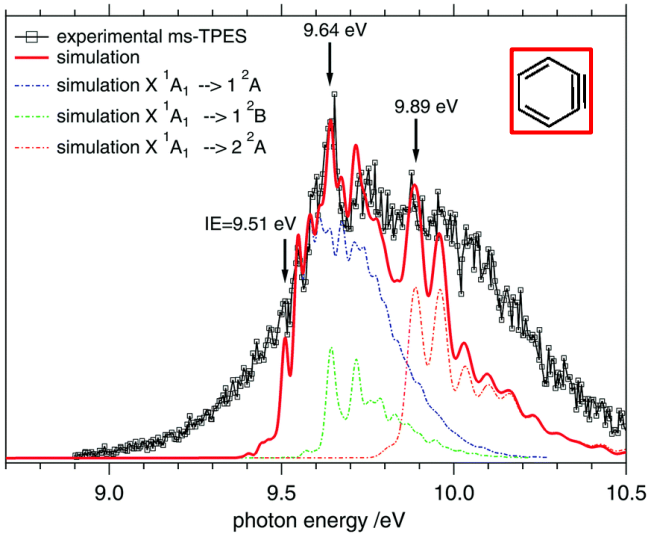
We use high-level computational approaches to investigate the spectroscopy of the organic biradicals *ortho*-benzyne and pentadiynylidene. Comparison with experimental data obtained from mass-selective threshold photoelectron spectroscopy highlights the varying goodness of different quantum-chemical approaches. For both systems, more approximative methods can be seen to fail even in the qualitatively correct prediction of the system's structure & properties. We highlight these potential pitfalls and conclude some key learning for the accurate prediction of ionization energies of biradicals.



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References

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