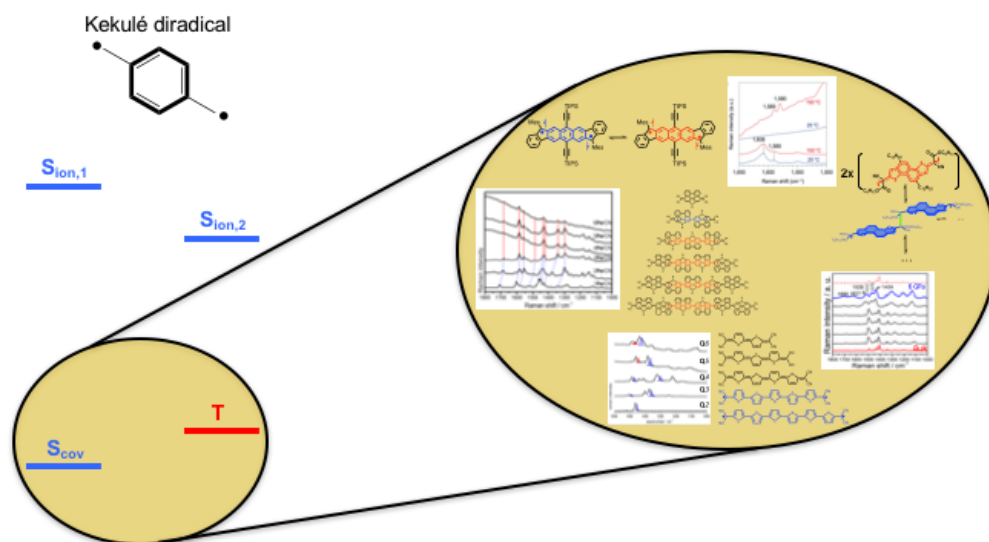


# Raman Spectroscopy as a Versatile Tool to Study Organic Biradicals

J. L. Zafra<sup>1</sup>, J. Casado<sup>1</sup>

<sup>1</sup> Department of Physical Chemistry, University of Malaga, 29071 Malaga, Spain  
([zafra@uma.es](mailto:zafra@uma.es))

In recent years, there has been a renewed interest in the study of open-shell polycyclic aromatic hydrocarbons (PAHs). Among them, biradicals are characterized by a four states energetic model for the low lying electronic states  $S_0$ ,  $S_1$ ,  $S_2$ ,  $T_1$ . Such a distribution is related to the attractive electronic, magnetic and optical properties which make biradicals promising candidates for a wide range of applications in organic electronics, such as nonlinear optics, molecular spintronics, energy storage and organic photovoltaic devices sensitized by singlet fission. Despite all the promising properties predicted for open-shell PAHs, a common drawback still needs to be overcome: the high reactivity of radicals, which implies that most open-shell species tend to be too short-lived for practical applications and even for characterization [1]. In this regard, Raman spectroscopy has shown to be a suitable tool for studying this kind of molecular systems, able to provide valuable information that could be used in the development of new synthetic approaches [2].



Herein we report the study of different open shell PAHs with biradical character with the aim to highlight how Raman spectroscopy can help us to elucidate the molecular structure and the electronic configuration of their ground states and how the molecular information provided can be used to rationalize their properties in the context of the four states model [3], [4], [5].

## References

- [1] *J. Mater. Chem.* **2012**, 22, 4151
- [2] *Angew. Chem. Int. Ed.* **2017**, 56, 2250
- [3] *Nat. Chem.* **2016**, 8, 753
- [4] *Angew. Chem. Int. Ed.* **2016**, 55, 14563
- [5] *Angew. Chem. Int. Ed.* **2015**, 54, 5888

