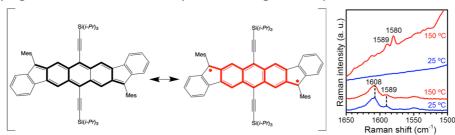
## RAMAN SPECTROSCOPY MEETS ORGANIC BIRADICALS. STUDY OF A NEW DIINDENO[B,I]ANTHRACENE DERIVATIVE

<u>J. L. Zafra</u><sup>1</sup>, G. Rudebusch<sup>2</sup>, K. Jorner<sup>3</sup>, G. López Espejo<sup>1</sup>, M. Peña-Álvarez<sup>4</sup>, I. Arretxea Marcos, <sup>1</sup>, R. Ponce Ortiz<sup>1</sup>, C. J. Gómez-García<sup>5</sup>, H. Ottoson<sup>3</sup>, M. M. Haley<sup>2</sup>, J. Casado<sup>1</sup>

- Department of Physical Chemistry, University of Malaga, 29071 Malaga, Spain (zafra@uma.es)
  Department of Chemistry and Materials Science Institute, University of Oregon, OR 97403-1253, USA
  - Department of Chemistry BMC, Uppsala University, Box 576, 751 23 Uppsala, Sweden
  - Department of Physical Chemistry, Complutense University of Madrid, 28040 Madrid, Spain
    ICMOL, Universidad de Valencia, 46980, Paterna, (Valencia) Spain

Raman, Quinoidal, Biradicals, Ambipolar, Electrochemistry, Pressure, Temperature

In recent years, there has been a renewed interest in the study of open-shell polycyclic aromatic hydrocarbons (PAHs). Among them, biradicals exhibit attractive electronic, magnetic and optical properties which make them 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 of 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 aplications and even for characterization <sup>[1]</sup>. In this regard, Raman spectroscopy has shown to be a suitable tool for studying this kind of molecular systems, being able to provide valuable information.



This work reports the study of a new biradical, diindeno[b,i]anthracene (DIAn)<sup>[2], [3]</sup>, highlighting the crucial role played by Raman Spectroscopy in the characterization of the ground electronic state as well as in the rationalization of the ambipolar behavior shown in OFETs. To this end, neutral and charged species has been studied by Raman spectroscopy as a function of excitation wavelength, temperatura and pressure.

## Referencias

- [1] Z. Sun, J. Wu. J. Mater. Chem. 2012, 22, 4151-4160.
- [2] G. E. Rudebusch, José L. Zafra, K. Jorner, K. Fukuda, J. L. Marshall, I. Arrechea-Marcos, Guzmán L. Espejo, R. Ponce Ortiz, Carlos J. Gómez-García, Lev N. Zakharov, M. Nakano, H. Ottosson, Juan Casado, Michael M. Haley, *Nat. Chem.* **2016**, *8.*, 753-759.
- [3] G. E. Rudebusch, Guzmán L. Espejo, José L. Zafra, M. Peña-Alvarez, S. N. Spisak, K. Fukuda, Z. Wei, M. Nakano, M. A. Petrukhina, Juan Casado, and Michael M. Haley, JACS. 2016, 138., 12648-12654.