

## PIEZOCROMIC PROPERTIES OF PYRIDIL DIVINYL ANTHRACENE DERIVATIVES: A JOINT RAMAN AND DFT STUDY

S. Fernández-Palacios<sup>1</sup>, M. Peña-Álvarez<sup>2</sup>, V. G. Baonza<sup>2</sup>, Bin Xu<sup>3</sup>, Suqian Ma<sup>3</sup>, J. T. López Navarrete<sup>1</sup>, M. Moreno Oliva<sup>1</sup>, M. C. Ruiz Delgado<sup>1</sup>

<sup>1</sup> Department of Physical Chemistry, University of Malaga, Campus de Teatinos s/n, 229071, Malaga, Spain, sarafpc@uma.es

<sup>2</sup> MALTA-Consolider Team, Department of Physical Chemistry, Chemistry Faculty, University Complutense of Madrid, 28040 Madrid, Spain

<sup>3</sup> State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Qianjin Street No. 2699, Changchun 130012, China.

**Palabras Clave:** *compuestos  $\pi$ -conjugados, piezocromismo, Raman, DFT*

Piezochromic materials, which show color changes resulting from external pressure or mechanical grinding, are of great interest from a scientific viewpoint owing to their potential applications as pressure-sensing and optical-recording systems.[1] It has been recently discovered solid-state fluorescence properties and piezochromic luminescence in a family of 9,10-Bis((E)-n-(pyrid-2-yl)vinyl)anthracene, BPnVA (n=2 orto-,3 meta- and 4 para-) compounds, see Figure 1.[2] The crystal structures indicate that the three compounds with varying position of the nitrogen on the external pyridyl exhibit different molecular packing modes. In this work, we aim at providing further insight into the interplay played by the molecular and supramolecular structural changes and the luminescence changes observed under pressure by using a combined experimental-theoretical approach that links Raman spectroscopy with DFT calculations.

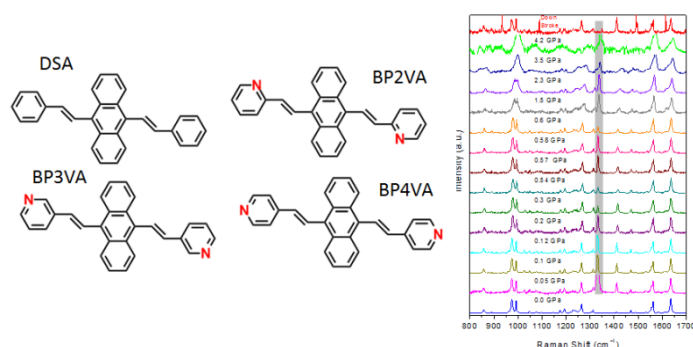


Figura 1. (Left) Chemical structures of the anthracene-based compounds under study and (right) Variable pressure Raman spectra of BP2VA.

### Referencias

- [1] M. Harun-UrRashid, T. Seki, Y. Takeoka, *Chem. Rec.* **2009**, *9*, 87.  
[2] a) J. Zhang, J. Chen, B. Xu, L. Wang, S. Ma, Y. Dong, B. Li, L. Ye and W. Tian *Chem. Commun.* **2013**, *49*, 3878. b) Y. Dong, B. Xu, J. Zhang, X. Tan, L. Wang, J. Chen, H. Lv, S. Wen, B. Li, L. Ye, B. Zou, W. Tian, *Angew. Chem.* **2012**, *124*, 10940–10943. c) Y. Dong, J. Zhang, X. Tan, L. Wang, J. Chen, B. Li, L. Ye, B. Xu, B. Zou and W. Tian *J. Mater. Chem. C*, **2013**, *1*, 7554.