Raman Spectroscopy as a Versatile Tool to Study Organic Biradicals

Juan Casado,[a] José Luis Zafra,[a] David Casanova,[b] Xiaozhang Zhu[c] y Samara Medina[a]

[a] *Department of Physical Chemistry, Faculty of Science, University of Málaga, Andalucía Tech, Campus de Teatinos, s/n 29071 Málaga, Spain.*
[b] *IKERBASQUE - Basque Foundation for Science (DC) & Donostia International Physics Center & Kimika Fakultatea, Euskal Herriko Unibertsitatea, Paseo Manuel de Lardizabal, 4, 20018 Donostia-San Sebastián, Euskadi, Spain.*
[c] *Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Organic Solids, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China. 4School of Chemistry and Chemical Engineering, University of Chinese Academy of Sciences, Beijing 100049, P. R. China*
samara@uma.es

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Since π-conjugated organic molecules were probed as potential semiconducting materials, suitable for replacing the widely used silicon technologies, their structural, optical and conductive properties have been under study to improve their application in organic electronics and to make possible their *ad hoc* synthesis. In this sense, the modification of the π-electron delocalization path is one of the available tools to tune the properties of the molecules to obtain the desired characteristics for the fabrication of these devices.

One of the parameters employed to tailor π-conjugated organic molecules for organic electronics is the diradical character. A progressive change in the diradical contribution to the ground electronic state structure can tune some of the main system features, highlighting the HOMO-LUMO energy gap and the aggregation mode. The main drawback of this approach is the loss of chemical stability when increasing the diradical character of these molecules.

On the other hand, the π-electron delocalization can be interrupted introducing a perpendicularly conjugated path. The competition of these two cross-conjugated patterns leads to a new 2-dimensional delocalization scenario that changes the electronic properties of the studied materials.

In this project, we present a stable quinoidal quaterthiophene diradical that possess outstanding stability and conductivity properties. [1] The combination of the diradical character together with the possibility to delocalize the electron density through two different perpendicular paths explain its exceptional behavior in comparison with the other members of the series, or with its linearly conjugated analogues. The balance between these two properties has been evaluated through UV-Vis-NIR electronic spectroscopy and Raman and IR vibrational spectroscopy in the neutral and charged forms of the target molecule and similar non-cross-conjugated samples.

References

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