Theoretical and experimental absorption spectra study of [(FeTPPbipy)\textsubscript{n}] by means of TD-DFT calculations

A. Fidalgo-Marijuan\textsuperscript{a}, G. Barandika\textsuperscript{b}, B. Bazán\textsuperscript{a}, M. K. Urtiaga\textsuperscript{a}, M. I. Arriortua\textsuperscript{a}

\textsuperscript{a}Department of Mineralogy and Petrology, University of the Basque Country (UPV/EHU), Apdo. 644, 48080 Bilbao (Spain)
\textsuperscript{b}Department of Inorganic Chemistry, University of the Basque Country (UPV/EHU), Paseo de la Universidad 7, 01006 Vitoria-Gasteiz (Spain)

Iron metallocorphyrins are paradigmatic examples of nanodevices used by natural systems like haemoglobin or cytochromes in oxygen transport, electron transfer and catalysis.\textsuperscript{1} Therefore, they can be thought to be developed as MOFs for several applications, and the UV-Vis spectra of metallocorphyrins is a powerful tool to understand their electronic behaviour analyzing the typical Soret and Q bands.

In this work, we have characterised the UV-Vis spectrum of [(FeTPPbipy)\textsubscript{n}]\textsubscript{=} (TPP= meso-tetraphenylporphyrin, bipy= 4,4’-bipyridine) neutral radical from both experimental and theoretical point of view. The later has been carried out by means of Time Dependent-Density Functional Theory (TD-DFT) calculations.\textsuperscript{2}

The interest of this compound lies on the presence of an unpaired electron per metallic centre that is delocalised on the phenyl groups of TPP. Moreover, the π-stacking of the crystal structure, is the crucial point on the behaviour of this compound.

**Introduction**

**Experimental**

![UV-Vis absorption spectrum](image)

A weak and broad band at 690 nm is in accordance with the presence of a porphyrinic radical.\textsuperscript{4}

**Theoretical**

![Theoretical spectra](image)

Conclusions

- The blue shifted Soret band indicates the presence of a radical specie.
- The π-stacking along the crystal structure is the responsible of the electron pairing.
- An important charge transfer takes place between the phenyl groups and the metal centre of the porphyrin.

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**References**