

# Segundo Simposio Iberoamericano de Química Orgánica (SIBEAQO-II)

## Libro de Abstracts



8-12 de Septiembre, 2010  
Santiago de Compostela, España

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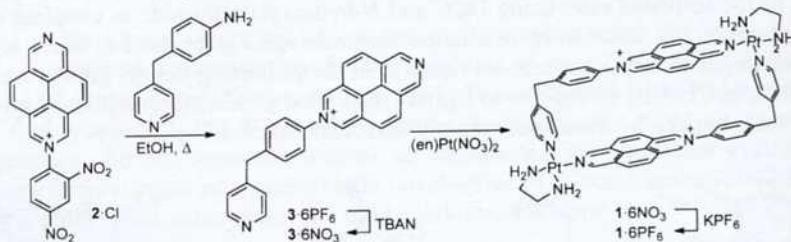
Luis A. Martínez

## COMPLEXATION AND EXTRACTION OF PYRENE TO THE AQUEOUS PHASE USING A DINUCLEAR Pt<sup>II</sup> DIAZAPYRENium-BASED METALLOCYCLE

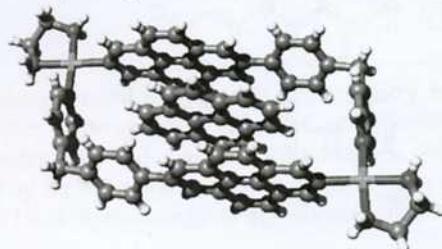
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Polycyclic aromatic hydrocarbons (PAHs) represent an important group of environmental pollutants owning two or more fused aromatic rings.<sup>1</sup> PAHs are characterized by its hydrophobicity and tendency to accumulate in the organic matter. Appropriate extraction techniques able to enhance the solubility of the compounds, in order to remove their entire labile fraction to an aqueous media, are highly required. Following our ongoing investigations on the complexation of PAHs in aqueous media,<sup>2</sup> we report here the synthesis and characterisation of a new dinuclear Pt<sup>II</sup> diazapypyrenium-based metallocycle (**1**), capable of forming 1:1 inclusion complexes with Pyrene (PYR) in organic and aqueous media.



The above-mentioned complexes PYR $\subset$ 1·6PF<sub>6</sub>/6NO<sub>3</sub>, in CD<sub>3</sub>CN and D<sub>2</sub>O, were studied by 1D and 2D NMR. The Job plot for PYR $\subset$ 1·6PF<sub>6</sub> in CH<sub>3</sub>CN was in good agreement with a 1:1 stoichiometry, that it was further confirmed by single crystal X-ray crystallography. The association constants in CH<sub>3</sub>CN (10704 $\pm$ 766 M<sup>-1</sup>) and H<sub>2</sub>O (5.59 $\times$ 10<sup>5</sup> M<sup>-1</sup>) were determined by U.V. dilution method and liquid-liquid extraction, respectively.



Crystal structure of PYR $\subset$ 1·6PF<sub>6</sub>. Solvent molecules and counterions omitted for clarity. Colour code: C, grey; H, light grey; N, blue; Pt, orange.

### Acknowledgements

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### References

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- (2) Peinador C, Pia E, Blanco V, García MD, Quintela JM. *Org. Lett.* **2010**, 12, 1380–1383.