Mini-Symposium

***ISIS** – 8, allée Gaspard Monge, 67000 Strasbourg*

Chirality – from molecular engineering to high resolution chiroptical spectroscopy

Tuesday, September 19th, 3 pm

at ISIS-2, entry from ISIS main building

15:00 **Jeanne Crassous**, *Univ. Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes)*

Properties of helicene-based supramolecular assemblies

15:45 **Anne Zehnacker**, *Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Université Paris-Saclay*

Spectroscopic studies of chiral molecules

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see abstracts below

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Properties of helicene-based supramolecular assemblies

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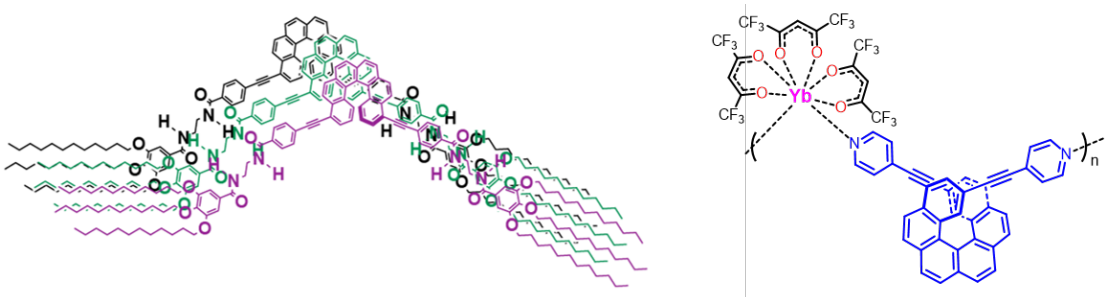
Ortho-fused aromatic rings form helically shaped chiral molecules such as carbo[6]helicenes, that wind in a left-handed (M) or a right-handed (*P*) sense.[1] The helical topology combined with extended π-conjugation provides helicenes with peculiar properties such as strong photophysical and chiroptical properties (high optical rotation values, intense electronic circular dichroism and circularly polarized emission). The molecular engineering of helicenes using organometallic and heteroaromatic chemistries offers a convenient way to generate supramolecular assemblies and to tune the properties of these helically shaped π-ligands architectures. Indeed, their combination with metallic or organic assembling units leads to chiral materials with appealing properties (circularly polarized phosphorescence, magnetochirality, spin selectivity) for applications in materials science (Circularly Polarized OLEDs, Chiroptical Switches, Spintronics). I will present a set of representative examples.[2]



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[2] a) R. Rodríguez, C. Naranjo, A. Kumar, P. Matozzo, T.-K. Das, Q. Zhu, N. Vanthuyne, R. Gómez, R. Naaman, L. Sánchez, J. Crassous, *J. Am. Chem. Soc.* **2022**, *144*, 7709 ; b) K. Dhbaibi, M. Grasser, H. Douib, V. Dorcet, O. Cador, N. Vanthuyne, F. Riobé, O. Maury, S. Guy, Amina Bensalah-Ledoux, B. Baguenard, Geert L. J. A. Rikken, C. Train, B. Le Guennic, M. Atzori, F. Pointillart, J. Crassous, *Angew. Chem. Int. Ed.* **2023**, 62, e202215558.

Spectroscopic studies of chiral molecules

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The two enantiomers of a chiral molecule can be distinguished by using a probe that is itself chiral. This probe can be of chemical nature, *i.e.* another molecule, a surface, or generally speaking a chiral environment, or of physical nature, *i.e.* a circularly polarised light. I will illustrate these two aspects with gas-phase spectroscopy experiments.

Spectroscopic studies of weakly bound molecular complexes isolated in the gas phase at low temperature provide information on the nature of the forces responsible for chiral recognition.[1] I will present the study of systems used in chiral stationary-phase chromatography[2] or involved in biological processes such as the transmission of nerve impulses.[3]

Photoelectron circular dichroism manifests itself by an asymmetry in the angle of electron ejection following the ionisation of a chiral molecule by a circularly polarised light. I will describe experimental results that show the sensitivity of PECD to molecular conformation and long-range interactions.[4, 5]

References

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2. Hirata K., Mori Y., Ishiuchi S. I., Fujii M., Zehnacker A. Chiral discrimination between tyrosine and beta-cyclodextrin revealed by cryogenic ion trap infrared spectroscopy. *Physical Chemistry Chemical Physics* **22**, 24887-24894 (2020).

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