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Fondation Jean-Marie Lehn

Open PhD thesis

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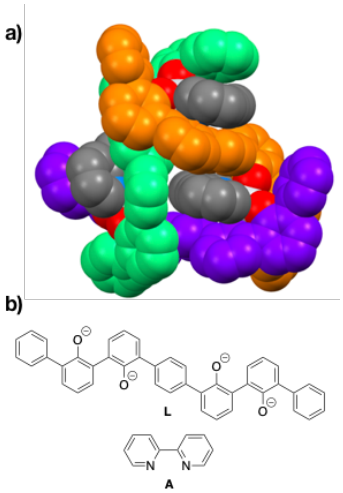

Figure 1. a) X-ray crystal structure of ΛΛΔ-[$Ti_3L_3(A)_3$] (C_1 symmetry) in space-fill model. For clarity, the strands L are differently colored (purple, orange, and green). Color code: carbon for the 2,2′-bipyridine ligand, dark gray; nitrogen, blue; oxygen, red; and titanium, light gray. Hydrogen atoms have been omitted for the sake of clarity. b) Representation of ligands **L** and **A**.

Project

This PhD project aims to propose a unique archetype of molecular device based on a homochiral-to-heterochiral reversible switch. The molecular systems involved in the project are self-assembled trinuclear Ti(IV)-based architectures constructed around chiral TiO_4N_2 nodes (Δ or Λ configuration) (figure 1).[1] We propose two approaches to render a stereochemical switch (represented in figure 2) more efficient and faster. The first approach implies the reduction of the size of the ligands surrounding the metallic centers within the trinuclear complex to facilitate the heterochiral (Δ, Δ, Λ or Λ, Λ, Δ) to homochiral (Δ, Δ, Δ or Λ, Λ, Λ) transformation. The second strategy deals with the formation of supramolecular complexes in the presence of an ammonium cation to displace the homochiral ⇄ heterochiral equilibrium towards the formation of the homochiral species ⊂ ammonium cation complex. Overall, we propose to develop a new prototype of molecular machinery relying on a reversible stereochemical transformation.

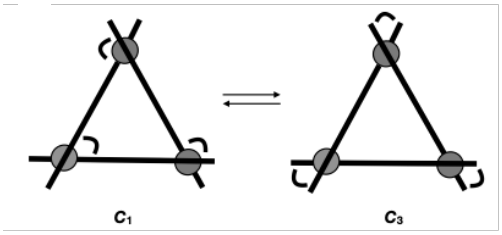

Figure 2. Schematic representation of the equilibrium between C_3-[$Ti_3\mathbf{L}_3(\mathbf{A})_3$] and C_1-[$Ti_3\mathbf{L}_3(\mathbf{A})_3$] in CH_2Cl_2. The straight lines symbolize the **L** ligand, the curved lines symbolize the nitrogen chelate **A**, and the round spots are Ti(IV).

Keywords

organic synthesis – coordination chemistry - metallosupramolecular system – computational simulation

Candidates

Organic synthesis, coordination chemistry and structure determination of new architectures are central tasks in daily work of this thesis. Successful candidates should have a solid experience in synthetic chemistry, an open mind for interdisciplinary research (physical chemistry, spectroscopy) autonomy and teamwork. In addition, the candidate will be involved in understanding dynamic phenomena using **computational simulations**. This part of the work will be supervised by Dr A. Chaumont (MSM team, UMR 7140). The candidate will be encouraged to present her/his results at national and international conferences. The thesis will be funded by the "foundation Jean-Marie Lehn" of the University of Strasbourg.

Contact

To apply, please send your cover letter, CV (with references), and the marks of the M1/M2 degree (if available) to Dr. P. MOBIAN (mobian@unistra.fr).

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[1] P. Mobian, D.-J. Pham, A. Chaumont, L. Barloy, G. Khalil, N. Kyritsakas, *J. Am. Chem. Soc.*, **2024**, 146, 20, 14067–14078.