

Towards improved lanthanide-based single-molecule magnets based on novel sandwich complexes with polyaromatic hydrocarbons

Single molecule magnets (SMMs) are nanoscale materials which retain magnetization for relatively long time in the absence of external magnetic field. In contrast to *e.g.* ferromagnets found in everyday life, for SMMs this property is not the consequence of collective ordering of paramagnetic centers, but it arises from their specific electronic structure resulting in magnetic anisotropy of the paramagnetic ion. Owing their potential applications in quantum computers or as memory carriers with extremely high storage density, there is an ongoing research to enhance the performance of such materials. The main problem to solve is to rise so called blocking temperature (T_b), which is the temperature below which the SMM character is observed. Until recently, these were temperatures as low as -260°C and currently the record value is 80 K (-193°C), *i.e.* 3°C above boiling point of liquid nitrogen. Design of novel SMMs with high T_b is a very demanding, but based on recent findings the most promising in this respect are lanthanide (Ln; like dysprosium or thulium) compounds where the central cation surrounding has uniaxial symmetry. The abovementioned record holder is the example of such a compound where dysprosium is placed between two 5-membered aromatic rings.

The project aims to synthesize a series of sandwich lanthanide (Ln) complexes with large ligands based on 6-membered ring polyaromatic hydrocarbons (PAH): truxene (Fig. 1) and triphenylene. Such complexes with 6-membered aromatic rings are still very rare for lanthanide cations. However, the advantages of the PAHs selected in this project include their size, flat geometry, stiffness as well as ability to modify their structure. This can be realized by *e.g.* reducing to anionic form with charges down to -3 or introduction of substituents varying in size or electron withdrawing/donating properties in different positions of the molecule. Aside of that, the properties of the final Ln-PAH complex are also influenced by the counteranion used to balance the overall charge. To screen this influence small halides, larger AlCl_4^- or very large weakly coordinating anions such as perfluorinated alkoxyaluminates or aryloborates will be used.

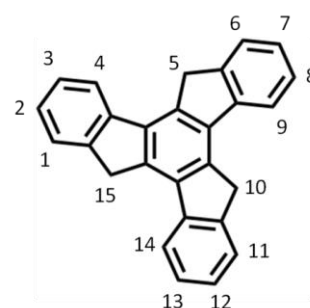


Figure 1. Structure of truxene molecule with numbering of carbon

The realization of this interdisciplinary project will include several tasks involving research groups from Poland (University of Warsaw) and Slovenia (Jožef Stefan Institute). The first step will be the synthesis of the above mentioned PAHs and their derivatives. These will be used in the second step, *i.e.* the synthesis and thorough characterization of Ln complexes, with the emphasis on determination of crystal structure and magnetic properties. Although this is not the main goal of the project, fluorescence measurements will also be performed, since compounds containing Ln and PAHs in spatial vicinity are known to be valuable luminescent materials. In parallel with experiments, theoretical studies will be carried out in order to gain insight into the nature of these systems and to understand the properties they exhibit.

The results of the project will make an important contribution to science. Judging from the recent research, the proposed compounds could have very good SMM performance. Moreover, the results obtained would be valuable for further research in this field by understanding the whole SMM phenomenon. If very high T_b values, *i.e.*, above 80 K, are obtained, it would bring the practical application of SMM closer. Aside of this, the complexes obtained will extend the coordination chemistry of the Ln-PAH family, which currently does not contain examples of PAHs larger than 4-ring molecules. This would be beneficial not only for coordination chemistry but also for research on key magnetic and luminescent materials.