

PNII-RU-TE-2012-3-0422

Chiral building-blocks in designing molecular magnetic materials



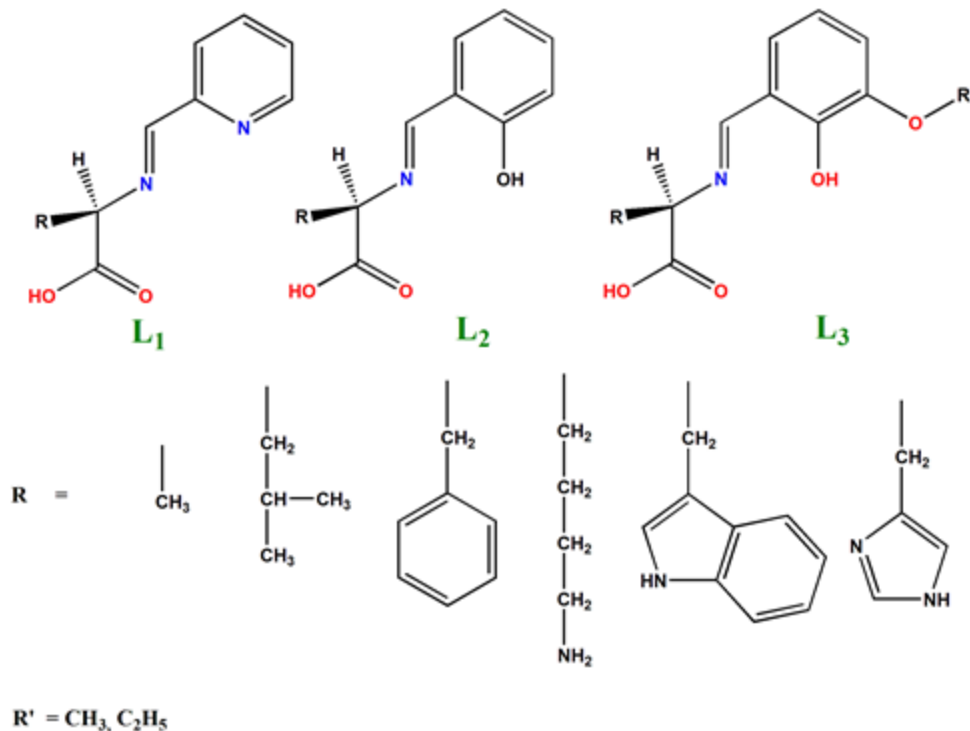
2013-2016



**Director de proiect,
CS III Catalin Maxim**

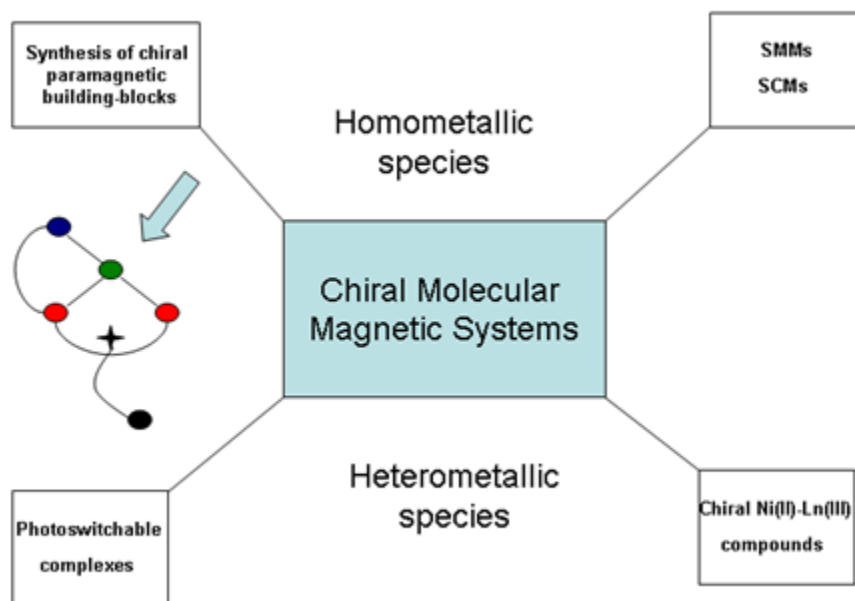
Project description

The present project will focus on the synthesis and characterization of new chiral molecular systems based on amino-acids derivatives using the molecular approach strategy to produce compounds of interest in materials science. Three families of the ligands will be obtained, using different chiral amino-acids



Methodology

The molecular approach allows to define a global designing scheme. Then the targeted building blocks can be synthesised and, to some extent, studied separately. A one-to-one interaction will lead to specific results that will be gathered to lead to the final processed materials.



Main objectives

1. Design of chiral tridentate Schiff Base.
2. Design of (i) new classical 3-D molecule-based magnets by combining magnetic properties with other properties (especially chirality); (ii) new homo-metal and heterometal Single Molecule Magnets by employing original ligands, including chiral ligands, as a prerequisite for obtaining, in a rational way, chiral magnets; (iii) Single Chain Magnets based on new chiral tectons.
3. Magneto-structural correlations in heterometallic complexes..
4. Design of novel chiral photomagnetic materials: Cu(II)-Mo(IV), Co(II)-Mo(V)
5. Design of photoswitchable heterobi- and heterotrimetallic Single Molecule Magnets and Single Chain Magnets.
6. Design of new chiral heterodinuclear systems Ni(II)-Ln(III).

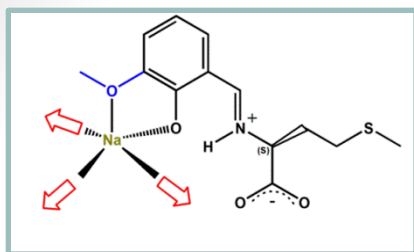
Project team

- CS III Catalin Maxim
- CS Ene Cristian Dumitru
- AC Dogaru Andreea
- AC Mocanu Teodora
- Tehn. Cazacu Stefana

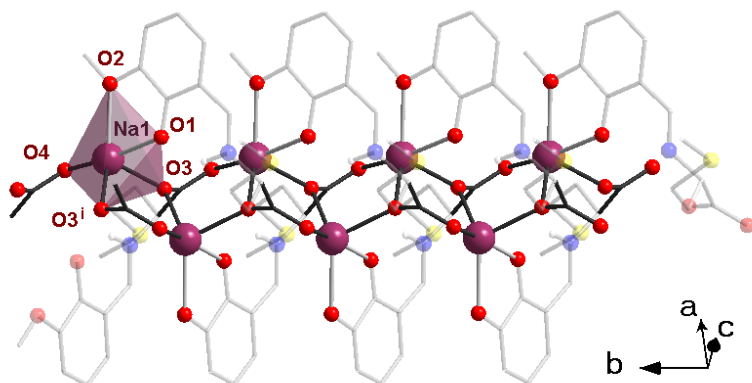
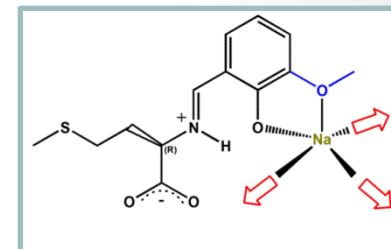
Project Budget

NR. CRT	DENUMIRE CAPITOL BUGET	TOTAL VALOARE 2013 (lei)	TOTAL VALOARE 2014 (lei)	TOTAL VALOARE 2015 (lei)	TOTAL VALOARE 2016 (lei)	TOTAL VALOARE (lei)
1.	CHELTUIELI DE PERSONAL	147583	125000	90000	15000	377583
2.	CHELTUIELI INDIRECTE (regie)	34500	24150	27000	10350	96000
3	CHELTUIELI DE DEPLASARE	5564,95	8000	10000	2000	25564,95
4.	CHELTUIELI DE LOGISTICĂ	76852,05	28000	80000	52000	236852,05
	TOTAL	264500	185150	207000	79350	736000

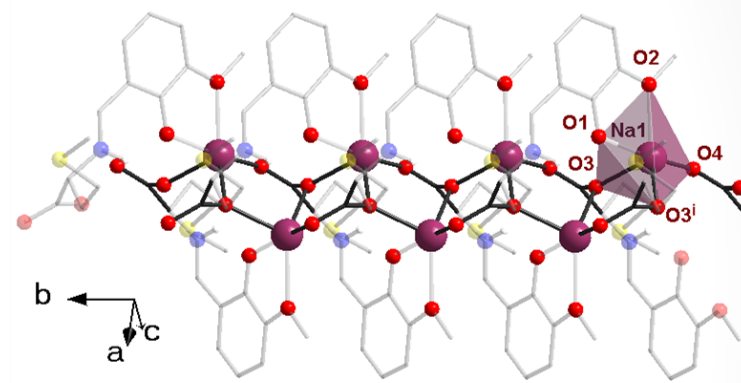
Design of new chiral tridentate Schiff Base.



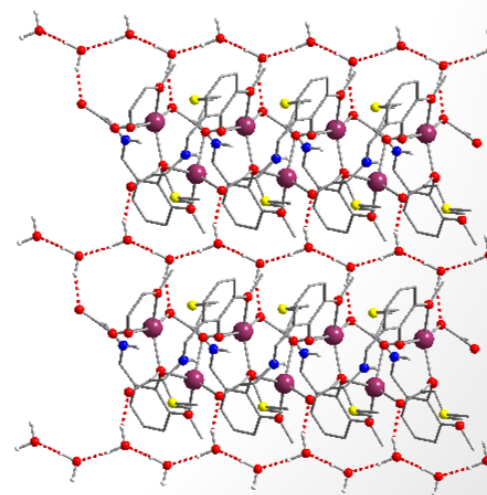
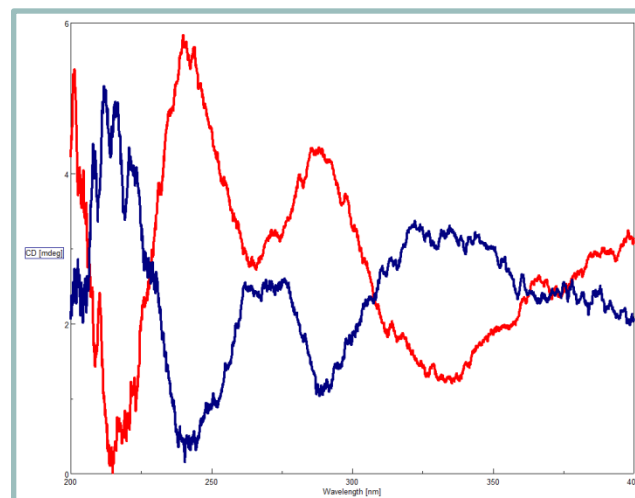
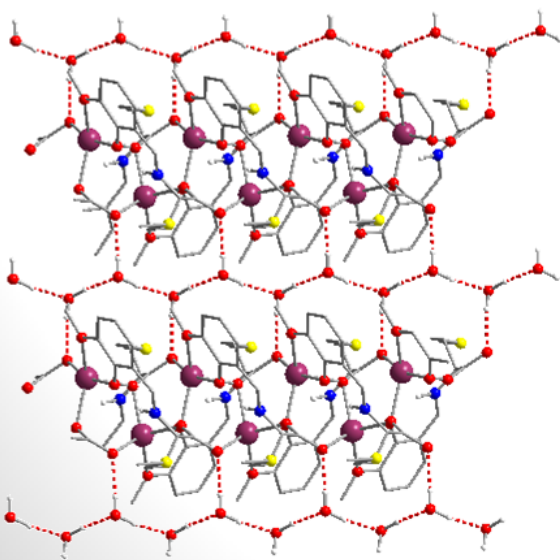
<i>Monoclinic</i>	Crystal System	<i>Monoclinic</i>
<i>P 2₁</i>	Space Group	<i>P 2₁</i>
11.227 (3)	<i>a</i> (Å)	11.132 (3)
4.8463 (11)	<i>b</i> (Å)	4.7999 (11)
15.658 (5)	<i>c</i> (Å)	15.493 (5)
90.00	α (°)	90.00
109.78 (2)	β (°)	109.84 (2)
90.00	γ (°)	90.00
801.7 (4)	<i>V</i> (Å ³)	778.7 (4)



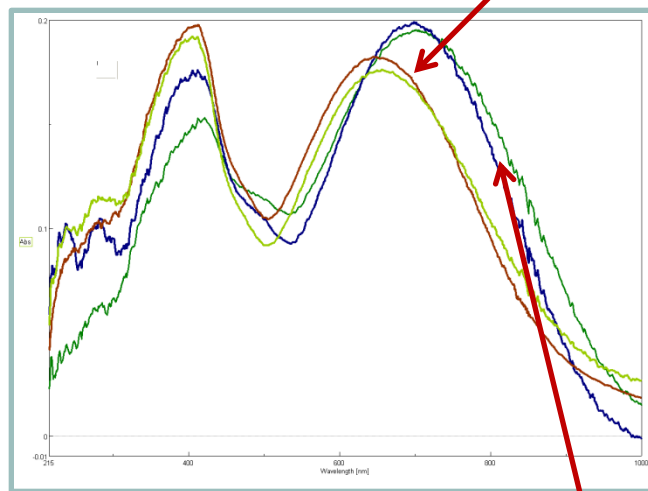
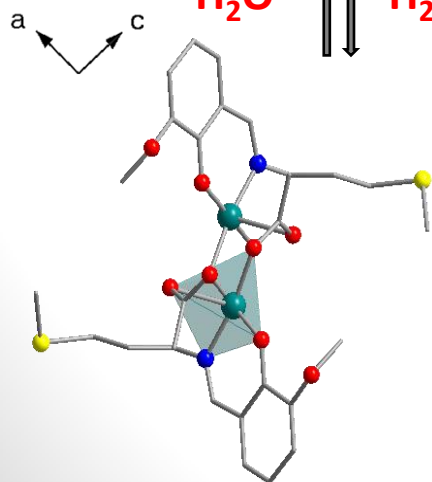
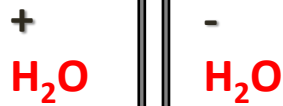
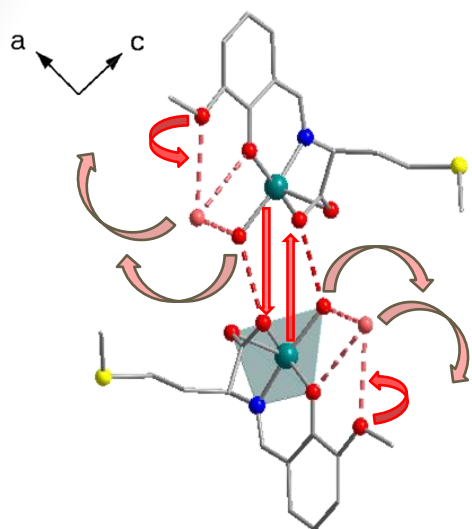
Na(Va-L-Met)



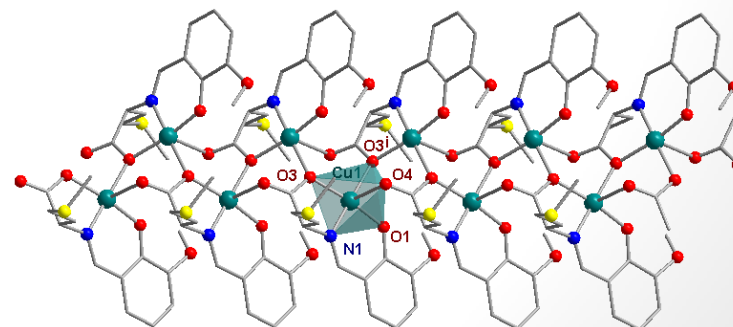
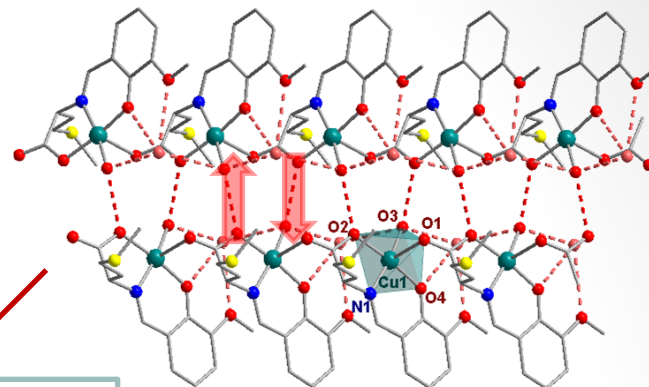
Na(Va-D-Met)

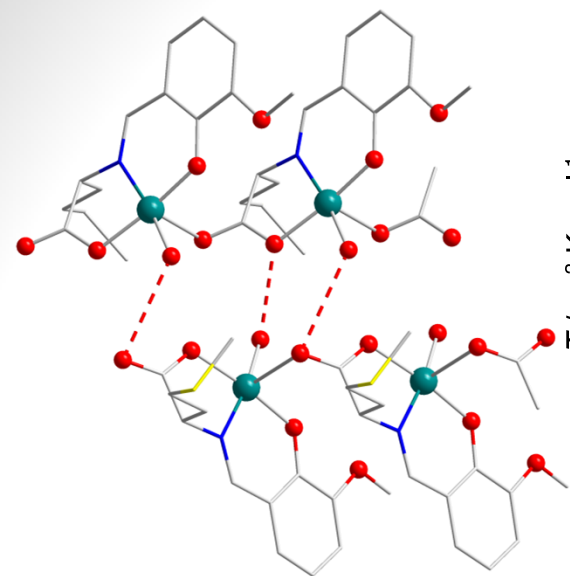


Reversible SCSC Transformation of a Chiral Chain Containing Tridentate Schiff Bases

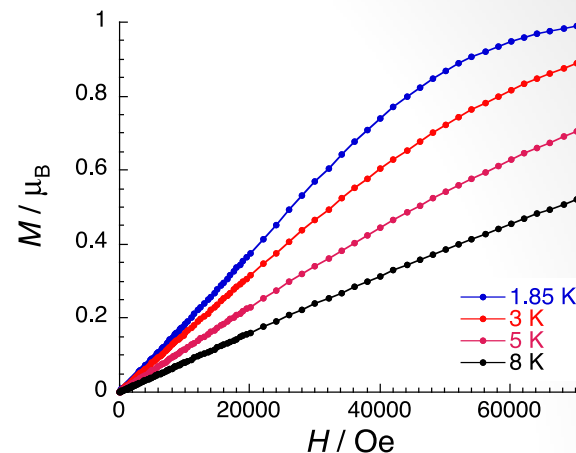
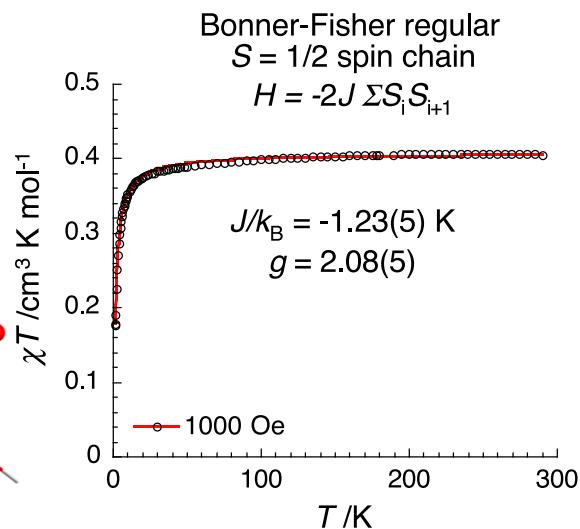


UV-VIS Spectra

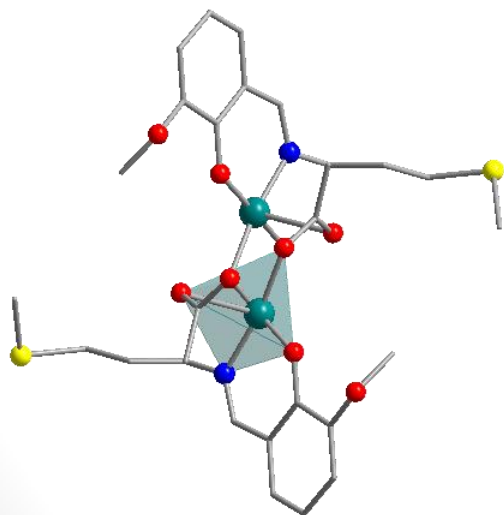




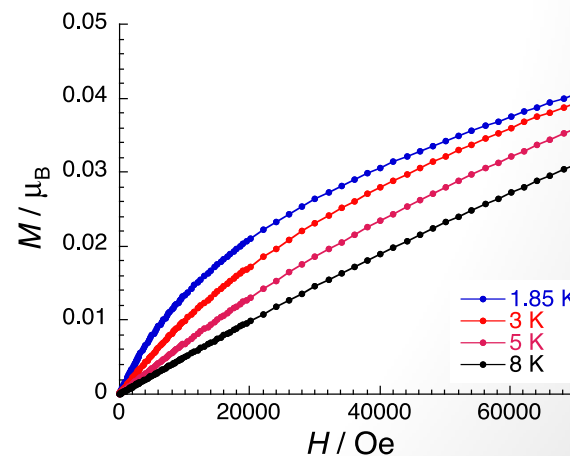
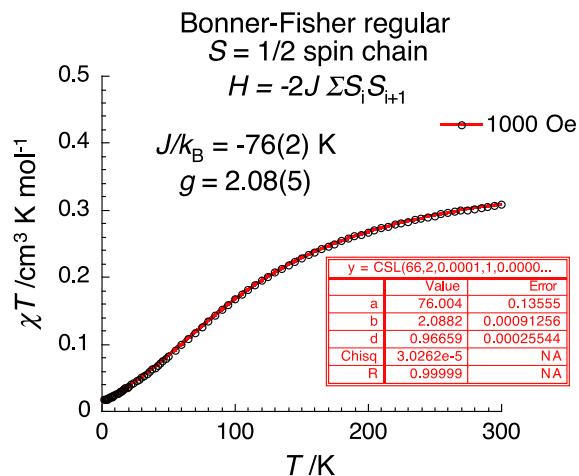
[Cu(Va-L-Met) H₂O] H₂O



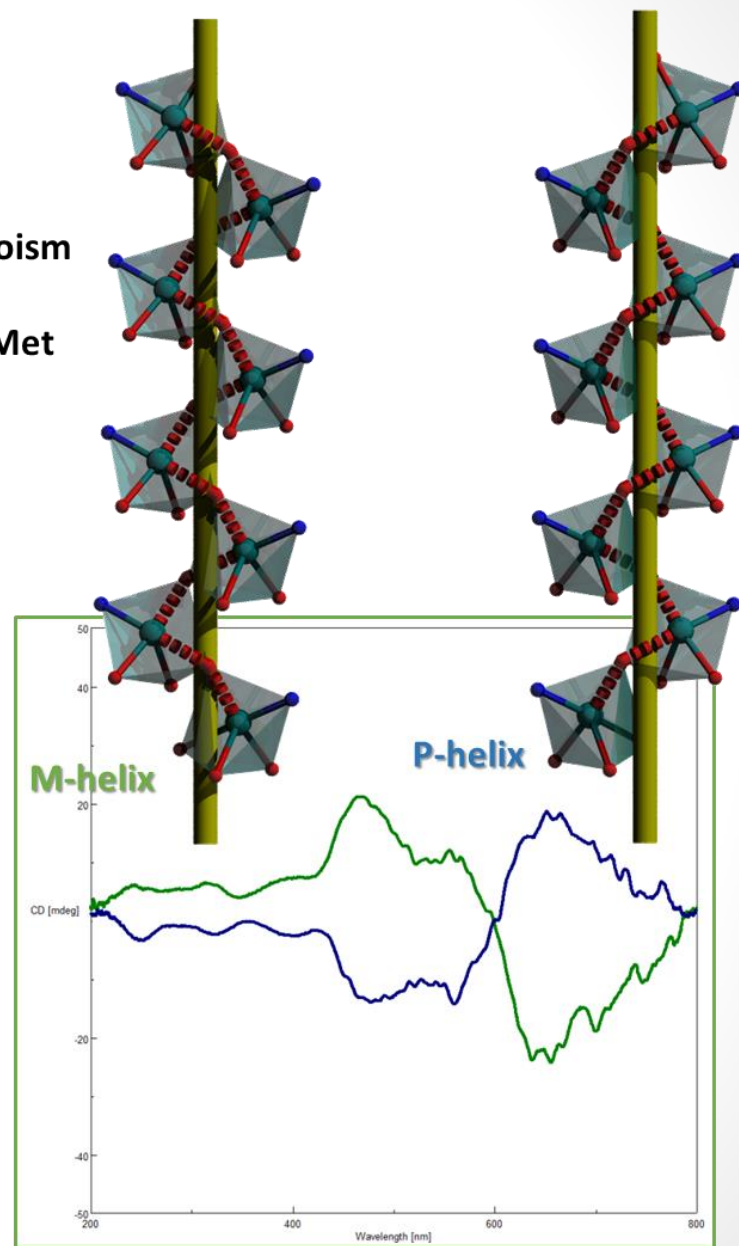
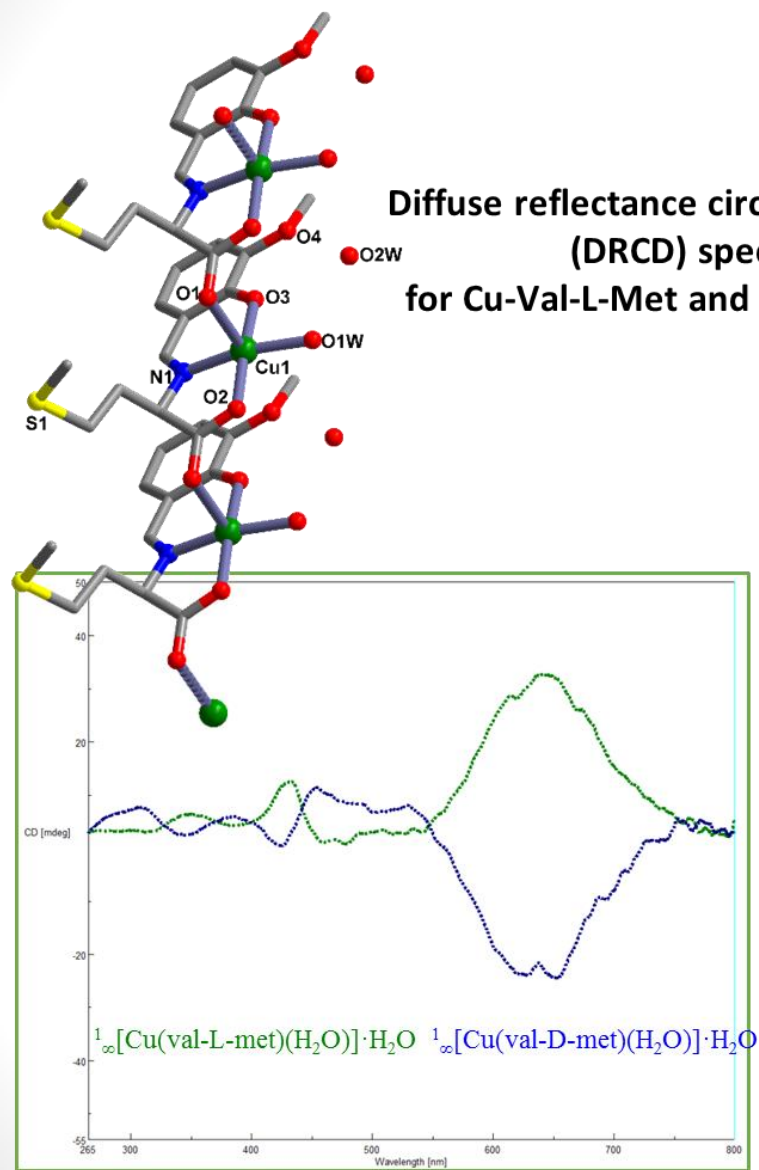
Dramatic change for magnetic interaction!!!!



[Cu(Va-L-Met)]

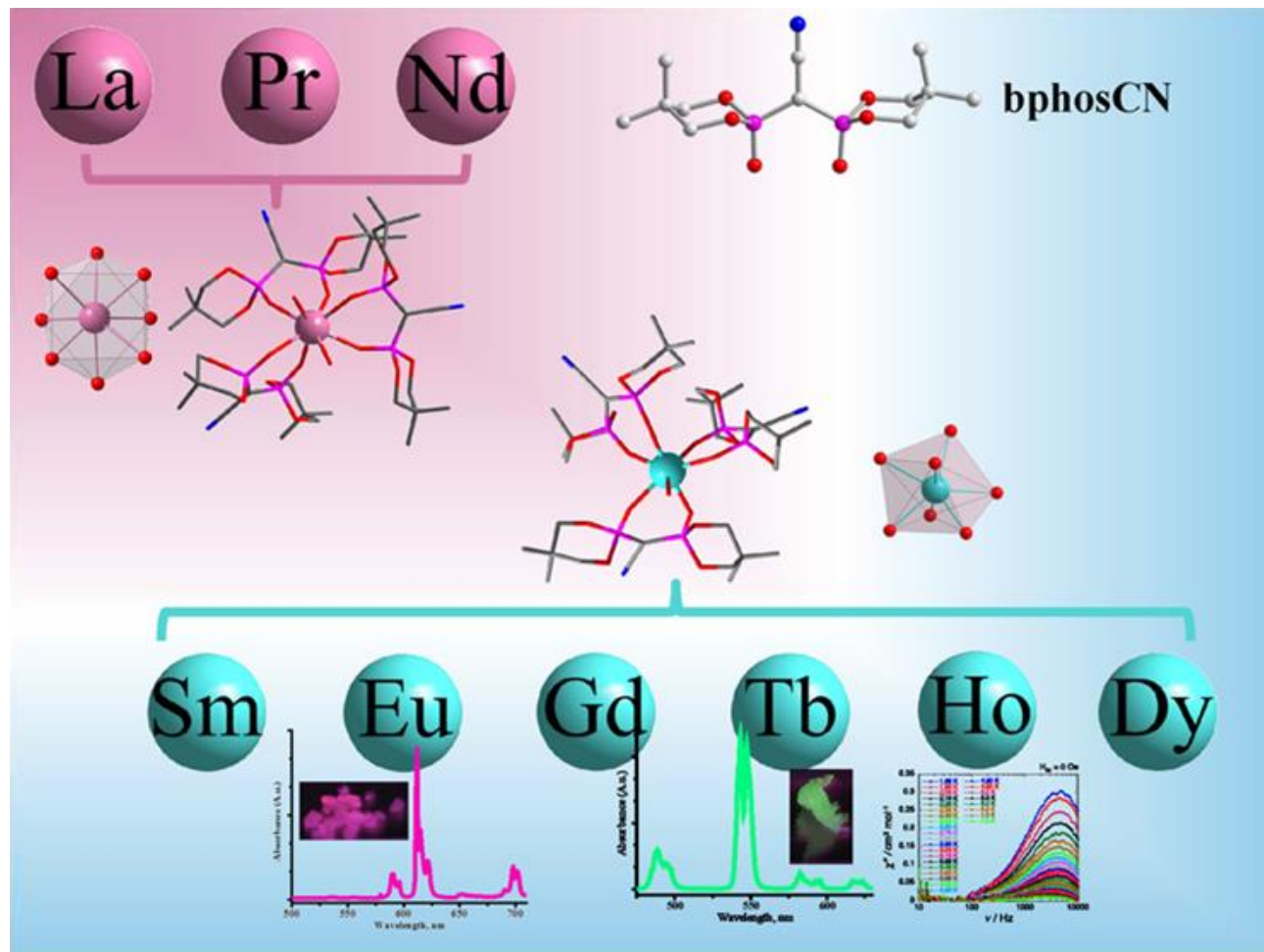


Chiroptical properties



Results

Cyanomethylene-bis(phosphonate)-Based Lanthanide Complexes:
Structural, Photophysical, and Magnetic Investigations



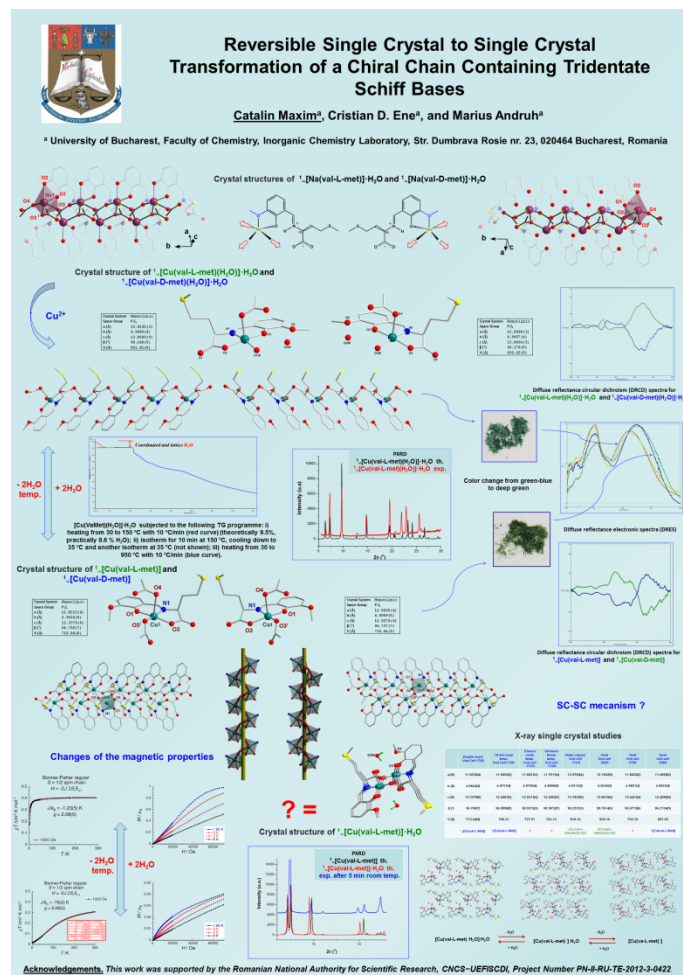
Catalin Maxim, Cristian D. Ene, and Marius Andruh, **Crystal Structures and Optical Properties of Enantiopure and Racemic Coordination Polymers Containing Tridentate Schiff Bases**, GECOM CONCOORD, Vers, 19-23 mai 2014

Cristian D. Ene, Catalin Maxim, Ioana Nicolau, and Ileana C. Farcasanu, **Copper(II) Complexes of Chiral Schiff Bases - from Coordination Building-Blocks to Biological Interactors**, GECOM CONCOORD, Vers, 19-23 mai 2014

Results 2015

Conferences

Catalin Maxim, Cristian D. Ene, and Marius Andruh, **Reversible SCSC Transformation of a Chiral Chain Containing Tridentate Schiff Bases**, GECOM CONCOORD, Lyon, 26-29 mai 2015



Results 2016

Papers

Inorg. Chim. Acta, **2016**, 440, 148–153

Eur. J. Inorg. Chem. **2016**, 4185–4193

Conferences

Workshop “Crystal Engineering of Multifunctional Molecule-Based Materials” Sinaia 2016,

„Multimetallic complexes obtained by single-crystal-to-single-crystal transformations” Catalin Maxim
Oral presentation

„Mononuclear lanthanide(III) complexes of symmetrical tripodal ligands - structural investigations to elucidate biochemical interactions”, Cristian D. Ene, Oral presentation.

International Conference on Coordination Chemistry, 2016, Brest

„Enantiopure coordination polymers containing tridentate Schiff bases ligands. Crystal structures, optical and magnetic properties”, Catalin Maxim Oral presentation.

International Conference of Physical Chemistry, ROMPHYSCHEM 16, Galati, 2016

"Chirality driven crystallization behavior of tridentate Schiff base complexes", Catalin Maxim,
Oral presentation