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Design, synthesis and physicochemical properties of ternary La(III) systems with dietary flavonoids

LABORATORY OF INORGANIC CHEMISTRY AND ADVANCED MATERIALS

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Abstract: The synthesis of well-defined crystalline compounds of lanthanides with flavonoids and ternary auxiliary ligand chelators presents itself as an opportunity for new materials with applications in a) medicinal applications targeting diagnosis, and b) potential therapeutic administration of disease. The fact that there is a striking similarity in size between lanthanum La(III) and Ca(II), projects potential similarities in the biological chemistry of the two different classes of metal ions, with equally important consequence in physiology and disease. Poised to delve into the development of new materials based on lanthanides and bearing properties enabling further biological investigation into physiological and pathological roles, the chemistry of ternary La(III)-chrysin-phenanthroline species was pursued and led to isolable crystalline material. Physicochemical characterization (FT-IR, elemental analysis, X-ray crystallography, tec.) combined with theoretical Hirshfeld analysis led to the formulation of a profile, justifying further inquiry into its biological role (e.g. antioxidant) in pathophysiological aberrations.

Introduction

Lanthanides are a series of 15 elements, extending from lanthanum (Z = 57) to the lutetium (Z = 71) (**Fig. 1A**), often referred to as the 4f block elements. Lanthanide complexes are characterized by high coordination numbers, rich coordination geometries and unique luminescence properties (long lifetime, narrow emission bands, etc.) [**1**]. Their size resemblance to Ca(II) (**Fig. 1B**) have since long been recognized as a factor, warranting further perusal of lanthanides into diagnosis and therapeutics of human health aberrations. On the other hand, flavonoids are phenolic compounds, fully incorporated in the plant kingdom, a) well-known for their biological properties as antioxidant, antitumor, antimicrobial, neuroprotective and cardioprotective agents, and b) exhibiting protective behavior against oxidative stress in a series of human diseases, like cancer, diabetes, neurodegeneration, etc. [**2**]. To that end, the design and synthesis of hybrid ternary metal-based flavonoid materials, containing naturally-occurring flavonoids (or derivatives thereof) in their coordination sphere, including combinations of the aforementioned metal ions (e.g. La(III) and selected flavonoids (e.g. chrysin, quercetin) are poised to provide new (metallo)drugs with well-defined biological profiles and improved pharmacological activities compared to parent flavonoids [**3**].

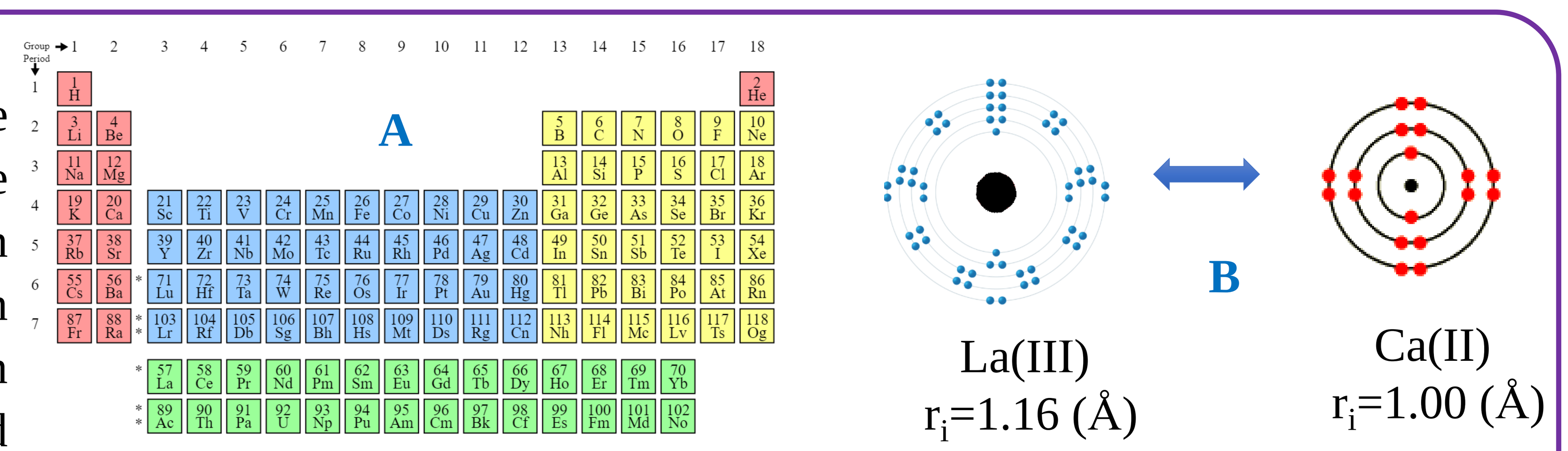
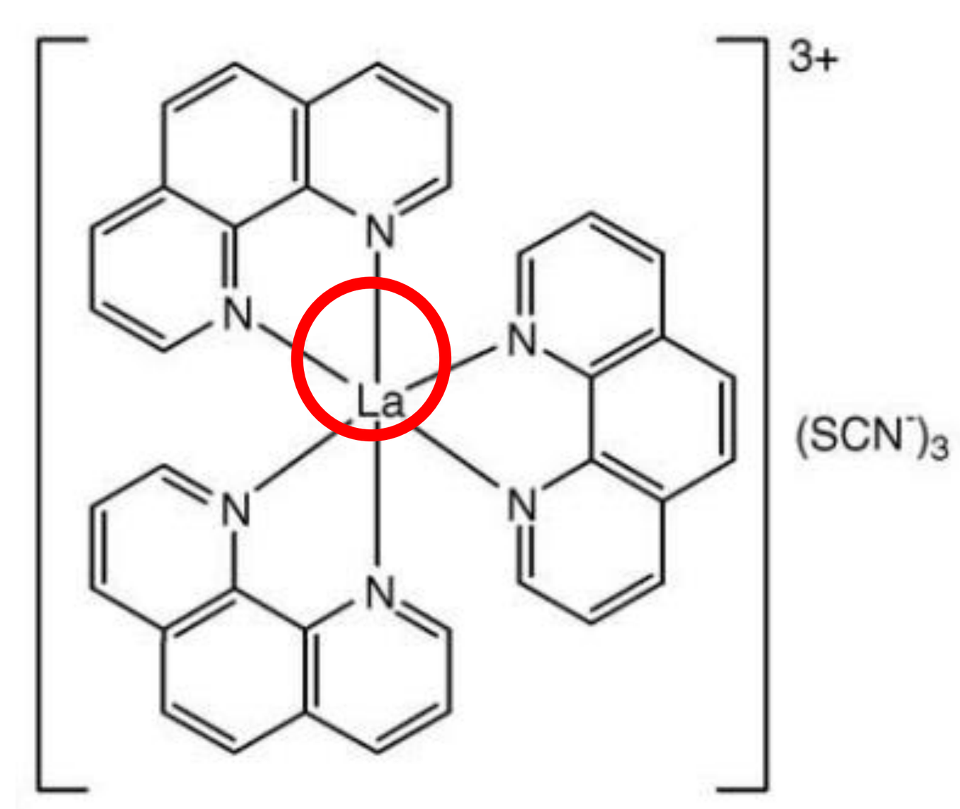


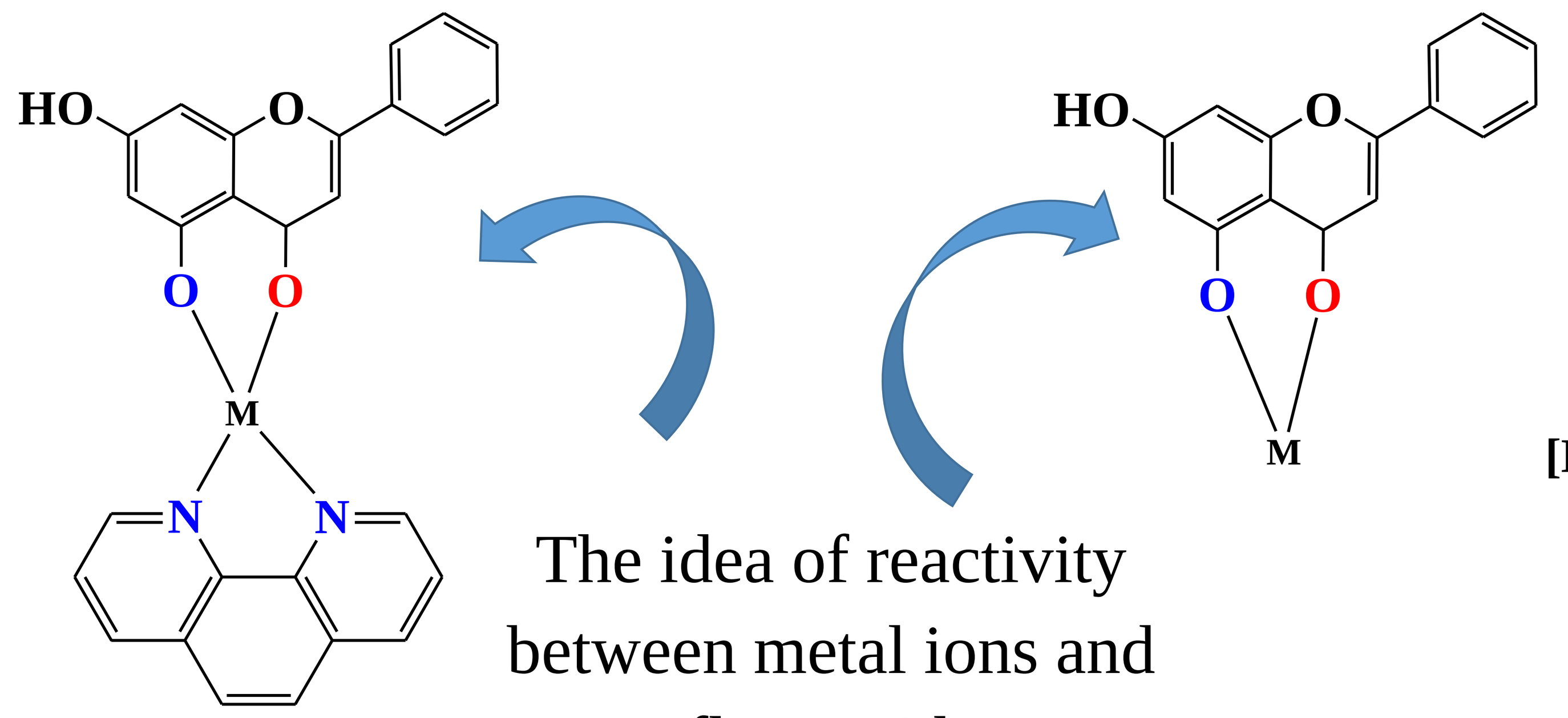
Fig. 1: Lanthanide physical property similarities

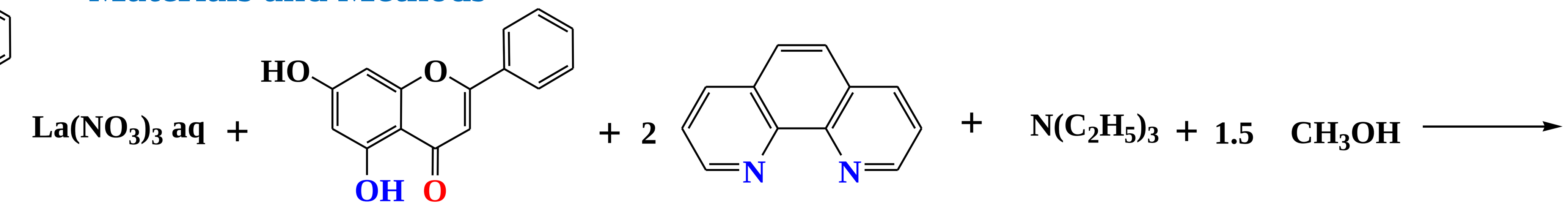


[Tris(1,10-phenanthroline)lanthanum(III)] thiocyanate

Fig. 2: Binary La(III) complex species

Materials and Methods

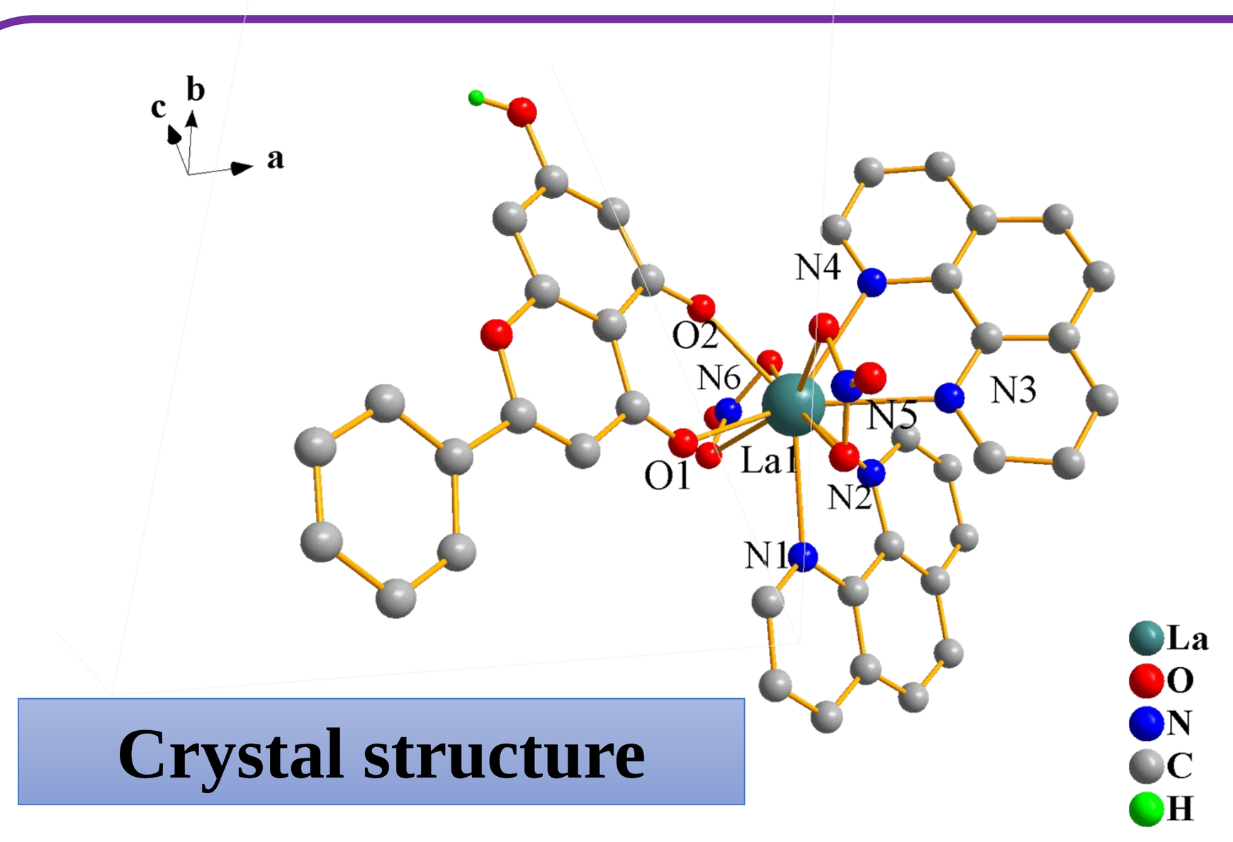


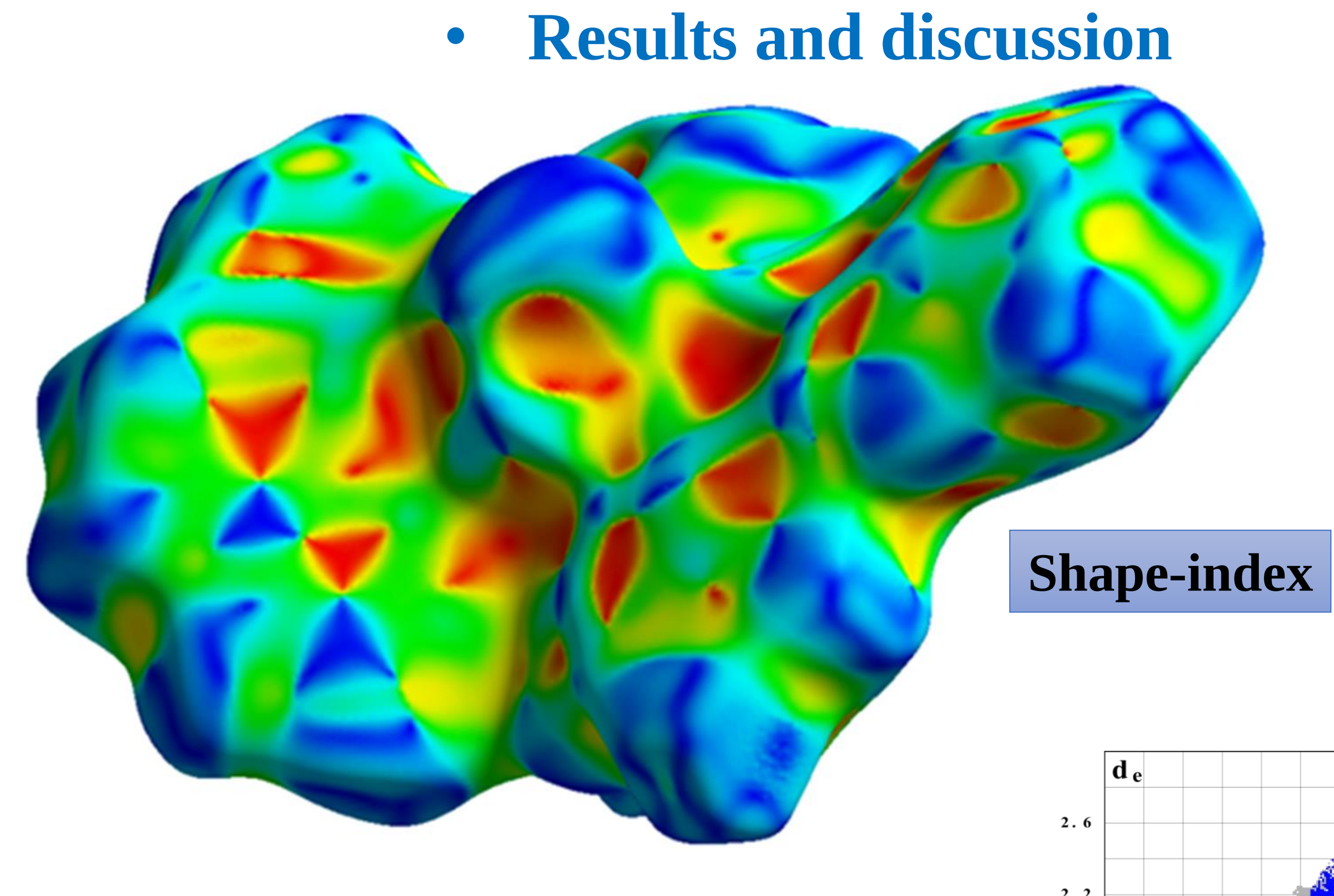


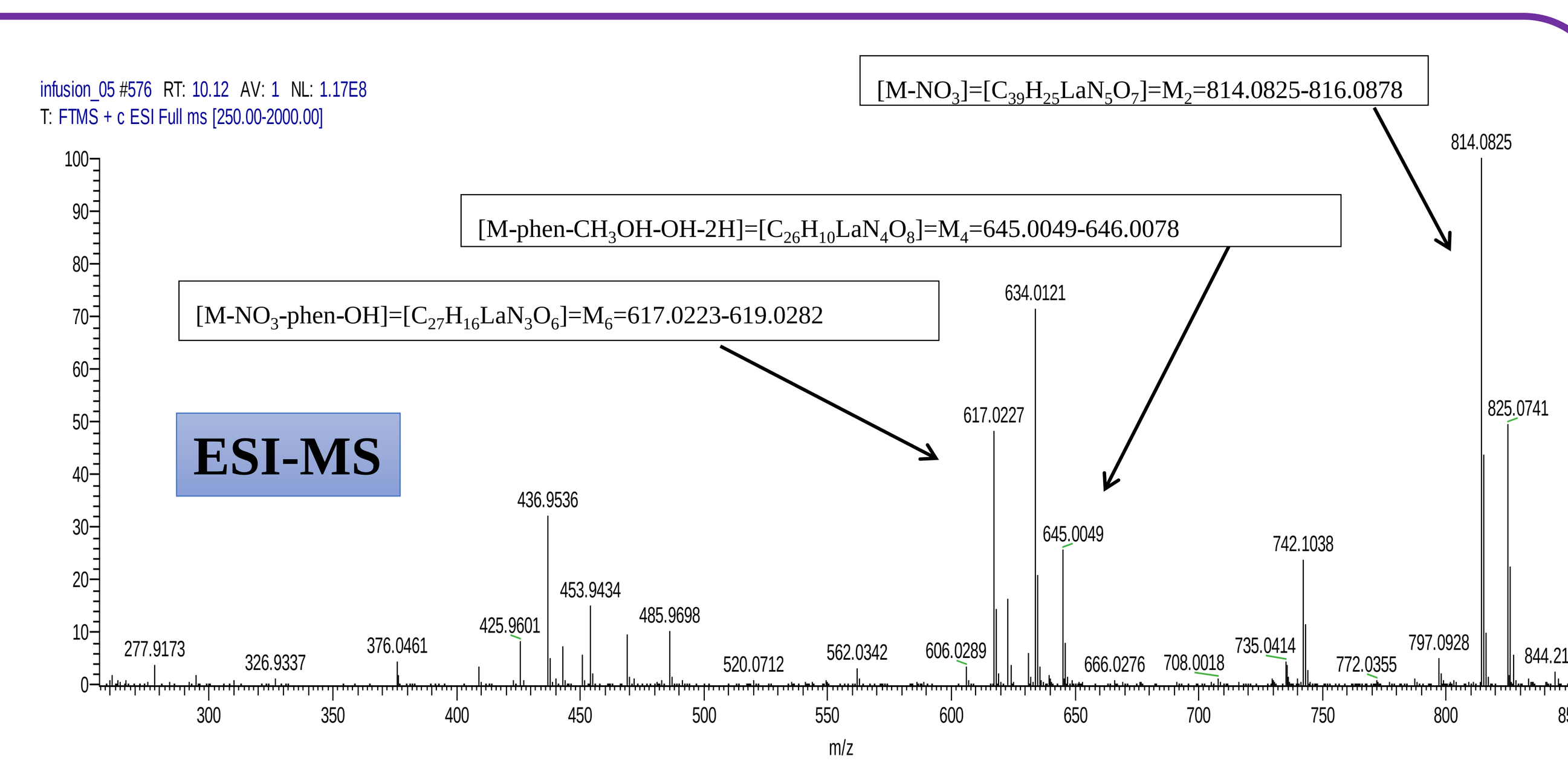
$[La(C_{15}H_9O_4)(C_{12}H_8N_2)_2(NO_3)_2]\bullet 1.5\ CH_3OH$ + $[(C_2H_5)_3NH]NO_3$ + x H_2O

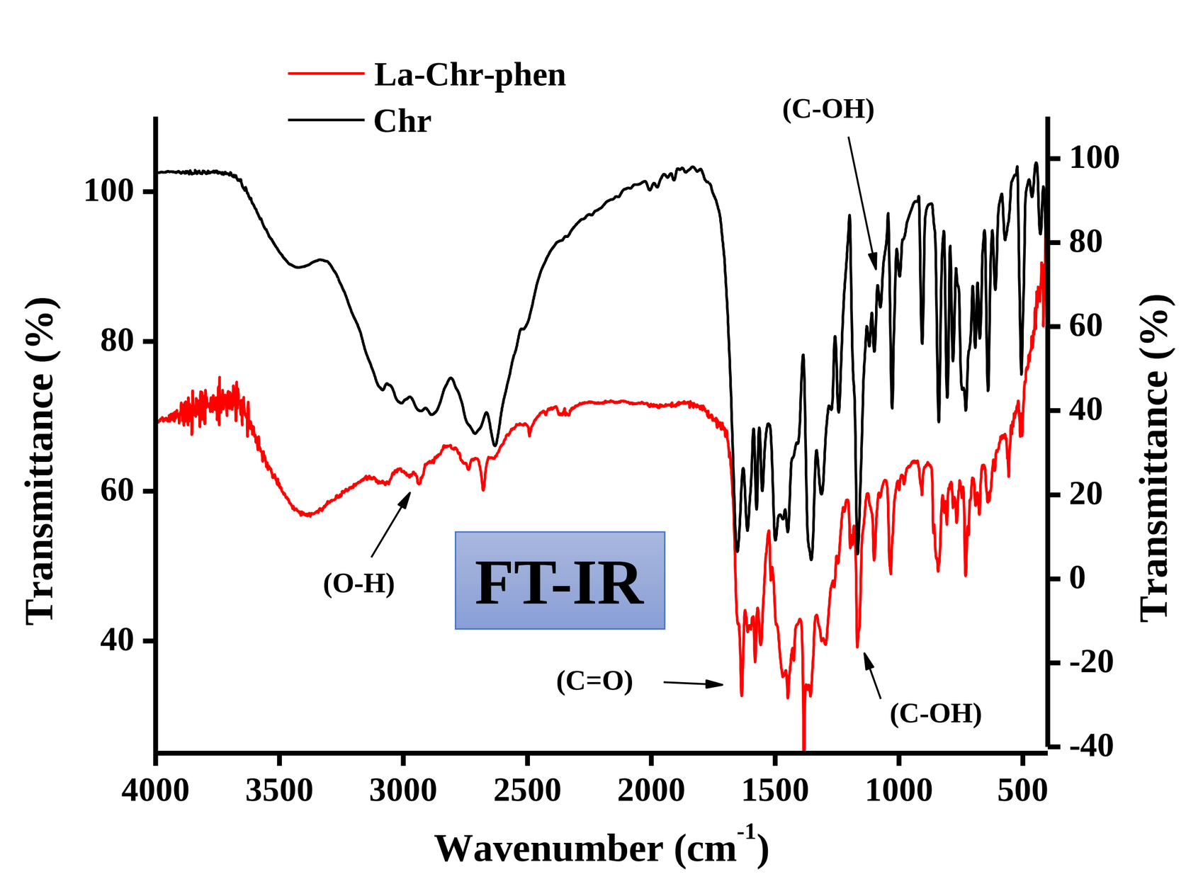
The isolated crystalline material was further subjected to spectroscopy and structural investigation, collectively justifying its nature and properties.

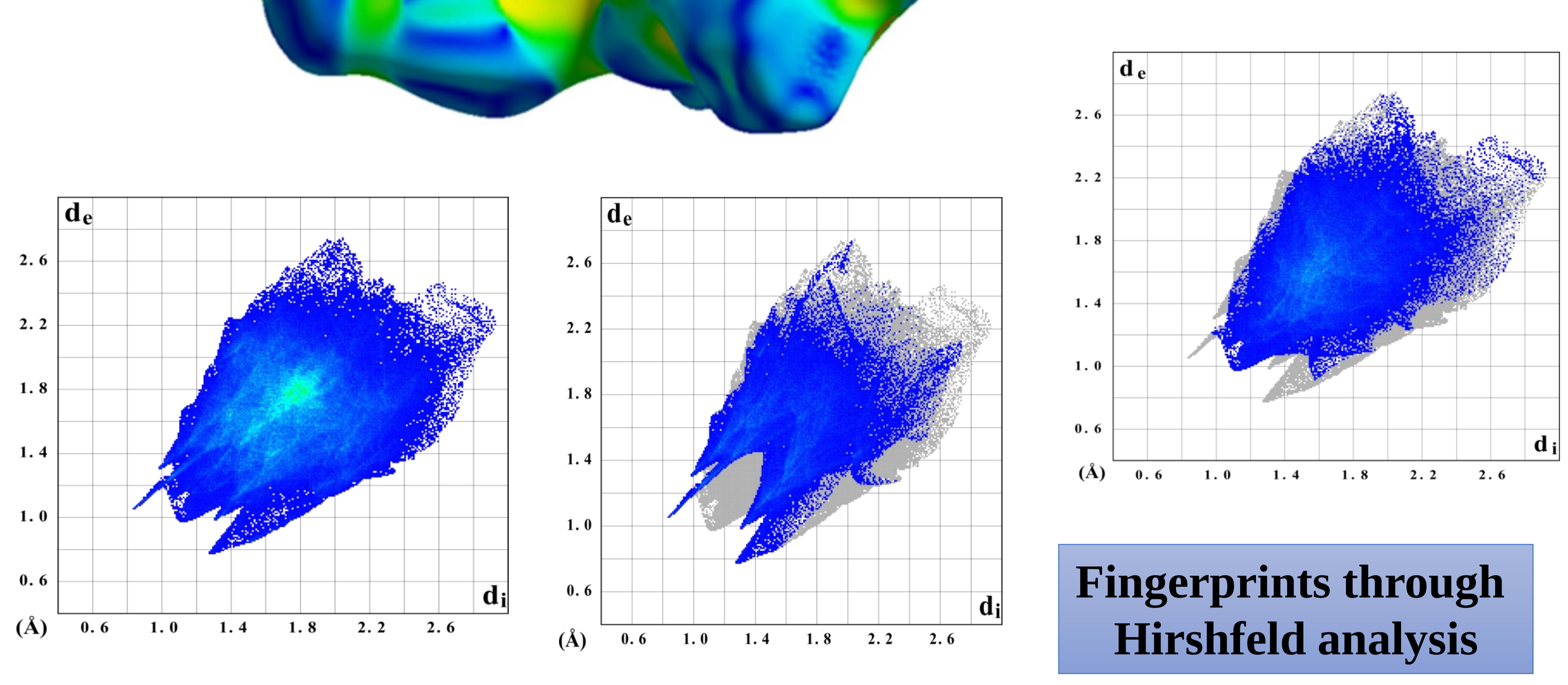
Results and discussion

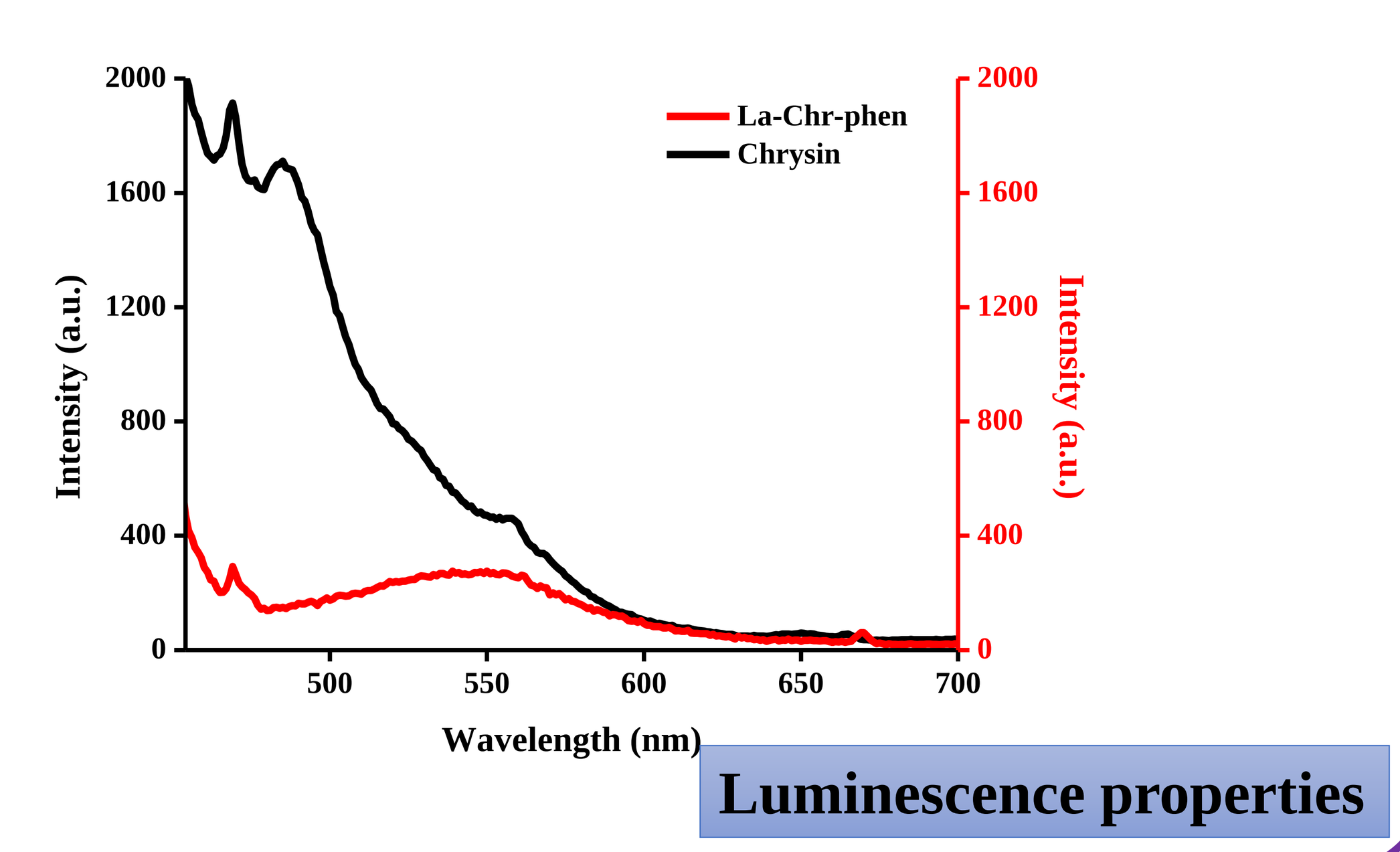












Conclusions

- ❖ Ternary La(III)-chrysin-phenanthroline chemistry ked to the isolation of crystalline material
- ❖ The Physicochemical properties reveal a well-defined profile for the La(III) species
- ❖ Theoretical investigation of the material supplements the experimental profile of the La(III) species
- ❖ The collective properties justify further biological perusal into the role(s) of La(III) into (patho)physiologies and potential use in applications

Literature

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[3]. H. Manman, C. Weilan, L. Zhimin, P. Liang, H. Lixia, C. Min, J. Inorg. Biochem. 195 (2019) 13-19.