



ACADEMIA ROMÂNĂ
SCOSAAR

Anexa nr.6

REZUMATUL TEZEI DE ABILITARE

**TITLUL: MATERIALE FUNCȚIONALE AVANSATE CU PROPRIETĂȚI
BIOLOGICE ȘI ADSORBTIVE**

Domeniul de abilitare: CHIMIE

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ABSTRACT

The habilitation thesis entitled “*Advanced functional materials with biological and adsorptive properties*” presents the main scientific and professional results obtained by the author after being awarded the scientific title of Doctor in the field of Exact Sciences – Chemistry by the Romanian Academy, in 2009.

The thesis is structured into three sections: I. Main professional, academic, and scientific achievements; II. Plan for the evolution and development of the author’s professional, scientific, and academic career; III. Bibliography.

The first section comprises two chapters (I.1 and I.2). Chapter I.1 presents the main professional and academic achievements obtained by the author after receiving the doctoral degree. Chapter I.2 presents the main scientific achievements, based on 10 representative ISI-ranked scientific articles published as principal author. This chapter is divided into two subchapters corresponding to the research directions addressed:

I.2.1 Coordination compounds of some transition metals and hybrid materials derived from them, with antitumor and antimicrobial properties.

I.2.2 Magnetic oxide materials with applications in water depollution processes.

Within the first research direction (Subchapter I.2.1), the synthesis, structural characterization, and evaluation of the biological activity of coordination compounds of transition metals with various organic ligands were addressed. The development of new efficient and selective bioactive agents remains a major challenge in the context of increasing drug resistance and the toxicity associated with current therapies, particularly in the treatment of neoplastic diseases and infections caused by multidrug-resistant bacteria. Over the past decades, coordination chemistry of transition metals has emerged as a field of major impact in biomedical research, offering substantial advantages over organic molecules due to the versatility of metal ion oxidation states, their coordination geometries, as well as the diversity of organic ligands, which exhibit multiple and various modes of coordination to the metal ions. The discovery of cisplatin marked the beginning of the clinical use of coordination compounds as antitumor agents; however, its adverse effects have driven research toward other metals. Among these, ruthenium complexes have stood out due to their favorable biological properties. In this context, new coordination compounds of ruthenium with Schiff base ligands obtained by condensation of salicylaldehyde/*o*-vanillin with various amines (diamines: ethylenediamine, *o*-phenylenediamine, 1,3-diaminopropane, 1,2-

diaminocyclohexane, 1,3-diamino-2-propanol, and organic molecules that contain a single primary amine group: N,N-dimethyl-ethylenediamine, 2-aminomethylpyridine, 2-aminoethylpyridine) were synthesized and characterized. The obtained compounds were investigated by various physicochemical and structural methods in order to establish their molecular formulas. Their cytotoxic and antitumor activities were evaluated using complementary short-term and long-term experiments on several tumor cell lines: HT29 (human colorectal carcinoma), Saos-2 (human osteogenic sarcoma), HeLa (human cervical carcinoma), LSR-SF-SR (rat sarcoma), as well as on a non-tumoral cell line, Lep3 (human embryonic fibroblasts).

Subsequently, nanostructured hybrid systems were developed by immobilizing ruthenium complexes within mesoporous silica matrices of the SBA-15 type. The hybrid materials obtained by immobilization and the Ru(III)/Ru(II) complexes, as well as the mesoporous SBA-15 silica support, were structurally, morphologically, and texturally characterized in order to identify the interactions established between the components of the final hybrid material. The cytotoxic activity of the obtained hybrid materials was investigated on A549 pulmonary tumor cells, normal lung fibroblasts (MRC-5), and HeLa tumor cells.

Another study was dedicated to the synthesis and characterization of a series of coordination compounds of Co(II), Ni(II), Cu(II), and Zn(II), using isoxicam - a representative of the oxicam class of nonsteroidal anti-inflammatory drugs - as ligand. Their cytotoxic activity was evaluated on four tumor cell lines (LSCC-SF-Mc29, LSR-SF-SR, MCF-7, HeLa) and one non-tumoral cell line (Lep-3).

The last study presented within this subchapter describes a new series of mononuclear coordination compounds of Co(II) and Cu(II) with mixed ligands—Schiff bases obtained by condensation of o-vanillin with amino acids (tryptophan, tyrosine, threonine, serine) and 2,2'-bipyridine as auxiliary ligand. Following physicochemical characterization and structural elucidation of the compounds, their cytotoxic activity was evaluated using two tumor cell lines: HeLa and LSR-SF-SR.

The second research direction (Subchapter I.2.2) focused on the synthesis, characterization, and performance evaluation of advanced magnetic materials designed to function as efficient adsorbents for the removal of heavy metal ions and organic dyes from contaminated waters. Through various experimental approaches, a series of functionalized magnetic materials based on cobalt ferrite, magnetite, mesoporous silica, chitosan, and active organic compounds were synthesized and characterized, exhibiting remarkable adsorption properties and efficient magnetic

separability. In a first study, the influence of the concentration of the surfactant cetyltrimethylammonium bromide (CTAB) on the formation of mesoporous cobalt ferrite was analyzed, and the adsorption capacity of the obtained materials for Pb^{2+} ions from aqueous solutions was comparatively evaluated. In another study, a cobalt ferrite–chitosan magnetic composite was developed and tested for the adsorption of Congo red and methyl orange dyes from aqueous solutions, both in single-component and binary systems. To elucidate the adsorption mechanisms, equilibrium adsorption and kinetic studies were performed. In addition, desorption tests demonstrated the possibility of reusing these materials in successive water treatment processes.

A distinct study within this direction concerns the development of magnetic adsorbents based on magnetite functionalized with polyamines. Three new magnetic adsorbents were synthesized by immobilizing di-, tri-, and tetra-amines on the surface of silica-coated magnetite nanoparticles, with the aim of introducing specific chelating groups for heavy metal ions. Their capacity to adsorb Cu^{2+} ions from aqueous solutions was comparatively evaluated, highlighting the influence of the polyamines structure on adsorption kinetics and capacity. The results demonstrated the potential of these materials as efficient, selective, and easily recoverable adsorbents, suitable for practical depollution applications.

Additionally, hybrid nanocomposites based on magnetite and mesoporous silica of the MCM-41 and SBA-15 types, functionalized with active organic groups such as *o*-vanillin and carboxyl groups, were developed. The integration of magnetite into mesoporous silica matrices enabled the obtaining of materials with high specific surface area, controlled porosity, and uniform distribution of active sites, leading to superior adsorption performance compared to conventional materials. High stability over repeated adsorption–desorption cycles and facile magnetic separation support their potential application in sustainable water treatment technologies.

Overall, the developed magnetic adsorbent materials are distinguished by high efficiency, easy magnetic separation, and real potential for practical applicability, supporting the relevance and impact of this research direction in the current context of environmental protection.

The second section of the habilitation thesis presents the plan for the evolution and development of the author's professional, scientific, and academic career, the proposed objectives, and future research directions. The habilitation thesis ends with the third section, which includes 190 bibliographic references.