INORGANIC CHEMISTRY

Pentacoordinated complexes of Ni(II).
supervisor: prof. RNDr. Juraj Černák, DrSc. (juraj.cernak@upjs.sk)
study form: full time
Annotation: Within the thesis new magnetically active complexes of Ni(II) with heteroleptic coordination sphere will be studied. The synthetic design, with the aim to achieve pentacoordination, will be based on the use of sterically demanding ligands in combinations of two- and three-donor ligands, or four- and mono-donor ligands. Beside commercially accessible ligands also new ligands will be synthesized within this work. Emphasis will be done on the preparation of the compounds in the single crystal form. Prepared complexes will be characterized by chemical and spectroscopic methods, and their crystal structures will be elucidated. Results of experimental magnetic studies will be correlated with the results of structure analyses.
Literature: A. K. Bara, C. Pichon, J.-P. Sutter, Coord. Chem. Rev., 308 (2016) 346–380.
I. Nemec, R. Herchel, I. Svoboda, R. Boča, Z. Trávníček, Dalton Trans., 44 (2015) 9551-9560.
S. Gómez-Coca, D. Aravena, R. Morales, E. Ruiz, Coord. Chem. Rev., 289–290 (2015) 379–392.

Complexes of transition metals with nitroderivatives of 8-quinolinol as antitumor drugs.
supervisor: doc. RNDr. Ivan Potočňák, PhD. (ivan.potocnak@upjs.sk)
study form: full time
Annotation: The aim of the thesis is to prepare and characterize (IR, UV-VIS, NMR, elemental analysis, thermal analysis, X-ray structure analysis) complexes of selected transition metals with both commercially available and synthesized nitroderivatives of 8-quinolinol. Their anti-tumor activity along with the selectivity will be studied against selected tumor cell lines. On the basis of the knowledge on the composition, structure and biological properties of the prepared compounds new compounds will be prepared and characterized in order to modify their structure and therefore their antitumor activity.
Literature: M. Fanelli et al., Coordination Chemistry Reviews 310 (2016) 41–79.
V. Oliveri, G. Vecchio, European Journal of Medicinal Chemistry 120 (2016) 252–274.
M. C. Mandewale et al., Beni-Suef University Journal of Basic and Applied Sciences 6 (2017) 354–361.
A. Casini et al., Metal-based Anticancer Agents, Royal Society of Chemistry, 2019.

Complexes with planar heterocyclic ligands exhibiting antiproliferative activity.
supervisor: doc. RNDr. Ivan Potočňák, PhD. (ivan.potocnak@upjs.sk)
study form: full time
Annotation: The aim of the thesis is to prepare and characterize (IR, UV-VIS, NMR, elemental analysis, thermal analysis, X-ray structure analysis) complexes of selected metals with both commercially available and synthesized planar N- and O-donor ligands, which are able to intercalate to the DNA and thus enable to exhibit antiproliferative activity of the prepared complexes. This will be assessed against selected tumor cell lines. On the basis of the knowledge on the composition, structure and biological properties of the prepared compounds new compounds will be prepared and characterized in order to modify their structure and therefore their antiproliferative activity.

Literature: M. Fanelli et al., Coordination Chemistry Reviews 310 (2016) 41–79.
V. Oliveri, G. Vecchio, European Journal of Medicinal Chemistry 120 (2016) 252–274.
M. Kubanik et al., Organometallics 34 (2015) 5658–5668.
M. C. Mandewale et al., Beni-Suef University Journal of Basic and Applied Sciences 6 (2017) 354–361.
A. Casini et al., Metal-based Anticancer Agents, Royal Society of Chemistry, 2019.

Influence of metal ions coordination sphere on their antimicrobial, cytostatic and toxic effect.

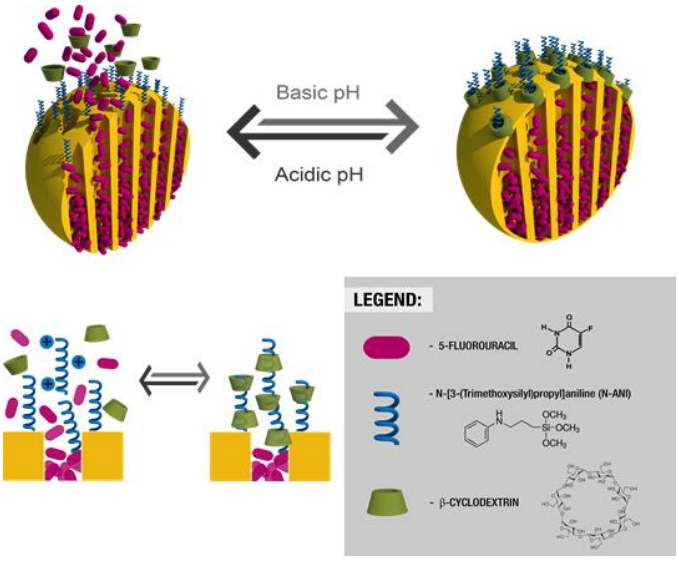
supervisor: doc. RNDr. Zuzana Vargová, PhD. (zuzana.vargova@upjs.sk)
study form: full time

Annotation: Thesis is focused on monitoring of influence of N, O, S-donor ligands coordination ability on biological activity and toxic effect of selected predominantly soft metal ions. The aim of the thesis is to determine their influence on metal ion function in the process of pathogenic microorganisms growth inhibition and their selectivity against beneficial microorganisms (potential antimicrobial agents with additional cytostatic effect) as well as in the process of reducing its toxic effect on the environment (potential chelating agents).

Nanoporous silica particles for targeted drug delivery.

supervisor: prof. RNDr. Vladimír Zeleňák, DrSc. (vladimir.zelenak@upjs.sk)
consultants: RNDr. Miroslav Almáši, PhD., doc. RNDr. Adriana Zeleňáková, PhD.
study form: full time

Annotation: The thesis is a follow-up to several years of research focused on the development of new intelligent drug delivery systems releasing bioactive substances in a targeted way by the influence of physical or chemical stimulus [1-3]. The theme of the PhD thesis is based on this knowledge and concept and its motivation is to design, prepare and test inorganic porous carriers based on silica matrix, transporting the drug to cancer cells by active targeting. For this purpose, the silica nanoparticles will be modified with ligands (e.g., folic acid derivatives) that, due to the specific ligand-receptor interactions on the surface of the cancer cell, allow preferential binding and internalization of such systems by cancer cells.

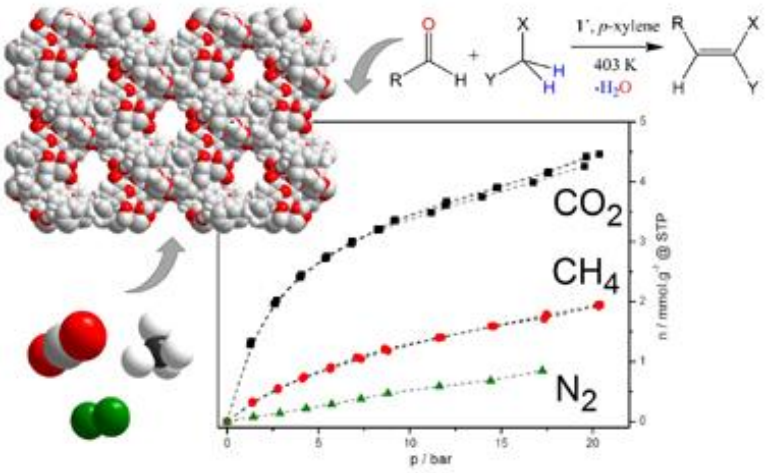


Literature: V. Zeleňák, E. Beňová, M. Almáši, D. Halamová, V. Hornebecq, V. Hronský, New Journal of Chemistry, 42 (2018) 13263-13271.
E. Beňová, D. Bergé-Lefranc, V. Zeleňák, M. Almáši, V. Huntošová, V. Hornebecq, Applied Surface Science, 504 (2020) 144028.
M. Almáši, E. Beňová, V. Zeleňák, B. Madaj, V. Huntošová, J. Brus, M. Urbanová, J. Bednarčík, V. Hornebecq, Materials Science and Engineering C, 109 (2020) 110552.

Metalo-organic frameworks for hydrogen adsorption.

supervisor: prof. RNDr. Vladimír Zeleňák, DrSc.(vladimir.zelenak@upjs.sk)
consultants: RNDr. Miroslav Almáši, PhD., doc. RNDr. Adriana Zeleňáková, PhD.
study form: full time

Annotation: Metal-organic networks (MOFs) or porous coordination polymers represent worldwide one of the key research topics of the last decade. One of the areas where MOF has great application potential is energy saving [1] and gas adsorption applications such as carbon dioxide or hydrogen adsorption [2]. Hydrogen adsorption and storage in MOF is given special attention today, as MOFs are one of the options for efficient hydrogen storage and transition to a carbon-free economy. The aim of the thesis is to design methods of modification of MOF, to prepare and test metal-organic networks that exhibit increased hydrogen adsorption enthalpy (more than 10 kJ / mol) and increased adsorption capacity under non-cryogenic conditions.



Literature: V. Zeleňák, M. Almáši, A. Zeleňáková, P. Hrubovčák, S. Bourelly, P. Llewellyn, Scientific Reports 9 (2019)15572.
M. Almáši, V. Zeleňák, R. Gyepes, S. Bourrelly, M.V. Opanasenko, P.L. Llewellyn, J. Čejka, Inorganic Chemistry, 57 (2018) 1774-1786.