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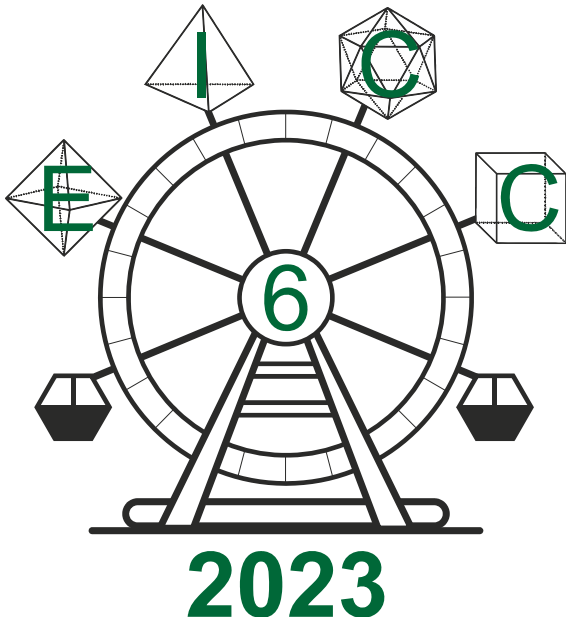

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WELCOME FROM THE CHAIRMEN OF THE 6TH EUCHEMS INORGANIC CHEMISTRY CONFERENCE

Dear Colleagues,

We wish to cordially welcome you to the 6th EuChemS Inorganic Chemistry Conference 2023 at the TU Wien. This series of meetings has been initiated in 2011 and since then developed to a true European event organized every two years. The 6th EICC covers all aspects of inorganic chemistry with special focus on coordination & supramolecular chemistry, organometallic chemistry & catalysis, magnetochemistry, energy & photochemistry, green & bioinorganic chemistry, inorganic materials & nanoparticles, nuclear chemistry and theoretical inorganic chemistry.

Ideally located in the center of Europe, Vienna has a long-standing tradition as a major conference site since the "Congress of Vienna" in 1815. Its unique atmosphere will provide inspiration for a fruitful scientific meeting, and the participants will have ample time to enjoy a wealth of culture and historical places in and around Austria's capital city.

We hope that you find the conference interesting and stimulating and wish you a pleasant stay in Vienna.

Sincerely,

Peter Weinberger and Karl Kirchner
Chairmen of 6th EICC

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SPIN STATES OF Mn(II) AND Fe(III) COMPLEXES WITH THIOSEMICARBAZONE

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[c]University of Belgrade – Faculty of Chemistry, Belgrade, Serbia

Mn(II) and Fe(III) complexes with condensation product of thiosemicarbazide and 2-acetylthiazole have been synthesized and characterized by single-crystal X-ray diffraction [1]. Two complexes have the same ligand system – bis tridentate coordination of the thiosemicarbazone ligand through the NNS donor set of atoms. Furthermore, the central metal ions in both cases have the same d^5 electronic configuration. However, measured magnetism and analysis of the crystal geometries show that these two complexes have a different number of unpaired electrons. We rationalized the results by electronic structure calculations based on density functional theory. High-spin Mn(II) complex has trigonal-prismatic geometry with ionic metal-ligand bonding. Hund's rule of maximum multiplicity is responsible for its sextet spin-ground state. On the other hand, low-spin Fe(III) complex has octahedral coordination and strong metal-ligand covalency with delocalization of spin density toward ligands. Low-spin, doublet state is favored because of the nephelauxetic effect, i.e., smaller pairing energy in Fe(III) complex.

Our results show that the difference in the electronic structure of the two complexes, i.e., different spin-ground states, directly affects these molecules' structure, magnetism, reactivity, and biological activities.

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[1] Stojičkov, M., Zlatar, M., Mazzeo, P. P., Bacchi, A., Radanović, D., Stevanović, N., Jevtović, M., Novaković, I., Anđelković, K., Sladić, D., Čobeljić, B., Gruden, M. (2023). Polyhedron, 237, 116389.