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Twenty-third Annual Conference

YUCOMAT 2022

&

Twelfth World Round Table Conference on Sintering

XII WRTCS

Program

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WRTCS 2022

International Institute for the Science of Sintering

TWENTY-THIRD ANNUAL CONFERENCE

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TWELFTH WORLD ROUND TABLE CONFERENCE ON SINTERING

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Hunguest Hotel Sun Resort, Herceg Novi, Montenegro
August 29 - September 2, 2022

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P.S.III.E.1.

Synthesis, characterization and DFT calculations of Schiff base Co(III) complexes

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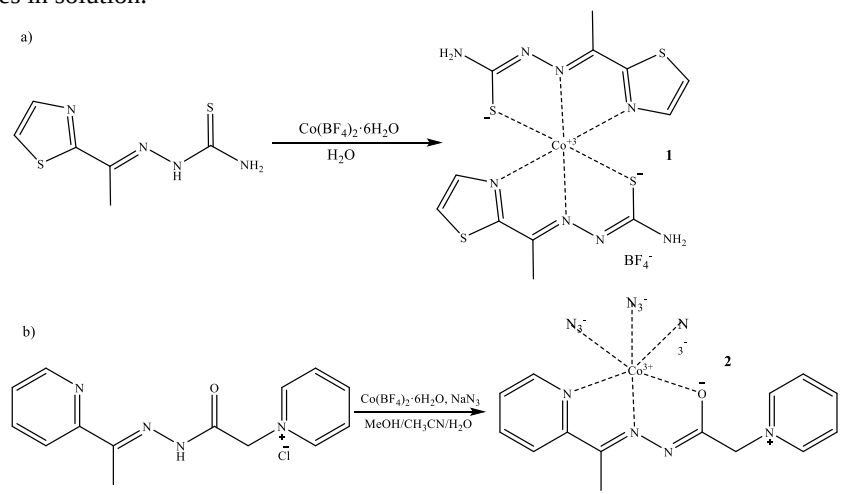
The Co(III) complex (**1**) was synthesized by the reaction of (E)-2-(1-(thiazol-2-yl)ethylidene)hydrazine-1-carbothioamide (**HL^1**) and $Co(BF_4)_2 \cdot 6H_2O$ in solvent mixture of $MeOH/H_2O$ (Scheme 1a). The Co(III) complex (**2**) was synthesized by the reaction of (E)-1-(2-oxo-2-(2-(1-(pyridin-2-yl)ethylidene)hydrazinyl)ethyl)pyridin-1-ium chloride (**HL^2**Cl) and $Co(BF_4)_2 \cdot 6H_2O$ in solution mixture $MeOH/CH_3CN/H_2O$. After complete dissolution of $Co(BF_4)_2 \cdot 6H_2O$ in the reaction mixture, NaN_3 was added (Scheme 1b). Obtained green crystals were characterized by SCXRD, elemental analysis. IR, NMR and UV/Vis spectroscopy. The Co(III) ions in **1** form mononuclear [Co**L^1**$_2$]BF_4 complex with two **L^1** ligands coordinated through thiazole and imine nitrogen atoms and enolate sulfur atom. The Co(III) ions in **2** form mononuclear [Co**L^2**$(N_3)_3$] complex with **L^2** ligand coordinated through thiazole and imine nitrogen atoms and enolate oxygen atom, while three remaining places are occupied by azide ions.
Density functional theory (DFT) calculations were performed to elucidate the structures of Co(III) complexes in solution.



*Scheme 1. Synthesis of complexes **1** and **2**.*