

Área: INO

## Spectroscopic and Structural Studies of Saccharin Complexes with Fe(II), Co(II), and Ni(II)

Camila A. Soares (PG),<sup>1\*</sup> Patricia Appelt (PQ),<sup>1</sup> Davi Back (PQ),<sup>2</sup> Fauze J. Anaissi (PQ),<sup>1</sup>

acorone.camila@gmail.com

<sup>1</sup>Departamento de Química, UNICENTRO.; Departamento de Química, UFSM.

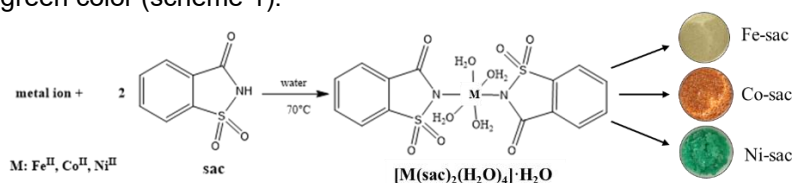
Palavras Chave: Coordination chemistry; Saccharin complexes; Transition metals; UV-Vis spectroscopy; Single crystal.

### Highlights

Saccharin forms stable octahedral complexes with Fe(II), Co(II), and Ni(II). UV-Vis spectra display distinct intra-ligand and *d-d* electronic transitions. Single-crystal data confirms monodentate coordination of saccharin through nitrogen. Structural parameters are consistent with reports, though space group variations are observed.

### Resumo/Abstract

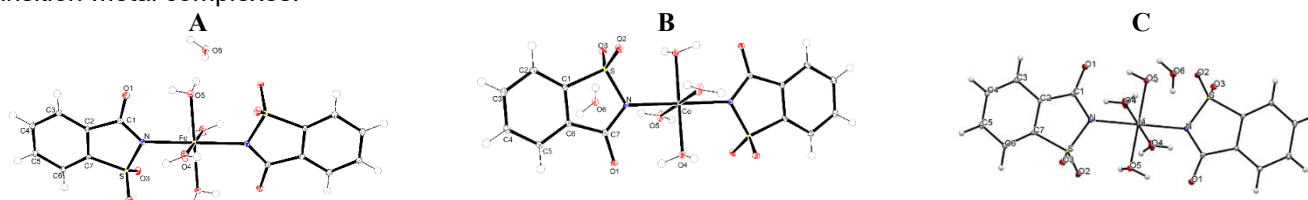
The saccharin ligand reacts with Fe(II), Co(II), and Ni(II) metal ions to form a complex with the general formula:  $[M(\text{sac})_2(\text{H}_2\text{O})_4] \cdot \text{H}_2\text{O}$ . The Fe-sac complex yielded a yellow color; the Co-sac complex yielded a salmon color; and the Ni-sac complex yielded a green color (scheme 1).



**Scheme 1.** Synthesis of complexes M-sac.

The coordination chemistry of saccharin with transition metals was investigated through UV-Vis spectroscopic and crystallographic methods. The UV-Vis spectra of all complexes display an intense intraligand band at 268 nm, attributed to saccharin  $\pi \rightarrow \pi^*$  transitions. For Co(II), an additional absorption at 511 nm corresponds to the  ${}^4\text{T}1\text{g}(\text{P}) \rightarrow {}^4\text{T}1\text{g}$  ligand field transition, consistent with an octahedral environment. The Ni(II) complex exhibits two characteristic absorptions: 668–735 nm range, assigned to the  ${}^3\text{T}1\text{g} \rightarrow {}^3\text{A}2\text{g}$  transition, and a spin-orbit coupling feature, in agreement with literature reports. The Fe(II) complex exhibited a low-energy band at 900 nm, corresponding to the  ${}^5\text{E}_\text{g} \rightarrow {}^5\text{T}2\text{g}$  transition and indicative of Jahn–Teller distortion in a high-spin state.

Single crystals of  $[M(\text{sac})_2(\text{H}_2\text{O})_4]$  ( $M = \text{Fe}, \text{Co}, \text{Ni}$ ) were obtained by slow methanol: diethyl ether evaporation. X-ray diffraction confirmed octahedral coordination in a symmetrical structure, with two saccharin binding monodentate via nitrogen in a trans position relative to each other (figure 1). Structural features were consistent with previously reported complexes, with space group  $\text{P}2_1/\text{c}$ , although variations were observed for Co(II), as they crystallized in a space group  $\text{P}2_1/\text{a}$ .<sup>1</sup> These results highlight the stability and reproducibility of saccharin-based coordination environments in transition-metal complexes.



**Figure 1.** Representation of the A) Fe-sac; B) Co-sac, and C) Ni-sac complexes (ellipsoids with 50% probability).

### Agradecimentos/Acknowledgments

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### Referências e notas

1. Appelt, P. et al. *J. Inorg. Biochem.*, 272, 2025.