

BOOK OF ABSTRACTS



ICNI - III

3rd INTERNATIONAL CONFERENCE ON NONCOVALENT INTERACTIONS

June 17th - 21st 2024
Belgrade, Serbia



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How selenium's electronic structure favor its participation in non-covalent interactions?

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Selenium is an exceptional chalcogen with distinct features that make it a valuable element in the study of non-covalent interactions. Firstly, selenium's ability to exist in different oxidation states allows for the formation of varying covalent bonds with neighboring atoms. Secondly, due to the anisotropic electronic shell, selenium atom enables its participation in non-covalent interactions as both a nucleophile and an electrophile. Thirdly, selenium's electron shell has a notable tendency to polarize, making it possible to adjust the electrophilicity/nucleophilicity of selenium compounds through intramolecular electronic effects and influence of environment (i.e. solvent, neighboring groups). Lastly, the abundance of the isotope selenium-77 makes it particularly well-suited for measuring NMR spectra, facilitating direct experimental observation of non-covalent interactions involving selenium.

In this presentation, we will cover various studies carried out by our research group focusing on non-covalent interactions with the selenium atom. We will delve into fundamental aspects, such as the distinctive electronic structure of selenium^[1] and the impact of external conditions.^[2,3] Additionally, we will discuss the reasons behind the effectiveness of selenium-containing proteins in human body's antioxidant defense.^[4] Furthermore, we will present an example highlighting the dual nature of selenium as an electrophile and nucleophile in the context of recently studied complexes.

References

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