



**UPO** UNIVERSITÀ DEL PIEMONTE ORIENTALE  
DIPARTIMENTO DI SCIENZE E INNOVAZIONE TECNOLOGICA

## EVENTI DiSIT

Seminario  
22/06/2023  
14:00-16:00  
Aula 205

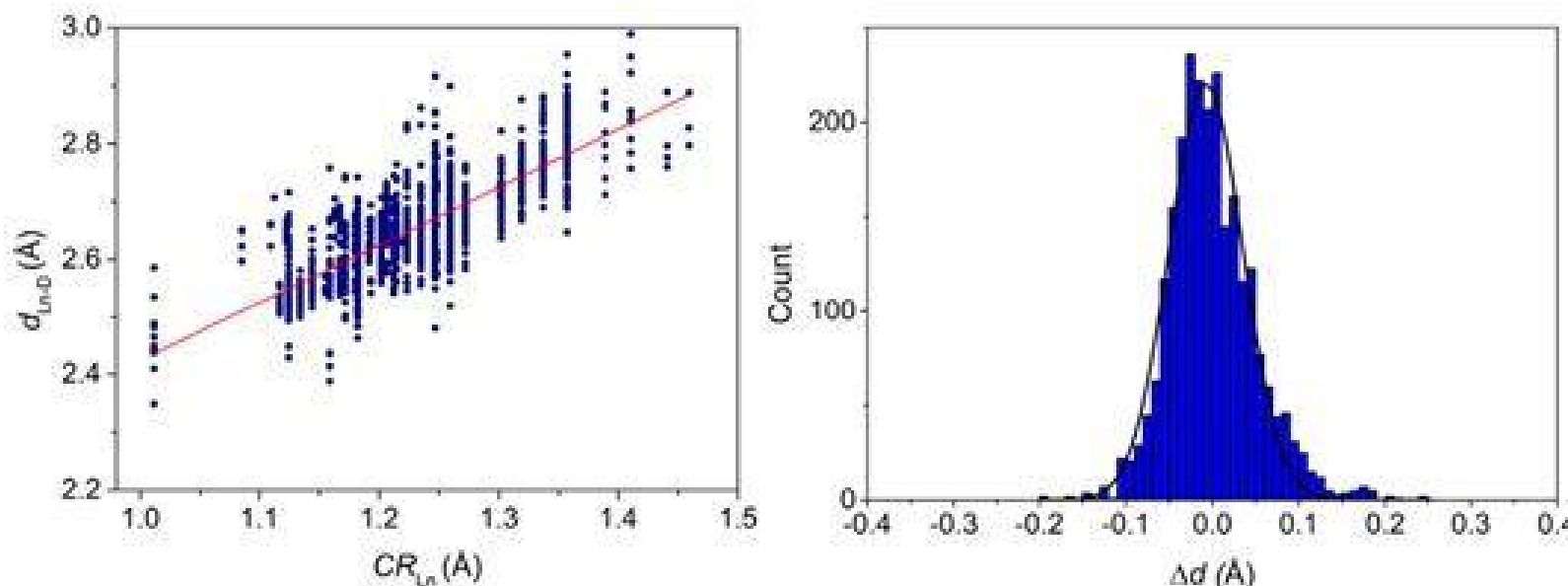
# Structural and Thermodynamic Descriptors to Rationalize Lanthanide Coordination Chemistry

[Prof. Carlos Platas Iglesias](#)

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University of A Coruña - Department of Chemistry





The analysis of the large body of structural data available in the Cambridge Structural Database allowed estimating donor radii for the most common groups present in complexes with the rare-earth ions. Our approach is based on the assumption that Ln donor distances can be broken down into contributions of the cation and the donor atom. Theoretical calculations using density functional theory (DFT) and wave function approaches (NEVPT2) support this assumption, as they show that the minimum in electron density along the Ln donor bond corresponds well with Shannon's crystal radii. Subsequent linear fits of the experimental bond distances for all rare earth cations (except Pm3+) afforded donor radii that allow predicting Ln donor distances regardless the nature of the rare-earth cation and its oxidation state (see Figure). This set of donor radii can be used to rationalize structural data and identify particularly weak or strong interactions, which has important implications as to understand the stability and reactivity of complexes of these metal ions. With a similar approach, we have demonstrated that the thermodynamic stability constants of Gd(III) complexes can be approximated from the contributions of the different donor groups present in the ligand structure.

EVENTO APERTO A:

Docenti, Borsisti, Assegnisti, Dottorandi

SEMINARIO IN LINGUA: INGLESE

