



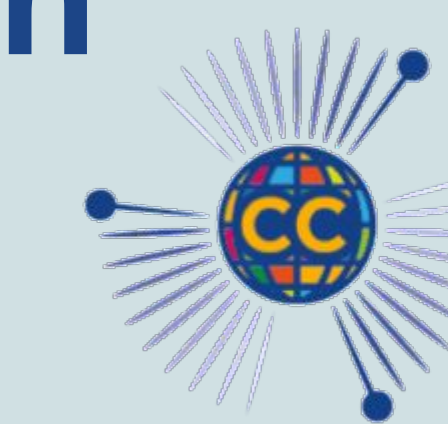
Application of Zirconium-EDTA Mixed Ligand Complexes for Anion Removal: A Theoretical Evaluation

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Introduction

Clean drinking water is a basic need for all living beings. With the rapid growth of the global population, the demand for clean drinking water is increasing. However, due to the growth of industrialization, agricultural activities, and all other human activities, available drinking water resources are getting contaminated with chemical wastes, including anions such as PO_4^{3-} , SO_4^{2-} , CO_3^{2-} , F^- , and Cl^- , resulting a global health concern.



Aim of the project

In this study, a theoretical investigation was carried out to evaluate the possible use of zirconium mixed-ligand complexes, which are possible to produce as value-added products from zirconium-containing mineral resources such as zircon and baddeleyite, for anion removal.

Methodology

Identifying the possible mixed complexes formed by Zr(IV) with EDTA and anionic ligands in aqueous medium

Generating the structures of the complexes
Software -Avogadro 2

Geometry Optimization with DFT calculations
Software-ORCA 5.0; Method- hybrid B3LYP functional
Basis set- def2-TZVP

Bond Order Analysis



Baddeleyite



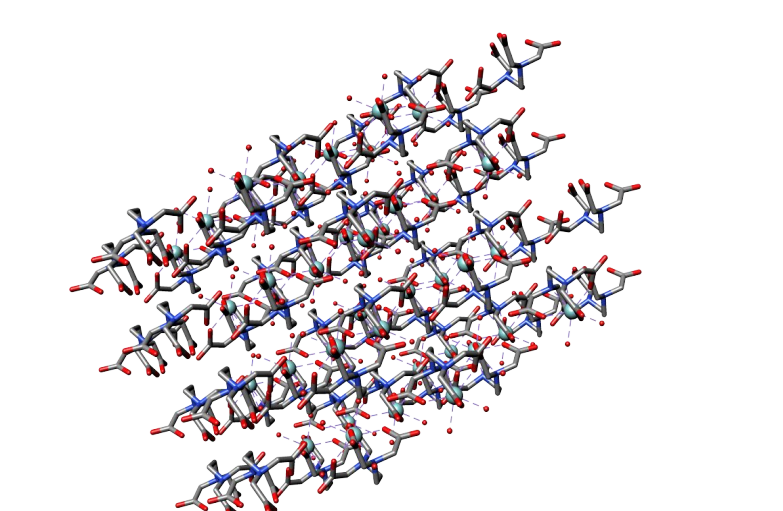
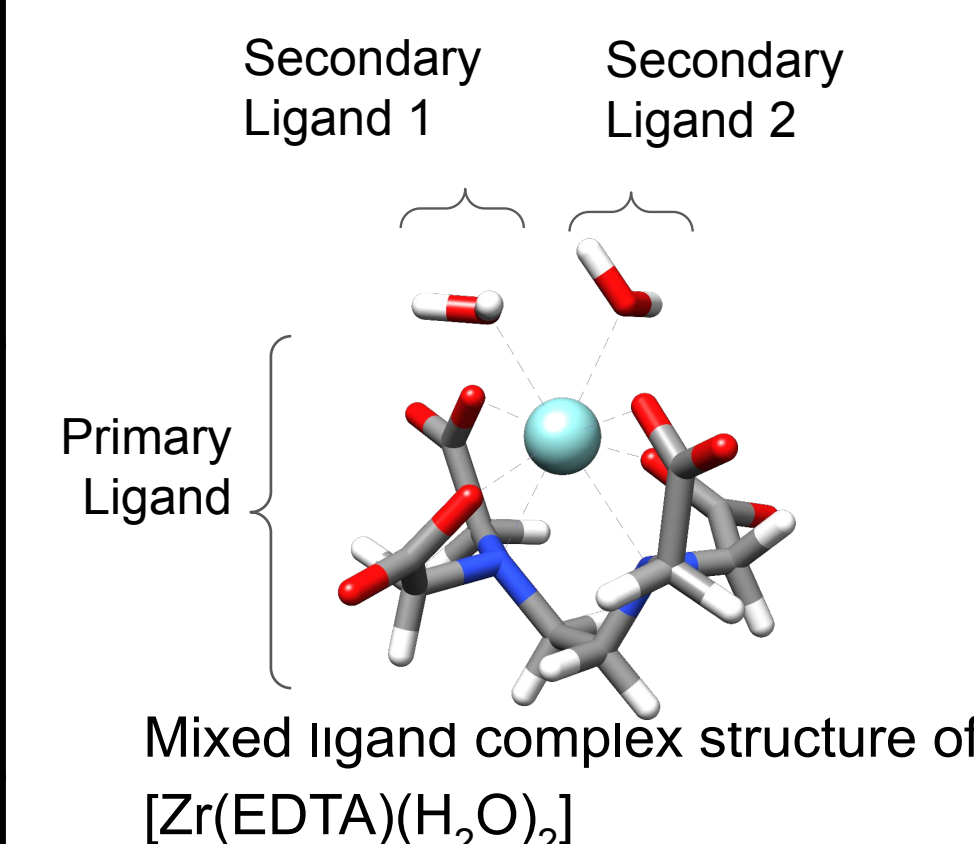
Zircon

Results

- Average bond order for Zr-OH₂- 0.314

Table1: Calculated bond orders for metal-anion bonds

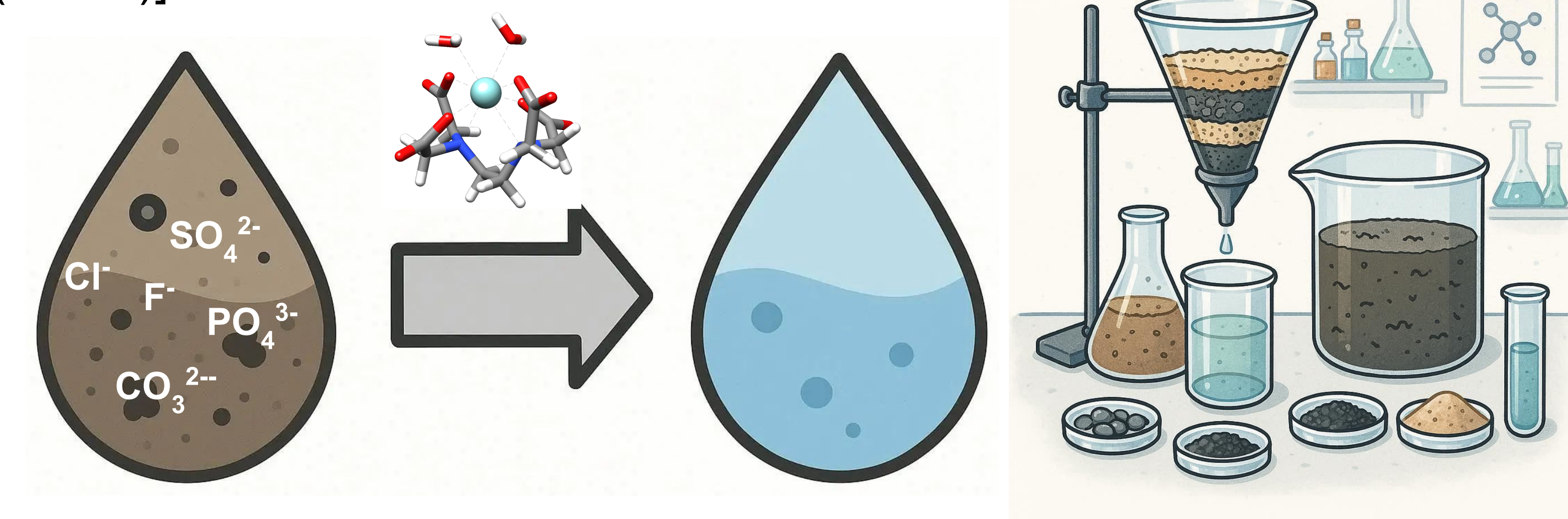
Anion	Complex	Average Bond Order (metal-anion)
Cl^-		0.690
		0.681
F^-		0.780
		0.761
SO_4^{2-}		0.472
CO_3^{2-}		0.587
PO_4^{3-}		0.737



Recorded crystal structure of $[\text{Zr}(\text{EDTA})(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$

Discussion

Based on the bond order analysis, bond order of Zr-anion bond are higher than that of Zr-OH₂ in $[\text{Zr}(\text{H}_2\text{O})_2(\text{EDTA})]$. Therefore, PO_4^{3-} , SO_4^{2-} , CO_3^{2-} , F^- , and Cl^- all have significantly stronger binding to Zr(IV) than H₂O. Hence, they can replace H₂O molecules in $[\text{Zr}(\text{H}_2\text{O})_2(\text{EDTA})]$.



Conclusion

The results showed that PO_4^{3-} , SO_4^{2-} , CO_3^{2-} , F^- , and Cl^- all have significantly stronger binding to Zr(IV) than H₂O. These findings suggest a promising approach to water purification using Zr-EDTA mixed ligand complexes, which can be synthesized as a value-added product from available zirconium mineral resources.

Acknowledgement

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Chemical Structures: Chimera
Image creation : Bing Image Creator

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