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June 2023

*Changing the World's Energy Future*

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**Prepared for the  
U.S. Department of Energy  
Under DOE Idaho Operations Office  
Contract DE-AC07-05ID14517**

# Exploring the speciation of actinide salts in the presence of contaminants related to molten salt reactors

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## Abstract

Molten salt reactors (MSRs) are up-and-coming Generation IV nuclear reactors with either coolant and/or radioactive fuel in molten salt form. Due to their improved safety, efficiency, affordability and convenient waste processing system, these reactors are considered a superior alternative to conventional ones. However, prior to commercial implementation, it is necessary to have an extensive understanding of the reactions occurring in the MSR. The safety parameters of the MSR are determined by the rheological properties such as density and viscosity of the molten salt and these properties are governed by the local structure of the molten salts. Due to the high operational temperatures of MSR's, corrosion plays an important role. Because of their influence, the container corrosion products become part of the fuel salt matrix. In this work, we are investigating how these corrosion products, e.g., Mo, Ni, Cr, would impact the speciation of the actinide metal centers. For the initial studies, lanthanides are used as a surrogate for actinides. Lanthanide chloride salts ( $\text{LnCl}_3$ ) are reacted with transition metals and excess of alkali or alkali earth metal salts or salt mixtures ( $\text{LiCl}$ ,  $\text{NaCl}$ ,  $\text{KCl}$ ) and analyzed using different characterization techniques.

## Project Overview

- **Knowledge Gap:** There is no work conducted to identify the impact of impurities on the local structure of the actinide
- **Hypothesis:** The speciation of lanthanide and actinide chlorides can be affected by the introduction of contaminants, which would impact the bulk properties
- **Scientific Question:** How the unintentional impurities such as corrosion byproducts and intentionally added materials such as graphite in a nuclear fuel reactor, would impact the speciation of lanthanide and actinide salts

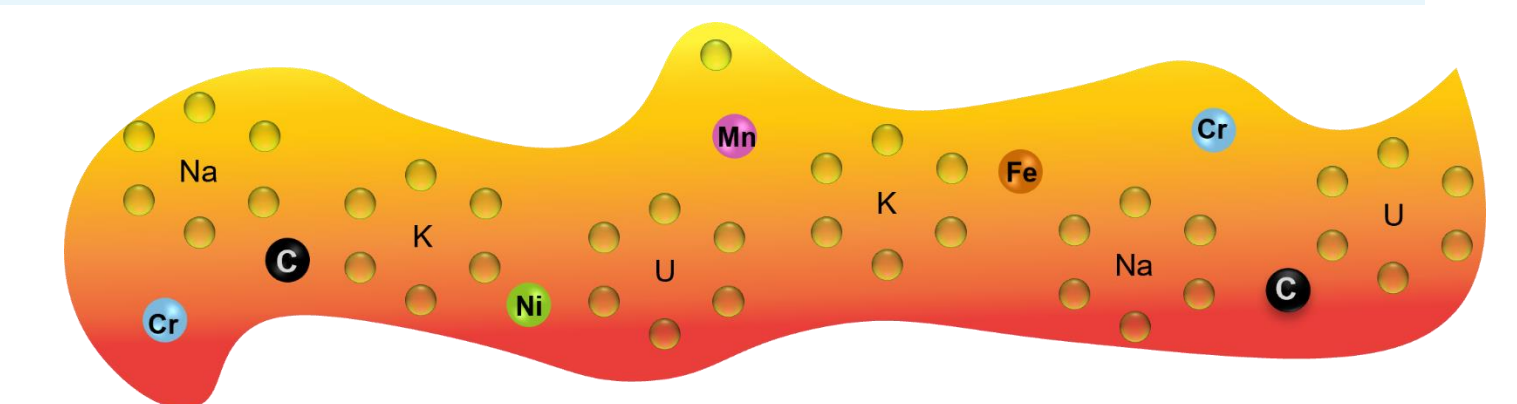


Figure 1: Corrosion products related to MSRs can modify the speciation of actinide salts

## Experimental Approach

The experiments are approached using two methods

(1)

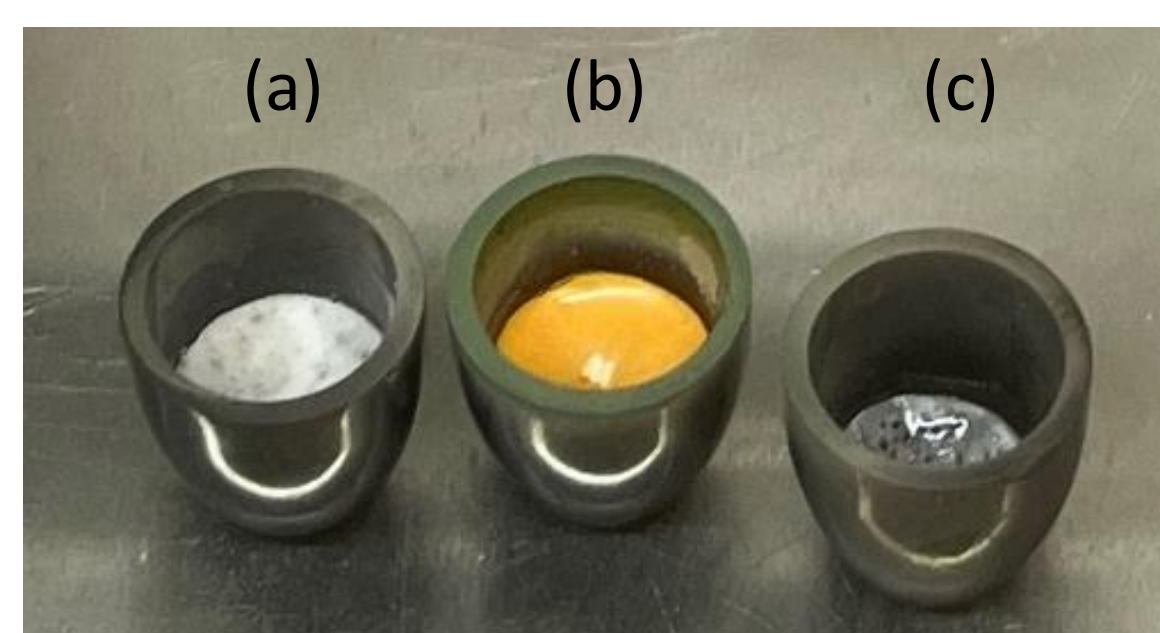


Figure 2: (a) Lithium chloride ( $\text{LiCl}$ )/cerium chloride ( $\text{CeCl}_3$ ), (b)  $\text{LiCl}/\text{CeCl}_3$ /nickel chloride ( $\text{NiCl}_2$ ), and (c)  $\text{LiCl}$  heated and cooled to room temperature in glassy-carbon crucibles

- Reactants are added to a glassy carbon crucible
- Heated up to  $\sim 800^\circ\text{C}$  and kept at that temperature for 12 hours
- Slowly cooled to room-temperature

(2)

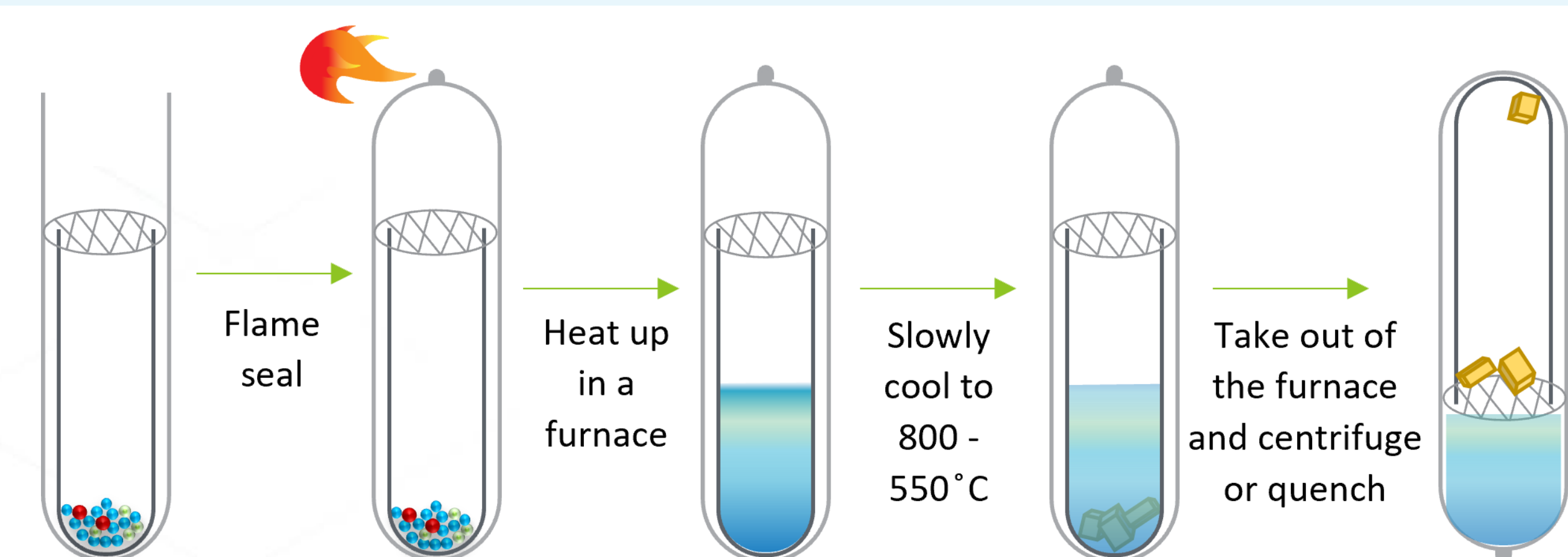


Figure 3: Reaction process when the reagents are placed inside a quartz tube

- Reactants are added into an alumina crucible and that is placed inside a quartz tube and flamed sealed under vacuum
- Heated up to  $\sim 1000^\circ\text{C}$  and kept at that temperature for 12 hours
- Slowly cooled to a desired temperature
- Taken out at that temperature and quenched

## Results and Discussion

The reactions conducted in glassy carbon crucibles led to the formation of polycrystalline materials

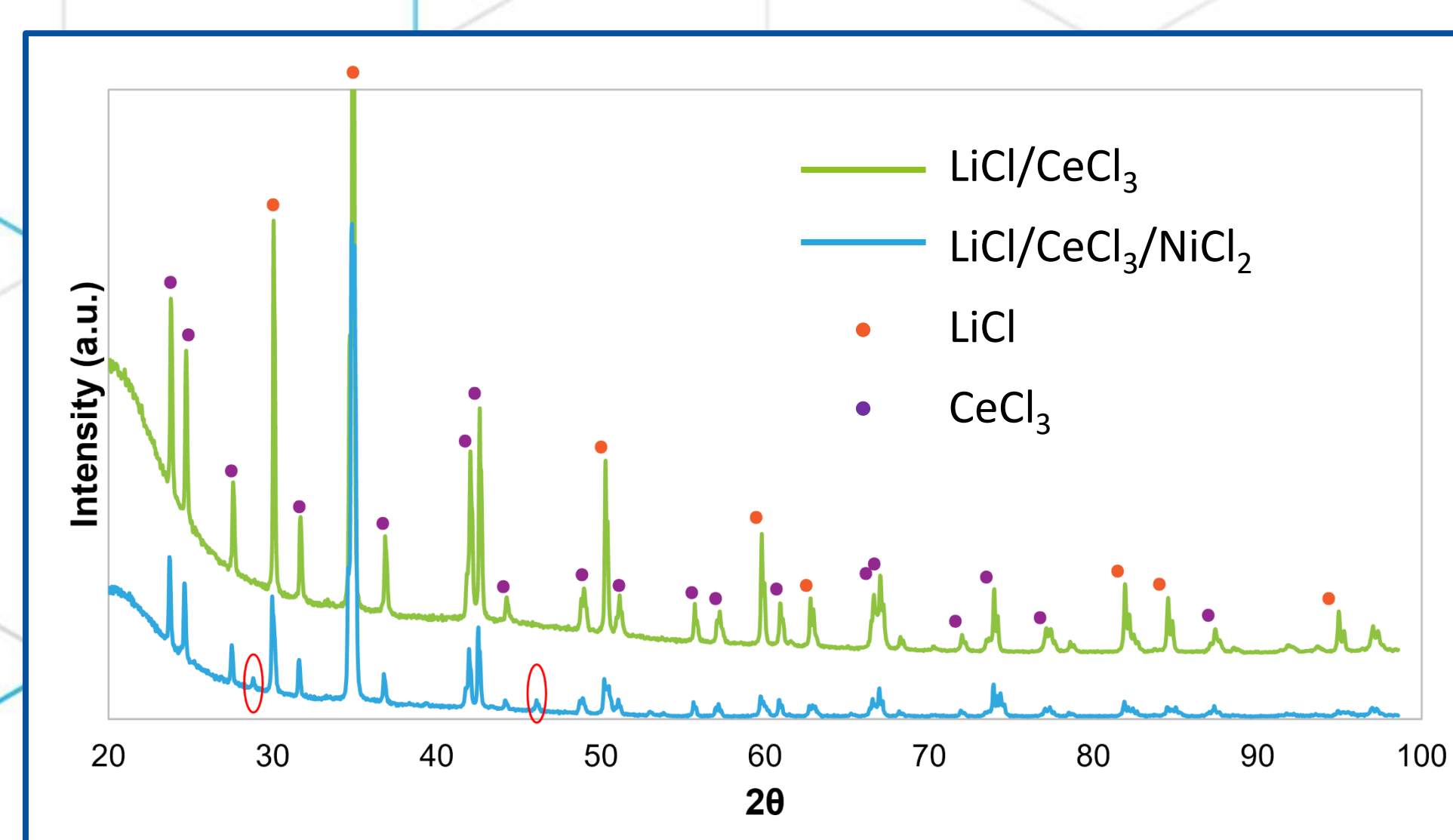


Figure 4: Powder X-ray diffractogram of  $\text{LiCl}/\text{CeCl}_3$  and  $\text{LiCl}/\text{CeCl}_3/\text{NiCl}_2$  samples. Unidentified peaks of the  $\text{LiCl}/\text{CeCl}_3/\text{NiCl}_2$  sample are circled in red.

Powder X-ray diffraction analysis identified the presence of  $\text{LiCl}$  and  $\text{CeCl}_3$ , but peaks related to  $\text{NiCl}_2$  were absent. However, there were two unidentified peaks present. It can be assumed that there might be a phase change once  $\text{NiCl}_2$  is heated to high temperatures in the presence of  $\text{LiCl}$  and  $\text{CeCl}_3$  and the new unidentified peaks might be related to this phase.

## Conclusion and Future work

- High temperatures seem to be affecting the speciation of the salts
- Samples will be analyzed using other characterization techniques such as Raman spectroscopy, FTIR spectroscopy, UV-Visible spectroscopy and ICP-MS

## Acknowledgement

This project was supported through the INL Laboratory Directed Research and Development (LDRD) Program (23P1077-002FP).

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