

# Final Thesis (M.Sc.)

## Synthesis and Solubility data of Fe-containing hydroxy and carbonate sodalites and cancrinite

Institut für Bauforschung (ibac)  
Lehrstuhl für Baustoffforschung  
Arbeitsgruppe Mikrostruktur und Modellierung

**Contact:**

Michael Wenzel, M.Sc.  
Schinkelstraße 3, Raum 254  
D-52062 Aachen  
Telefon 0241/80-95119  
[wenzel@ibac.rwth-aachen.de](mailto:wenzel@ibac.rwth-aachen.de)

**Date**

11/10/2022

**Background:**

To produce sustainable cements substitutes for fly ash and blast furnace slag are needed. Intense research is targeting the reutilization of currently unused metallurgical wastes like Bauxite Residue (BR) to close material cycles.

Bauxite residue is generated in significant quantities (150 Mio.t/a) for the application in industrial cements. It's initial reactivity is mostly related to the so called desilication product, which makes up to 20 wt.% of the BRs mass (e.g. shown by Peys et al 2021). The main mineral phases of the desilication product are sodalite and/or cancrinite.

It is important to know which hydrate phases they form and how their presence affects the cements phase assemblage to exclude internal durability issues. Thermodynamic modelling e.g. with GEMs or similar software can help to answer the question of the contribution of sodalites and cancrinites to hydration reactions.

The solubility data currently used for thermodynamic modelling have been determined on stoichiometrically ideal OH-sodalite that does not form under the conditions of a Bayer process.

This thesis aims at generating solubility data of sodalites closer to those found in BRs. The work is separated in a theoretical and experimental part. The latter will focus on synthesizing sodalites of varying Si/Al ratios and including iron traces via hydrothermal synthesis. In a two-step synthesis cancrinite will be synthesized using sodalite as intermediary product. The

synthesized zeolites will be characterized in collaboration with a PhD student. Finally, solubility experiments are carried out to determine solubility products. The theoretical part will focus on understanding the characterization techniques and applied synthesis pathways.

**Your tasks:**

- **Literature research including the topics.**
  - o Basics of the Bayer process
  - o Sodalite/Cancrinite structures observed in Bauxite Residue
  - o Synthesis of Sodalites/Cancrinites
  - o Published Solubility Data for these zeolites
- **Experiments and Discussion**
  - o Synthesis of Sodalites and Cancrinite
  - o Characterization of the synthesized phases
  - o Determination of solubility products at room temperature

**Requirements:**

- You are studying chemistry/ material science or a related engineering discipline
- Interest in analytical work and chemistry
- Either fluent in English or German

**Beneficial are:**

- Practical experience in chemical or physical laboratories
- Basic knowledge of cement chemistry/ zeolite chemistry or physical chemistry

The experimental matrix has been developed for 6 months (writing included) but can be adapted to the requirements of your colloquium.