

THERMAL SAFETY & STRUCTURE-RELATED REACTIVITY INVESTIGATION

R&D project

Context

- A family of 5-membered cyclic sulfamidates was studied to characterize and model the thermal behaviour of individual compounds as a function of their structures

Objectives

- Design and develop a milliliter-scale reaction calorimeter, and use it to classify a family of compounds in terms of their thermal reactivity with strong bases
- Use multivariate data analysis and machine learning to model the reactivity of the compounds as a function of their structures

Outcome

- A mini-calorimeter was built and validated for accuracy
- The compounds were characterized in terms of reaction enthalpy and risk class
- The multivariate model was shown to predict correctly the risk class of new compounds
- This approach provides early safety evaluation potential for development and scale-up

