SUSE

Sustaining Carbonic Esters Synthesis with Carbon Dioxide Feedstock

CP2D 2008

AGENCE NATIONALE DE LA RECHERCHE

ANR

A French-Finnish Consortium:

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"***Matériaux Nanostructurés : Phénomènes à l'Interface***" (MaNaPI/University of Burgundy-Dijon) - Prof. Frédéric Bernard,

"***Chimiométrie et Modélisation moléculaire***" (CHEMOD/University Claude Bernard Lyon I) - Prof. Henry Chermette,

*"**Mass and Heat Transfer Process Laboratory**" (OU/*University of Oulu) - Prof. Riitta Keiski,

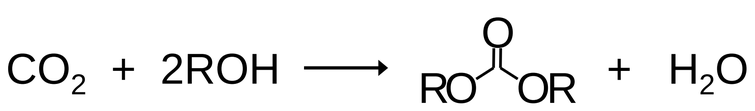
*"**Laboratory of Industrial Chemistry and Reaction Engineering***" (ÅA/Åbo Akademi) - Prof. Jyri-Pekka Mikkola.

Carbon Dioxide: a Source of Carbon for a Sustainable Chemistry

The development of new and innovative reaction methodologies based on CO_2 as feedstock is a significant area of interest in both academic and industrial research boosted by the Sustainable Chemistry and Engineering challenge. In addition to replacing fossil fuels with biomass- and non-carbon based energy sources, direct or indirect utilization of CO_2 can also contribute to reducing CO_2 accumulation to the atmosphere. The utilization of CO_2 as feedstock for producing chemicals is also an interesting challenge to explore new concepts and new opportunities for catalysis and industrial chemistry. This project addressed basic issues in the design of reaction routes to benign carbonic esters taking advantage on a multi-disciplinary cooperation between Finnish and French research groups.

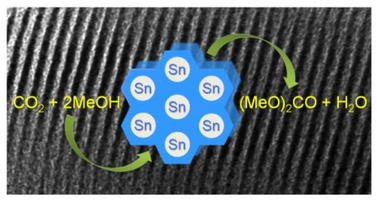
Direct Synthesis of Carbonic Esters from Carbon Dioxide and Alcohol

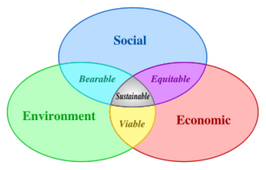
Carbonic esters are an important class of commodity chemicals that find applications in a variety of sectors. Nonetheless, their primary synthesis pathway still relies on the use of hazardous phosgene, one of the most acutely toxic substances used on industrial scale. The alternative route, the catalytic oxidative carbonation of methanol, allows responding to the current demand in dimethyl carbonate. However, these technologies intrinsically limit the production due to engineering and safety constraints. Therefore, substitution strategies are highly desirable in meeting the following criteria of the "12 Principles of Green Chemistry": (1) waste prevention, (2) atom economy, (4) design of safer chemicals, (5) safer solvents, (7) use of renewable feedstocks, and (9) catalysis. The SUSE project explored innovative hybrid catalysis for carbonic esters synthesis in shifting to carbon dioxide and alcohols co-reagents.

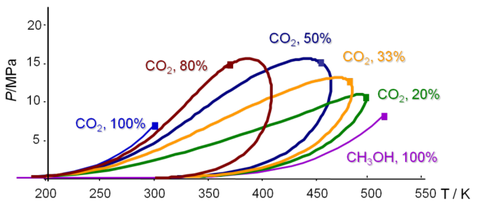


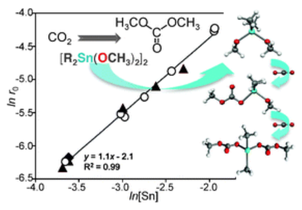
A Multidisciplinary Approach

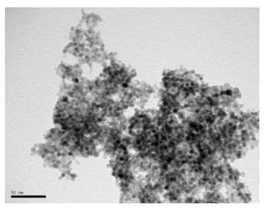
To carry out this project, the research activity was organized in six work-tasks, shared out among the French and Finnish partners, targeting several aspects of the challenge, and including in particular: thermodynamic calculations and simulations, the development and characterization of new catalysts, catalytic evaluation for the reaction target, molecular modeling and reaction mechanisms, reactor design and the identification of sustainability indicators.











Impacts:

- A comprehensive approach,
- A various range of new pre-catalytic materials for the selective synthesis of carbonic esters,
- A notable increase in the activity of catalyst precursors,
- A better understanding of the mechanisms of insertion of carbon dioxide in the Sn-OR bond,
- Modeling of a complete catalytic cycle by DFT calculations.

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