EHLCATHOL

Chemical transformation of enzymatic hydrolysis lignin (EHL) with catalytic solvolysis to fuel commodities under mild conditions

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W2: Mechanism-EHL solvolysis and potential condensation reactions

Catalytic hydrogenation and hydrodeoxygenation of selected model compounds



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Catalytic hydrogenation/hydrodeoxygenation of model compounds



- Development of heterogeneous base metal catalysts
- Reaction optimization for selective hydrogenation/hydrodeoxygenation processes
- Application of the established protocol for other EHL-derived model compounds







R. V. Jagadeesh, A.-E. Surkus, H. Junge, M.-M. Pohl, J. Radnik, J. Rabeah, H. Huan, V. Schünemann, A. Brückner and M. Beller, Science, 2013, 342, 1073. R. V. Jagadeesh, K. Murugesan, A. S. Alshammari, H. Neumann, M. Pohl, J. Radnik, M. Beller, Science, 2017, 358, 326.

Catalytic hydrogenation/hydrodeoxygenation



- B is the targeted product-Complete hydrogenation/hydrodeoxygenation
- Catalyst showed more selectivity towards product B (99%)



• In all the cases complete conversion and 99% selectivity were achieved



Catalytic hydrogenation/hydrodeoxygenation



• Reaction in n-hexane or n-heptane or n-octane

- Reaction in i-PrOH
- i-PrOH is found to be the good caping agent



Planned mechanistic investigations



- To study the initial kinetics and mechanism, we will select fist EHL derived monomer and then dimer or oligomer (these will be provided by W4).
- Solvolysis, hydrogenolysis, hydrogenation reactions will be applied.
- In situ-IR or in situ-NMR studies will be conducted.
- Based on these studies, product distribution and suitable caping agents will be find out to protect/deactivate functional groups.
- We will look for the possible condensation or re-condensation reactions.



Summary and outlook

- We developed Ni-catalyzed hydrodeoxygenation process for the conversion of ketones, ethers and phenols to (cyclo)alkanes.
- Hydrodeoxygenation of lignin and EHL-derived model compounds, dimers and oligomers will be tested.
- Mechanistic and kinetics investigations for the reaction of model EHL-derived model compounds will be made.

