Aqueous Phase Hydroalkylation and Hydrodeoxygenation of Phenol by Dual Functional Catalysts Comprised of Pd/C and H/La-BEA

Abstract:
Aqueous phase catalytic phenol hydroalkylation and hydrodeoxygenation have been explored using Pd/C combined with zeolite H-BEA and La-BEA catalysts in the presence of H-2. The individual steps of phenol hydrogenation, cyclohexanol dehydration, or alkylation with phenol were individually investigated to gain insight into the relative rates in the cascade reactions of phenol hydroalkylation. The hydroalkylation rate, determined by the concentrations of phenol and cyclohexanol in phenol hydroalkylation, required the hydrogenation rate to be relatively slow. The optimized H+/Pd ratio was 21, which allowed achieving comparable cyclohexanol formation rates via phenol hydrogenation and consumption rates from alkylation with phenol in phenol hydroalkylation. La-BEA was shown to be more selective for hydroalkylation than H-BEA in combination with Pd/C, because cyclohexanol dehydration was retarded selectively compared to alkylation of phenol. This indicates that dehydration is solely catalyzed by Bronsted acid sites, while alkylation can be achieved in the presence of La3+ cations.

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