Technology Offer

Bifunctional Catalyst for Phenol Production via Decarboxylation

Ref.-No.: 1001-6599-LC

Abstract

This technology enables the selective transformation of aromatic carboxylic acids into substituted phenols through a novel catalytic system combining bimetallic iron-ruthenium nanoparticles with amine-functionalized supported ionic liquid phases ($Fe_{(25)}Ru_{(75)}$@SILP+IL-NEt_2). The catalyst performs two chemical transformations in tandem: decarboxylation and selective reduction or hydrodeoxygenation. This bifunctional system delivers excellent selectivity and yield, particularly when applied to lignin-derived substrates. Operating under hydrogen pressure, it enables direct access to valuable phenol derivatives and anilines from renewable feedstocks. The system is recyclable, retains its structural integrity over multiple cycles, and demonstrates broad applicability across various substituted hydroxy- and aminobenzoic acids. It provides a promising route for sustainable phenol production in the pharmaceutical, agrochemical, and specialty chemical sectors.

Background

Current phenol production relies heavily on the cumene process using fossil-derived benzene and propene, which poses environmental and economic challenges. Alternative synthetic routes such as direct alkylation, amination, and lignin depolymerization are either inefficient, require harsh conditions, or suffer from limited selectivity and substrate scope. Recent attempts to decarboxylate hydroxybenzoic acids using Cu-based catalysts or ionic liquids achieved poor yields (<50%). Moreover, integrating decarboxylation with reduction/hydrodeoxygenation in one step remains an unmet challenge. There is a critical need for multifunctional catalysts that perform clean and efficient transformations of bio-based molecules into high-value chemicals under mild conditions.

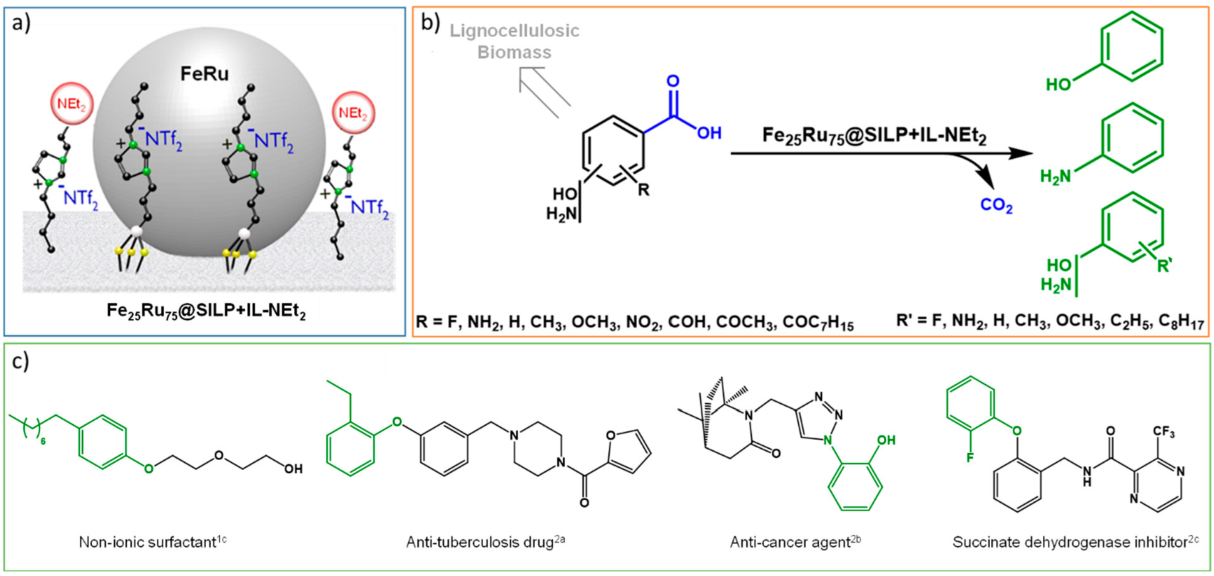

Figure 1: Multifunctional Catalyst Concept and Applications. **(a)** Structural illustration of the bifunctional $Fe_{25}Ru_{75}$@SILP+IL-NEt_2 catalyst combining metal nanoparticles with basic ionic liquids. **(b)** Selective decarboxylation of lignin-derived aromatic acids into phenols and anilines. **(c)** Example applications of the resulting phenol derivatives in surfactants, pharmaceuticals, and agrochemicals.

Max-Planck-Innovation GmbH
Arnulfstr. 58
80335 München
www.max-planck-innovation.de

Technology

The patented technology features a multifunctional catalyst composed of bimetallic $Fe_{(25)}Ru_{(75)}$ nanoparticles immobilized on a silica support modified with amine-functionalized ionic liquids (IL-NEt_2). The catalyst is synthesized by in situ reduction of iron and ruthenium precursors on a supported ionic liquid phase (SILP), followed by physisorption of IL-NEt_2. This design brings metal and amine sites into close proximity, facilitating synergistic catalysis. The catalyst operates under hydrogen at moderate temperatures (150–175 °C) and pressures (50 bar), converting hydroxy- and aminobenzoic acids to phenols and anilines with >99% selectivity. Tandem reactions are possible, converting substrates with formyl, acyl, or nitro groups into more reduced phenol derivatives. Structural and catalytic integrity is maintained over at least five reuse cycles, with no significant metal leaching or catalyst deactivation. Mechanistic studies confirm the cooperative action of the metallic and basic components during hydrogen activation and CO_2 elimination.

Advantages

- **High product selectivity**: >99% yield for phenols and anilines from diverse aromatic acids.
- **Multifunctional catalysis**: Performs decarboxylation and reduction/hydrodeoxygenation in a single step.
- **Sustainable feedstock compatibility**: Efficient conversion of lignin-derived and bio-based substrates.
- **Catalyst recyclability**: Maintains performance over multiple cycles with no structural degradation.
- **Operates under mild conditions**: Active under moderate temperature and hydrogen pressure without aromatic ring hydrogenation.

Potential applications

- **Pharmaceutical synthesis**: Production of phenol-derived intermediates for drugs (e.g., anticancer, anti-TB agents).
- **Agrochemical manufacturing**: Synthesis of fungicide and pesticide building blocks.
- **Lignin valorization**: Conversion of biomass waste into high-value chemicals.
- **Fine and specialty chemicals**: Custom phenol and aniline derivatives for dyes and resins.
- **Surfactant production**: Generation of alkylphenols for nonionic surfactant synthesis.

Patent Information

PCT (WO2024194467A2, 22.03.2024); EP application

Publications

Levin, N., Goclik, L., Walschus, H., Antil, N., Bordet, A., & Leitner, W. (2023). Decarboxylation and tandem reduction/decarboxylation pathways to substituted phenols from aromatic carboxylic acids using bimetallic nanoparticles on supported ionic liquid phases as multifunctional catalysts. *Journal of the American Chemical Society*, *145*(41), 22845-22854.

Contact

Dr. Lars Cuypers

Senior Patent- & License Manager, Chemist
Phone: +49 (0)89 / 29 09 19 – 21
eMail: cuypers@max-planck-innovation.de

Max-Planck-Innovation GmbH
Arnulfstr. 58
80335 München
www.max-planck-innovation.de