ELECTROPHOTOCATALYZED FRAGMENTATION OF LIGNIN MODELS

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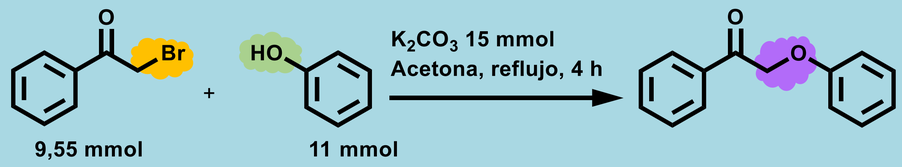
GOALS

To study the reductive fragmentation reaction of lignin models through electro-photoredoxcatalysis (e-PRC) within the lignin oxidation-reduction depolymerization strategy.

- To synthesize oxidized lignin model compounds..
- To study a model reaction of reductive fragmentation of the C_β–O bond.
- Computational modeling of the reaction mechanism.

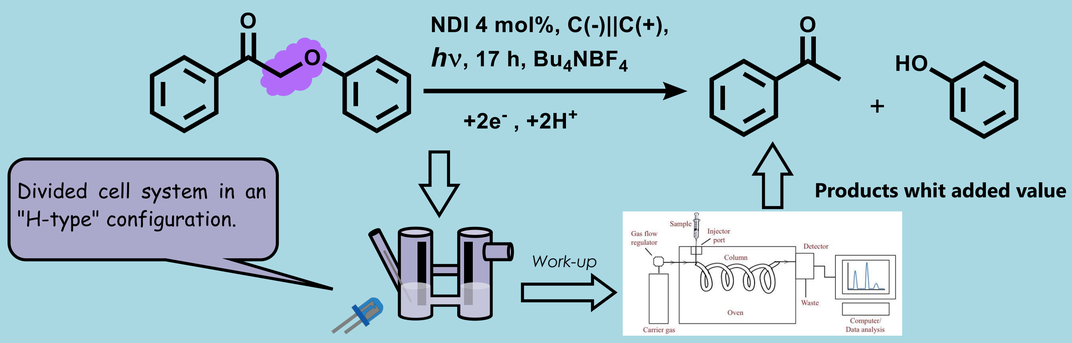
EXAMPLES

Synthesis of 2-phenoxy-1-phenylethan-1-one



Use of simple reagents and solvents for a reaction with good atom economy.

Examples experimental



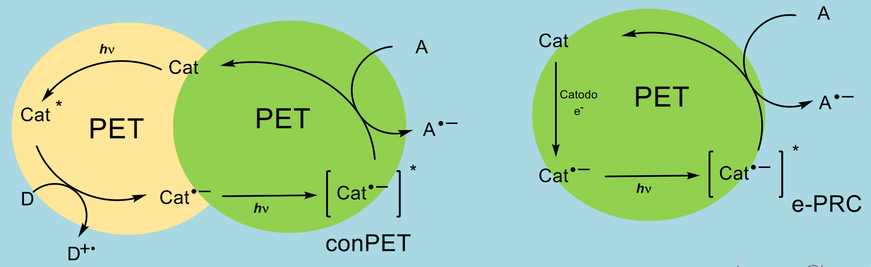
ADVANTAGES

- Use of a catalyst to achieve reactions below -1.5 V (vs. SCE).
- Easy isolation of high value-added products.
- Possibility of functionalizing the products.
- Potential use of more benign electrolytes.

DISADVANTAGES

- Use of halogenated electrolytes
- Long reaction time.

CONCEPT: Use electrical current and visible light to fragment the C–O bond at a low potential, minimizing the use of reagents.



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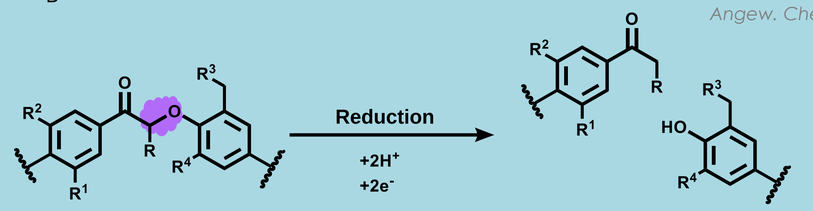
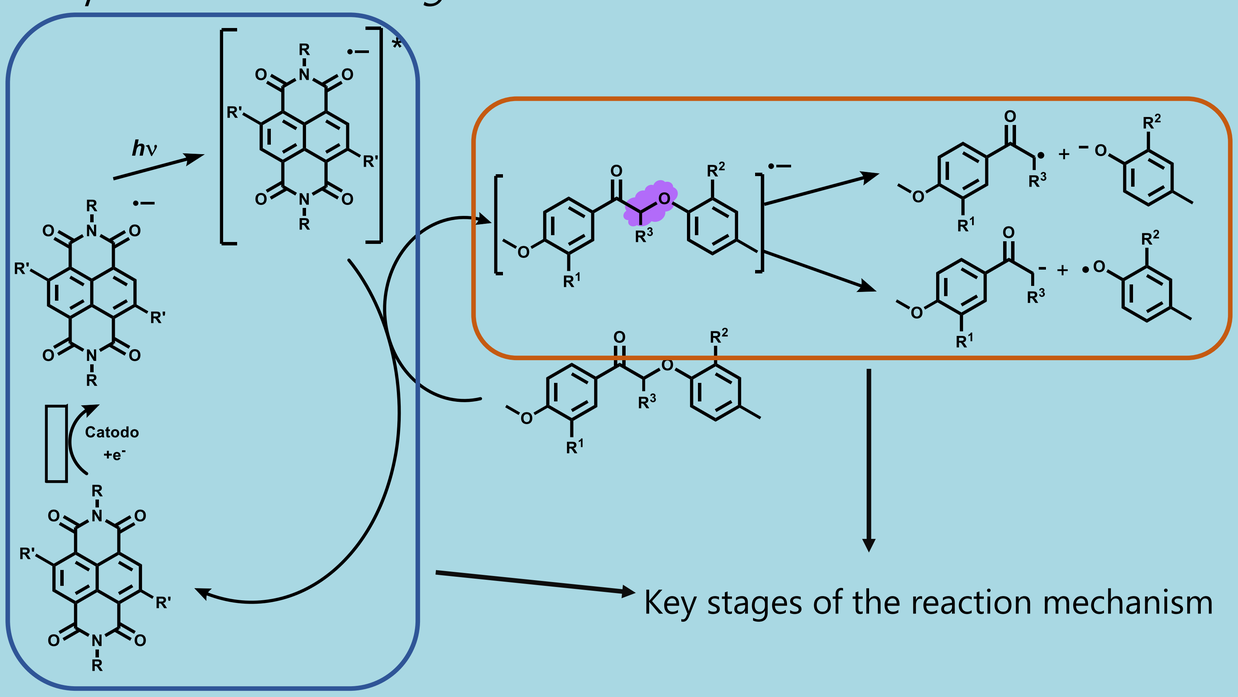


Chem. Rev., **2023**, 123, 4510–4601.

Computational modeling of the reaction mechanism



ADVANTAGES

- Explore the reaction mechanism and study the key stages in complex models.
- Avoid using reagents and energy unless the reaction is thermodynamically and kinetically feasible.

DISADVANTAGES

- Loss of intrinsically experimental data in complex models.
- Need to readjust reaction conditions for the depolymerization of lignin extracted from biomass derived from peanut waste.

Relation to Green Chemistry

❖ The use of electricity and visible light as "clean reactants" eliminates the need for stoichiometric amounts of chemical reagents that generate waste. Furthermore, this research the replacement of toxic metal catalysts, with safer organic photocatalysts. The methodology allows operations under mild conditions, reducing energy consumption and saving purification steps through combined depolymerization and functionalization processes, which maximize resource efficiency. Lastly, this research promotes the valorization of agro-industrial waste, offering a sustainable solution to current challenges.