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Selective Nucleophilic α -C Alkylation of Phenols with Alcohols via Ti=C Intermediate on Anatase TiO₂ Surface

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Nucleophilic C-Alkylation of Phenols with Alcohols Promoted by Anatase TiO₂

Category

Polymer-Supported Synthesis

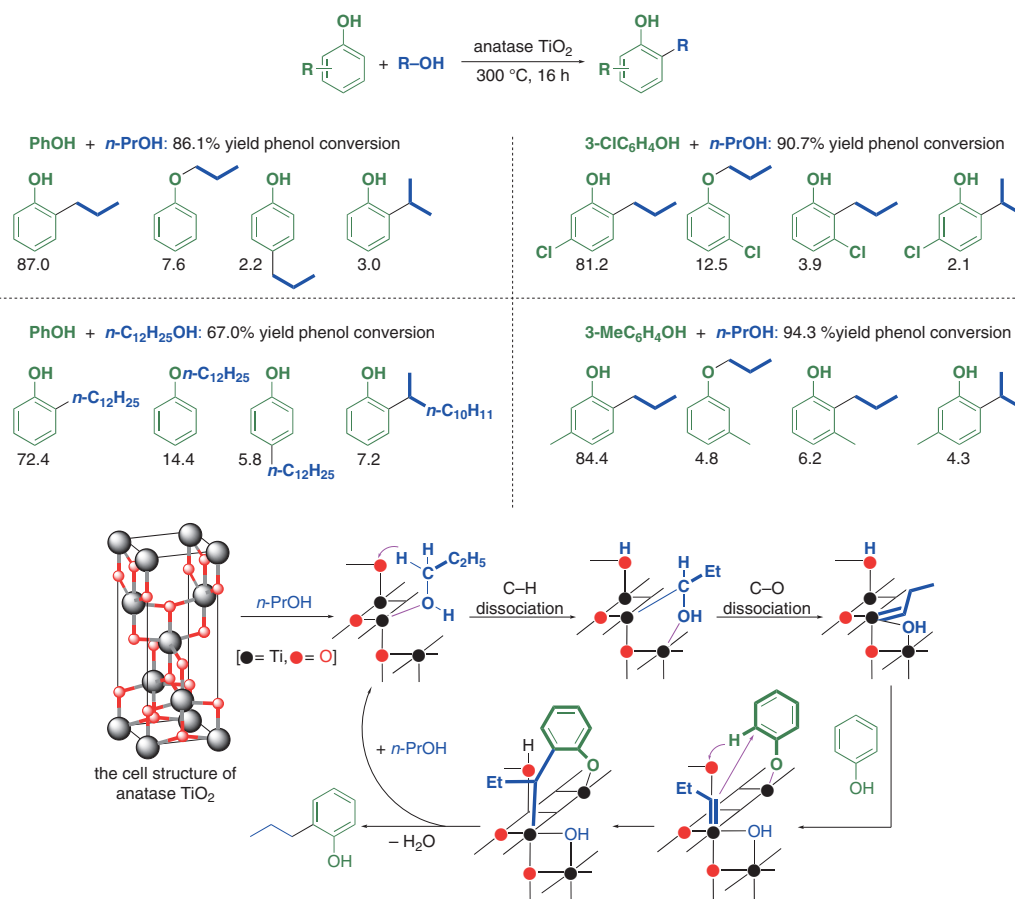
Key words

aromatic alkylation

anatase TiO₂

nucleophilic aromatic functionalization

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Significance: C-alkylation of phenols with alcohols was promoted by anatase TiO₂ at 300 °C. Phenol reacted with *n*-propyl alcohol to give 2-propylphenol with 87% selectivity. Rutile TiO₂, a stable polymorph of titania, did not promote the C-alkylation (ca. 0% phenol conversion). Phenols bearing 3-chloro and 3-methyl substituents showed a similar trend of selectivity for the alkylation, although they have opposite electronic effects.

Comment: DFT calculations as well as experimental observations indicate that the main reaction pathway of C-alkylation is different from the conventional Friedel-Crafts alkylation. The authors have proposed that the reaction proceeds via a Ti=C intermediate which reacted with a Ti-activated phenol nucleophilically at the *ortho*-position.

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