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Isooctane Synthesis by Mimicking of Geological Reaction Conditions

Background

Isooctane (2,2,4-trimethylpentane) is an important ingredient in hydrocarbon fuels that power countless modern machines. One conventional method for synthesizing isooctane is through the alkylation process. Alkylation starts with isobutane and isobutene and requires large quantities of sulfuric acid or hydrofluoric acid to achieve dimerization, which in turn generates toxic waste that is costly to remediate. Another conventional way to synthesize isooctane is to dimerize isobutene with a supported acid catalyst, followed by hydrogenation with one of several metal hydrogenation catalysts (e.g., platinum or palladium). In addition to also generating costly waste, the rare metals used in the hydrogenation step of the supported acid catalyst method present significant material costs.

Invention Description

Researchers at Arizona State University have developed a greener and more economical two-step process for isooctane synthesis from isobutene, tert-butanol, or isobutanol. This method is novel in that it uses circumneutral hot water as the only solvent, requiring no additional acid or base catalysts to dimerize the isobutene. The intermediate is reduced to isooctane using inexpensive Earth-abundant reagents and catalysts as opposed to the rare and expensive metal catalysts typically employed, such as platinum or palladium.

The use of circumneutral water as the solvent is free from the environmental hazards associated with conventional methods that involve volatile, toxic, and/or flammable solvents. Since the reaction requires no added acids, bases, or other aqueous reagents, the water can be recycled for use in future synthesis reactions, and produces no toxic waste requiring remediation. The fundamental chemical transformations involved in this process (i.e., alkene dimerization and alkene reduction) can be performed for analogous hydrocarbon synthesis reactions.

Potential Applications

- Hydrocarbon fuels
- Isooctane synthesis

Benefits and Advantages

- Environmentally friendly
- Cost effective