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Chemoselective hydrodehalogenation and high efficiency birch reduction using two-dimensional inorganic electride dicalcium nitride ([Ca_2n] +·e-) as a reducing agent

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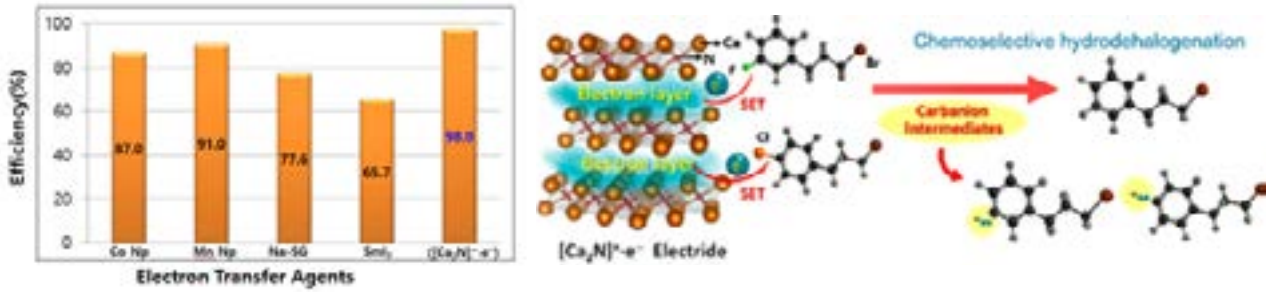
Polycyclic aromatic and halogenated organic compounds are known as a functional material which has applications in chemical industry, biology, pharmacology. Inspite of the utility of polycyclic aromatic and halogenated hydrocarbons, it has concerns about human health such as carcinogenic or mutagenic risk and considerable environmental pollution. In hydrogenation of polycyclic aromatic hydrocarbons (Birch reduction) and dehalogenation reactions, the consecutive single-electron transfer from reducing agents generates the radical and corresponding carbanion and removes the halogen atom and π–conjugated electron in polycyclic aromatic compounds. The most prominent feature of two-dimensional electride [Ca_2N] +·e^-- is powerful electron donating nature as reductant originated from high electron concentration and low work-function. The electron donating ability of two-dimensional electride was demonstrated through single electron transfer involving chemical reactions such as pinacol coupling reaction, trifluoromethylation, transfer hydrogenation. Herein, we report a new strategy for efficient chemoselective hydrodehalogenation through the formation of stable carbanion intermediates, which are simply and birch reduction of polycyclic aromatic rings by using the anionic electrons of two dimensional inorganic electride [Ca_2N]+·e^--with effective electron transfer ability. The consecutive single-electron transfer from inorganic electride [Ca_2N] +·e^-- stabilized free cabanions, which is a key step in achieving the selective reaction. The control of equivalent of inorganic electride [Ca_2N] +·e^--and reaction condition provided exceptional reactivity in comparison with other reducing agents such as cobalt nanoparticle, manganese nanoparticle, Samarium iodide (SmI_2) and sodium silica-gel. Also, a determinant more important than leaving group ability is the stability control of free carbanions according to the s character determined by the backbone structure. We anticipate that this approach may provide new insight into selective chemical formation, including hydrodehalogenation.



Biography

Byung Il Yoo got his Bachelor's degree in Department of Chemistry from Korea Advanced Institute of Science and Technology in 2014. Since 2016, he joined prof. Sung Wng Kim's group of Sungkyunkwan University as Post-Graduate student. He research interest includes synthesis new type of inorganic electride, chemical application of inorganic electride.

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