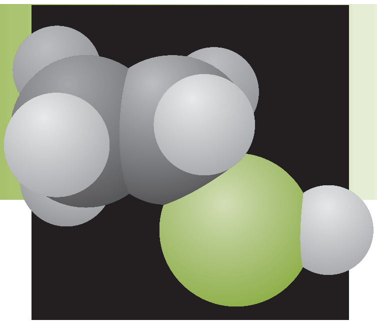
CHEMICALS

Project Fact Sheet



Alkane Functionalization Catalysis

Benefits

- Energy savings of nearly 7 trillion Btu per year by 2020
- Decreased production of carbon dioxide by 600,000 tons in 2020
- More efficient use of an abundant, inexpensive hydrocarbon feedstock (alkanes)
- Lower operating costs, increased safety, and reduced pollutant emissions

Applications

Alkane functionalization catalysts for direct conversion of alkanes could replace current methods of methanol synthesis and allow production at a significantly lower cost. Considerable opportunities also exist for the extension of the system to other alkanes, and conversion of methane at petroleum drilling sites.

Homogeneous catalyst system could produce commodity chemicals with substantial energy savings and waste reduction

Despite being the most abundant and least expensive hydrocarbon feedstock available, alkanes (e.g., methane, ethane, propane) are rarely used as chemical building blocks because few viable methods exist for their direct conversion into valuable products. Methanol, for example, is not produced directly by oxidation of methane, but by high-temperature, energy-intensive steam reforming and subsequent hydrogenation processes which date back to the 1920's.

A homogeneous catalyst system is under development that will enable direct oxidation of methane to methanol at ambient temperatures, offering considerable reductions in energy use and waste generation over current processes. The new system will use catalysts that operate in environmentally-benign media (e.g., water or dense-phase carbon dioxide), and will eliminate the byproduct formation of carbon dioxide, which occurs during conventional steam reforming. Another major application of the technology would be conversion of methane to methanol at petroleum drilling sites. Methane at these sites is often flared or reinjected rather than utilized because of prohibitive transportation costs (methane must be compressed for transport). Conversion of these considerable methane reserves (about 3 million tons in 1995) would obviate the need for methane flaring and eliminate the associated emissions of carbon dioxide, which are considerable.

Homogeneous Catalyst System

Rapid throughput energy containment reactor boosts catalyst discovery and testing rates.

Project Description

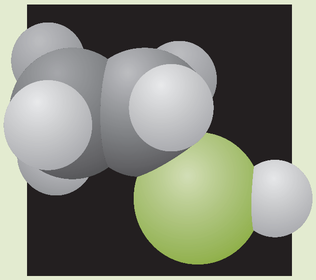
Goal: Replace the current energy-intensive, methanol synthesis process with Alkane Functionalization Catalysis.

The proposed process will develop a near-ambient temperature route for direct selective oxidation of methane (alkanes) to the commodity chemical methanol. Robust platinum complexes, with chelating nitrogen ligands show promise as homogeneous catalysts for the process, but a practical system has yet to be identified. Focus will be on rapid synthesis and testing of chelating nitrogen ligands and their new platinum and palladium complexes to provide for rapid development of more robust and practical oxidation catalysis.

Principal innovations are (1) rapid throughput synthesis of new diamine ligands by amine coupling; (2) ligand binding/electro-chemical studies of palladium and platinum complexes; (3) application of a unique high-pressure, multi-well reactor to monitor catalysis; (4) catalyst optimization in benign solvents; and (5) integration of the above with computational and mechanistic studies.

Progress and Milestones

- New families of diamine ligands and corresponding platinum catalyst precursors have been prepared.
- Current research is focusing on a single catalyst system that will activate an alkane, undergo oxidation by oxygen to a Pt(IV) species, and allow nucleophilic attack by water at an alkyl group to produce the desired alcohol product.
- Process development is scheduled to be complete by 2005 with expansion into new alkane activation processes finalized by 2020.
- This process is expected to be available for implementation by private industry in 5 to 10 years.



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February 1999