United States Environmental Protection Agency
Office of Pollution Prevention and Toxics Washington, DC 20460
EPA744F-93-005 April 1993

Design for the Environment
Chemical Design Project

Why Focus on Research in Organic Chemistry?

The moment a chemist puts pencil to paper to design a synthetic sequence for a chemical product, he also intrinsically makes decisions about whether that sequence will use or generate hazardous substances that require treatment, recycling, transportation or disposal. There are literally hundreds of different chemical reactions that can be utilized to construct a desired organic chemical, some which provide more pollution prevention benefits than others. With proper forethought and analysis, organic chemists can avoid many of the environmental problems and liabilities chemical producers face before they arise.

What environmental concerns are associated with the synthesis of chemicals?

The traditional approach to chemical design has been to search for synthetic pathways or reaction steps that produce the greatest yield at the least cost. Many approaches that produce high yields, however, also generate toxic by-products or use high-risk substances as feedstocks, solvents, and catalysts. When these chemicals are used or produced in large volumes in their industrial applications, the associated cost to human health and the environment can be high. The development of alternative synthetic pathways which avoid or reduce the use of toxic chemicals will provide chemical producers with powerful tools for pollution prevention. Companies can save money by lowering disposal costs, avoiding regulatory problems and reducing health hazards for employees.

What is the Chemical Design Project?

EPA's Chemical Design Project aims to change the way organic chemists approach the design of synthetic pathways for chemical production. EPA is encouraging consideration of alternative synthetic pathways through: (1) grant awards to academic institutions; (2) discussion at national symposia; and (3) use of computer programs which assist in the design of chemical pathways.

What is EPA doing to encourage academic research in this area?

In 1992, EPA awarded six grants to fund basic research projects which consider environmental impacts, and not just yield, in the design of chemical synthetic pathways. Now EPA is joining forces with the National Science Foundation (NSF) through a memorandum of understanding to award approximately two million dollars in additional grants. By fostering this kind of basic research in organic chemistry, EPA and NSF hope to bring about a paradigm shift in the way chemists, in both academia and the chemical industry, think about the design and manufacture of chemicals.

What kinds of research constitute alternative synthesis?

The six research projects funded by the 1992 EPA grants provide excellent examples of novel approaches that minimize or eliminate hazardous feedstocks, catalysts, solvents, or by-products.

Replacing Heavy Metal Catalysts

Catalysts are of utmost importance to the industrial production of chemicals, yet they often have toxic components, including silver and mercury, that contribute to hazardous waste disposal problems when discarded. The University of Connecticut's research project, directed by Dr. Gary Epling, is considering the effectiveness of a more environmentally benign alternative: molecules that can be activated by inexpensive artificial light sources. This research is developing large-scale methodology for the light-induced cleavage of dithianes and benzyl ethers, reactions commonly used in the dye industry.

New Synthesis of Styrene

Styrene is a high volume chemical that has hundreds of applications in everyday products. UCLA's research project, lead by Dr. Orville Chapman, is developing an alternative synthetic method for the manufacture of styrene. The proposed method uses less toxic chemicals as substitutes for problem environmental chemicals including the known carcinogen benzene, which presently serves as a basic feedstock of styrene.

Visible Light to Replace the Friedel-Crafts Reaction

Dr. George Krauss is leading Iowa State University's research into an innovative photochemical alternative to the Friedel-Crafts reaction, one of the top ten most used chemical reactions. The use of visible light as a mechanism for initiating the reaction could provide an economic incentive for replacing a well-known reaction step that uses toxic pollutants.

Elimination of Tin Based Catalysts

Dr. Barry Snider of Brandeis University is working to reduce the hazard posed by radical cyclization reactions which use highly toxic tin-based catalysts by substituting a recyclable catalyst that will not accumulate in waste effluents. The improved synthetic selectivity of this approach should result in greater yields of the target compound and fewer impurities that enter the waste stream.

Replacing Benzene with Simple Sugars

Benzene is a basic ingredient in many commercially important industrial chemicals including hydroquinone and benzoquinone. Although benzene is an extremely useful petrochemical, it is a known carcinogen and problem pollutant. Dr. John Frost o[f] Purdue University is working on a new, environmentally benign method of producing hydroquinone and benzoquinone, that replaces the use of benzene. This method utilizes a genetically engineered bacterium that produces quinic acid fro[m] D-glucose. The quinic acid is converted into hydroquinone and benzoquinone under more environmentally safe conditions.

Alternative for Toxic Solvents

Dr. James Tanko at the Virginia Polytechnic Institu[te] and State University is evaluating the utility of supercritical carbon dioxide (carbon dioxide betwee[n] liquid and gaseous states) as the solvent for certain free-radical chemical reactions. This approach ma[y] provide an economic incentive for private industry make the transition away from the currently used problem solvents such as chlorofluorocarbons, carbon tetrachloride and benzene.

Is there additional information available on the Chemical Design Project?

For more information contact EPA's Pollution Prevention Information Clearinghouse (202) 260-1023 or Paul Anastas, Economics and Technology Division (TS-779), Office of Pollution Prevention and Toxics, U.S. EPA, 401 M Street, S.W. Washington, D.C. 20460; (202) 260-2659.