



Project Summary

Substitution Reactions for the Detoxification of Hazardous Chemicals

Fred K. Kawahara

Recent literature on substituting chemical reagents that will convert toxic halogenes to their nontoxic hydrocarbons was surveyed. Within this category of chemical substitution, three types of reactions are discussed: superoxide ion radical reactions, polyethylene glycol (PEG) transformations of PCBs, and catalytic hydrogen transfer reactions.

This Project Summary was developed by EPA's National Risk Management Research Laboratory, Cincinnati, OH, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Background

Chemical substitution is one of several techniques available to treat hazardous chemicals that can threaten the environment. In the report, briefly summarized here, chemical treatment is substituting hydrogens for halogens so as to convert the halogenated organics to hydrocarbons or to mineralize the organic to carbon dioxide, water, or other component(s).

Three types of reactions applicable to the conversion of hazardous chlorohydrocarbons to their respective nontoxic hydrocarbons are discussed:

- superoxide ion radical reactions,

- dehalogenation of polyhaloaromatics and polyhaloalkanes with PEGs; and
- catalytic hydrogen transfer reactions.

Some fundamental aspects of these reactions are reported.

With O_2 representing molecular oxygen, a one-electron reduction in its valence yields the ion radical $O_2^{\cdot-}$. Studies are cited that demonstrate reactions caused by this superoxide ion radical, e.g., PCB oxygenation.

Use of PEG, together with a base such as potassium hydroxide, has been found to be a promising technique. On reporting on processes involving PEG's use, how PEG functions as the reactive agent to dechlorinate PCB is developed.

With the catalytic transfer hydrogenation reactions, organic acceptor molecules are catalytically reduced with hydrogen donated by another organic molecule. The literature review of catalytic transfer hydrogenation is restricted to certain reaction conditions and solvent effects and to some details in molecular donor and acceptor structures. Studies on the effects of temperature, solvents, solvents in heterogeneous systems, homogeneous catalysis, and heterogeneous catalysis on transfer reductions are included.

The full report is a valuable survey of recent literature (incorporating almost 100 citations) on this subject; it is not intended as a manual on technical application.



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The complete report, entitled "Substitution Reactions for the Detoxification of Hazardous Chemicals," (Order No. PB98-177876; Cost: \$25.50, subject to change) will be available only from:

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