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Project Summary

Environmental Fate Constants for Organic Chemicals Under Consideration for EPA's Hazardous Waste Identification Projects

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Under Section 301 of the Resource Conservation and Recovery Act (RCRA), EPA's Office of Solid Waste (OSW) is in the process of identifying chemicals to be considered in projects called the hazardous waste identification projects. At this time, there are some 200 chemical constituents identified in these projects. This publication addresses environmental fate constants and chemical hydrolysis pathways for the 189 organic chemicals already identified. Chemical hydrolysis rate constants for parent compounds and products including structural presentation of the pathways are presented. Redox rate constants are given for selected compounds. Sorption coefficients are presented for parents and products in terms of the octanol/water partition coefficient and the organic-carbon-normalized sediment/water partition coefficient. The ionization constant is given when this process affects sorption in the environmental pH range.

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report (see Project Report ordering information at back).

Introduction

Assessment of potential risk posed to humans by man-made chemicals in the environment requires the prediction of environmental concentrations of those chemicals under various environmental reaction conditions. Whether mathematical models or other assessment techniques are employed, knowledge of equilibrium and kinetic constants (fate constants) is required to predict the transport and transformation of these chemicals.

Under Section 301 of RCRA, EPA's OSW has identified wastes that may pose a substantial hazard to human health and the environment. RCRA requires that EPA develop and promulgate criteria for identifying and listing hazardous wastes, taking into account, among other factors, persistence and degradability in the environment of selected chemicals.

EPA continues to believe that the Agency must assure continuity of the hazardous waste program while developing appropriate revisions. While fully preserving existing hazardous waste identification rules, EPA is considering alternatives to take an initial step towards defining wastes that do not merit regulation under Subtitle C and that can and will be safely managed under other regulatory regimes.

In the course of developing appropriate revisions, OSW is in the process of identifying chemicals to be considered in projects called the hazardous waste identification projects. At this time, there are some 200 chemical constituents identified. The 189 proposed organic chemicals are addressed in this report.

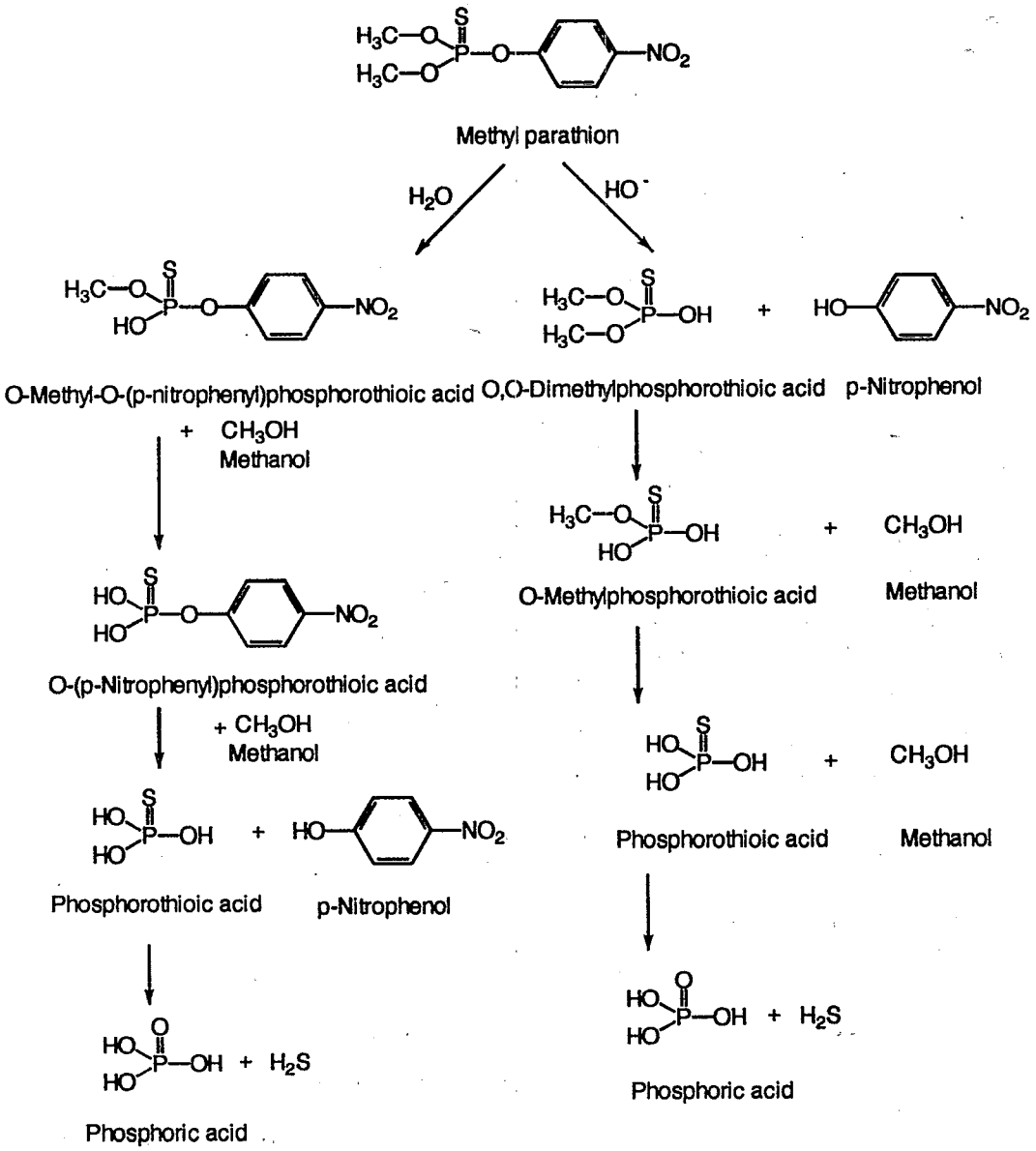
Synopsis of Report

This report is composed of two parts. Part I includes text and data on chemical hydrolysis, sorption, and redox reactions. In the hydrolysis section, hydrolysis kinetics are elucidated for the chemical classes of halogenated aliphatics, organophosphorus esters, carboxylic acid esters, amides, carbamates, and nitriles. In the sorption section, the sorption of neutral and ionizable organic compounds is addressed including computational techniques. In the redox section, the kinetics of the unexplored area of heterogeneous redox reactions is elucidated. Part I concludes with a table listing hydrolysis products (intermediate and final) including rate constants for parents and intermediates, and sorption data for parents and for intermediate and final products, and a table listing computed redox rate constants at different levels of organic carbon for selected halogenated aliphatics and nitroaromatics. Part II includes text and structural pathways of chemical hydrolysis for all organics that undergo this process. Non-hydrolyzing organics are identified and their structures are given.

As an illustration of the data provided, two pages from the complete report are reproduced in this summary. The example organic compound is methyl parathion.

141. Methyl parathion

Hydrolysis of methyl parathion may occur through either reaction with H_2O (neutral hydrolysis) or reaction with HO^- (base-mediated hydrolysis). Nucleophilic substitution by H_2O occurs in sequence at the two methoxy carbons to yield *O*-methyl-*O*-(*p*-nitrophenyl)-phosphorothioic acid (diester) and *O*-(*p*-nitrophenyl)phosphorothioic acid (monoester), respectively. Loss of the second methyl group from the disubstituted ester would be at a rate approximately a factor of 10 less than the loss of the methyl group from the triester. Hydrolysis of the monosubstituted ester [*O*-(*p*-nitrophenyl)phosphorothioic acid] would proceed through cleavage of the P-O bond at a rate of approximately one-half the rate of the parent triester. Hydroxide-ion-mediated hydrolysis of methyl parathion proceeds through initial attack of the hydroxide ion on the phosphorus atom with displacement of the *p*-nitrophenylate ion. Loss of the two methyl groups from the *O*,*O*-dimethylphosphorothioic acid will proceed as described above. The phosphorothioic acid generated in each hydrolytic pathway will eventually degrade to phosphoric acid and hydrogen sulfide.



Common Name	Chemical Abstract Service No.	Sorption Log K_{oc}	Sorption Log K_{ow}	Chemical Hydrolysis k_a $M^{-1}Y^{-1}$	Chemical Hydrolysis k_n Y^{-1}	Chemical Hydrolysis k_b $M^{-1}Y^{-1}$	Comment	References K_{oc} / K_{ow} / k_h
140. Methyl methacrylate	80-62-6	0.74	1.06	0	0	1.9E6	RATE	/ 4 / 24
Methacrylic acid (pK_a=4.45)	79-41-4	-1.53	0.470	0	0	0	NHFG	/ 4 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
141. Methyl parathion	298-00-0	2.47	2.79	NG	2.8	NG	n	/ 4 / 39
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-Methyl-*O*-(*p*-nitrophenyl)-phosphorothioic acid (pK_a=1.3)	7699-30-1	-2.5	-0.5	0	0.2	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-(*p*-Nitrophenyl)phosphorothioic acid (pK_a=1.1)	18429-96-4			0	1	0	z	/ / 0
Phosphorothioic acid (pK_a=1.5)	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
p-Nitrophenol (pK_a=7.0)	100-02-7	1.2	1.85	0	0	0	NHFG	/ 4 / 0
p-Nitrophenol (pK_a=7.0)	100-02-7	1.2	1.85	0	0	0	NHFG	/ 4 / 0
O,O-Dimethylphosphorothioic acid (pK_a=1.6)	1112-38-5	-3	-1	0	0.2	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
O-Methylphosphorothioic acid (pK_a=1.5)	1111-99-5	-4	-2.0	0	1	0	z	/ 29 / 0
Methanol **	67-56-1	-1.08	-0.764	0	0	0	NHFG	/ 4 / 0
Phosphorothioic acid (pK_a=1.5)	13598-51-1	-5	-3.0	0	3	0	bb	/ 29 / 64
Phosphoric acid	7664-38-2	NA	NA	0	0	0	NHFG	/ 0 / 0
Hydrogen sulfide	7783-06-4	NA	NA	0	0	0	NHFG	/ 0 / 0
142. Naphthalene	91-20-3	3.11	3.36	0	0	0	NHFG	38 / 38 / 0
143. 2-Naphthylamine (pK_b=9.8)	91-59-8	1.77	2.09	0	0	0	NHFG	/ 4 / 0
144. Nickel (and compounds N.O.S.)	7440-02-0							

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The complete report, entitled "Environmental Fate Constants for Organic Chemicals Under Consideration for EPA's Hazardous Waste Identification Projects," (Order No. PB93-221646AS; Cost: $27.00; subject to change) will be available only from:

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

The EPA Project Officer can be contacted at:

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