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MICROBIAL TRANSFORMATION RATE CONSTANTS OF STRUCTURALLY DIVERSE MAN-MADE CHEMICALS

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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient analytical tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact and control of environmental contaminants, the Measurements Branch develops microbial transformation rate constants for use in exposure and risk assessment models.

The U.S. Environmental Protection Agency reviews hundreds of new and existing chemicals each year to determine their impact on the environment. key process in the fate of these chemicals is microbially mediated transformation. In this report, second-order microbial transformation rate constants are provided for 35 chemicals of diverse chemical structure. The data are intended for use in mathematical models that are used in evaluating chemical risk.

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ABSTRACT

To assist in estimating microbially mediated transformation rates of man-made chemicals from their chemical structures, all second order rate constants that have been measured under conditions that make the values comparable have been extracted from the literature and combined with rate constants not reported before to compile a comprehensive list of second order rate constants for chemicals of diverse structures. Chemicals for which constants are presented include seven chlorinated carboxylic acid esters of 2,4-dichlorophenoxyacetic acid (2,4-D), phenol and seven substituted phenols, three phthalate esters, three anilines, seven amides, and seven acetanilides. The 35 constants were measured in the laboratory by a protocol that measures disappearance of the chemical substrate as a function of time in the presence of suspended natural populations from unpolluted aquatic systems. Second order rate constants, k_2 (L org.$^{-1}$ hr.$^{-1}$), range from 4.2×10^{-8} for the hexyl acid ester of 2,4,-D to 4.2×10^{-15} for the di-ethylhexyl phthalate ester.

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INTRODUCTION

The U.S. Environmental Protection Agency's Office of Toxic Substances (OTS) reviews about 1800 new chemicals and about the same number of existing chemicals annually to determine their potential impact on the environment. A principal consideration in the review process is the chemical's persistence in the ambient environment. For many man-made chemicals, a major mechanism for transformation is microbially mediated transformation. Therefore, it is necessary to assess the rate at which chemicals under review will undergo microbial transformation under environmental conditions (3). Information on microbial transformation rates is provided to OTS for only about 2 percent of the chemicals submitted for review, and relevant information on microbial transformation is sparse in the literature.

In the absence of measured microbial transformation rate constants, the OTS reviewers must estimate the rate on the basis of chemical structure (1). To assist OTS in predicting microbial transformation from chemical structure, this report lists second order microbial transformation rate constants, measured in the laboratory using the same protocol, for 35 chemicals of diverse chemical structure. Included in the data are rates for 7 para-substituted acetanilides not reported previously.

THE MEASUREMENT PROTOCOL

The protocol used for measuring the second-order rate constants is described in detail by Steen (10). A flow diagram of the procedure is presented in Figure 1. This report will include only a brief summary of the protocol.

Collection of microbiota is accomplished by a grab-sampling technique—3.8-liter amber glass jugs are immersed in the appropriate aquatic source until full. The aquatic sites chosen for study had no known history of exposure to the organic chemical being investigated. At sampling, water temperature is recorded. Samples are transferred immediately to the laboratory. Population densities and pH are measured from sub-samples taken after arrival at the laboratory. Physical, chemical, and biological properties or characteristics of the waters are recorded.

Methodologies for determining suspended population densities, for measuring parent chemical disappearance, for preparing of sterile and non-sterile treatments, and for analyzing metabolites and products are covered in detail by Steen (10). Treatment of the aquatic samples in the laboratory takes one of two courses prior to determination of the experimental second-order rate constant. Based on preliminary investigations and determination of the rate of disappearance of the test chemical using unconcentrated natural populations, a decision is made either to determine rate constants using initial population densities or to concentrate the population when the initial rate proves too slow to measure reproducibly or permit adequate estimation.

For unconcentrated populations, a test chemical is added and chemical disappearance as a function of time is measured. When concentration of microbial population is required, larger volumes of the aquatic source are sampled. This is necessary because bacterial populations in water samples may be concentrated 10-fold by filtering 22 liters through a 0.22-μm-pore-diameter membrane filter (Nucleopore or equivalent) prewashed with sterile distilled water. Following filtration, filters are collectively placed in 3-liter, wide-mouth, cotton-plugged Erlenmeyer flasks containing 2.2 liters of the original aquatic source. Sterile aqueous stock solutions of nutrients are prepared to yield concentrations (g/L) of NH_4Cl (0.5), $(NH_4)_2SO_4$ (0.5), Na_2HPO_4 (0.5), KH_2PO_4 (0.5), $MgSO_4$ (0.001), and $FeCl_3$ (0.001). No more than 1 ml of each nutrient then is added to the concentrated bacterial population resuspended from the filters to the aqueous phase. Bacterial suspensions are incubated for 48 hours at 22°C in a temperature-controlled shaker (150 to 200 rpm) prior to the addition of supplemental nutrients. This procedure effects a 10- to 100-fold enhancement of the natural bacterial population and allows for maintenance of the population over the incubation period. Concentrating the populations enables measurement of rates of transformation of chemicals that would otherwise be difficult to measure at the low indigenous population levels normally encountered in the aquatic sources.

Procedures for calculating the second-order microbial transformation rate stant have been covered in detail by Paris et al. (5) and Steen (10). The e equation used for this determination is:

$$-d[S]/dt = k_2[B][S] \quad (1)$$

re [S] is the concentration of the chemical, [B] is the concentration of suspended bacterial population, and k_2 is the second-order rate constant ressed as L org.$^{-1}$ hr.$^{-1}$. The second-order rate constants were determined forcing the overall reaction to proceed in a pseudo first-order fashion by ntaining the microbial population in great excess relative to the centration of the chemical substrate.

UMPTIONS AND LIMITATIONS

Four assumptions are made in application of the protocol. First, the centage of degrader organisms for newly encountered, man-made chemicals is umed to be about the same in all natural, unpolluted surface waters. While s assumption needs much more study, the work of Paris et al. (5) provides stantial support for this assumption. Second, it is assumed that ptation time is ignored in calculating rates. For most chemicals estigated, adaption time (if not an artifact of the measurement protocol) short (less than 50%) relative to total transformation time. Third, the strate (test chemical) concentration is assumed to be much less than the oretical Ks half-saturation concentration and the reaction kinetics are umed to be first-order with respect to substrate concentration. Fourth, carbon and energy contributions from the test chemical are assumed to be ufficient to cause measurable growth of the constitutive populations.

These assumptions and limitations notwithstanding, the data presented in s report should provide a reliable basis for comparing the relative radation rates of the chemicals measured by the same protocol, and the ues developed should contribute substantially to estimation of microbially iated transformation on the basis of chemical structure. Justification for rapolation of results beyond the conditions listed in the references has been fully established. The use of a standard protocol, a consistent set assumptions, and a bench mark chemical approach for determination of ative degradation rates was addressed by Newton et al. (4).

SOURCES OF CHEMICALS

Chemicals used in all of the microbiological investigations were obtained from analytical stocks of major chemical manufacturers, from the analytical chemical repository of EPA's Pesticides and Industrial Chemicals Repository, Research Triangle Park, North Carolina, or from analytical stocks of the Environmental Research Laboratory, Athens, Georgia. In all cases, chemicals investigated were in excess of 95 percent purity. All spike solutions were prepared under aseptic conditions from these analytical stocks. Co-chromatography, gas chromatography-infrared spectroscopy, and gas chromatography-mass spectrometry were used to identify or confirm known or speculated products/metabolites.

RESULTS AND DISCUSSION

The microbial transformation rate constants presented in this report were measured as a part of eight different studies. The most significant thing about the constants from the standpoint of using them to estimate the reaction rates of other compounds is that they were all measured in the same way Tables 1 through 4 reflect historical data generated for the purpose of testing the second-order mathematical expression as an adequate predictor of microbial transformation rates in natural aquatic systems. Rate constants likewise, were used in the development of property-reactivity relationships (relationships between chemical properties and biological reactivity). Tables 5 and 6 summarize rate constants generated by a standard protocol developed from previous experimental efforts (literature cited) for measurement of relative microbial transformation rates using standard methodologies, an aquatic source extensively characterized, and for the development of property-reactivity relationships.

The first series of chemicals tested (Table 1) were those presented by Paris et al. (5) in a study to determine the variability in rate constants measured by a protocol in which the total microbial population was measured to provide the value for [B] in Equation 1. Microbial transformation rate constants were measured for three chemicals representing somewhat diverse structures. These comparisons also were made between and among some 40 natural freshwater aquatic sites encompassing a wide variety of aquatic systems. Additionally, the waters spanned a fairly wide range of temperatures. For the three chemicals investigated, butoxyethyl ester of 2,4-dichlorophenoxyacetic acid (2,4-DBE), malathion (an organophophorous insecticide), and chlorpropham (CIPC), microbial transformation rate constants were not measurably different from site to site. Mean values of second-order microbial transformation rate constants for the 40 natural aquatic sites were 5.4 ($\pm$2.7) X 10^{-10}, 4.4 ($\pm$2.9) X 10^{-11}, and 2.6 ($\pm$1.3) X 10^{-14} liter org.$^{-1}$ hr.$^{-1}$ for 2,4 DBE, malathion and CIPC, respectively. Results of these investigations also suggested strongly that the second-order rate expression could be used to describe microbiological transformation of xenobiotics at low concentrations, which was the focus of the investigation. Rate constants (k_2) for the three chemicals were reproducible (Coefficient of Variation approximately 65%). An additional investigation by Rogers et al. (9) showed significantly larger variations in measured second-order rate constants using

similar methods. The reasons for these differences are not clear and should be investigated in future studies.

Results of an early study of property-reactivity reported by Paris et al. (7) provided microbial transformation rates for phenol and seven substituted phenols: *p*-methylphenol, *p*-methoxy phenol, *p*-chlorophenol, *p*-bromophenol, *p*-acetylphenol, *p*-cyanophenol, and *p*-nitrophenol. Table 2 provides a summary of the mean microbial rate constants for the eight phenols studied in waters from five different sites. The variation from site to site is apparently well within the approximate 65% coefficient of variation presented by Paris et al. (5). This study involved a different microbiological pathway (microbial oxidation) from the hydrolytic pathways investigated to this point.

The study of three phthalate esters by Steen et al. (12) to determine the effects of sediment sorption on microbial transformation provided the data in Table 3. For these three chemicals, the major microbial transformation occurred in the aqueous phase.

Tables 4 through 7 present results from studies related to property-reactivity correlations, which are becoming more and more important as the need to predict microbial transformation rates for man-made chemicals continues to increase and the number of laboratory measurements remains relatively small. Tables 4 and 5 contain measured transformation rate constants for a series of chlorinated carboxylic acid esters and a series of substituted anilines studied by Paris et al. (8) and Paris and Wolfe (6). In both studies, property/reactivity relationships were sought. The relationship between microbial transformation and hydrophobicity using K_{ow} was examined for the esters of chlorinated carboxylic acids. For the substituted anilines, microbial transformation was related to bulk substituent steric properties such as Vander Waals radii. The esters of the chlorinated carboxylic acids were transformed via classical microbiological hydrolytic processes, whereas the substituted anilines were transformed through different enzymatic mechanisms dioxygenases classed as oxidation processes.

Steen and Collette (11) developed what has been described as a highly promising departure from traditional property-reactivity relationships (2). The rate constants for seven amides presented in Table 6 were used to relate infrared spectral characteristics to microbial transformation. To extend this concept to para-substituted acetanilides, Steen is reporting the rate constants in Table 7 for the first time in this report. A thorough analysis of the results will be presented in a subsequent report. For the para-substituted acetanilides, the initial attack by suspended bacterial populations is assumed to be an hydrolytic reaction at the N-C-O bond to yield para substituted aniline as the primary metabolite/product. Based on co-chromatography with known analytical standards, this appears to have been the case. This observation will be confirmed by spectroscopic analysis.

Microbial transformation rates are currently being measured for two additional classes of organic chemicals, halogenated aromatic and aliphatic ethers and sulfonyl urea-based chemicals under development for use as herbicides.

Table 8 is a compilation of all of the rate constants for the 35 chemicals which the measurement protocol has been applied. This relatively small umber of compounds represents the largest number of chemicals for which aboratory measurement of second order microbial transformation rates have een performed by the same protocol and are therefore comparable for use in redicting microbial transformation based on chemical structure.

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Figure 1. RATE CONSTANT MEASUREMENT FLOW SCHEME

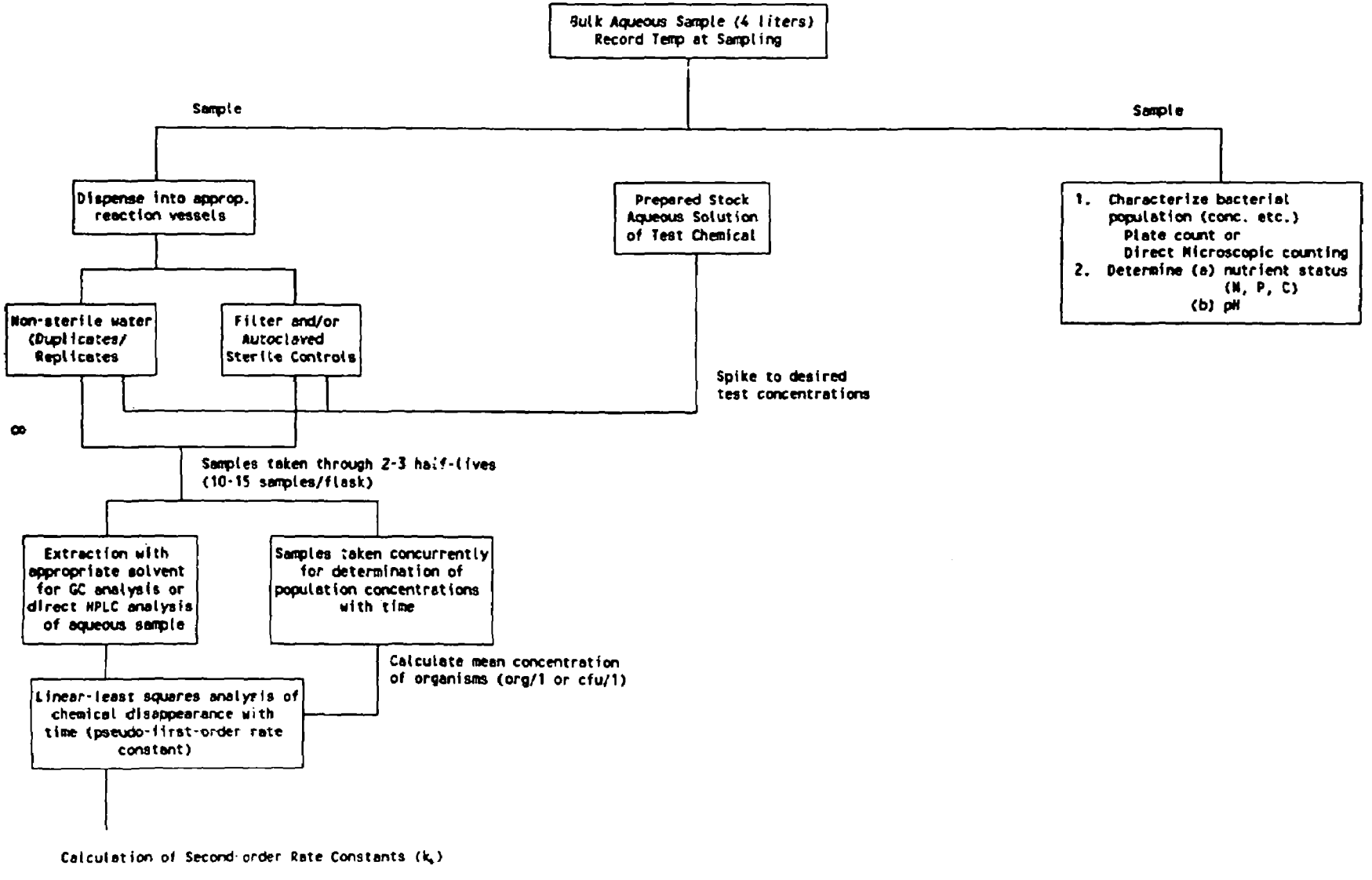

Table 1. MICROBIAL TRANSFORMATION RATE CONSTANTS IN AQUATIC SYSTEMS FROM ACROSS THE CONTINENTAL UNITED STATES*

Size	Temp (°C)	k_t (liters organism^{-1}h^{-1})		
		2,4-DBE	Malathion	CIPC
Northeast				
John's Creek	19	$(2.4 \pm 1.0) \times 10^{-10}$		
Potts Mt. Creet	20	$(8.6 \pm 4.5) \times 10^{-10}$		
Roanoake River	21	$(3.9 \pm 2.2) \times 10^{-10}$		
Augusta Creek	10	$(6.5 \pm 1.8) \times 10^{-10}$		
Sautatuck River (a)	10	$(1.5 \pm 0.3) \times 10^{-10}$		
Carnegie Lake	2	$(1.6 \pm 0.4) \times 10^{-10}$	$(2.9 \pm 1.1) \times 10^{-11}$	
Oneida Lake	16	$(6.7 \pm 2.1) \times 10^{-10}$	$(6.2 \pm 3.7) \times 10^{-11}$	$(1.8 \pm 1.3) \times 10^{-14}$
Princeton Canal	7			$(3.0 \pm 2.3) \times 10^{-14}$
Southeast				
Hickory Hills Pond	26		$(5.5 \pm 3.3) \times 10^{-11}$	$(1.7 \pm 1.2) \times 10^{-14}$
Oconee River	20	$(3.1 \pm 1.9) \times 10^{-10}$	$(5.3 \pm 2.9) \times 10^{-11}$	$(1.3 \pm 1.0) \times 10^{-14}$
Black Warrior River	22		$(5.9 \pm 2.3) \times 10^{-11}$	
U.S. Department of Agriculture pond	25	$(5.0 \pm 2.7) \times 10^{-10}$		
Weiss Reservoir	27		$(2.7 \pm 2.0) \times 10^{-11}$	
Manchester Creek	19	$(4.7 \pm 3.2) \times 10^{-10}$		
Shoals Creek	20	$(6.7 \pm 4.6) \times 10^{-10}$		
Richland Creek	17	$(6.4 \pm 2.2) \times 10^{-10}$		
Overlook Lake	25	$(1.6 \pm 0.6) \times 10^{-10}$	$(2.5 \pm 1.4) \times 10^{-11}$	
Okefenokee Swamp	20	$(7.6 \pm 4.7) \times 10^{-10}$		
Walker's Prong	26	$(11.5 \pm 8.9) \times 10^{-10}$		
Mississippi River	18	$(12.0 \pm 5.6) \times 10^{-10}$	$(2.0 \pm 1.6) \times 10^{-10}$	
Guntersville Lake	29	$(5.9 \pm 2.0) \times 10^{-10}$		
Escambia Bay (a)	24		$(6.3 \pm 3.2) \times 10^{-11}$	
Coweeta Creek	17	$(5.2 \pm 2.7) \times 10^{-10}$		$(2.2 \pm 1.6) \times 10^{-14}$
Coosa River	28			$(2.1 \pm 1.5) \times 10^{-14}$
Wheeler's Lake	27	$(4.9 \pm 1.4) \times 10^{-10}$		
Tennessee River	27	$(1.7 \pm 0.6) \times 10^{-10}$	$(3.6 \pm 2.9) \times 10^{-11}$	
Gulf Breeze (a)	27	$(5.6 \pm 2.9) \times 10^{-10}$		
Northwest				
Willamette River	20			$(2.9 \pm 2.1) \times 10^{-13}$
Duluth water treatment	17	$(5.4 \pm 1.0) \times 10^{-10}$		
St. Louis River	18	$(6.0 \pm 1.7) \times 10^{-10}$		
Pond Oregon	20	$(8.0 \pm 1.3) \times 10^{-10}$		
Columbia River	20	$(6.8 \pm 2.6) \times 10^{-10}$	$(4.2 \pm 3.6) \times 10^{-11}$	
Blue River (summer) (b)	26	$(37 \pm 12) \times 10^{-10}$	$(5.2 \pm 1.0) \times 10^{-11}$	
Blue River (winter)	1	$(7.1 \pm 6.3) \times 10^{-10}$		
Lake Superior	16		$(4.9 \pm 3.0) \times 10^{-11}$	$(4.9 \pm 4.1) \times 10^{-14}$
Southwest				
Ada	20	$(6.3 \pm 3.1) \times 10^{-10}$		$(3.1 \pm 2.1) \times 10^{-13}$
Searsville	15	$(5.5 \pm 1.8) \times 10^{-10}$		
Trinity River	12	$(3.6 \pm 1.6) \times 10^{-10}$		
Lake Travis	22	$(2.3 \pm 1.3) \times 10^{-10}$	$(4.0 \pm 3.0) \times 10^{-11}$	$(3.9 \pm 1.8) \times 10^{-14}$
Lake Mead	22	$(3.8 \pm 1.5) \times 10^{-10}$	$(4.4 \pm 2.2) \times 10^{-11}$	
MEAN	19.5 ± 6.7	$(5.4 \pm 2.7) \times 10^{-10}$	$(4.4 \pm 2.9) \times 10^{-11}$	$(2.58 \pm 1.29) \times 10^{-14}$

* Data taken from Paris et al., 1981.
a Marine waters.
b Not included in mean value or statistical analysis.

Table 2. MICROBIAL TRANSFORMATION RATE CONSTANTS FOR A SERIES OF SUBSTITUTED PHENOLS[a]

Compound	k_2 (L org.$^{-1}$hr.$^{-1}$) (mean (± S.E.)[b] Mean for all sites
Phenol	$(3.3 \pm 1.2) \times 10^{-10}$
p-Methylphenol	$(2.7 \pm 1.3) \times 10^{-10}$
p-Methoxyphenol	$(2.2 \pm 1.1) \times 10^{-11}$
p-Chlorophenol	$(7.1 \pm 1.6) \times 10^{-11}$
p-Bromophenol	$(9.1 \pm 1.0) \times 10^{-11}$
p-Acetylphenol	$(2.0 \pm 1.0) \times 10^{-10}$
p-Cyanophenol	$(4.2 \pm 1.7) \times 10^{-12}$
p-Nitrophenol	$(3.8 \pm 1.4) \times 10^{-11}$

a Extracted from Paris et al., 1983.

b Mean value of eight determination per site with the standard error of the estimate.

3. MICROBIAL TRANSFORMATION OF A SERIES OF PHTHALATE ACID ESTERS IN NATURAL AQUATIC SYSTEMS

Compound	k_2 (L org.$^{-1}$hr.$^{-1}$)*
Di-butyl phthalate	$(3.1 \pm 0.8) \times 10^{-11}$
Di-octyl phthalate	$(3.7 \pm 0.6) \times 10^{-13}$
Di-ethyl hexyl phthalate	$(4.2 \pm 0.7) \times 10^{-15}$

* Extracted from Steen et al., 1979.

Table 4. SECOND-ORDER RATE CONSTANT FOR ESTERS OF 2,4 DICHLOROPHENOXYACETIC ACID IN 5 SITES[a]

2,4 D ester	k_2 (L org.$^{-1}$hr.$^{-1}$ ± S.E.) mean of all sites[b]
Methyl	$(5.8 \pm 0.9) \times 10^{-10}$
Ethyl	$(5.2 \pm 1.6) \times 10^{-10}$
Propyl	$(2.9 \pm 1.2) \times 10^{-9}$
Butyl	$(4.1 \pm 1.2) \times 10^{-9}$
Hexyl	$(4.2 \pm 3.3) \times 10^{-8}$
Octyl	$(3.2 \pm 1.1) \times 10^{-8}$

a From Paris et al., 1984.

b Mean of eight determinations per site.

Table 5. TRANSFORMATION RATE CONSTANTS FOR THREE ANILINES AND THREE SITES[a]

	k_2 (L org.$^{-1}$hr.$^{-1}$)[b]
Compound	Mean k_2 for all sites
Aniline	$(1.1 \pm 0.8) \times 10^{-11}$
3-Chloroaniline	$(2.2 \pm 1.7) \times 10^{-12}$
3-Nitroaniline	$(4.6 \pm 0.1) \times 10^{-13}$

a Paris and Wolfe, 1987.

b Mean value of eight determinations per site ± standard error of the estimate.

Table 6. SECOND-ORDER RATE CONSTANTS FOR SEVEN AMIDES

Amide	Second-order Rate Constant (k_2) (L org.$^{-1}$hr.$^{-1}$)[a]
Propachlor (1918-16-7)	(1.1 ± 0.9) X 10^{-9}
Propanil (709-98-8)	(5.0 ± 2.7) X 10^{-10}
2-Acetamidofluorene (53-96-3)	(4.8 ± 2.8) X 10^{-11}
Benzanilide (93-98-1)	(2.4 ± 0.7) X 10^{-12}
Monalide (7287-36-7)	(6.0 ± 2.3) X 10^{-13}
Pronamide (23950-58-5)	(5.0 ± 2.3) X 10^{-14}
Niclosamide (50-65-7)	(2.0 ± 0.8) X 10^{-14}

a Steen and Collette, 1989.

Table 7. SECOND-ORDER RATE CONSTANTS FOR p-SUBSTITUTED ACETANILIDES[a]

Acetanilide	k_2 (L org.$^{-1}$hr.$^{-1}$)[b]
Cl	(1.11 ± 0.65) X 10^{-10}
CH_3	(1.70 ± 0.57) X 10^{-10}
Br	(3.85 ± 2.27) X 10^{-11}
H	(1.48 ± 1.02) X 10^{-11}
NO_2	(2.20 ± 0.68) X 10^{-12}
OCH_3	(8.51 ± 3.99) X 10^{-13}
CN	(1.45 ± 1.19) X 10^{-13}

a Unpublished data.

b Mean ± S.E. for four determinations.

Table 8. COMPILATION OF SECOND-ORDER MICROBIAL TRANSFORMATION RATE CONSTANTS MEASURED AT ATHENS ENVIRONMENTAL RESEARCH LABORATORY FOR 35 ORGANIC CHEMICALS

Chemical Class	CAS No.	k_s (L org.$^{-1}$ hr.$^{-1}$)
Carboxylic Acid Esters of 2,4-D		
Butyl	(94-80-4)	$(4.1 \pm 1.2) \times 10^{-9}$
Butoxy ethyl	(1929-73-3)	$(5.4 \pm 2.7) \times 10^{-10}$
Ethyl	(533-23-3)	$(5.2 \pm 1.6) \times 10^{-10}$
Hexyl	(1917-95-9)	$(4.2 \pm 3.3) \times 10^{-9}$
Methyl	(1928-38-7)	$(5.8 \pm 0.9) \times 10^{-10}$
Octyl	(1928-44-5)	$(3.2 \pm 1.1) \times 10^{-9}$
Propyl		$(2.9 \pm 1.2) \times 10^{-9}$
Phenols		
Phenol	(108-95-2)	$(3.3 \pm 1.2) \times 10^{-10}$
p-acetyl	(99-93-4)	$(2.0 \pm 1.0) \times 10^{-10}$
p-bromo	(106-41-2)	$(9.1 \pm 1.0) \times 10^{-11}$
p-chloro	(106-48-9)	$(7.1 \pm 1.6) \times 10^{-11}$
p-cyano	(767-00-0)	$(4.2 \pm 1.7) \times 10^{-12}$
p-nitro	(100-02-7)	$(3.8 \pm 1.4) \times 10^{-11}$
p-methoxy	(150-76-5)	$(2.2 \pm 1.1) \times 10^{-11}$
p-methyl	(106-44-5)	$(2.7 \pm 1.3) \times 10^{-10}$
Phthalate ester		
di-butyl	(84-74-2)	$(3.1 \pm 0.8) \times 10^{-11}$
di-ethylhexyl	(117-81-7)	$(4.2 \pm 0.7) \times 10^{-13}$
di-octyl	(117-84-0)	$(3.7 \pm 0.6) \times 10^{-13}$
Anilines		
Aniline	(62-53-3)	$(1.1 \pm 0.8) \times 10^{-11}$
3-chloro	(108-42-9)	$(2.2 \pm 1.7) \times 10^{-12}$
3-nitro	(99-09-2)	$(4.6 \pm 0.1) \times 10^{-13}$
Amides		
2-acetamidofluorene	(53-96-3)	$(4.8 \pm 2.8) \times 10^{-12}$
benzanilide	(93-98-1)	$(2.4 \pm 0.7) \times 10^{-12}$
Monalide	(7287-36-7)	$(6.0 \pm 2.3) \times 10^{-13}$
Niclosamide	(50-65-7)	$(2.0 \pm 0.8) \times 10^{-14}$
Pronamide	(23950-58-5)	$(5.0 \pm 2.3) \times 10^{-14}$
Propachlor	(1918-16-7)	$(1.1 \pm 0.9) \times 10^{-9}$
Propanil	(709-98-8)	$(5.0 \pm 2.7) \times 10^{-10}$
Acetanilides		
Acetanilide	(103-84-4)	$(1.48 \pm 1.02) \times 10^{-11}$
p-bromo	(103-88-8)	$(3.85 \pm 2.27) \times 10^{-11}$
p-chloro	(539-03-7)	$(1.11 \pm 0.65) \times 10^{-10}$
p-cyano	(35704-19-9)	$(1.45 \pm 1.19) \times 10^{-13}$
p-methoxy	(51-66-1)	$(8.51 \pm 3.97) \times 10^{-13}$
p-methyl	(103-89-9)	$(1.70 \pm 0.57) \times 10^{-11}$
p-nitro	(104-04-1)	$(2.20 \pm 0.68) \times 10^{-12}$