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Project Summary

Microbial Transformation Rate Constants of Structurally Diverse Man-made Chemicals

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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 x 10^{-8} for the hexyl acid ester of 2,4,-D to 4.2 x 10^{-15} for the di-ethylhexyl phthalate ester.

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 of the same title (see Project Report ordering information at back).

Overview

For many man-made chemicals, a major mechanism determining persistence in the ambient environment is microbially mediated transformation. As the U.S. Environmental Protection Agency reviews chemicals to determine their potential impact on the environment, information is required concerning the rates at which new and existing compounds will undergo microbial transformation under environmental conditions. Relevant information for individual chemicals is sparse in the literature.

In the absence of measured microbial transformation rate constants, reviewers must estimate the rate on the basis of chemical structure. To assist 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 (see Table 1). Included in the data are rates for seven *para*-substituted acetanilides not reported previously.

Table 1. Second-order Microbial Transformation Rate Constants for 35 Organic Chemicals

Chemical Class	CAS No.	k_2(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)	$(4.2 \pm 3.3) \times 10^{-8}$
Methyl	(1928-38-7)	$(5.8 \pm 0.9) \times 10^{-10}$
Octyl	(1928-44-5)	$(3.2 \pm 1.1) \times 10^{-8}$
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)	$(4.2 \pm 0.7) \times 10^{-15}$
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)	$(2.20 \pm 0.68) \times 10^{-12}$

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The complete report, entitled "Microbial Transformation Rate Constants of Structurally Diverse Man-made Chemicals," (Order No. PB91- 181 958/AS; Cost: $15.00, 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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