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LITERATURE STUDY OF THE BIODEGRADABILITY OF CHEMICALS IN WATER

Volume 1. Biodegradability Prediction, Advances in and Chemical Interferences with Wastewater Treatment

by

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16. ABSTRACT

Post-1974 literature on wastewater treatment was retrieved by on-line searching of eight databases. From 1,000 articles critically examined, 600 were used to generate a three-tiered permutated index keyed to, and presented with the 600 article bibliography in Volume 2; the three levels of the index are name of chemical, name of microbe affecting or affected by said chemical, and treatment process involved. These same 600 articles were used to generate separate biodegradable and nonbiodegradable lists of chemicals, on which a successful feasibility study was carried out to create an algorithm to predict biodegradability using only substructural fragments and molecular weight. The results of this study, in Volume 1, indicated 93% accuracy for biodegradables, but only 70% for nonbiodegradables due to the inadequate selection available. Also in Volume 1 is a report on technological advances in wastewater treatment gleaned from the 1,000 documents. In the same section, in tabular format, are references to commercial literature and some journal articles, supplied with this report to EPA, obtained by canvassing Japanese and West German manufacturers in this field. Rounding out Volume 1 is a condensation of abstracts from the 1913-1974 literature dealing only with adverse effects of chemicals on wastewater treatment, also in tabular format; it is intended to complement references to this topic in the permutated index.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Biodeterioration Chemical removal Indexes (documentation) Mathematical prediction Sewage treatment Waste treatment	Permutated index	Field - Group 12 A 13 B 68 D

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FOREWORD

The U. S. Environmental Protection Agency was created because of increasing public and government concern about the dangers of pollution to the health and welfare of the American people. Noxious air, foul water, and spoiled land are tragic testimonies to the deterioration of our natural environment. The complexity of that environment and the interplay of its components require a concentrated and integrated attack on the problem.

Research and development is that necessary first step in problem solution; it involves defining the problem, measuring its impact, and searching for solutions. The Municipal Environmental Research Laboratory develops new and improved technology and systems to prevent, treat, and manage wastewater and solid and hazardous waste pollutant discharges from municipal and community sources, to preserve and treat public drinking water supplies, and to minimize the adverse economic, social, health, and aesthetic effects of pollution. This publication is one of the products of that research and provides a most vital communications link between the researcher and the user community.

Franklin Research Center has collaborated with Genesee Computer Center to demonstrate the feasibility of developing a statistical model of chemicals based on certain substructural elements and molecular weight, for the eventual purpose of enabling industrial chemists, water treatment plant engineers, and other environmentalists to predict biodegradability. In addition Franklin Research Center has collected wastewater treatment technology advances over the period 1974-1979, and in a separate volume, created a three-tiered permutated index of the world's literature over the same time period correlating chemical, degrading microorganism, and wastewater treatment process.

Francis T. Mayo, Director
Municipal Environmental Research
Laboratory

ABSTRACT

This report is mainly the result of a compilation of post-1974 wastewater treatment literature to study correlation of chemical biodegradability with molecular substructure, discover technological advances, and create a three-tiered permutated index.

The first volume of the report contains sections on (1) a feasibility study of using discriminant equations for distinguishing biodegradable from nonbiodegradable chemicals, (2) review of post-1974 wastewater treatment techniques, and (3) examination of inhibitory effects of chemicals on wastewater treatment techniques during the period 1913-1974. The second volume contains the three-tiered permutated index. A brief description of each volume follows.

Volume 1 contains three autonomous sections outlined as follows:

1. Supplied with three lists of chemicals, selected from the articles used to create the permutated index, and given biodegradability rankings of "yes", "no", and "no-uncertain", Genesee Computer Center of Rochester, NY applied repetitive discriminant analysis and ridge regression using molecular weight and Wiswesser Line Notation-based substructural fragments to derive an algorithm with a predictability accuracy of 93% for biodegradability and 70% for nonbiodegradability.

2. This section is concerned with post-1974 developments in wastewater treatment techniques. In addition tabular presentations are made of Japanese and West German commercial literature.

3. The toxic or inhibitory effects of chemicals on wastewater treatment from 1913-1974 literature are presented as abstracts appended to an alphabetical listing of chemicals. The list is intended to complement more recent references presented in the permutated index in Volume 2.

Volume 2 consists of a permutated index structured around chemical wastes in water, microbial activity in wastewater treatment systems, and specific wastewater treatment schemes, all keyed to a bibliography of 600 articles.

This report was submitted in fulfillment of Grant No. R806699-01 by Franklin Research Center under the sponsorship of the U. S. Environmental Protection Agency. This report covers the period July 15, 1979 to April 30, 1981, and work was completed as of April 30, 1981.

CONTENTS

ACKNOWLEDGMENTS

Section 2, Structure-Activity Analysis, was prepared under subcontract to the Genesee Computer Center, Rochester, N.Y., Mr. Kurt Enslein, director. The chemical compounds provided for their evaluation were selected and categorized by Dr. Richard Mason, Principal Literature Scientist, of the Franklin Research Center staff. Dr. Mason was also responsible for furnishing Wiswesser Line Notations (WLN) for the compounds.

Mr. John Geating, Senior Information Analyst of the Franklin staff, was responsible for the Section 3, Recent Technology Appendix, which includes new technologies and processes in wastewater treatment. Mr. Geating also compiled the information included in Section 4, the chemical contaminants and water treatment section.

SECTION 1

INTRODUCTION

The task of providing a literature study of the biodegradability of chemicals in water was divided into three separate sections to provide easy access. The three approaches are discussed in more detail in the following subsections.

STRUCTURE-ACTIVITY STUDY

A major aspect of the subject of the biodegradability of waste chemical substances in water is the potential correlation which may exist between various structures, functional groups, or positional relationships within the structure. The obvious advantages of foretelling the potential of any specific compound to degrade (or not) in a specific wastewater treatment system is sufficient reason to conduct such a study.

The raw material needed to obtain chemical compounds for the study was derived from the articles obtained for the Permutated Index found in Volume 2 of this report. A total of eight databases (see Table 1) were accessed resulting in 6,861 citations ordered. These citations were perused, duplicate articles eliminated, and ultimately, approximately 1,000 hard copies obtained. Each one of these papers was critically examined for all compounds with adequate data for the structure-activity study.

These data were originally intended to be presented for substructural analysis as a list of compounds designated degradable, and a list designated non-degradable. Unfortunately, it became immediately obvious that the literature in this field is not presented in such a manner as to allow such clear-cut interpretations of results. Consequently, a third list of compounds, designated non-degradable/qualified, was created. Its entries were transferred to the other two lists when more reliable data came to light. The remaining entries on this third list were of no use in constructing the predictability algorithm.

Compounds were placed in the biodegradable category when sufficient evidence was presented by the author to infer this. The author need not have specifically commented on each compound presented, no matter how oblique the "presentation." Complete mineralization or complete conversion to a partially degraded metabolite was not required, as there are too many factors which could legitimately interfere with this and not be necessary to the author's purpose. Essentially the only requirement for acceptance of the data was that the author had taken precaution against mere physical removal of the compound from the detection/assay device.

Compounds were placed in the nondegradable category when degradation was limited to 0-5% in a time period exceeding 10 days. The nondegradable/qualified category was reserved for observations of 0% degradation in a time period below 10 days. Use by the author of adapted microbe(s) or co-study of similar compounds occasionally influenced otherwise borderline decisions.

RECENT TECHNOLOGY APPENDIX

The previous EPA Report, issued in May 1975 (NTIS PB-243-825), entitled "Rēview and Evaluation of Available Techniques for Determining Persistence and Routes of Degradation of Chemical Substances in the Environment" was updated by inclusion of new or re-clustered wastewater treatment processes and equipment. These inclusions were uncovered through searches of published literature reports, review of manufacturers' advertisements and material on file in a national professional association, Water Pollution Control Federation in Washington, DC, and through recommendations as a result of direct contact with professionals, e.g., manufacturer's representatives, consultants and operating engineers.

In addition, the literature of commercial wastewater technology from West Germany and Japan was searched for relevant contributions.

TABLE 1. DATA BASES ACCESSED FOR LITERATURE STUDY

Data Base	File No.	Time Periods Searched	Citations Ordered
1. ERIC	1	66 thru Nov. 79	81
2. DISS ABST	-	1861 thru Nov. 79	119
3. AQUATIC SCI ABST	-	78 thru Oct. 79	430
4. AGRICOLA	110	70 thru 78	775
	10	79 thru Nov.	100
5. CAB ABST	-	74 thru Sept. 79	264
6. CA	4	74 thru 76	820
	3	77 thru Mar. 80	1,908
7. BIOSIS	-	74 thru Dec. 78	1,216
8. SCISEARCH	94	74 thru 77	675
	34	78 thru Mar 80	473
Total			6,861

TABLE OF CHEMICAL CONTAMINANTS WITH ADVERSE EFFECTS ON WATER TREATMENT PROCESSES (1913-1974)

This compilation focused on specific chemical contaminants found in wastewaters and reported in earlier publications (1913-1974) to have had negative impact, i.e., toxicity and/or inhibition, within municipal or industrial wastewater treatment systems. The list of chemicals was derived from two sources:

a. A database prepared to the U.S. Environmental Protection Agency entitled: Oil and Hazardous Materials· Technical Assistance Data System (OHM · TADS);

b. A report prepared for the EPA by the Allegheny County Sanitary Authority entitled: Effect of Hazardous Material Spills on Biological Treatment Process, Dec. 1977.

These reports did not contain solely nonbiodegradable and/or toxic chemicals; therefore, it was necessary to eliminate the "non-problem" chemicals.

The retained chemicals, their CAS Registry Number, effects, and the literature sources, where given, were intermeshed alphabetically for ease of accession by the user.

SECTION 2

STRUCTURE-ACTIVITY STUDY

INTRODUCTION

The purpose of the work to be described in this report was to determine the feasibility of developing a structure-activity model that would distinguish between biodegradable and nonbiodegradable chemicals. Similar structure-activity models have been developed in the past for a variety of biological endpoints, including rat oral LD50(1), mutagenicity(2), carcinogenicity (3), and teratogenicity(4). While one usually does not consider biodegradability as a single endpoint due to the diverse nature of the reactions, if one considers that, for example in rat oral LD50, the animals can die due to a large variety of reasons, and that for teratogenicity the endpoint can be positive for any number of reasons, the distinction between biodegradability and these endpoints is very much reduced. Thus we feel confident that biodegradability can be handled as an endpoint, though one would, of course, wish to have different models for different modes of action. This is, however, not possible due to the relative scarcity of data.

THE DATA SET

Generally, compounds were classified into three categories:

biodegradable
nonbiodegradable
nonbiodegradable/qualified

Obviously, the degree of confidence that a compound was not biodegradable in the qualified set is less than for a compound in the unqualified category.

By far the largest number of compounds were found to be biodegradable. For this reason a subset of these compounds was selected at random and was used in the structure-activity models. Thus we have the following number of compounds in each one of the categories:

biodegradable	296
nonbiodegradable	61
nonbiodegradable/qualified	73

PARAMETERS

Three types of parameters were considered in the models to be described:

Molecular weight
The octanol-water partition coefficient (log p)
Wiswesser Line Notation (WLN)-based substructural keys

Molecular weight is, of course, self-evident. The partition coefficient was to be used initially, but due to the great difficulty in obtaining accurate numbers for a sufficient number of compounds in time for completion of the project, was not used in the finally developed models. The WLN-based keys are based on a major modification of the CROSSBOW program(5) and are fully described in Appendix B.

STATISTICAL METHODOLOGY

The statistical methodology employed in the development of these models consisted of stepwise discriminant analysis(6) and ridge regression(7) procedures. Typically, in stepwise discriminant analysis variables are allowed to enter the equation with very low F to enter and high F to remove. After all the possible candidate variables are entered into the equation, backward stepping is begun and those variables which contribute least to the discrimination are removed, one variable at a time, until no variable with an F to remove less than 1.7 is left in the equation. After the more important variables are thus identified a ridge regression experiment is performed to determine those parameters which contribute to instability of the discriminant equation. At the same time, compounds which appear to be consistent outliers in both the ridge regression and discriminant analysis are removed. Finally, after the ridge regression and discriminant analysis results are combined, a final discriminant analysis is performed.

THE MODEL

In view of the fact that there are two categories of nonbiodegradables, it is possible to develop three separate models, i.e., biodegradables vs. the nonbiodegradables, biodegradables vs. the nonbiodegradables/qualified, and biodegradables vs. the two nonbiodegradables combined. It became evident during the development of these three different models that the nonbiodegradable/qualified group was responsible for the introduction of a fair amount of noise, i.e., led to relatively poor discriminability between the two sets of compounds. This, of course, is not too surprising since the qualified group was composed of compounds for which a clear distinction between biodegradability and nonbiodegradability could not as readily be made. Thus the more elaborate model development was limited to contrasting the biodegradables with the nonbiodegradable group.

Biodegradable vs. Nonbiodegradable Model

The data set including the substructural keys that were generated for each of the compounds is shown in Appendix A. Compounds identified only by CAS number in Appendix A are listed alphabetically by Principal name or synonym in Appendix F. In Table 2 we show the initial discriminant equation contrasting the biodegradable compounds with the nonbiodegradable chemicals. In this table, the parameters are listed in decreasing order of importance, i.e., power in distinguishing between the two groups. Another way of portraying the equation is in the more conventional form below:

Discriminant score = 3.50 - (12.1 if Key 81 is present) - (13.7 if Key 142 is present) - ... - (2.76 if Key 43 is present)

Examples of the mechanics of manually determining a probability of biodegradability from the limited data set in this feasibility study are presented in Appendix E. These examples employ compounds which were used to develop the data in Table 3.

The next step consisted of a ridge regression run in which the parameters identified in Table 2 were used. From this run the following Keys were identified as contributing to instability of the discriminant equations:

K22 - Generic halogen
K138 - Two benzene rings
K139 - More than 2 benzene rings
K141 - Two carbocyclic rings
K144 - Two heterocyclic rings
K145 - More than two heterocyclic rings

From the ridge regression computation and the previous discriminant equation, compounds which were misclassified in both runs were identified. A few compounds that had been identified as definitely being non-degradable were reclassified as actually belonging to the qualified group. A "final" data base was then generated. A listing of this data base is shown in Appendix C. From this data base another discriminant analysis equation was generated, by forcing in all the variables that remained after the ridge regression run. A backward stepping procedure was then used to remove those variables which had an F of less than 1.7. The final discriminant equation was thus obtained and this is shown in Table 3.

In Table 4 we display the performance of this discriminant equation. Into the indeterminate group we place those compounds whose probability of classification is too near 0.5 to be effectively used. From Table 4 one can see that 92.5% of the compounds identified as degradable are so classified by the discriminant equation, and 68.4% of the non-degradables are correctly classified. The false positives amount to 15.8% and the false negatives, i.e., compounds which are in fact degradable but are called non-degradable by the equation, amount to 2.1%. Some 21.3% of the compounds cannot be classified by the equation.

TABLE 2. INITIAL DISCRIMINANT EQUATION CONTRASTING BIODEGRADABLE WITH NONBIODEGRADABLE COMPOUNDS

Key No.	Frequency: Biodegradable	Frequency: Nonbiodegradable	Description	Coefficient	F
81	0	8	Single occurrence of sulphur in a ring	-12.1	27.3
142	1	5	More than 2 carbocyclic rings	-13.7	24.9
318	0	3	Halogenated aromatic	-16.3	19.5
67	17	1	One -C=O group (substituent fragment)	5.97	19.2
21	30	0	Alkyl chain $(CH_2)_n$ or $CH_3(CH_2)_{n-1}$ where n=10 or more (chain frag.)	4.98	18.8
334	2	1	Pyrimidine analog	-17.3	17.6
61	0	3	More than one -N= or HN= group (sub. frag.)	-11.7	17.4
144	2	2	Two heterocyclic rings	-23.8	17.1
127	2	0	True bridge indicator (ring linkage)	23.8	16.0
138	27	18	Two benzene rings	-16.1	15.2
85	7	1	Single occurrence of carbonyl in a ring	8.16	14.2
139	8	2	More than two benzene rings	-16.1	13.6
22	9	6	Generic halogen (chain frag.)	-19.2	13.0
181	1	1	Substituent primary amide	-12.1	11.9
315	9	15	Haloalkane	16.5	11.1
97	169	48	Aromatic 6-membered ring (s)	12.9	10.8
1	20	2	Atoms other than C,H,O,N,S or halogens	5.43	10.7
188	1	0	Barbiturate (sub. frag.)	19.2	10.6
199	0	1	Substituent hydroxylamine	-15.4	10.5
149	7	3	Presence of suffix	-4.90	9.54
106	4	1	More than 3 heteroatoms in one ring	-11.2	9.19
137	125	13	One benzene ring	-11.8	9.06
69	28	3	One $-\overset{O}{\overset{\parallel}{C}}-OH$ (acid) group (sub. frag.)	2.82	8.58
3	19	7	Branching terminal nitro-group-NO_2 outside of ring	-2.96	8.18
19	41	3	Ethyl/ethylene group (chain frag.)	2.63	7.57
331	9	18	Fused polynuclear aromatic	-12.6	7.54

(continued)

TABLE 2 (continued)

Key No.	Frequency Biodegradable	Nonbiodegradable	Description	Coefficient	F
36	9	2	More than one -O- group (chain frag.)	-4.96	7.12
130	4	8	Bilinkage	6.77	6.47
42	13	0	More than one $-\overset{O}{\overset{\|}{C}}-OH$ (acid) group (chain frag.)	3.47	5.86
20	30	2	Alkyl chain $(CH_2)_n$ or $CH_3(CH_2)_{n-1}$ where n=3-9 (chain frag.)	2.39	5.86
141	6	5	Two carbocyclic rings	-16.8	5.76
57	4	0	More than one -NH- group (sub. frag.)	10.3	5.14
65	41	4	One -OH group (sub. frag.)	1.89	4.90
45	39	5	One methyl/methylene group (sub. frag.)	1.75	4.66
39	14	1	One -C=O group (chain frag.)	3.05	4.65
145	1	0	More than two heterocyclic rings	-16.5	4.40
35	11	2	One -O- group (chain frag.)	-3.10	4.25
152	2	0	Chain tertiary amide	-6.23	4.14
175	4	0	Chain phosphonyl	-6.43	3.83
114	5	5	One carbo/carbo fusion	13.2	3.64
102	16	3	Heterocyclic 6-membered ring(s)	7.03	3.63
98	4	1	Carbocyclic 5-membered ring(s)	-5.17	3.45
MWT	-	-	Molecular weight	-0.0057	3.37
101	11	10	Heterocyclic 5-membered ring(s)	6.30	3.37
16	0	1	Triple bond outside of a ring	-9.88	3.30
66	22	1	More than one -OH group (sub. frag.)	2.00	3.27
33	5	1	One chlorine (chain frag.)	5.10	3.24
7	3	6	One 3-branch carbon atom outside of ring	-3.34	3.09
75	2	0	Single occurrence of oxygen in more than one ring	9.87	2.70
38	15	1	More than one -OH group (chain frag.)	2.15	2.28
143	25	11	One heterocyclic ring	-4.76	2.04

(continued)

TABLE 2 (continued)

Key No.	Frequency Biodegradable	Nonbiodegradable	Description	Coefficient	F
17	39	4	One methyl/methylene group (chain frag.)	1.17	2.02
148	8	5	More than one 3-branch carbon atom (extension)	-2.14	1.98
43	5	1	More than one methyl/methylene group (chain frag.)	-2.76	1.95
			Constant	3.50	

TABLE 3. FINAL DISCRIMINANT EQUATION CONTRASTING BIODEGRADABLE WITH NONBIODEGRADABLE COMPOUNDS

Key No.	Frequency		Description	Coefficient	F
	Biodegradable	Nonbiodegradable			
81	0	8	Single occurrence of sulphur in a ring	-13.9	50.4
142	1	5	More than 2 carbocyclic rings	-10.5	28.0
21	30	0	Alkyl chain (CH_2) or CH_3 $(CH_2)_{n-1}$ where n=10 or more (chain frag.)	5.03	21.7
137	125	10	One benzene ring	3.94	21.3
61	0	3	More than one -N= of HN= group (sub frag.)	-12.1	20.1
67	17	1	One -C=O group (sub. frag.)	4.71	13.9
1	20	2	Atoms other than C,H,O,N,S or halogen	5.01	13.2
65	41	1	One -OH group (sub. frag.)	3.03	13.1
199	0	1	Substituent hydroxylamine	-16.4	12.4
85	7	1	Single occurrence of carbonyl in a ring	6.16	12.0
181	1	1	Substituent primary amide	-11.0	11.4
149	7	3	Presence of suffix	-4.80	10.4
36	9	2	More than one -O- group (chain frag.)	-5.44	9.69
127	2	0	True bridge indicator (ring linkage)	12.8	9.43
334	2	1	Pyrimidine analog	-11.1	9.31
3	18	6	Branching terminal nitro-group-NO_2 outside of ring	-3.19	9.22
19	41	3	Ethyl/ethylene group (chain frag.)	2.57	7.99
42	13	0	More than one $-\overset{O}{\overset{\|}{C}}-OH$ (acid) group (chain frag.)	3.85	7.74
318	0	3	Halogenated aromatic	-8.45	7.52
97	166	45	Aromatic 6-membered ring (s)	-2.36	7.06
106	4	1	More than 2 heteroatoms in one ring	-7.35	6.30
7	3	6	One 3-branch carbon atom outside of ring	-4.30	6.23

(continued)

TABLE 3 (continued)

Key No.	Frequency		Description	Coefficient	F
	Biodegradable	Nonbiodegradable			
148	8	5	More than one 3-branch carbon atom (extension)	-3.37	6.20
20	30	2	Alkyl/chain $(CH_2)_n$ or $CH_3\,(CH_2)_{n-1}$ where n=3-9 (chain frag.)	2.29	6.01
69	28	3	One $-\overset{O}{\overset{\|}{C}}-OH$ (acid) group (sub frag.)	2.11	5.21
39	14	1	One -C=O group (chain frag.)	2.73	5.11
188	1	0	Barbiturate (sub. frag.)	12.5	5.03
175	4	0	Chain phosphonyl	-6.61	4.74
143	25	11	One heterocyclic ring	2.34	4.45
152	2	1	Chain tertiary amide	-6.20	4.41
35	11	2	One -O- group (chain frag.)	-2.98	4.27
114	4	5	One carbo/carbo fusion	-3.40	4.24
38	15	1	More than one -OH group (chain frag.)	2.78	3.68
98	4	1	Carbocyclic 5-membered ring(s)	-5.09	3.62
MWT	-	-	Molecular weight	-.005	2.87
16	0	1	Triple bond outside of a ring	-8.25	2.62
57	4	0	More than one -NH- group (sub. frag.)	4.83	2.30
66	20	1	More than one-OH group (sub. frag.)	1.60	2.27
43	5	1	More than one methyl/methylene group (chain frag.)	-2.46	1.66
130	4	8	Bilinkage	-2.10	1.55
			Constant	3.42	

TABLE 4. DEGRADABLE VS. NONDEGRADABLE CLASSIFICATION MATRIX

		Discriminant equation evaluation					
		Degradable		Indeterminate (.3-.699)		Nondegradable	
		N	%	N	%	N	%
Actual Classification	Degradable	270	92.5	16	5.5	6	2.1
	Nondegradable	9	15.8	9	15.8	39	68.4

TABLE 5. MISCLASSIFICATIONS IN RANGES

Probability of biodegradability	No. of compounds in range	Proportion misclassified	Misclassifications: Actual N	Misclassifications: Actual Cumulative	Misclassifications: Expected Cumulative
.9 - 1.000	255	.0157	4	4	12.75
.8 - .899	13	.077	1	5	14.7
.7 - .799	11	.36	4	9	17.45
.6 - .699	5	.20	1	10	19.2
.5 - .599	7	.43	3	13	22.35
.4 - .499	4	.75	3	16	24.15
.3 - .399	9	.56	5	21	27.3
.2 - .299	2	.50	1	22	27.8
.1 - .199	1	1.00	1	23	27.95
.0 - .099	42	.0952	4	27	30.05

In Table 5 we show another way of looking at these results. From this Table it can be seen that in the extreme probability ranges the proportion of compounds misclassified is 1.6% and 9.5%. Based on the data in this Table a two sample Kolmogorov-Smirnov (K-S) test was performed to determine whether the misclassifications were randomly distributed. The test statistic was not significant, thus indicating that the equation shown in Table 3 is unbiased. The fact that the K-S test is not significant is conducive to substantial confidence in the quality of the equation.

In Tables 6a through 6d we show the compounds that were misclassified or determined to be in the indeterminate range, as well as their posterior probabilities of classification. It does not appear that the compounds which are in these Tables are clustered in any obvious way.

Biodegradable vs. Nonbiodegradable/Qualified Classification

The initial discriminant equation is shown in Table 7, with the resulting classification matrix in Table 8. While the results on the surface look better than for the results of Table 4, had this equation been optimized, one would have found that the classification accuracy would have been poorer than if only the clearly nonbiodegradable compounds had been used.

Biodegradable vs. Nonbiodegradable/Both Sets

The results for this equation which combined all the nonbiodegradable compounds irrespective of subclassification and compared them with all biodegradable compounds are shown in Table 9, with the classification matrix shown in Table 10. The classification accuracy is clearly not as good as for the results shown in Table 4. The classification accuracy would further deteriorate if the optimization process carried out for Table 4 had been performed.

CONCLUSIONS

Feasibility

It is feasible to develop discriminant equations to distinguish biodegradable from nonbiodegradable compounds. The level of accuracy achievable for this discrimination is around 93% for the biodegradable compounds and approximately 70% for the nonbiodegradable compounds, after making allowance for 5.5 and 15.8% respectively for compounds whose probability of degradability cannot be determined. Approximately 16% of the compounds judged to be non-degradable are called degradable by the discriminant equation (false positives), and 2.1% of compounds in fact degradable are called non-degradable (false negatives) by the equation.

TABLE 6a. MISCLASSIFIED BIODEGRADABLE COMPOUNDS

CAS #	Name	Posterior Probability
72435	Ethane, 1,1,1-trichloro-2,2-bis (p-methoxyphenyl)-	.007
85472	1-Naphthalenesulfonic acid	.032
92875	Benzidine	.124
115322	Benzhydrol, 4,4'-dichloro-alpha-(trichloromethyl)-	.022
309002	Aldrin	.244

TABLE 6b. MISCLASSIFIED NONBIODEGRADABLE COMPOUNDS

CAS #	Name	Posterior Probability
67685	Methyl sulfoxide	.057
75014	Ethylene, chloro-	.043
88744	Aniline, o-nitro-	.247
99650	Benzene, m-dinitro-	.275
100254	Benzene, p-dinitro-	.275
104030	Benzeneacetic acid, 4-nitro-	.273
121471	Metanilic acid	.016
620928	Phenol, 4,4'-methylenebis-	.160
622479	Benzeneacetic acid, 4-methyl-	.017

TABLE 6c. NONBIODEGRADABLE COMPOUNDS CLASSIFIED AS "INDETERMINATE"

CAS #	Name	Posterior Probability
83056	Acetic acid, bis(p-chlorophenyl)-	.463
90971	Benzenemethanol, 4-chloro-alpha-(4-chloro-alpha-phenyl)-	.431
117340	Benzeneacetic acid, alpha-phenyl-	.431
119562	Benzenemethanol, 4-chloro-alpha-phenyl-	.691
366187	2,2'-Bipyridine	.623
728870	Benzhydrol, 4,4'-dimethoxy-	.476
1883325	Benzeneethanol, beta-phenyl-	.682
3026662	Pyridinium, 1-dodecyl-, iodide	.587
10450698	9-Octadecen-1-aminium, N,N,N-trimethyl-, chloride, (Z)-	.699

TABLE 6d. BIODEGRADABLE COMPOUNDS CLASSIFIED AS "INDETERMINATE"

CAS #	Name	Posterior Probability
61905	Leucine, L-	.354
72184	Valine, L-	.370
90153	1-Naphthol	.537
90437	2-Biphenylol	.676
91010	Benzenemethanol, alpha-phenyl-	.477
96413	Cyclopentanol	.631
101815	Methane, diphenyl-	.555
135193	2-Naphthol	.494
140727	Pyridinium, 1-hexadecyl-, bromide	.362
567180	2-Naphthalenesulfuric acid, 2-hydroxy-	.342
612000	1,1-Biphenylethane	.649
831812	Benzene, 1-chloro-4-(phenylmethyl)-	.502
1698608	3(2H)-Pyridazinone, 5-amino-4-chloro-2-phenyl-	.319
2785548	Pyridinium, 1-tetradecyl-, chloride	.423
27697514	Ethanaminium, N,N,N-trimethyl-, chloride	.507
38775223	Benzenesulfonic acid, 2-(1,1'-biphenyl)-4,4'-diyldi-(2,1-ethenediyl)bis-	.695

TABLE 7. DISCRIMINANT EQUATION CONTRASTING BIODEGRADABLE WITH NONBIODEGRADABLE/QUAL. COMPOUNDS

Key No.	Frequency		Description	Coefficient	F
	Biodegradable	Nonbiodegradable			
318	0	8	Halogenated aromatic	-16.2	86.3
85	7	0	Single occurrence of carbonyl in a ring	8.24	16.3
57	4	0	More than one -NH- group (substituent frag.)	-7.13	16.1
148	8	11	More than one 3-branch carbon atom (extension)	-4.67	15.4
77	12	1	1 single occurrence of nitrogen in a ring	18.2	15.2
73	5	4	Single occurrence of oxygen in a ring	18.0	14.5
72	10	0	More than one $-\overset{O}{\overset{\|}{C}}-O$ (ester) group (sub. frag.)	5.86	14.1
321	0	4	Epoxide	-11.1	13.6
112	8	12	One single carbocyclic ring	-4.88	13.2
1	20	0	Atoms other than C,H,O,N,S or halogens	3.96	13.0
143	25	7	One heterocyclic ring	-16.3	12.1
138	27	9	Two benzene rings	3.58	11.8
167	1	3	Chain methoxy	-7.55	11.8
42	13	1	More than one $-\overset{O}{\overset{\|}{C}}-OH$ (acid) group (chain frag.)	4.39	11.7
44	4	0	More than one $-\overset{O}{\overset{\|}{C}}-O$ (ester) group (chain frag.)	7.41	11.1
41	39	6	One $-\overset{O}{\overset{\|}{C}}-OH$ (acid) group (chain frag.)	2.52	9.72
14	8	7	One double bond, excluding -C=S, -N=, or C=O outside of a ring	-3.63	7.74

(continued)

TABLE 7 (continued)

Key No.	Frequency Biodegradable	Frequency Nonbiodegradable	Description	Coefficient	F
89	0	1	Single occurrence of exocyclic double bond in a ring	-13.1	7.38
18	43	23	More than 1 methyl/methylene group (chain frag.)	-2.25	7.18
48	2	4	Alkyl chain $(CH_2)_n$ or $CH_3(CH_2)_{n-1}$ where n=3-9 (sub. frag.)	-9.36	7.13
123	0	1	More than 1 hetero/hetero fusion in a ring	-11.1	7.05
63	11	2	One -O- group (sub. frag.)	-3.30	6.76
11	4	2	More than 1 sulphur atom outside of a ring	-4.77	6.43
78	8	1	Multiple occurrence of nitrogen in a ring	11.4	5.71
16	0	1	Triple bond outside of a ring	-9.88	5.60
100	0	3	Carbocyclic ring(s) other than 5 and 6-membered	-6.18	5.41
25	0	1	Bromine (chain frag.)	-9.25	4.87
331	9	3	Fused polynuclear aromatic	-3.22	4.56
317	39	12	Haloalkane	6.94	4.36
20	30	12	Alkyl chain (CH_2) or $CH_3(CH_2)_{n-1}$ where n=3-9 (chain frag.)	-1.81	4.23
9	7	2	Greater than 3-branch nitrogen atom (outside of ring)	3.54	3.98
50	39	8	Generic halogen (sub. frag.)	1.56	3.96
65	41	3	One -OH group (sub. frag.)	1.45	3.78
21	30	1	Alkyl chain (CH_2) or $CH_3(CH_2)_{n-1}$ where n=10 or more (chain frag.)	1.98	3.77
137	125	12	One benzene ring	1.44	3.51

(continued)

TABLE 7 (continued)

Key No.	Frequency: Biodegradable	Frequency: Nonbiodegradable	Description	Coefficient	F
188	1	0	Barbiturate (sub. frag.)	8.48	3.27
101	11	2	Heterocyclic 5-membered ring(s)	3.14	3.25
3	19	0	Branching terminal nitro-group	1.88	3.23
4	13	4	Dioxo (excluding NO_2) outside of ring	4.22	2.97
151	2	2	Chain secondary amide	-3.70	2.94
8	15	1	3-branch nitrogen atom outside of ring	2.10	2.88
36	9	0	One -O- group (chain fragment)	2.74	2.74
30	15	1	One $-NH_2$ group (chain frag.)	1.95	2.71
19	41	16	Ethyl/ethylene group (chain frag.)	-1.18	2.43
7	3	3	4-branch carbon atom outside of a ring	-2.84	2.40
43	5	0	One $-\overset{\overset{O}{\|}}{C}-O$ (ester) group (chain frag.)	3.01	2.28
47	2	1	Ethyl/ethylene group (sub. frag.)	-3.60	2.13
325	1	0	3 or 4 membered β-Lactam	-6.55	1.90
34	1	0	Unusual carbon atom (chain frag.)	5.87	1.80
			Constant	1.88	

TABLE 8. DEGRADABLE VS. NONDEGRADABLE/QUAL.

		Discriminant equation evaluation					
		Degradable		Indeterminate (0.3-0.699)		Non/qual.	
		N	%	N	%	N	%
Actual Classification	Degradable	258	87.2	30	10.1	8	2.7
	Non/qual.	7	9.5	13	17.6	54	73.0

Improvements

The most serious deficiency of these models lies in the relatively small number of nonbiodegradable compounds. While this may be a desirable state of affairs from a naturalistic viewpoint, it is not the best of all possible worlds statistically inasmuch as the variety of chemicals represented in the nonbiodegradable category is relatively small. Of course, nature may be such that there is not in fact a large variety of such structures, but a larger number of nonbiodegradable compounds would undoubtedly improve the accuracy of classification of the equations.

It may also be that greater accuracy could be achieved if the organisms used in the different biodegradability experiments were identified and used as additional parameters in the development of the equations.

Until additional work is done, the results of this feasibility study may only be applied to compounds containing any of the 39 Keys listed in Appendix D plus the following nonquantified Keys, which were eliminated from the final model for lack of sufficient influence on it: 17, 33, 45, 75, 101, 102. As previously indicated the presence of Keys 22, 138, 139, 141, 145, or 315 has been shown to have an unacceptably variable influence on the model, so that compounds containing one of these as the only "guess" Key should be exempted from the inevitable attempts at extrapolation.

Finally, due to time constraints, we were unable to use partition coefficients. In future developments the use of such coefficients could at least be attempted. In the same vein, parameters such as molecular connectivity indices should also be explored.

TABLE 9. DISCRIMINANT EQUATION CONTRASTING BIODEGRADABLE WITH NONBIODEGRADABLE/BOTH SETS COMPOUNDS

Key No.	Frequency		Description	Coefficient	F
	Biodegradable	Nonbiodegradable			
81	0	9	Single occurrence of sulphur in a ring	-10.3	52.7
142	1	5	More than 2 carbocyclic rings	-7.96	22.2
141	6	8	2 carbocyclic rings	-5.83	19.1
21	30	1	Alkyl chain $(CH_2)_n$ or $Ch_3\ (CH_2)_{n-1}$ where n=10 or more (chain fragment)	3.13	19.0
42	13	1	More than one $-\overset{O}{\overset{\parallel}{C}}-OH$ (acid) group (chain frag.)	4.16	17.1
85	7	1	Single occurrence of carbonyl in a ring	6.15	16.7
112	8	13	One single carbocyclic ring	-5.14	16.4
72	10	0	More than one $-\overset{O}{\overset{\parallel}{C}}-O$ (ester) group (substituent fragment)	4.66	16.4
148	8	16	More than one 3-branch carbon atom (extension)	-3.52	16.0
65	41	7	One -OH group (sub. frag.)	2.25	13.4
318	0	11	Halogenated aromatic	-10.1	12.3
61	0	3	More than one -N= or HN= group (sub. frag.)	-6.58	10.4
57	4	1	More than one -NH- group (sub. frag.)	8.54	10.4
1	20	2	Atoms other than C,H,O,N,S or halogens	4.32	9.50
14	8	10	1 double bond, excluding -C=S, -N=, or -C=O	-2.94	9.45
199	0	1	Substituent hydroxylamine	-10.1	8.31
127	2	0	True bridge indicator (ring linkage)	7.22	7.73
44	4	0	More than one $-\overset{O}{\overset{\parallel}{C}}-O$ (ester) group (chain frag.)	4.64	7.04
67	17	2	One -C=O group (sub. frag.)	2.45	6.83
167	1	3	Chain methoxy	-4.68	6.71

(continued)

TABLE 9 (continued)

Key No.	Frequency: Biodegradable	Frequency: Nonbiodegradable	Description	Coefficient	F
310	35	9	Aromatic amino	2.44	6.29
317	2	0	Haloalkane	9.15	6.23
41	39	10	One $-\overset{\text{O}}{\overset{\|}{\text{C}}}-\text{OH}$ (acid) group (chain frag.)	1.53	5.82
188	1	0	Barbiturate (sub. frag.)	10.6	5.73
123	0	1	More than one hetero/hetero fusion in a ring	-8.37	5.70
63	11	5	One -O- group (sub. frag.)	-2.49	5.35
134	39	44	1 ring system	1.99	5.06
79	0	1	Single occurrence of nitrogen in more than one ring	-11.1	4.93
69	28	8	One $-\overset{\text{O}}{\overset{\|}{\text{C}}}-\text{OH}$ (acid) group (sub. frag.)	1.47	4.62
10	18	11	1 sulphur atom outside of a ring	1.62	4.50
181	1	1	Substituent primary amide	-5.60	4.16
334	2	1	Pyrimidine analog	-6.66	4.06
50	39	19	Generic halogen (sub. frag.)	1.77	3.96
25	0	1	Bromine (chain frag.)	-6.38	3.47
152	2	1	Chain tertiary amide	-4.29	3.40
7	3	9	4-branch carbon atom outside of a ring	-2.04	3.23
45	39	9	One methyl/methylene group (sub. frag.)	1.05	3.20
30	15	5	One $-NH_2$ group (chain frag.)	1.62	3.08
66	22	3	More than one -OH group (sub. frag.)	1.35	2.95
100	0	3	Carbocyclic ring (s) other than 5 and 6-membered	-3.72	2.90
6	41	20	One 3-branch carbon atom outside of a ring	-0.95	2.69
58	19	7	One $-NH_2$ group (sub. frag.)	-1.86	2.47
149	7	4	Presence of suffix	-2.26	2.35
89	0	1	Single occurrence of exocyclic double bond in a ring	-6.14	2.34

(continued)

TABLE 9 (continued)

Key No.	Frequency: Biodegradable	Frequency: Nonbiodegradable	Description	Coefficient	F
151	2	2	Chain secondary amide	-2.93	2.12
48	2	4	Alkyl chain $(CH_2)_n$ of $CH_3(CH_2)_{n-1}$ where n=3-9 (sub. frag.)	-2.22	2.06
172	11	1	Chain phenoxy	1.80	2.04
321	0	4	Epoxide	-4.43	1.96
34	1	0	Unusual carbon atom(chain frag.)	4.98	1.95
11	4	2	More than 1 sulphur atom outside of a ring	-2.20	1.90
52	21	18	More than one chlorine (sub. frag.)	-2.49	1.90
39	14	7	One -C=O group (chain frag.)	1.38	1.90
106	4	1	More than 2 heteroatoms in one ring	-3.89	1.83
9	7	4	Greater than 3-branch nitrogen atom outside of a ring	2.19	1.80
180	2	11	Biphenyl (chain frag.)	3.45	1.76
111	1	1	More than 1 single heterocyclic ring	4.70	1.66
16	0	2	Triple bond outside of a ring	-3.21	1.65
103	2	4	Heterocyclic ring(s) other than 5 and 6-membered	-3.54	1.64
78	8	4	Multiple occurrence of nitrogen in a ring	-2.37	1.55
5	18	2	Terminal oxygen (not carbonyl) (outside of ring)	-1.83	1.54
18	43	35	More than 1 methyl/methylene group (chain frag.)	-0.78	1.53
			Constant	0.54	

TABLE 10. DEGRADABLE VS. NONDEGRADABLE/BOTH SETS

		Discriminant equation evaluation					
		Degradable		Indeterminate (0.3-0.699)		Non/both sets	
		N	%	N	%	N	%
Actual Classification	Degradable	243	82.1	37	12.5	16	5.4
	Non/both sets	18	13.3	23	17.0	94	69.6

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SECTION 3

RECENT TECHNOLOGY APPENDIX

PROLOGUE

Despite the abundance of electronic, chemical and electro-mechanical technology currently being applied to municipal and industrial wastewater treatment, the ubiquitous bacterium remains the stable backbone of all sanitary treatment programs. Nevertheless, this presents something of a paradox to the practicing sanitary engineer, facility planner, or applied scientist. On the one hand it represents a simple, direct treatment process that will reduce domestic and industrial wastes through its metabolic activity. On the other hand, the complex, interdependent conditions which promoted success at one plant are too often insufficiently understood to allow successful application of that approach to another treatment facility. In other words, a design/system which demonstrated highly successful results in one facility, i.e., efficient reduction of solid/chemical wastes, is all too often only mediocre or poor at another.

This is not to say that electronic, chemical and electro-mechanical technology is too risky or uncertain to use. It means that each treatment facility must, in the end, adapt those techniques and methods which can support their individual needs, based on their specific problems and requirements. Ultimately, the solution will be found in the successful synthesis of past experience, judicious laboratory studies, and informed and careful shopping for complementary technology.

Superimposed on the previous comments is the overriding need to study and plan for these facilities and processes with a full understanding of today's radically changing energy, economic and social situations. It is obvious that wastewater treatment plants will have to depend less and less on the traditional fossil fuels and concentrate more on renewable energy sources. In addition, the designers should explore ways to employ natural processes which work in conjunction with each other, e.g., aerobic bacterial action, aquaculture, and evaporation/condensation. The re-use of the end products of the treatment process, whether it involves using the sludge as mulch or extracting heavy metals from plant roots, must be added to the challenge of the planners' and operators' tasks.

The papers presented were selected with the foregoing comments in mind. They were intended to serve as a basis for stimulation of the possibilities which exist, not necessarily as absolute techniques.

SOLAR-DEPENDENT TECHNIQUES

Algae-Bacterial Systems

A paper by John (1979) describes a technique of using the controlled growth of a *Chlorella* sp. in wastewater lagoons that removes 80% COD, 65% of the nitrogen and 75% of phosphorus with an optimum ratio of algae to bacteria of 60:40. An examination by Shelef (1978) compares an intensive algal wastewater treatment system for an urban population which compares favorably with the activated sludge technique. The paper discusses resource recovery, water for irrigation and proteins for animal feed. The continuing examination by Shelef (1978a) provides additional information concerning the economic and design considerations for the algal system described. The author presents data to show that the oxygen, produced by the algae through photosynthesis, surpasses the BOD of the raw sewage, thus significantly reducing the energy requirement for aeration.

Another algal system which harvests the plants for animal feed, Garrett (1978), is used in treating animal wastes slurry. The salient feature of this design is characterized by high productivity, resulting from the suppression of glycolate excretion and photo-respiration in the algae due to CO_2 enrichment by the indigenous bacterial community. Lincoln *et al*. (1978) describe the use of plankton (free-floating microalgae) to convert animal wastes into high grade plant protein as a low-cost wastewater treatment project.

Aquaculture

A test plant project is reported by Naegel (1977) which used nutrients from fish wastewater (mainly oxidized nitrogenous compounds) for algal production coupled with an activated sludge system for water purification. Lettuce and tomatoes were grown in the recirculated water.

Hepher *et al*. (1975) discuss the benefits, hazards, and limitations of the integrated waste treatment and aquaculture system. Fresh water lagoons, which are stocked with fish, were infused with domestic sewage at a rate which diluted the high BOD levels to concentrations which could be utilized by the fish.

Another study on the cost-effectiveness of aquaculture by Wert (1978) uses a two-fold approach to promote the addition of this technique to wastewater treatment facilities, especially those of smaller municipalities of about 2,000 population. The first approach employs a matrix consisting of strategies vs. objectives which highlights the advantages of aquaculture. The second details the financial and economic aspects of the technique as they apply to the matrix. A considerable saving (up to 28% of conventional costs) is predicted for all strategies incorporating an aquaculture system, using either most "optimistic" or most "pessimistic" cost evaluations.

Plant Culture

Wolverton and McDonald (1977) present information on the use of water hyacinths to treat wastewater containing high concentrations of silver resulting from photographic laboratory discards. Design and operational considerations are discussed, including the proposed recovery of silver which is highly concentrated in the roots of the hyacinths.

A comprehensive discussion of the use of water hyacinth culture for wastewater treatment is presented by Dinges (1976) of the Texas Department of Health Resources, Division of Wastewater Technology and Surveillance. This extensive paper presents a total view of the system from design to operation, including technical and financial data.

Distillation

A pilot operation of domestic waste treatment by solar distillation and plant culture is presented by Quasim (1978). The paper presents data obtained from a preliminary domestic solar still-greenhouse in the treatment of sewage, recovery of high quality distillate, and utilization of the nutrients contained in the sewage for plant culture.

RECYCLE/REUSE TECHNIQUES

Sludge

Wong (1977) presents a paper which discusses the use of extracts of activated/digested sludge as a medium for cultivating algae in the laboratory. Growth rates of *Chlorella* sp. cultured in the extracts were higher than with conventional medium.

A commercial process for treating sludge uses chemical fixation and solidification to modify waste material. Solid TeK, operating from Morrow, GA offers a wide range of services, products and systems on a specialized basis to deal with a variety of wastes resulting from the end-products from waste treatment plants. The process employs specifically formulated chemicals which render materials ranging from wastewater sludge to fly ash from precipitators acceptable for introduction to a landfill or other disposal.

Effluent Water

Neilson (1977) presents an extensive review (137 citations), and the practicalities and conclusions reached as a result of experience in using combinations of electromagnetic radiation techniques with and without chemical treatment. The review supports the argument that synergistic activity can be achieved by the serendipitous application of various combinations of these techniques. Data from operating treatment plants show essentially sterile water following programmed exposure of the effluent waste to gamma radiation. The author cites the relatively inexpensive availability of cesium 137 as the result of waste fuel from nuclear power plants as a source of gamma emitters. Safety practices and considerations are discussed.

PROCESS TREATMENT CONTROLS

Phosphorus and Nitrogen Removal via Chemical Treatment

Schwartz (1976) presents data from studies which used activated carbon and an equilibrium-regenerated spent fluid cracking catalyst (alumina silicate) impregnated with x-zeolite to increase the removal of phosphorus. The activated carbon was instumental in increasing the sludge settling rate, as well as the clarity, and promoted significant reductions in BOD and COD in a municipal sewage treatment plant. The regenerated catalyst was shown to be more promising when employed in a refinery activated sludge system than with the municipal treatment plant.

A paper by Long (1975) presents the results of research directed towards the development and evaluation of a combined chemical-biological process of phosphorus removal in a pilot plant. The process utilized the addition of timed quantities of alum (aluminum sulfate) and sodium aluminate as precipitating agents. Automated chemical addition, related to the influent rate, was discovered to be an important facet of the process.

The removal of phosphorus from domestic sewage by using ferrous iron and ferric chloride from a metal finishing plant (pickle liquor waste) is described by Azkona (1979). Significant reductions of phosphorus without deterioration of the bacterial population were described.

Phosphorus removal by simultaneous precipitation with ferrous sulfate heptahydrate (Bio-Denitro process) is discussed by Bundgaard (1978). The process is carried out in tandem with an activated sludge process.

A new high-rate activated sludge process employing activated carbon is described by Besik (1977). With a mixed microbial population and a mixture of powdered and granular activated carbon, the process is capable of removing the total nitrogen along with bio-oxidation of organics encompassing efficiencies up to 90% for both soluble organic carbon and nitrogen.

Aerobic Treatment

Benefield (1977) presents the results of an applied research program designed to investigate the differences surrounding growth and substrate utilization kinetics displayed between air- and oxygen-aerated sludge systems. Results indicated that the standard tests used to quantify these experiments, e.g., VSS test, were unable to distinguish between proliferating, active but non-proliferating, and inactive cellular material. When these deficiencies are recognized, the differences largely disappear.

Garber (1977) sees the controversy between air and oxygen aerated systems as a result of the nature of the type of influent waste - oxygen is beneficial when high carbonaceous loadings are encountered (as in fruit and vegetable canning areas) - and where plant space limitations present acute problems.

Jeris et al. (1977) describe fluidized beds as an efficient variation of the activated sludge/trickling filter technology which appears to combine the best features of both. These beds require less than 5% of the reactor space required for conventional facilities and exhibit high efficiencies for the removal of carbonaceous BOD and nitrogen.

Anaerobic Treatment

Schammel (1976) presents a paper which seeks to highlight the inefficiency of aerobic effluent treatment, especially with respect to the needless expenditure of energy during the disposition of potentially valuable resources contained in the wastes. In contrast, anaerobic digestion converts over 80% of the BOD to methane, which is usable as a fuel source, and carbon dioxide. It also reduces the production of sludge to one-fifth that of the aerobic process. New technology development, in the author's opinion, removes earlier disadvantages associated with this method and provides a way of allowing the process to pay for itself. Economic and mathematical data are presented.

Biological Acceleration/Inhibition

In a paper about waste treatment from the carbonization industry (coke, etc.) where high concentrations of thiocyanate are present, Catchpole (1978) discusses the significant accelerating effect upon activated sludge activity through small additions of para-aminobenzoic acid (PABA) or glucose to the aeration tank. It is postulated that the PABA or glucose was likely to be exerting its influence on the enzyme systems involved in thiocyanate oxidation and not by a change in the microbiological population. Conversely, when catechol was present in the activated sludge mixture, the retention times are significantly increased. These results and their impact upon the treatment of carbonization liquors are discussed.

MANAGEMENT OF ELECTRICAL PROPERTIES

Grutsch (1978) describes the complex electrical properties associated with colloidal waste material (suspended solids) and the need to apply understanding of these properties when optimizing unit operations. All suspended solids, whether colloidal or not, carry a negative electrical surface charge. Inert and slowly biologically-oxidized colloids and suspended matter contribute to increasing the amount of fine particles in the sludge mass. Increasing the sludge age increases their accumulation, thereby contributing to the deterioration in sludge flocculating properties. Removing colloids and suspended matter before the activated sludge process results in an excellent activated sludge at very high sludge age.

A permanent magnet, encased within the pipe carrying effluent wastewater, is claimed by the marketing organization - Super Ion Corp., Orlando, FL - to significantly increase the clarity and improve the sludge settleability in the final wastewater treatment tanks. The product is used in boiler systems to prevent scale formation and to remove existing scale, and in cooling tower applications for the same purpose. The phenomena has been employed in the USSR for 25 years and is postulated to work by controlling the ionization of the carbonates and thus preventing scale buildup; the mode of operation thus appears to relate to aspects of the previous paper in this section.

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JAPANESE LITERATURE/EQUIPMENT SURVEY

Tables 11-18 represent a compilation of selected commercial equipment/processes and periodical references relating to wastewater treatment from Japan. Note that the population density and geographical character of the Japanese Islands have made the issue of efficient wastewater treatment and management critical. Consequently, activity in this area appears to have been more intensive with possibly more imaginative and broad-based commercial offerings, especially for small to medium-sized communities. The "Ref. No." are identification numbers for the particular documents, mainly company literature, supplied to EPA with this report.

Table 11, Total Treatment System, ranges in municipal equipment from multi-family dwellings on up, in industrial plants from food processing through textiles to heavy chemicals, and in technology from activated carbon to iron powder. Brochures or journal articles from 22 companies are listed.

Table 12, Liquid-Solid Separation Equipment, ranges over belt presses, centrifuges, filters, and flocculants. Thirty-four companies are represented.

Table 13, Biological Treatment Process concentrates on the activated sludge processes, including forced aeration. Thirty-three companies are represented.

Table 14, Sludge Disposal, covers drying, freeze-thawing, composting, and incineration. Material from 33 companies is referenced.

Table 15, Oil Removing, covers skimmers, and both on- and offshore treatment of oily shipboard waste. Seven companies are listed.

Table 16, Tertiary Treatment Process, covers such diverse concepts as reverse osmosis, hydroponics, and ion-exchange as conceived by 11 companies.

Table 17, Meters/Analyzers, covers chlorine through cyanide to oil detectors, and the BOD-TOC type meters, from 16 companies.

Table 18, Others, covers such equipment as deodorizers, pumps, and activated carbon reactivators from 11 companies.

TABLE 11. TOTAL TREATMENT SYSTEM

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
1-1	Mitsubishi-Lurgi Waste Water Treatment Process "GYLOFLOC"	Mitsubishi Hvy. Industries, Ltd.	Co. Brochure	KH-319
1-2	Mitsubishi Sewage Treatment Plant (Secondary Treatment)	"	"	KH-385
1-3	Mitsubishi Rotary Disk Type Waste Water Treatment Process	"	"	KH-434
1-4	Mitsubishi Community Sewage Treatment Plant	"	"	KH-375
1-5	Mitsubishi water Treatment System for Exudation from Reclaimed Land	"	"	KH-443
1-6	Mitsubishi Laboratory Waste Water Treatment System	"	"	KH-378
1-7	Mitsubishi-Lurgi Water Recycling System for a Building	"	"	KH-289
1-8	Mitsubishi Methane Gas Producing/ Waste Liquids Treatment System	"	"	KH-399
1-9	MKK Night Soil Treatment System	Mitsubishi Kakoki Kaisha, Ltd.	"	02-76-BAP
1-10	MKK Industrial Waste Water Treatment System for Machining/ Metal-working Factories	"	"	WP-62-003
1-11	MKK Industrial Waste Water Treatment System for Pulp Plant	"	"	"
1-12	MKK Industrial Waste Water Treatment System for Paper Mfg. Plant	Mitsubishi Kakoki Kiasha, Ltd.	"	WP-62-003
1-13	MKK Industrial Waste Water Treatment System for Food Processing Plant	"	"	"

(continued)

TABLE 11 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
1-14	MKK Industrial Waste Water Treatment System for Ironworks	"	"	"
1-15	MKK Industrial Waste Water Treatment System for Chemical Plant	"	"	"
1-16	MKK Industrial Waste Water Treatment System for Oil Refinery	"	"	"
1-17	MKK Industrial Waste Water Treatment System for Coke Oven Gas Mfg. Plant	"	"	"
1-18	MKK Industrial Waste Water Treatment System for Textile Mill	"	"	"
1-19	Effluent Treatment/Reuse System for Commercial Bldg.	Mitsubishi Rayon Engineering Co., Ltd.	"	5312-20
1-20	Waste Water Treatment System for Dyeing Plant	"	"	5403-30(H)
1-21	Community Sewage Treatment System	"	"	"
1-22	Large-capacity Waste Water Treatment System, "DAIAMARUSU SYSTEM"	"	"	554-3-5-000
1-23	Biochemical Water Treatment Plant	Suido Kiko Kaisha, Ltd.	Co. Brochure	G3-145
1-24	Silk Refinery Effluent Treatment	"	"	"
1-25	Effluent Treatment System for Activated Carbon or Fire-proof Board Mfg. Plant	"	"	"
1-26	Effluent Treatment System for Broiler Plant	"	"	G-3.145
1-27	Effluent Treatment System for Paper	"	"	"

(continued)

TABLE 11 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
1-28	Effluent Treatment System for Electroplating Plant	"	"	"
1-29	Effluent Treatment System for Fruit & Juice Canning Plant	"	"	"
1-30	DOWA Iron-powder Method for Treatment of Laboratory Effluent	The Down Mining Co., Ltd.	1. Co. Brochure 2. Quarterly Review on Environment, No. 25 Sept. 1979	GJ-0048A
1-31	Water Treatment Plant Using SIL-B Process	Risui Kagaku K.K.	Co. Brochure	CW901
1-32	ShinkoPfaudler Water Treatment System	Shinko-Pfaudler Co., Ltd.	Co. Catal. No.	Hai-7902-2
1-33	Industrial Waste Water Treatment Process	Hitachi, Ltd.	Co. Brochure	AA-045
1-34	Sewage Treatment Process	Hitachi, Ltd.	Co. Brochure	AA-045
1-35	Water Treatment System for Effluent & Sludge from Purification Plant	Japan Organo Co., Ltd.	Cat. No.	Y-1
1-36	Water Treatment System for Effluent from Metal Surface Treatment Plant	"	"	A-11-4
1-37	Water Treatment System for Effluent from Thermal Power Plant	"	"	"
1-38	Water Treatment System for Industrial Waste Water Containing Heavy Metals	"	"	"
1-39	Water Treatment System for Effluent from Surface Treatment Plant	"	"	"
1-40	Water Treatment System for Effluent from Chemical Textile Plant	"	"	"

(continued)

TABLE 11 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
1-41	Water Treatment System for Effluent from Maritime Products Processing	"	" "
1-42	Water Treatment System for Effluent from Sugar Refining Plant	"	" "
1-43	Water Treatment System for Effluent from Food Processing Complex	"	" "
1-44	Water Treatment System for Effluent containing synthetic detergent	"	" "
1-45	Water Treatment System for Effluent from Dyeing Plant	Japan Organo Co., Ltd.	Cat. No. A-11-4
1-46	Night-soil Treatment Plant	"	Cat. No. A-34
1-47	Small-scale Community Sewage Treatment Plant called "Hodaka System"	J. Oguchi Hodaka Town Office	J. Solid Waste, 10(7): 21-29, 1980
1-48	Energy-saving Measures for Effluent Treatment Facilities at Sodegaura Oil Refinery	Fuji Seikyu K.K.	The 1980 Collection of Energy-saving Measures, Energy Conservation Center, Tokyo:737-744, 1980
1-49	Improved Operation of Total Waste Water Treatment System at Aichi Oil Refinery	Idemitsu Kosan K.K.	" :875-881
1-50	Energy Conservation by re-examining Water Treatment Processes for Effluent at Mishima Plant	Daiwo Seishi K.K.	" :1407-1416
1-51	Organic Wastewater Treatment System "BIOBLOCK R"	Kurita Water Industries, Ltd.	J. Japan Sewage Works Assoc., 16(182):10-12, 1979

(continued)

TABLE 11 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
1-52	Fixed Bed Type Activated Sludge Treatment System for Organic Effluents	Biseibutsu Kogaku Kenkyusho K.K.	PPM 11(5):Kozen-6, 1980
1-53	Two-stage Aeration Wastewater Treatment Process for Effluent from Orange Canning Plant	T. Mohri, Toyo Shokuhin J. College	PPM 11(6):25-38, 1980
1-54	Practical Application of "Low-dilution 2-stage Activated Sludge" Water Treatment Process	Y. Ichiki, Ebara-Infilco Co., Ltd.	PPM 11(6):48-62, 1980
1-55	Batch Operation Type Activated Sludge Process for Treatment of Laundry Effluent	Y. Ishida, et al, Japan Construction Metal Products Co., Ltd.	PPM 11(6):63-70, 1980
1-56	FA (Furukawa-Arsendorf) System Night Soil Treatment Plant	Furukawa Co., Ltd.	PPM 11(9):34-40, 1980
1-57	Biological Water Treatment System "BIOLEX"	Ebara-Infilco Co., Ltd.	EPCEI (Environmental Pollution Control Equipment Index), 1980:p. 21
1-58	Rotary Aeration Type Wastewater Treatment System, "BIOTRIX"	Asahi Engineering Co., Ltd.	PECEI, 1980: p. 21
1-59	Small- & Medium-scale Community Sewage Treatment Plant	Hitachi Shipbuilding & Engineering Co., Ltd.	Co. Brochure E-113
1-60	Soaked Filter Bed Type Wastewater Treatment System	"	" E-112
1-61	Laboratory Waste Water Treatment System for Tsukuba Univ.	"	" E-122
1-62	Wastewater Treatment System for Univ. & Labs.	"	" E-110
1-63	Water Treatment/Reuse System for Commercial Bldg.	"	" E-119

(continued)

TABLE 11 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
1-64	Water Treatment/Reuse System for Multi-family Bldg.	Hitachi Shipbuilding & Engineering Co., Ltd.	Co. Brochure	E-119
1-65	Water Treatment/Reuse System for Manufacturing Plant	"	"	"
1-66	Water Treatment System for Wastewater Containing Heavy Metal Discharged from Refuse Incineration Plant	"	"	E-115
1-67	"HYDREX", Water Treatment System with Activated Carbon Continuously Replaced with Reactivated One	"	"	E-123
1-68	On-shore Waste Water Treatment Plant for Oily Effluent from Ships	"	"	E-108

TABLE 12. LIQUID-SOLID SEPARATION EQUIPMENT

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
2-1	Mitsubishi Grit Chamber Equipment	Mitsubishi Heavy Industries, Ltd.	Co. Brochure	KH-415
2-2	Mitsubishi Settling Basin Equipment	"	"	KH-414
2-3	Mitsubishi Clarifiers	"	"	KH-401
2-4	Mitsubishi Pressure Flocculating Concentrator	"	"	KH-402
2-5	Mitsubishi-Bird Centrifuge Concentrator	"	"	KH-403
2-6	Mitsubishi Belt Press	"	"	KH-441
2-7	Mitsubishi Double-layer Pressure Sand Filter	"	"	KH-416
2-8	Mitsubishi Trickling Filter System "BIOPACK"	"	"	KH-254
2-9	"Trash Rake Car" Screen	Mitsubishi Kakoki Kaisha, Ltd.	"	W-02-00
2-10	Bar Screen	"	"	"
2-11	Swing Rake Bar Screen	"	"	"
2-12	Grit Collector	"	"	"
2-13	Circular Clarifier	"	"	"
2-14	Scum Skimmer	"	"	"
2-15	Thickener with Sludge Collector	Mitsubishi Kakoki Kaisha, Ltd.	"	W-02-00
2-16	Flotation Treatment Tank for Thickening	"	"	"
2-17	Bar Screen W/Rakes & Traveling Water Screen	"	"	78.04BHA

(continued)

TABLE 12 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
2-18	Mitsubishi-Zurn Strain-O-Matic	"	"	"
2-19	MKK-Bamag Deep Filter Tank	"	"	W-61-01
2-20	MKK Corrugated Plate Flocculator (CPF	"	"	WP-62-006
2-21	MKK Tiltable Plate Flotator (TPF)	"	"	WP-66-03
2-22	MKK Tiltable Plate Interceptor (TPI)	"	"	WP-66-01
2-23	Mitsubishi KM Decanting Centrifuge	"	"	U-01-05
2-24	MKK 3-stage Belt Press	"	"	U-02-07
2-25	Mitsubishi KM Drum Filter	"	"	U-02-03
2-26	Mitsubishi-Zurn Micro-matic System	"	"	
2-27	Mitsubishi-Zurn Strain-O-matic Strainer 593 Series	"	"	W-52-03
2-28	MKK Swing Disk Screen	"	"	W-51-05
2-29	Floating Scum Skimmer	Mitsubishi Kakoki Kaisha, Ltd.	"	W-30-01
2-30	Fine-meshed Rotary Strainer/Filter "MAISUTO"	Suido Kiko Kaisha, Ltd.	"	G3-145
2-31	Pressure Flotation Treatment Tank for Thickening	"	"	"
2-32	Flocculation/Sedimentation Thickener "SEDI-THICKENER"	"	"	"
2-33	High-speed Filter System "PIONEER PRE-T FILTER"	"	"	G3-145
2-34	Oxidation Promoting/Filtering Material "HECHIMARON"	Shinko Nylong Co., Ltd.	"	

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TABLE 12 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
2-35	IK Screen Skimmer, Model ST	Ichikawa Woolen Textile Co., Ltd.	"
2-36	High-molecular Coagulants, IK-Floc	"	"
2-37	IK-LT Dehydrator	"	"
2-38	Rotary Diaphragm Press	Shinko-Pfaudler Co., Ltd.	Cat. No. Hai-7902-2
2-39	SP Filter Press, MF & UF Types	"	" Ge-7803
2-40	Test Filter	Nihon Rakasochi Co., Ltd.	Co. Brochure
2-41	One-man Filter Press & Frame	"	"
2-42	Portable Filter Press	"	"
2-43	Closed Type Rotary Filter "CLEAN FILTER"	Nihon Rokasochi Co., Ltd.	Co. Brochure
2-44	Diaphragm Filter Press	"	"
2-45	High-molecular Flocculant "ORFLOC"	Japan Organo Co., Ltd.	Cat. No. Y-1
2-46	Gravity Filter Basin, "W Type Aquazur Filter"	"	Cat. No. A-30-2
2-47	Gravity Filter Basin, "Monopack Filter"	"	"
2-48	Grit Chamber & Screen for Sewage Treatment	"	" A-18-3
2-49	Primary & Final Clarifiers and Sludge Collector for Sewage Treatment	"	"
2-50	Sprinkling Filter Bed	"	"
2-51	Sludge Thickener	"	"

(continued)

TABLE 12 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
2-52	Pressure Filter, Automatic Type	"	" S-5-3
2-53	Pressure Filter, Manual Type	"	"
2-54	Belt Press Type Dehydrator with Aquapelletizing Pretreatment Process "DEHYDROL"	Ebara-Infilco Co., Ltd.	J. Japan Sewage Works Assoc., 16(182):Ko-3, 1979
2-55	Kurita Jet Press Filter, Model JMF	Kurita Kikai K.K.	" :KO-26, 1979
2-56	SUIWO MFG Type Activated Carbon Adsorption Equipment	Suido Kiko Kaish-a, Ltd.	" :KO-31, 1979
2-57	Comminuter & Bar Screen	Comminutor Service Co., Ltd.	" :KO-44, 1979
2-58	Clean Filer	Narita Koki K.K.	PPM 11(5):Kozen-39, 1980
2-59	"AUTO-SCREEN", an Automatically-controlled Screen Device for Pre-treatment of Wastewater	Ikunamu Kensetsu K.K.	" :Kozen-66, 1980
2-60	Compact Filter/Dehydrator	Daiden Setsubi Sekkei K.K.	" :Kozen-69, 1980
2-61	Wastewater Treatment Device	Kubota, Ltd.	Jap. Patent Tokko Sho 54-18068 PPM 11(5):97-98, 1980
2-62	Suito's All-automatic Filter Press	Saito Kakoki K.K.	PPM 11(6):Kozen-8, 1980
2-63	Rotary Filter with Long-nap Filter Cloth	Toyama Kikai K.K.	PPM 11(7):99, 1980
2-64	Self-cleaning Tiltable Wedge Wire Screen	Nihon M.C. Boeki Co., Ltd.	" :101, 1980
2-65	Helios Dehydrator	Nitto Engineering Service Co., Ltd.	" :103, 1980
2-66	Toray TH Screen	Toray Industries Inc.	PPM 11(9):Kozen-11, 1980

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TABLE 12 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
2-67	Moving Filter Bed Type Sand Filter	Takuma Co., Ltd.	PPM 11(9):99, 1980
2-68	Filter Devices (an overview report)	M. Shimamura, Mitsubishi Kakoki Kaisha, Ltd.	Ind. Poll. Control 16(6):587-593, 1980
2-69	Flotation Separation (" ")	K. Otsubo, Hitachi Plant Construction Co., Ltd.	" :594-600, 1980
2-70	Single Type Automatic Filter Press for Two-stage Dehydration	Ishigaki Mechnical Industry Co., Ltd.	Jap. Ind. & Technol. Bull., 8(5):16-17, 1980
2-71	Screened Scum Dehydration Press	Nippon Inka K.K.	EPCEI (Environmental Pollution Control Equipment Index) 1980:12
2-72	Rolling Screen	Iwase Tekko K.K.	EPCEI, 1980:14
2-73	Nakagawa Filter Press	Nakagawa Kagaku Sochi K.K.	" " :15
2-74	Bar Screen	Kato Tekko K.K.	" " :16
2-75	NKK Unit System Sludge Dehydrator	Nippon Kokan K.K.	" " :30
2-76	Belt Press	Sumitomo Jukikai Environtec Co. Ltd.	" " :30
2-77	KOBELCO/ALFA-LAVAL Decanter Type Centrifuge	Kobe Steel, Ltd.	" " :31
2-78	Belt Press Type Dehydrator "Sevel Roller"	Doriko K.K.	" " :32
2-79	Inka High-speed Belt Press	Nippon Inka K.K.	" " :33
2-80	Mitsubishi Vacuum filter	Mitsubishi Heavy Industries, Ltd.	Co. Brochure KH-383
2-81	Mitsuabishi Sludge Filter Press	"	" KH-423
2-82	Mitsubishi-Bird High-speed Centrifuge	"	" KH-194

TABLE 13. BIOLOGICAL TREATMENT PROCESS

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
3-1	Mitsubishi-Lurgi Waste Water Treatment Process "GYLOFLOC"	Mitsubishi Heavy Industries, Ltd.	Co. Brochure	KH-319
3-2	Mitsubishi-Lurgi Surface Aerator "GYROMIX"	"	"	"
3-3	Mitsubishi-Lurgi Pendulum Scraper	"	"	"
3-4	Mitsubishi-Lurgi Flocculating Sedi-mentation Equipment "SEDIMAT" MH 6A	"	"	KH330
3-5	Mitsubishi Sewage Treat ment Plants (Secondary Treatment Process)	"	"	KH-385
3-6	Mitsubishi Rotary Disk Type Waste Water Treatment Process	"	"	KH-434
3-7	Mitsubishi Community Sewage Treatment Plant	"	"	KH-375
3-8	Mitsubishi Water Treatment System for Exudation from Reclaimed Land	"	"	KH-443
3-9	Mitsubishi Sewage Sludge Digestion System	"	"	KH-432
3-10	Mitsubishi Trickling Filter System "BIOPACK"	"	"	KH-254
3-11	Mitsubishi Laboratory Wastewater Treatment System	Mitsubishi Heavy Industries, Ltd.	"	KH-378
3-12	Mitsubishi-Lurgi Water Recycling System for Building	"	"	KH-289
3-13	Mitsubishi Methane Gas Producing/ Waste Liquids Treatment System	"	"	KH-399

(continued)

TABLE 13 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source	Literature
3-14	Cross-flow Flocculator	Mitsubishi Kakoki Kaisha, Ltd.	"	W-02-00
3-15	Swing Diffuser	"	"	
3-16	Spring Air Diffuser	"	"	
3-17	Deep Aerator	"	"	
3-18	Gas Recirculation System for Digestion Tank	"	"	
3-19	Digestor Heating System	"	"	
3-20	MKK Night Soil Treatment System	"	"	
3-21	MKK Industrial Waste Water Treatment System for Food Processing Plant	"	"	WP-62-003
3-22	MKK Industrial Waste Water Treatment System for Oil Refinery	"	"	"
3-23	MKK Industrial Waste Water Treatment System for Coke Oven Gas Mfg. Plant	"	"	"
3-24	MKK Industrial Waste Water Treatment System for Textile Mill	Mitsubishi Kakoki Kaisha, Ltd.	Co. Brochure	WP-62-003
3-25	Mitsubishi-ICI Deep Shaft Process	"	"	W-68-01
3-26	SURFACT Process: BIO-SURF Air Drive System	"	"	
3-27	AERO-SURF Process: BIO-SURF Air Drive System	"	"	
3-28	Waste Water Treatment System for Dyeing Plant	Mitsubishi Rayon Engineering Co., Ltd.	"	5403-30(H)
3-29	Community Sewage Treatment System	"	"	

(continued)

TABLE 13 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
3-30	Biochemical Water Treatment Plant	Suido Kiko Kaisha, Ltd.	"	G3=145
3-31	Silk Refinery effluent Treatment Plant	"	"	"
3-32	Effluent Treatment System for Activated Carbon or Fire-proof Boards Mfg. Plant	"	"	"
3-33	Effluent Treatment System for Broiler Plant	"	"	"
3-34	Effluent Treatment System for Paper Mfg. Plant	"	"	"
3-35	Effluent Treatment System for Electroplating Plant	Suido Kiko Kaisha, Ltd.	"	G3-145
3-36	Effluent Treatment System for Fruit & Juice Canning Plant	"	"	"
3-37	Submersible Aerators, Model TR, TRN & TRNG	Tsurumi Mfg. Co., Ltd.	1. Tsurumi Technical Manual 2. Co. Brochure TSURUMI-2	
3-38	Toshibe Aerator	Tokyo Shibaura Electric Co., Ltd.	Co. Brochure	KSA-99091
3-39	Toshiba Ozonizer	"	"	KSA-99107
3-40	Industrial Waste Water Treatment Process	Hitachi, Ltd.	Hitachi Brochure AA-045	
3-41	Sewage Treat ment Process	"	"	
3-42	Water Treatment System for Effluent from Sugar Refining Plant	Japan Organo Co., Ltd.	Cat. No. A-11-4	
3-43	Water Treatment System for Effluent from Food Processing Complex	"	"	
3-44	Night-soil Treatment Plant	"	Cat. No. A-34	

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TABLE 13 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
3-45	Small-scale Community sewage Treatment Plant called "Hodaka System"	Ebara Mfg. Co., Ltd.	J. Solid Wastes, 10(7): 21-29, 1980
3-46	Improved Operation of Total Waste Water Treatment System at Aichi Oil Refinery	Idemitsu Kosan K.K.	The 1980 Collection of Energy-saving Measures, Energy Conservation Center, Tokyo:875-881
3-47	Energy Consevation by Re-examining Wazter Treatment Processes for Effluent at Mishima Plant	Daiwo Seishi K.K. (Paper Mfg.)	" :1407-1416
3-48	Organic Wastewater Treatment System "BIO-FLOCK R"	Kurita Water Industries, Ltd.	J. Japan Sewage Works Assoc., 16(182):KO-3, 1979
3-49	Pure Oxygen Aeration in Open Tanks	Ataka Construction & Engineering Co., Ltd.	" :KO-13, 1979
3-50	Air Blow Nozzle	Daicel Ltd.	" :KO-29, 1979
3-51	Fixed Bed Type Activated Sludge Treatment System for Organic Effluent	Biseibutsu Kogaku Kenkyusho K.K.	PPM 11(5):Kozen 6, 1980
3-52	Energy-saving JAS Jet Aeration System	Nishihara Environmental Sanitation Research Corp., Ltd.	" :Kozen 31, 1980
3-53	Packing Material for Aeration	Tsutsunaka Plastics Kogyo K.K.	" :Kozen 41, 1980
3-54	Two-stage Aeration Wastewater Treatment Process for Orange-canning Effluent	T. Mohri, Toyo Shokuhin J. College	PPM 11(6):25-38, 1980
3-55	Practical Application of "Low-dilution 2-stage Activated Sludge" Water Treatment Process	Y. Ichiki, Ebara-Infilco Co., Ltd.	PPM 11(6):48-62, 1980
3-56	Batch Operation Type Activated Sludge Process for Treatment of Laundry Effluent	Y. Yoshida, et al, Japan Construction Metal Products Co., Ltd.	" :63-70, 1980

(continued)

TABLE 13 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
3-57	Water Treatment Process for Wastewater Containing Formaldehyde	Mitsubishi Gas-Chemical Co., Inc.	Japan. Pat. Tokko Sho 54-22022 PPM 11(6):107-108, 1980
3-58	Improved Activated Sludge Treatment System	Mitsubishi Chemical Industries, Ltd.	Japan. Pat. Tokko Sho 54-22702 PPM 11(6):108-109, 1980
3-59	Wastewater Treatment System Using Activated Sludge and Carbon Powder	Nittesu Kakoki K.K.	Japan. Pat. Tokko Sho 54-22707 PPM 11(6):109-110, 1980
3-60	Small-sized, Noiseless Underwater Blower	Shin Meiwa Industry Co., Ltd.	PPM 11(7):97, 1980
3-61	FA (Furukawa-Arsendorf) System Night-soil Treatment Plant	Furukawa Co., Ltd.	PPM 11(9):34-40, 1980
3-62	Wastewater Neutralization Process (an Overview Report)	J. Sakagami, Fuji Kasui Kogyo, K.K.	Ind. Poll. Control, 16(6):579-582, 1980
3-63	Precipitators (an Overview Report)	M. Suito, Sumitomo Jukikai Envirotec Co.	" :583-586, 1980
3-64	Activated Sludge Process (an overview report)	K. Sono, Shinko-Pfaudler Co., Ltd.	16(6):601-609, 1980
3-65	Biological Wastewater Treatment System, "BIOLEX"	Ebara-Infilco Co., Ltd.	EPCEI (Environmental Pollution Control Equipment Index), 1980:4
3-66	Rotary Aeration Type Wastewater Treatment System, "BIOTRIX"	Asahi Engineering Co., Ltd.	" :21
3-67	Toray Aerator	Toray Industries Inc.	" :22
3-68	Jet Aeration System, JAS	Nishihara Environmental Sanitation Research Corp., Ltd.	" :23

(continued)

TABLE 13 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
3-69	Small- & Medium-scale Community Sewage Tertiary Treatment Plant	Hitachi Shipbuilding & Engineering Co., Ltd.	Co. Brochure	E-113
3-70	Soaked Filter Bed Type Waste Water Treatment System	"	"	E-112
3-71	Waste Water Treatment System for Univ. & Labs.	"	"	E-110

TABLE 14. SLUDGE DISPOSAL

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
4-1	Mitsuabishi Belt Press	Mitsubishi Hvy. Industries, Ltd.	Co. Brochure	KH-441
4-2	Mitsubishi-Lurgi Fluidized Bed Type Sludge Furnace	"	"	KH-368
4-3	Conveyor Sludge Collector	Mitsubishi Kakoki Kaisha, Ltd.	"	W-02-00
4-4	Double-floor Type Sludge Collector for Primary Clarifier	"	"	"
4-5	Double-floor Type Sludge Collector for Final Clarifier	"	"	"
4-6	Sludge Dehydrator	"	"	"
4-7	Sludge Incinerator	"	"	"

(continued)

TABLE 14 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
4-8	"REGRAN" (Return Grade Nature) Composting System	Nippon Shoryokki Seisakusho K.K.	Co. Brochure
4-9	Princiner K Series Incinerators	"	"
4-10	SIL-B Process - Pre-dehydration Treatment Using Silicic Flocculant for Sludge Disposal	Risui Kagaku K.K.	1. Co. Brochure CW303 2. Tech. Booklet
4-11	Sludge Dehydrator	Japan Organo Co., Ltd.	Cat. No. A-18-3
4-12	Sludge Incinerator	"	"
4-13	Sludge Treatment by the Freeze-Thawing Process	Japan Organo Co., Ltd.	Cat. No. A-24
4-14	Small-sized Freeze-Thawing Type Sludge Treatment Equipment "OR-FREEZER"	"	" 3HA 79-11
4-15	Belt Press Type Sludge Dehydrator	"	" A-19-3
4-16	Sewage Sludge Composting Process	NGK Insulators, Ltd.	Research Results on Reuse of Sludge as Resource compiled by "The Council on Reuse of Sewage Sludge as Resources":pp 4-7, Nov. 1979 (Japan Sewage Works) Assoc.)
4-17	High-speed Composting System "HITACHI BIOCELL"	Hitachi Kiden Kogyo K.K.	" :7-8, Nov. 1979
4-18	Hitachi Sludge Drying/Incinerating System	Hitachi Metals, Lt d.	" :8-10, Nov. 1979

(continued)

TABLE 14 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
4-19	Sludge Drier	Ohkawara Seisakusho K.K.	1978 Directory of Member Companies of Council on Reuse of Sewage Sludge as Resources, Japan Sewage Works Assoc.: pp. 19-21, 1979
4-20	Kyowa Sludge Drier	Kyowa Kako K.K.	1978 Directory of Member Companies of Council on Reuse of Sewage Sludge as Resources, Japan Sewage Works Assoc.: pp. :25-27, 1979
4-21	Kurita Sludge Composting System	Kurita Water Industries, Ltd.	":29-32, 1979
4-22	Kobe Steel, Ltd. Process for Disposal of Sewage Sludge	Kobe Steel, Ltd.	":33-36, 1979
4-23	High-speed Sewage Sludge Composting Equipment, "Negative Pressure Pelletizing/Fermenting System"	Sekisui-Okumura Kikai K.K.	":38-40, 1979
4-24	Sludge Incinerator with Waste Heat Boiler	Takuma Co., Ltd.	":44-47, 1979
4-25	Niigata Engineering's Sewage Sludge Treatment/Disposal System	Niigata Engineering Co., Ltd.	":51-54, 1979
4-26	Hitachizosen Sludge Drier/Incinerator	Hitachi Shipbuilding & Engineering Co., Ltd.	":67-68, 1979
4-27	Fluid Bed Type Sludge Incinerator	"	":68-70, 1979
4-28	High-speed Fermentation/Composting System	"	":70, 1979
4-29	Sludge Dehydrator, "KURIMOTO CLAM PRESS"	Kurimoto Iron Works, Ltd.	PPM, 11(5):Kozen-32, 1980

(continued)

TABLE 14 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
4-30	"WS Filter", Sludge Dehydrator Using No Chemicals	Nichiyu Koki K.K.	" :Kozen-66, 1980
4-31	Sludge Freezing Device for Sludge Freeze-Thawing Process	Fuji Electric Co., Ltd.	Japan. Pat. Tokko Sho 54-18863 PPM, 11(5):95-97, 1980
4-32	Kanebo's Sludge Dehydrator	Sekisui-Kanebo Environment K.K.	PPM, 11(6):Kozen-9, 1980
4-33	"BULKLESS", a Chemical to Remove Bulking of Activated Sludge	Mizushori Kagaku Kenkyusho K.K.	" :Kochu-6, 1980
4-34	Sludge Activity Stabilizer (O2-ϕ System)	Reika Kogyo K.K.	" :101, 1980
4-35	Toray TH-CSD (Coagulation/Separation/ Dehydration) System	Toray Industries Inc.	PPM, 11(9):Kozen-11, 1980
4-36	Disposal of Sludge (an Overview Report)	H. Kurose, Ebara-Infilco Co., Ltd.	Ind. Poll. Control, 16(6):611-618, 1980
4-37	Sludge Incinerators (" ")	A. Yasuda, Taguma Sogo Kenkyusho K.K.	" :619-625, 1980
4-38	Single Type Automatic Filter Press for 2-stage Dehydration	Ishigaki Mechanical Industry Co., Ltd.	Jap. Ind. & Technol. Bull., 8(5)16-17, 1980
4-39	Sludge Drier	Ohkawara Seisakusho K.K.	EPCEI (Environmental Pollution Control Equipment Index) " :27, 1980
4-40	Sludge Composting Tank	Ebara-Infilco Co., Ltd.	" :28, 1980
4-41	NKK Unit System Sludge Dehydrator	Nippon Kokan K.K.	EPCEI (Environmental Pollution Control Equipment Index :30, 1980
4-42	Belt Press	Sumitomo Jukikai Envirotec Co., Ltd.	" :30, 1980

(continued)

TABLE 14 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
4-43	KOBELCO/ALFA-LAVAL Decanter Type Centrifuge	Kobe Steel, Ltd.	" :31, 1980	
4-44	Belt Press Type Dehydrator "Seven Roller"	Doriko K.K.	" :32, 1980	
4-45	Inka High-pressure Belt Press	Nippon Inda K.K.	" :33, 1980	
4-46	Mitsubishi Sludge Filter Press	Mitsubishi Hvy. Industries, Ltd.	Co. Brochure	KH-423

TABLE 15. OIL REMOVING

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
5-1	Mitsubishi Oily Water Purifier	Mitsubishi Hvy. Industries, Ltd.	Co. Brochure	KH-437
5-2	Mitsubishi Oily Water Purifier for Ships	"	"	KH-384
5-3	MKK Waste Oil Treatment Plant	Mitsubishi Kakoki Kaisha, Ltd.	"	11.76AA
5-4	MKK Oily Water Treatment System	"	"	05-76.C.A.
5-5	MKK Oil-containing Waste Water Treatment System	"	"	09-76.B.N.
5-6	Oily Water Treatment Agent "DIA-MARUSU"	Mitsubishi Rayon Engineering Co.,	"	S54-3-5-00

(continued)

TABLE 15 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
5-7	"Skim Chemissor", Oil Skimming Pump	World Chemical Co., Ltd.	"
5-8	"Manhole Chemissor", Oil-skimming Pump	"	"
5-9	"Skim Suction", Oil-skimming Pump	"	"
5-10	"Skim Boat", Oil-skimming Boat	"	"
5-11	"OS Chemissor", Oil-skimming Pump	"	"
5-12	IK Oil Skimmer	Ichikawa Woolen Textile Co., Ltd.	"
5-13	Oil/Scum Collector	Toyo Giken K.K.	PPM, 11(6):Kozen-35
5-14	On-shore Waste Water Treatment Plant for Oily Effluent from Ships	Hitachi Shipbuilding & Engineering Co., Ltd.	Co. Brochure E-108

(continued)

TABLE 16. TERTIARY TREATMENT PROCESS

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
6-1	Mitsubishi Reverse Osmosis Desalination Plant	Mitsubishi Hvy. Industries, Ltd.	Co. Brochure KH-409
6-2	MKK Tertiary Treatment Process	Mitsubishi Kakoki Kaisha, Ltd.	" W-00-09
6-3	Tertiary Treatment System	Mitsubishi Rayon Engineering Co., Ltd.	" " :5403-30(H)
6-4	Advanced Waste Water Treatment System - Toshiba Aquaponic System	Tokyo Shibaura Electric Co., Ltd.	Toshiba Leaflet
6-5	Tertiary Filter	Taiyo Sanso Co., Ltd.	Co. Brochure
6-6	Ion-exchange Water Treatment Process	Japan Organo Co., Lt d.	Cazt. No. A-11-4
6-7	Toray Reverse Osmosis Module	Toray Industries Inc.	EPCEI (Environmental Poll. Control Equipment Index), :38, 1980
6-8	Unitika Wastewater Treatment/Heavy Metal Recovery System (Chelating Resin Method)	Unitika, Ltd.	" :38, 1980
6-9	Reverse Osmosis Module "HOLLOWSEP"	Toyobo Co., Ltd.	" :39, 1980
6-10	Compact Forced Settling/Adsorption Equipment	Elepon Kakoki K.K.	" :40, 1980
6-11	Small- & Medium-scale Community Sewage Tertiary Treatment Plant	Hitachi Shipbuilding & Engineering Co., Ltd.	Co. Brochure E-113
6-12	Tertiary Waste Water Treatment System	"	" E-120

TABLE 17. METERS/ANALYZERS

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
7-1	Water Quality Monitoring System Model WARA-22	Horiba, Ltd.	Horiba Bull. ME-0001G
7-2	Automatic COD Analyzers CODA-111/112	"	"
7-3	Simplified BOD Monitor, MODEL BOD-1	"	"
7-4	Organic Pollutant Monitor, Model UVOC-1	"	"
7-5	Water Pollution Analysis System for Mass Control of Pollutants	"	"
7-6	Water Quality Checker, Model U-7	"	"
7-7	Oil Content Alarm Monitor, Model OCMA-34	"	"
7-8	Oil Content Monitor (for Land Use)	"	"
7-9	Oil Content Monitor, Model OCMA-32A	"	"
7-10	Oil Content Analyzer, Model OCMA-200	"	"
7-11	TOSWACS - Toshiba New Waterac & Clearac System Series 100 thru 700	Tokyo Shibaura Electric Co., Ltd.	Co. Brochure KSP-1303
7-12	Automatic BOD Meter with Recorder	Japan Organo Co., Ltd.	Cat. No. S-5-3
7-13	Maintenance-free, Automatic SVI (Sludge Volume Index) Meter	Meidensha Electric Mfg. Co., Ltd.	J. Japan Sewage Works Assoc., 16(182):KO-14, 1979
7-14	Computerized Central Control System for Sewage Treatment Plant	Shinko Electric Co., Ltd.	J. Japan Sewage Works Assoc., 16(182):KO-19, 1979
7-15	Hokoshin Composite Sampler WLS401	Hokushin Electric Works, Ltd.	PPM 11(5):Kozen-9, 1980
7-16	SHARP's Automatic COD Measuring Device	Sharp Corporation	PPM 11(5):Kozen-25, 1980
7-17	Ultra-violet Ray Type Organic Pollution Monitoring Equipment	Shimadzu Seisakusho, Ltd.	PPM 11(6):104, 1980

(continued)

TABLE 17 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
7-18	Automatic Total Cyanide Monitoring Equipment	Matsushita Communication Industrial Co., Ltd.	PPM 11(6):104, 1980
7-19	Continuous-Cyanide Analyzer, VS-3900A	"	PPM 11(7):100, 1980
7-20	JEMIC Oil Spill Monitoring Devices	Nippon Sokki K.K.	EPCEI (Environmental Poll. Control Equipment Index), :4, 1980
7-21	Hitachi-Horiba pH Meter	Horiba, Ltd.	" :65, 1980
7-22	Ion Meter - Ion Electrode	"	" :65, 1980
7-23	Horiba Oil Content Densitometer	"	" :66, 1980
7-24	Horiba Automatic Water Quality Analyzer	"	" :67, 1980
7-25	Composite Sampler	Toray Industries, Inc.	" :68, 1980
7-39	Portable Residual Chlorine Meter RC-3	"	EPCEI (Environmental Poll. Control Equipment Index), :76, 1980
7-40	Automatic COD Measuring Equipment	Kawatetsu Keiryoki K.K.	" :77, 1980
7-41	ASTRO System TOC, TOD Measuring Equipment	"	" :77, 1980
7-42	Arithmetic Unit AW for Computation of COD Load	Ando Denki K.K.	" :78, 1980
7-43	"Sensor" System Defoamer Type Densitometer	Shibaura System Co., Ltd.	" :80, 1980
7-44	Microanalyzer for Nitrogen Content for Water	Yanagimoto Seisakusho K.K.	" :80, 1980
7-45	Portable COD Meter HC 207	Central Kagaku K.K.	" :81, 1980

TABLE 18. OTHERS

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature	
8-1	Mitsubishi Filter Sand Cleaner	Mitsubishi Hvy. Industries, Ltd.	Co. Brochure	KH-435
8-2	Mitsubishi-Lurgi Reactivation Furnace for Spent Activated Carbon	"	"	KH-424
8-3	Mitsubishi Sodium-Hypochlorite Dis-infection System (MSDS)	"	"	KH-342
8-4	Mitsubishi Deodorization Equipment, Activated Carbon Method	"	"	KH-364
8-5	Mitsubishi Deodorization Equipment, Ozone Catalyst Method	"	"	KH-332
8-6	Mitsubishi Marine Growth Preventing System, "M.G.P.S."	"	"	KH-380
8-7	Waste Liquid Incinerator	Asahi Engineering Co., Ltd.	Tech. Info. Booklet No. 1, Asahi, Engineer-ing Co.	
8-8	Chemical Injector	Suido Kiko Kaisha, Ltd.	Co. Brochure	G3-145
8-9	Submersible Ejectors, Model BR & BER	Tsurumi Mfg. Co., Ltd.	Tsurumi Tech. Manual II.	
8-10	Submersible Cutter Pumps, CE/C/CA Series	"	Cat. No. (D)7811-1	

(continued)

TABLE 18 (continued)

Ref. No.	Equipment/Process	Manufacturer (or Author)	Source Literature
8-11	Submersible Pumps & Blowers	Hitachi, Ltd.	Hitachi Brochure AA-045
8-12	Sewage Pump Speed Controller "Flow Matcher"	Nishihara Environmental Sanitation Research Corp., Ltd.	J. Japan Sewage Works Assoc. 16(182):KO-4, 1979
8-13	Sludge Pump, Model SPN	Furukawa Co., Ltd.	" :KO-5, 1979
8-14	Submersible Pumps	Sakuragawa Pump Mfg. Co., Ltd.	" :KO-35, 1979
8-15	Speed-variable Underwater Pumps, Model COP (Hydraulic)	Shin Meiwa Industry Co., Ltd.	" :KO-39, 1979
8-16	Instantaneous Evaporator for Effluent Containing Valuable Solids, "Drum Drier"	Mizuho Kogyo K.K.	PPM 11(5)Centerfold, 1980
8-17	Variable-speed Underwater Pump	Nishihara Environmental Sanitation Research Corp., Ltd.	Jpn. Ind. & Technol. Bull., 8(2):8, 1980

GERMAN WASTEWATER EQUIPMENT SURVEY

The following Company-Reference-by-Category lists represent the compilation of selected commercial equipment/processes relating to wastewater treatment from West Germany. The numbers are identification numbers for the particular documents, mainly company literature, supplied to EPA with this report.

Clarification Plants

1-1 High Efficiency Biofiltration
Hoechst AG

1-2 Wastewater Filtration
Vereinigte Kesselwerke AG

1-3 Method of Treating Dye Effluents
Vereingte Kesselwerke AG

1-4 Water Clarification Technology Instrumentation
Vereingte Kesselwerke AG

1-5 High Rate Biofiltration Processes
Grabowski

Aeration of Sludge

2-1 Organization and Design of Activated Sludge Plant According to the Schumacher Activated Sludge System
Schumacher

2-2 Countercurrent Aeration
Schreiber

2-3 Biological Wastewater - Purification by the Pipe Reactor System with Oxygen Aeration
Messer Griesheim

2-4 The Menzel Air Regulation System for Sludge Sterilization
Menzel Co.

2-5 Menzel Rotoflow Circular Flow Aeration System with True Sludge Rotation
Menzel Co.

2-6 Wastewater Purification with Oxygen - Supply of Oxygen
Linde Ag.

2-7 Wastewater Purification with Oxygen - System for Economical Control
Linde Ag.

2-8 Wastewater Purification with Oxygen - Special Oxygen Probe
Linde Ag.

2-9 Development and Objective of Waste Water Handling from the Viewpoint of Conservation
Linde Ag.

2-10 System for Biological Wastewater Purification
Linde Ag.

2-11 Revolutionary Aeration System
F.G.W. Fuchs AG

2-12 Superior Surface Aerator/Rotator
Vereinigte Kesselwerke AG

Flotation Equipment

3-1 Construction of Roedizer Flotation Systems in Communities and Industrial Areas
Roedizer AG

3-2 Reduced Tension Flotation
Vereinigte Kesselwerke AG

Automatic Control Technology

4-1 Control, Design and Distribution Technology
Schreiber

4-2 Computer Programs for Wastewater Purification
Schreiber

Denitrification as an Energy Saving Process

5-1 Observations on Energy Cost Savings with Purifications Through Denitrification
Menzel

5-2 Denitrification as a Necessary Demand with Weak Activated Sludge Process
Menzel

5-3 Energy Savings with Denitrification
Menzel

Sludge Drainage

6-1 Drainage Systems
Westfalia Separator AG

6-2 High Energy Sludge Dewatering
IWKA-Keller

6-3 Full Casing Centrifuge with Worm Gear
ATS Aquatic System

Sludge Utilization

7-1 Process for Utilization of Sewage, Especially from Dry & Clear Sludge
Patent Specification to Gebruder Weiss KG

7-2 Clarification & Decomposition of Sludge
Biologische Abfallverwertungs-Gesellschaft MBH & Co.

7-3 Rapid Band - Method for Sludge Clarification and Other Liquid Organic Waste Through Roedizer Fermentation Technology System
Roediger

SECTION 4

TABLE OF CHEMICAL CONTAMINANTS WITH ADVERSE EFFECTS ON WATER TREATMENT PROCESSES (1913-1974)

The following list of chemicals and the supporting bibliographic references represent an attempt to provide a listing of the negative effect of various chemical entities on the wastewater treatment process. The study was aimed primarily at listing those chemicals which had, or were perceived to have interfered with, or were responsible for a reduction in, the effectiveness of any of the commercial wastewater treatment techniques. Two extensive review works on the subject were employed.

O Oil & Hazardous Materials. Technical Assistance Data System (OHM-TADS)
U.S. Environmental Protection Agency
Oil & Special Materials Controls Division
Office of Water Program Operations
Washington, DC 20460

and

E Effect of Hazardous Material Spills on Biological Treatment Processes
Pajak, Andrew P. and Edward J. Martin
Environmental Quality Systems, Inc.
Rockville, MD 20850

with

Brisko, George A. and Frederick J. Erny
Allegheny County Sanitary Authority
Pittsburgh, PA 15233
U.S. Dept. of Commerce, NTIS PB-276 724

The letter "O" is used to designate those chemicals which were derived from the OHM-TADS list. The letter "E" refers to the Allegheny County study. Letter-number or number entries in parenthesis refer to the two bibliographies at the end of the listing.

The following lists those chemicals, together with the CAS registry number, from the two sources defined above, which exhibit a negative impact on wastewater treatment systems. The time period covered by the two sources represents papers appearing in the literature between 1913 through 1974.

Acetaldehyde 75070

O 230 mg/L req. to suppress oxygen utilization by synthetic sewage 50%. (C-10)

Acetanilide 103844

O Diluted solutions show no inhibitory effect on sewage organisms but 600-1000 ppm inhibit. (E-75)

Acetic Acid 64197

O High concentrations may cause extremely low pH, killing biota and interfering with coagulation. (R-118)

Acetic anhydride 108247

O High concentrations may cause extremely low pH which can destroy biota and interfere with coagulation.

Acetone 67641

O 0.5% had no appreciable effect on digestion. (R-118) (Q-10) (E-85) (E-75) (C-10)

Acetonitrile 75058

O Oxygen consumption inhibited by 490 mg/L of chemical; 50 to 70 mg/L reduced efficiency to the threshold of poor performance, i.e., toxic or inhibitory during oxidation periods up to 672 hr. (41) (43) (52)

Acetyl chloride 75365

O Acid can disrupt sewage treatment and increase reagent demand for coagulation in water treatment.

Acrolein 107028

O 1.5 ppm toxic to sewage organisms, 18 ppm toxic to acclimated sewage organisms, 20-50 mg/L is non-substrate limiting to anaerobic processes. (R-66) (E-76)

Acrylic acid 79107

O May cause low pH and subsequent coagulation problems. > 500 mg/L sodium acrylate is nonsubstrate limiting to anaerobic processes. (R-166) (E-86) (E-75)

Acrylonitrile 107131

O Toxic to anaerobic digestion mechanisms, 150-500 mg/L substrate limiting, 100 mg/L non-substrate limiting. (R-66) (R-92) (E-85)

Aldrin[R] 309002

E Aldrin was not significantly degraded. Less than 5% of COD exerted. (53)

Allyl alcohol 107186

O Appears fairly resistant to biodegration, but exposure to sun and air should break up unsaturated bond producing propyl alcohol which is more readily biodegradable. (R-66) (E-90) (E-85) (E-75)

Aluminum fluoride 7784181

O Aluminum may add to the bulk of sludge brought down in process. Fluoride may poison biota.

Aluminum hydroxide 21645512

O Will add greatly to sludge volumes.

Aluminum sulfate 10043013

O 18 ppm inhibited sewage organisms 50%. May add to volume of sludges, or may drop pH too low for coagulation practices at normal dose levels.

Americium 241 14596102

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Aminotriazole 61825

E No significant biodegradation of chemical. (53)

Ammonium benzoate 1863634

O If neutralized, amenable to biological treatment at a municipal sewage treatment plant.

Ammonium bifluoride 1341497

O When neutralized and diluted, amenable to biological treatment at municipal sewage treatment plants.

Ammonium bisulfite 10192300

O If neutralized and oxidized, amenable to biological treatment at a municipal sewage treatment plant.

Ammonium bromide 12124979

- O If neutralized and diluted, is amenable to biological treatment at municipal sewage treatment plant.

Ammonium citrate, dibasic 3012655

- O If neutralized, amenable to biological treatment at municipal sewage treatment plants.

Ammonium fluoride 12125018

- O When neutralized and diluted, amenable to biological treatment at a municipal sewage treatment plant.

Ammonium pentaborate 12007895

- O If neutralized and diluted, may be amenable to biological treatment at a municipal sewage treatment plant.

Ammonium sulfite 10196040

- O When oxidized and neutralized, amenable to biological treatment at a municiapl sewage treatment plant.

Ammonium tartrate 14307438

- O When neutralized and diluted, amenable to biological treatment at a municipal sewage treatment plant.

Ammonium thiocyanate 1762954

- O Excess of 5000 ppm required to lower BOD of sewage.

Ammonium thiosulfate 7783188

O When neutralized and diluted, amenable to biological treatment at a municipal sewage treatment plant.

Ammonia 7664417

E Deleterious effect on activated sludge process. Inhibition is greater at higher pH values. (46)

sec-Amyl acetate 626380

O Amenable to biological treatment when diluted at a municipal sewage treatment plant.

tert-Amyl acetate 625161

O Amenable to biological treatment at a municipal sewage treatment plant when diluted.

Amyl alcohol 123513

O 0.1% had little effect on digestion while 0.5% retarded it. (C-10) (E-85)

E Toxic threshold for aquatic organisms (treatment process) was approximately 350 mg/L. (46)

sec-Amyl benzene 538681

E 500 mg/L concentration toxic during 24 hours of aeration. (45)

tert-Amyl benzene (tert-Pentylbenzene) 2049958

E 500 mg/L concentration toxic during 24 hours of aeration. (45)

Aniline 62533

E At concentrations of 10 and 20 mg/L, the increased chemical concentrations increased chlorine demand. At 500 mg/L, toxic and inhibiting effects were exhibited for up to 72 hours. (44)

Anthracene 120127

E 500 mg/L was toxic or inhibitory for up to 24 hours; after this period, sludge acclimated and chemical was slowly oxidized. In other tests chemical was slowly oxidized - up to 12.6% of TOD exerted after 144 hours of oxidation. (44)

Antimony 122 14374799

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Antimony 124 14683104

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Antimony 125 14234356

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Antimony pentachloride 7647189

O Amenable to biological treatment at a municipal sewage treatment plant if chemically treated and neutralized first.

Antimony tribromide 7789619

0 Not acceptable at sewage treatment plant.

Antimony trioxide 1309644

0 Will add greatly to sludge volume.

Argon 37 13994713

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Arsenic 74 14304780

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Arsenic 76 15575209

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Arsenic 77 14687617

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Arsenic disulfide 1303328

O Not acceptable at sewage treatment plant.

Arsenic trichloride 7784341

O Not acceptable at sewage treatment plant.

Arsenic trioxide 1327533

O Anticipate possible arsine generation. Greater than normal amounts of activated carbon may be required.

Arsenic trisulfide 1303339

O Odor of hydrogen sulfide should be anticipated. Greater than normal amounts of activated carbon may be required.

Barium 7440393

O Will increase sludge load.

E Greater than 100 mg/L caused significant inhibition of oxygen consumption. (15) (1)

Barium 131 14914751

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Barium 133 13981414

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Barium 137 13981970

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Barium 140 14798084

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Barium carbonate 513779

O May add considerably to sludge volume.

Barium chloride 10361372

O May increase sludge load considerably.

Barium hydroxide 17194002

O May increase sludge volume considerably.

Barium nitrate 10022318

O May increase sludge load considerably.

Benzaldehyde 100527

E At 500 mg/L chemical was oxidized slowly for 6 hours; oxidation increased between 24 and 72 hours with 60% of TOD exerted after 144 hours. A 4% solution was toxic. (44) (15)

Benzamide 55210

E At 500 mg/L chemical was inhibitory or very slowly oxidized for first 6 hours, then rapid oxidation between 24 and 72 hours with 60% of TOD exerted after 144 hours. (44)

Benzene 71432

O Chlorinated benzenes are more toxic than benzene and detectable to taste at lower concentrations. 0.1% seriously retarded sewage digestion.

E Chemical showed varying toxicities at times from 6 hours to 144 hours. After 6 hours up to 0.7% of TOD was exerted; however after 144 hours of oxidation up to 53.5% of TOD exerted. Also, chemical exhibited various degrees of toxicity to various activated sludges. (9) (33) (44) (29)

Benzenethiol (Thiophenol) 108985

E At 500 mg/L the chemical inhibited O_2 uptake for up to 144 hours of oxidation. (44)

Benzidine 92875

E At 500 mg/L, chemical inhibited oxygen uptake for 144 hours of oxidation. (44)

Benzoic acid 65850

O >300 mg/L sodium benzoate is non-substrate limiting for anaerobic processes. (R-66) (C-10) (E-85) (Q-10)

Benzonitrile 100470

O 10 ppm inhibits sewage organisms. (E-191)

E Toxic or inhibitory effects exhibited for first 72 hours of oxidation with up to 40% TOD exerted after 144 hours; sludge acclimation was noted. (43) (44)

Benzylamine 100469

E Chemical inhibited oxygen uptake for up to 144 hours at 500 mg/L initial concentration. (44)

Beryllium 7 13966024

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Beryllium fluoride 7787497

O Not acceptable at municipal sewage treatment plant.

Bismuth 207 13982382

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Bismuth 210 14331794

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Boric Acid 10043353

O To produce a 50% inhibition of the 5 day oxygen utilization of synthetic sewage, >1000 ppm of boric acid was required.

Similar results were obtained in one study with 480 ppm. (R-90)

Boron (Borates) 7440428

Concentrations of 0.05 to 10 mg/L produced inhibition of activated sludge process. At pH 7, activated sludge would adsorb 25 mg of boron/g of sludge in 1 mg/L boron soln. at 31°C. Increased boron resulted in increased adsorption. Lower temperatures may result in increased adsorption. At >100 mg/L of boron, the settling characteristics of the sludge were adversely affected. (15) (46) (3) (4) (39)

Bromine 7726956

O Disinfectant - capable of killing active biota.

Bromine 82 14686692

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Butanedinitril (Succinonitrile) 110612

E 500 mg/L of chemical was reported to be toxic for up to 72 hours of oxidation, a similar concentration was readily, but slowly, oxidized in 24 hours. (43) (49)

Butanenitrile (Butyronitril) 109740

E 500 mg/L inhibited oxidation for up to 24 hours; after 72 hours, up to 10.5% of TOD was exerted. Another study reported slow but steady oxidation occurred at same concentration. (43) (49)

tert-Butyl acetate 540885

O Amenable to biological treatment at a municipal sewage treatment plant when diluted.

n-Butyl alcohol 71363

O Chlorination causes greater odor problem. 0.1% had little effect on digestion but 0.5% retarded it.

sec-Butylamine 13952846

O Amenable to biological treatment at a municipal sewage treatment plant when diluted. Inhibits oxygen uptake.

tert-Butylamine 75649

O Amenable to biological treatment at a municipal sewage treatment plant when diluted. Inhibits oxygen uptake.

n-Butylbenzene 136607

E Not susceptible to biodegradation at 100 mg/L initial concentration. (11)

sec-Butylbenzene 135988

E 500 mg/L toxic during 24 hours aeration. (45)

tert-Butylbenzene 98066

E 500 mg/L toxic during 24 hours of aeration. (45)

n-Butyl phthalate 84742

O May clog filters and exchange beds.

Cadmium (Cd^{+2}) 7440439

E Greater than 1 ppm significantly inhibited oxygen uptake. Inhibitory effects start to decrease rapidly as pH approches 7.4.. (8) (15) (51)

Cadmium 109 14109321

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Cadmium 115 14336686

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Cadmium acetate 543908

O Between 1 and 10 mg/L of cadmium significantly inhibits oxygen consumption.

Cadmium bromide 7789426

O Between 1 and 10 mg/L of cadmium significantly inhibits oxygen consumption.

Cadmium/Manganese mixture

E Mixture, 10 ppm Cd, 100 ppm Mn, was more inhibitory than similar concentrations of the individual elements. (15)

Cadmium sulfate 10124364

O 142 ppm inhibited sewage organisms 50%.

Cadmium/Zinc mixture

E Mixture, 10 ppm Cd, 10 ppm Zn, was more inhibitory than a similar concentration of either element individually. (15)

Calcium 45 13966057

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Calcium 47 14391992

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Calcium arsenite 52740166

O Not acceptable at municipal sewage treatment plant

Calcium carbide 75207

O Lime may produce additional sludge. Acetylene trapped in pipes and sewers poses a major explosion threat.

Calcium chromate 13765190

O Not acceptable at municipal sewage treatment plant.

Calcium dodecylbenzene sulfonate 26264062

O 8 ppm ABS inhibits water softening by coagulation. 300 ppm ABS causes the development of reducing flora resulting in the formation of sulfides, 60 ppm retarded the development of protolytic bacteria, 150 ppm retarded the growth of denitrifying bacteria. ABS interferes with uptake of oxygen and causes foam.

Calcium hypochlorite 7778543

O Will kill active biota.

Calcium phosphate 10103465

O May add considerably to sludge volume.

Calcium phosphide 1305993

O Lime may add considerable to sludge volume.

Captan[R] 133062

E Fungicide was not degradable. Inhibition was observed. (53)

Camphor 76222

O May clog filters.

Carbofuran 1563662

O May affect BOD, otherwise no adverse effects anticipated.

Carbon 14 14762755

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Carbon tetrachloride 56235

O 7.05% inhibited sewage digestion.

Cerium 141 13967743

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Cerium 144 14762788

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Cesium 131 14914762

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Cesium 134 13967709

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Cesium 137 10045973

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Chlorates 14866683

E >10 mg/L chlorates significantly inhibited oxygen consumption. (15)

Chloranil 118752

E At 10 mg/L the chemical inhibited oxygen consumption. (47)

Chlorine 7782505

At 200 and 500 mg/L, chlorine detrimentally affected sludge filterability. (69)

Chlorine 36 13981436

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Chloroform 67663

O No effect on sewage organisms.

4-Chloro-3-methylphenol (4-Chloro-m-cresol) 59507

E At 10 mg/L the chemical was mildly inhibitory; at 100 mg/L, effect was toxic. (47)

Chlorpyrifos 2921882

O Not amenable to biological treatment at municipal treatment plant. Ozone water treatment will increase the toxicity of chlorpyrifos due to the replacement of the P:S bond with the more toxic P:O bond. (I-83)

Chromic acetate 1066304

O 5 ppm hexavalent chromium is threshold for retardation of digestion.

Chromic acid 7738945

O 5 ppm hexavalent is threshold for retardation of digestion.

Chromic sulfate 10101538

O Not acceptable at municipal sewage treatment plant.

Chromium 7440473

O 5 ppm hexavalent is threshold for retardation of digestion. 2000 ppm trivalent retarded digestion 11%.

E A 10 mg/L slug of chromium had little affect on activated sludge process, but nitrification was inhibited. Large amounts of Cr immobilized by the sludge. A 500 mg/L slug dose of 4 hour duration significantly affected system; recovery time was 4 days. Hexavalent Cr was more toxic than trivalent chromium. (5) (28) (58) (12) (46) (2) (6) (8) (15)

Chromium 51 14392020

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Chromium/copper mixture

E Mixture was slightly more toxic (inhibition of O_2 uptake) than was copper alone, but significantly more toxic than was chromium alone. (15)

Chromium/Iron mixture

E Mixture was more toxic (oxygen uptake depression) than either element individually. (15)

Chromous chloride 10049055

O Not acceptable at municipal sewage treatment plant.

Chromyl chloride 14977618

O Not amenable to biological treatment at municipal water treatment plant.

Citric acid 77929

E Chemical was biodegradable but depressed oxygen consumption, increased pH, and increased suspended solids. (52)

Cobalt (ionic) 7440484

E No concentration tested showed stimulation; 0.08 to 0.5 mg/L inhibited growth. (39)

Cobalt 57 13981505

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Cobalt 58 13981389

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Cobalt 60 10198400

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria. 2,000,000 rad was required to give complete destruction of microorganisms in sewage, 90 percent kills of most organisms were achieved at 70,000 rad.

Cobalt chloride 7646799

0 64 ppm inhibits sewage organisms 50%. (E-206) 1000 mg/L was non-substrate limiting to anaerobic processes. (R-66)

Cobalt nitrate 10141056

0 24-29 ppm inhibits sewage degradation 50%. 1000 mg/L was non-substrate limiting to anaerobic processes. (R-66)

Cobaltous bromide 7789437

0 0.08 to 0.5 mg/L may inhibit growth of sewage organisms. (I-62)

Cobaltous sulfamate 14017415

0 0.08 to 0.5 mg/L may inhibit growth of sewage organisms (I-62)

Cobalt sulfate 10124433

0 24-29 ppm inhibits sewage degradation 50%. 1000 mg/L was

non-substrate limiting to anaerobic processes. (R-66)

Coconut oil 8001318

O Will interfere with settling and floc formation. May plug filters and exchange beds.

Copper 7440508

O 1 ppm inhibited sewage organisms 35%.

E A 30 mg/L slug dose caused a detrimental effect on activated sludge organic removal efficiency with recovery in 24 hours; a 75 mg/L 4 hour duration slug caused a 24 hour effect. Copper removal generally was good with large amounts found in the sludge. As organic loading increased copper removal decreased. (46) (17) (5) (12) (39) (1) (6)

Copper 64 13981254

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Copper/Cyanide mixture

E Mixture was more toxic than was copper alone, but less toxic than was cyanide alone. (15)

Copper/Iron mixture

E The Cu-Fe mixture was more toxic or inhibitory than iron alone, but less toxic than was Cu alone. (15)

Copper/Nickel mixture

E Cu-Ni mixture was more toxic than was either metal individually. (15)

m-Cresol 108394

O Taste threshold drops greatly with chlorination.

o-Cresol 95487

O 940 ppm inhibited 50% sewage organisms. Subject to chlorination and subsequently lower taste thresholds.

Crotonaldehyde 4170303

O 200 mg/L is substrate limiting and 50-100 mg/L is non-substrate limiting to anaerobic processes. (R-66) (E-85)

Cupric acetate 142712

O Material will color the water a dark green even at low concentrations. A 30 mg/L slug dose caused a detrimental effect on activated sludge organic removal efficiency with recovery in 24 hrs. A 75 mg/L 4 hr. duration slug caused a 24 hr effect. Copper removal generally was good with large amounts found in the sludge. As organic loading increased copper removal decreased. (I-62)

Cupric acetoarsenite 12002038

O A 30 mg/L slug dose caused a detrimental effect on activated sludge organic removal efficiency with recovery in 24 hrs. A 75 mg/L 4 hr. duration slug caused a 24 hr effect. Copper removal generally was good with large amounts found in the sludge. As organic loading increased copper removal decreased. (I-62)

Cupric chloride 7447394

O When dilute and neutralized, amenable to biological treatment at a municipal sewage treatment plant.

Cupric nitrate 3251238

O 8.4-35 ppm inhibits sewage treatment 50%.

Cupric oxalate 5893663

O A 30 mg/L slug dose caused a detrimental effect on activated sludge organic removal efficiency with recovery in 24 hrs. A 75 mg/L 4 hr. duration slug caused a 24 hr effect. Copper removal generally was good with large amounts found in the sludge. As organic loading increased copper removal decreased. (I-62)

Cupric sulfate 7758987

O Concentrations of 1250 ppm have sterilizing effect on microorganisms in drinking water. Oxygen utilization in a 5 day BOD test was decreased by 50% by 31 ppm $CuSO_4$. 0.05 ppm is used for control of plankton, 1.0 ppm for control of algae & protozoa, 0.6 ppm for control of duckweed & pond weed, 2.0 ppm to kill snails. The amount to control algae depends on the temperature.

Cupric sulfate 10380297

O Material will color the water a dark green even at low concentrations. A 30 mg/L slug dose caused a detrimental effect on activated sludge organic removal efficiency with recovery in 24 hrs. A 75 mg/L 4 hr. duration slug caused a 24 hr effect. Copper removal generally was good with large amounts found in the sludge. As organic loading increased copper removal decreased. (I-62)

Cupric tartrate 815827

O 1 mg/L produces effect on microorganisms; 75 mg/L is lowest 4 hour duration slug dose which produces a 24 hour effect on the effluent. Amenable to biological treatment at a municipal sewage treatment plant when dilute and neutralized.

Cyanide 57125

E At 2 to 3 mg/L there was little tendency of activated sludge to acclimate to chemical; however, recovery from slug load of 40 mg/L occurred in about 2 days. (24) (50)

Cyanide/Nickel mixture

E Mixture, at 100 ppm cyanide and 10 ppm Ni, was more toxic or inhibitory (O_2 uptake) than was Ni alone, but less than cyanide alone. (15)

Cystine 56893

E At 1000 mg/L concentration, O_2 consumption was completely inhibited and solids production stopped. (52)

DDT 50293

E Chemical was not significantly degraded. (53)

Diazinon[R] (Dimpylate) 333415

E Insecticide was not significantly degraded. (53)

1,2,5,6 Dibenzanthracene 53703

E Chemical was slightly inhibitory but slowly oxidized at 500 mg/L initial concentration; up to 8% TOD exerted after 144 hours. (44)

Dicamba 1918009

O Not amenable to biological treatment at a municipal sewage treatment plant.

Dichlobenil 1194656

O Not amenable to biological treatment at a municipal sewage treatment plant.

Dichlone 117806

O Not amenable to biological treatment at a municipal sewage treatment plant.

Dichlorobenzene 25321226

O Will undergo biochemical, chemical, and photochemical attack to form 2,5-dichlorophenol, dichloroquinol, and conjugates. (R-203) (C-10)

Dichlorvos 62737

O Not amenable to biological treatment at a municipal sewage treatment plant. (I-66) (I-29)

2,4-Dichlorophenol 120832

O 100 ppm inhibits BOD in sewage organisms 50%. (R-91) (E-196) (C-1)

2,4-Dichlorophenoxypropionic acid 120365

E No evidence of significant degradation of chemical after 7 days with initial concentration of 186 ppm. (66)

Dieldrin 60571

E Insecticide was not significantly degraded. (53)

Diethanolamine 111422

O Nontoxic to sewage organisms. (R-118) (R-45) (E-76) (E-90) (C-10) (E-84)

Diethylene glycol 111466

O 1000 mg/L was not non-substrate limiting to anaerobic processes. (R-66) (R-118) (E-90) (E-85) (E-75) (E-80)

Dimethylamine 124403

O Chlorination results in formation of toxic chloramines. (Q-17)

d,d'-Diethylstilbenediol (Diethylstilbestrol) 56531

E Chemical demonstrated inhibitory effects at 500 mg/L concentration. (44)

7,9-Dimethylbenz(c)acridine 963893

E At 500 mg/L, two out of three sludges showed toxic effects; third slowly oxidized the chemical; 4% TOD exerted after 144 hours. (44)

7,10-Dimethylbenz(c)acridine 2381400

E At 500 mg/L the chemical was toxic. (44)

m-Dinitrobenzene 25154545

O Not amenable to biological treatment at a municipal sewage treatment plant.

p-Dinitrobenzene 100254

O Not amenable to biological treatment at a municipal sewage treatment plant.

2-4-Dinitrophenol 51285

O At 100 ppm, can produce 50% inhibition of oxygen utilization. Phenols can be chlorinated at water treatment intakes and produce unacceptable tastes at low concentrations. (C-10)

E Chemical concentrations of 1 and 5 mg/L reduced the oxygen uptake rate and solids production; greater than 15 hour aeration required for 90% COD removal. (65)

2,4-Dinitrotoluene 121142

O Amenable to biological treatment at sewage treatment plant when dilute.

Diquat 85007

O Not amenable to biological treatment at a municipal sewage treatment plant.

Disulfoton 298044

O Not amenable to biological treatment at a municipal sewage treatment plant. Ozone water treatment will increase the activity of disulfoton due to the replacement of the P:S bond with the more toxic P:O bond (I-83) (I-29)

Dodecylbenzenesulfonic acid 27176870

O 8 ppm inhibits water softening by coagulation. 300 ppm ABS causes the development of reducing flora resulting in the formation of sulfides, 60 ppm retarded the development of proteolytic bacteria, 15-60 ppm retarded the growth of aerobic bacteria, 150 ppm retarded the growth of denitrifying bacteria. May cause foaming. (C-10)

Dulcitol (Galactitol) 608662

E At a 2% solution, chemical was slightly inhibitory. (15)

Dysprosium 159 14280343

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

EDTA 60004

O 500 ppm inhibits unacclimated sewage organisms. (R-46) (E-85) (R-45)

Endosulfan 115297

O As a sulfite, up to 500 mg/L can be oxidized if system is acclimated, but increased oxygen is required. (I-62) Otherwise not acceptable at a municipal sewage treatment plant. (I-65)

Endrin 72208

E Chemical was not significantly degraded. (53)

Erbium 15840128

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

1,2-Ethanediol (Ethylene glycol) 107211

E At 500 mg/L a 1 to 3 hour lag resulted before oxidation began. Oxygen consumption was significantly depressed. (52)

Ethion 563122

O Ozone water treatment will increase the activity of ethion due to the replacement of the P:S bond with the more toxic P:O bond. (I-83) (I-74)

Ethyl acetate 141786

O 1000 mg/L was not substrate limiting to anaerobic processes. (R-66)

Ethyl acrylate 140885

O Chlorination appears to aggravate odor. 600-1000 mg/L substrate limiting and 300-600 mg/L nonsubstrate limiting to anaerobic processes. (R-66)

Ethyl alcohol 64175

O 0.1% had little effect on digestion while .5% retarded it. (R-118)

Ethyl benzene 100414

O 1000 mg/L was not substrate limiting to anaerobic processes. (R-66)

Ethylene 74851

O Reactive gas dangerous in presence of chlorine.

Ethylenediamine 107153

O 100-300 mg/L nonsubstrate limiting to anaerobic processes. (R-66)

Ethylene dichloride 107062

O Highly toxic to anaerobic digestion even in minute quantities. 150-500 mg/L substrate limiting. (R-66)

Ethyl ether 60297

O Up to 0.5% stimulates digestion.

Ethyl phthmalate, phthmalol, phthalic-acid-diethylester 84662

O May plug filters and exchange beds.

Europium 152 14683239

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Europium 154 15585101

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Europium 155 14391163

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Ferric ammonium citrate 1185575

O More than 100 ppm causes inhibition of oxygen uptake; amenable to biological treatment at a municipal sewage treatment plant when dilute and neutralized.

Ferric ammonium oxalate 2944674

O More than 100 ppm causes inhibition of oxygen uptake; amenable to biological treatment at a municipal sewage treatment plant when dilute and neutralized.

Ferric chloride 7705080

O Will add considerably to sludge volume. Wastewater sludge digestion was affected at 300 mg/L Fe but significant inhibition did not occur until 500 mg/L. Total inhibition was evidenced above 1000 mg/L. No gas was produced at 1500-2000 mg/L Fe. (R-212)

Ferric fluoride 7783508

O More than 100 ppm causes inhibition of oxygen uptake; amenable to biological treatment at a municipal sewage treatment plant when dilute and neutralized.

Ferric hydroxide 1309337

O Will add considerably to sludge volume. Wastewater sludge digestion was affected at 300 mg/L Fe but significant inhibition did not occur until 500 mg/L. Total inhibition was evidenced above 1000 mg/L. No gas was produced at 1500-2000 mg/L Fe. (R-212)

Ferric nitrate 10421484

O More than 100 ppm causes inhibition of oxygen uptake; amenable to biological treatment at a municipal sewage treatment plant when dilute.

Ferric sulfate 10028225

O Will add considerably to sludge volume. Wastewater sludge digestion was affected at 300 mg/L Fe but significant inhibition did not occur until 500 mg/L. Total inhibition was evidenced above 1000 mg/L. No gas was produced at 1500-2000 mg/L Fe. (R-212)

Ferrous ammonium sulfate 10045893

O More than 100 ppm causes inhibition of oxygen uptake; amenable to biological treatment at a municipal sewage treatment plant when oxidized, neutralized, diluted.

Ferrous chloride 7758943

O More than 100 ppm causes inhibition of oxygen uptake; amenable to biological treatment at a municipal sewage treatment plant when dilute.

Ferrous hydroxide 18624447

O Will add to sludge volume. Wastewater sludge digestion was affected at 300 mg/L Fe but significant inhibition did not occur until 500 mg/L. Total inhibition was evidenced above 1000 mg/L. No gas was produced at 1500-2000 mg/L Fe. (R-212)

Ferrous sulfate 50820241

O Will add to sludge volume. Wastewater sludge digestion was affected at 300 mg/L Fe but significant inhibition did not occur until 500 mg/L. Total inhibition was evidenced above 1000 mg/L. No gas was produced at 1500-2000 mg/L Fe. (R-212)

2—Fluorenamine 153786

E At 500 mg/L chemical was slowly oxidized, but inhibitory. (44)

Fluoride 16984488

E At 30 mg/L there was no chemical removal by air aerated lagoon. (37)

Fluorine 7782414

O Can act as disinfectant and kill active biota.

Formaldehyde 50000

O 740 ppm caused 50% inhibition of sewage organisms. Concentrations above 120 mg/L inhibit activated sludge. (R-201) 50-100 mg/L are substrate limiting in anaerobic processes. (R-66)

E Chemical concentrations of from 50 to 720 mg/L demonstrated lag periods greater than 2 days before oxidation began. Following acclimation, 95% removal was achieved at 1750 mg/L initial formaldehyde concentration. By buffering with $NaHCO_3$, formaldehyde concentrations of up to 1500 mg/L were only slightly inhibitory. (52) (21) (16) (49)

Formic acid 64186

O 550 ppm caused 50% inhibition of sewage organisms.

Furfural 98011

O May plug filters or exchange bed.

Gadolinium 14276654

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Gallium 68 15757149

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Gallium 72 13982224

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Germanium 71 14374813

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Gold 195 14320935

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Gold 198 10043499

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Gold 199 14391118

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Hafnium 181 14900211

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Heptachlor 76448

E Insecticide was slightly degraded. (53)

Heptane 142825

O Toxic to sewage organisms.

Hexachlorocyclopentadiene 77474

O Not amenable to biological treatment at a municipal sewage treatment plant.

Hexane 110543

O Toxic to sewage organisms.

Holmium 166 13967652

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Hydracrylonitrile 109784

E Less than 10% reduction achieved in aerated lagoon. (9)

Hydrochloric acid 7647010

O May prevent coagulation by some agents through pH reduction.

Hydrogen 3 10028178

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Hydrogen cyanide 74908

O 4 ppm inhibited sewage digestion.

E A 500 mg/L concentration was toxic for 72 hour oxidation period. (43)

Hydrogen sulfide 7783064

E Causes corrosion above water line because it volatilizes and then condenses in moisture on walls. It is then converted to H_2SO_4 by bacterial activity. (46)

Hydroquinone 123319

O Chlorination drops taste threshold considerably. Chlorination degrades hydroquinone to p-benzoquinone. (Q-17) A concentration of 100 ppm will inhibit an unacclimated sewage system, but not an acclimated one. (R-45)

4-Hydroxybenzene carbonitrile (p-Hydroxybenzonitrile) 767000

E At 500 mg/L concentration, the chemical was toxic for up to 72 hours. (43)

Indium 113 14885780

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Indium 114 13981550

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Iodine 7553562

E Chemical was inhibitory at concentrations greater than 10 mg/L - inhibition of oxygen uptake. (15)

Iodine 125 14158317

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Iodine 129 15046841

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Iodine 130 14914024

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Iodine 131 10043660

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Iridium 192 14694690

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Iridium 194 14158351

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Iron 7439896

O Wastewater sludge digestion was affected at 300 mg/L Fe, but significant inhibition did not occur until 500 mg/L. Total inhibition was evidenced above 1000 mg/L. No gas was produced at 1500-2000 mg/L Fe. (R-212)

E Oxygen uptake was inhibited at concentrations greater than 100 mg/L. (15)

Iron 55 14681595

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Iron 59 14596124

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Iso-butyl acetate 110190

O Amenable to biological treatment at a municipal sewage treatment plant when diluted.

Iso-butyric acid 79312

O Amenable to biological treatment at a municipal sewage treatment plant when neutralized. Readily oxidized.

Isophorone 78591

O 1000 mg/L was not substrate limiting to anaerobic processes. (R-66)

Isopropanolamine dodecylbenzene sulfonate 42504461

O Amenable to biological treatment at a municipal sewage treatment plant when diluted at sewage treatment plant.

Kepone 143500

O Not amenable to treatment at a municipal sewage treatment plant.

Krypton 85 13983272

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Lactic acid 50215

O May be corrosive to equipment.

Lactonitrile 78977

E System unable to handle concentrations greater than 140 mg/L without acclimation. (41)

Lanthanum 140 13981287

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Lead 7439921

E Concentrations greater than 10 mg/L caused inhibitory effects. (15) (39)

Lead 210 14255040

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Lead acetate 301042

O 1 ppm Pb toxic to aerobic bacteria. 0.1-0.5 ppm inhibits bacteria. (C-1)

Lead chloride 7758954

O 1 ppm Pb toxic to aerobic bacteria. 0.1-0.5 ppm inhibits bacteria. (C-1)

Lead fluoborate 13814965

O Bacterial decomposition of organic matter is inhibited by 0.1 ppm lead.

Lead fluoride 7783462

O Concentrations greater than 10 mg/L inhibit growth of sewage organisms.

Lead iodide 10101630

O Concentrations greater than 10 mg/L inhibit growth of sewage organisms.

Lead nitrate 18256989

O 1 ppm Pb toxic to aerobic bacteria. 0.1-0.5 ppm inhibits bacterial action. (C-1)

Lead stearate 7428480

O Concentrations greater than 10 mg/L inhibit growth of sewage organisms.

Lead sulfate 15739807

O 1 ppm toxic to aerobic bacteria. 0.1-0.5 ppm inhibits bacterial action. (C-1)

Lead sulfide 1314870

O Concentrations greater than 10 mg/L inhibit growth of sewage organisms.

Lead thiocyanate 592870

O Bacterial decomposition of organic mater is inhibited by 0.1 ppm lead.

Lead thiosulfate 26265656

O Not amenable to biological treatment at a municipal sewage treatment plant.

Lindane 58899

O 10 ppm reduces activated sludge treatment efficiency 20%. (R-56)

E Insecticide was not significantly degraded. (53)

Linoleic acid 60333

O 3-4 ppm inhibits nitrification. (C-1)

Lithium chromate 14307358

O Not acceptable at municipal sewage treatment plant.

Lutetium 177 (Lutecium) 14265759

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Magnesium 7439954

O May add greatly to sludge volume and render it more difficult to dewater.

Magnesium 28 15092714

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Magnesium acetate 142723

O Will add greatly to sludge volume.

Magnus 53763443

O Inhibits biological systems at >50 ppm. (Q-17)

Malathion 121755

O In low loadings, stimulates growth of sewage organism. In higher loadings, may inhibit or destroy organisms. Load is a function of malathion per unit organisms not malathion per unit water.

E Insecticide was not significantly degraded. (53)

Maleic acid 110167

O pH lowered from 8.0 to 5.8. 128 mg/L of turbidity was coagulated and removed by this compound.

Malonic Acid 141822

E At 500 mg/L the chemical inhibited oxygen uptake. A 1/120 N solution stimulated oxygen uptake. (15) (49)

Manganese 13966319

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

E Approximately 10 mg/L caused inhibition of oxygen uptake by activated sludge. (39) (15)

Manganese/Zinc mixture

E Mixture was more inhibitory than either element alone. (15)

Mercaptodimethur 2032657

O May affect BOD, otherwise no adverse effects anticipated.

Mercuric cyanide 592041

O Toxic or inhibitory at concentrations greater than 5 mg/L of mercury, mercury is removed by uptake in sludge. Concerning the cyanide ion, there is little tendency of activated sludge to acclimate to the chemical, however, recovery from a slug dose of 40 mg/L occurred in about 2 days. (I-62)

Mercuric sulfate 7783359

O Toxic or inhibitory at concentrations greater than 5 mg/L of mercury. Mercury is removed by uptake in sludge. (I-62)

Mercuric thiocyanate 592858

O Toxic or inhibitory at concentrations greater than 5 mg/L of mercury. Mercury is removed by uptake in sludge. (I-62)

Mercurous Nitrate 10415755

O Toxic to sewage organisms. Demonstrated inhibition at 1 mg/L and toxicity at 200 mg/L in one study. In another study it was toxic or inhibitory at concentrations greater than 5 mg/L. Mercury was removed by uptake in sludge. (I-62)

Mercury 7439976

E Chemical demonstrated inhibition at 1 mg/L and toxicity at 200 mg/L in one study. In another, it was toxic or inhibitory at concentrations greater than 5 mg/L. Mercury was removed following uptake in sludge. (34) (22)

Mercury 197 13981516

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Mercury 203 13982780

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Methanol 67561

O No toxic effect on sewage organisms. 0.1% had little effect on digestion while 0.5% retarded it.

E Chemical could be removed by biological systems, but at 500 mg/L a 3 to 5 hour lag period was observed before oxidation could commence. At 1000 mg/L oxygen uptake was severely depressed. (9) (52) (33)

7-Methyl-1,2-benzanthracene 2541697

E At 500 mg/L, the chemical inhibited oxygen uptake for at least 24 hours. (44)

2-Methylbenzene carbonitrile (p-Tolunitrile) 104858

E At 500 mg/L the chemical was toxic for up to 72 hours. (43)

20-Methylcholanthrene (3-Methylcholanthrene) 56495

E At 500 mg/L the chemical showed inhibitory effect but could be slowly oxidized. (44)

2-Methyl-5-ethyl pyridine 104905

O 1000 mg/L is not substrate limiting, but 100 mg/L is nonsubstrate limiting to anaerobic processes. (R-66)

E Less than 30% removal achieved by aerated lagoon treatment. (9)

Methyl isobutyl ketone 108101

O 0.1% is not substrate limiting, but 100-300 mg/L is nonsubstrate limiting to anaerobic processes. (R-66)

Methyl mercaptan 74931

O Eliminate all ignition sources. Add HOCl bleach to chlorine residual and neutralize to pH 7 if necessary. May then be amenable to treatment at a municipal sewage treatment plant.

Methylparathion 298000

E Insecticide was not significantly degraded. (53)

Mexacarbate 315184

O Not amenable to biological treatment at a municipal sewage treatment plant.

Michler's Ketone (4,4-bis-(dimethylamino)benzophenone) 90948

E At 500 mg/L lag periods up to 72 hours were experienced before slow oxidation began. (44)

Molybdenum 99 14119154

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Naled 300765

O Not amenable to biological treatment at a municipal sewage treatment plant.

Naphthalene 91203

O Can be toxic to sewage organisms at 2500 ppm.

2-Napthylamine 91598

O Toxic to most sewage sludges at 2500 ppm. (E-8) (E-78)

E A 500 mg/L concentration of the chemical was toxic. (44)

Neodymium 14269740

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Neptunium 237 13994202

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Nickel 7440020

O 500 ppm retarded sewage digestion 9.4%. A nickel concentration of 3.6 ppm caused 50% reduction in oxygen utilization from synthetic sewage.

E Greater than 5 mg/L continuous dose significantly reduces efficiency of biological systems. A 200 mg/L, 4 hour slug dose produced a 24 hour effect with 40 hours necessary for recovery. Activated sludge removal of Ni was poor but was improved by lime addition. (46) (58) (5) (1) (12) (6)

Nickel 63 13981378

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Nickel ammonium sulfate 15699180

O 27 ppm Ni from nickel ammonium sulfate caused a 50% reduction in oxygen utilization of synthetic sewage.

Nickel chloride 37211055

O 15 ppm Ni as $NiCl_2$ inhibits BOD of sewage by 50%.

Nickel hydroxide 12054487

O Greater than 5 mg/L significantly reduces efficiency of biological systems. A 200 mg/L 4 hour slug may produce a 24 hour effect with 40 hours necessary for recovery.

Nickel nitrate 14216752

O A nickel concentration of 3.6 ppm caused a 50% reduction in the oxygen utilization from synthetic sewage.

Niobium 95 13967765

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Nitric acid 7697372

O May upset pH enough to interfere with coagulation.

Nitrilotriacetic acid (NTA) 139139

O NTA does not interfere with normal treatment processes. (E-189)

Nitrite 14797650

E Concentrations greater than 10 mg/L inhibited oxygen uptake. (15)

Nitrobenzene 98953

O 630 ppm inhibited sewage organisms 50%.

E At 500 mg/L chemical was toxic, inhibiting oxygen uptake for 144 hours. (44) (47) (45)

Nitrogen dioxide 10102440

O Can change pH and interfere with coagulation.

o-Nitrophenol 88755

- O Use 10-35 lb of carbon per lb of material. Additional treatment will be necessary to alleviate the phenolic taste in water. The chlorinated phenols present problems in drinking water supplies because phenol is not removed efficiently by conventional water treatment and can be chlorinated during the final water treatment process to form persistent odor producing compounds. (I-02)

p-Nitrophenol 100027

- O Use 10-35 lb of carbon per lb of material. Additional treatment will be necessary to alleviate the phenolic taste in water. The chlorinated phenols present problems in drinking water supplies, because phenol is not removed efficiently by conventional water treatment and can be chlorinated during the final water treatment process to form persistent odor producing compounds. (I-02)

Nitrotoluene 99081

- O May be amenable to biological treatment at a municipal sewage treatment plant.

o-Nitrotoluene 88722

- O Amenable to biological treatment at municipal sewage treatment plants when diluted.

p-Nitrotoluene 99990

- O May be amenable to biological treatment at a municipal sewage treatment plant.

Nitroxylene 89872

- O May plug filters and exchange beds.

o-Nitroxylol 99514

0 May plug filters and exchange beds.

p-Nitroxylol 89587

0 May plug filters and exchange beds.

Nonanol 143088

0 Initially can be toxic to sewage organisms.

1-Octanol 111875

0 500-1000 mg/L is substrate limiting in anaerobic process. (R-66)

Oleic acid 112801

E A 1/120 N solution inhibited oxygen uptake. (15)

Osmium 191 14119245

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Oxalic acid 144627

0 43 ppm caused no inhibition of sewage organisms.

E At 250 to 720 mg/L oxygen consumption was significantly inhibited. (49)

Oxydipropionitrile 53467097

0 < 6 ppm inhibits oxygen uptake of sewage for 5 days or more.

Palladium 103 14967681

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Palladium 109 14981647

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Parathion 56382

0 In low shock loadings stimulated growth of sewage organisms (i.e 1 mg/32 mg organisms). Higher doses inhibited and destroyed organisms. Loading was found to be a function of mass parathion per unit mass organism rather than per unit mass water.

E Insecticide was not significantly degraded. (53)

Pentachlorophenol 87865

0 Bacteria is inhibited by 4-225 pp,/ (R-90)

E At 150 mg/L chemical inhibited oxygen uptake and was not significantly degraded. (53)

Pentamethylbenzene 700129

E At 500 mg/L chemical was toxic or inhibitory during initial 24 hours of aeration. (45)

Pentane 109660

E At 500 mg/L pentane was resistant or very slowly oxidized. (43)

Pentanedinitrile (Glutaronitrile) 544138

E At 500 mg/L, chemical was toxic or very slowly oxidized. (43)

1-Pentene 109671

O Can be toxic to sewage organisms initially. (C-10) (E-80)

Perchloric acid 7601903

O May drop pH too low for adequate coagulation.

Perchloromethyl mercaptan 594423

O May plug filters and exchange beds.

Phenol 108952

O 1000 mg/L is not substrate limiting, but 400 mg/L is non-substrate limiting to anaerobic processes. (R-66)

E Although phenol was inhibitory without sludge acclimation, once acclimated, the biological systems could achieve almost complete phenol removal. (46) (47) (37) (32) (43) (44)

p-Phenylazoaniline (p-Aminoazobenzene) 60093

E At 500 mg/L chemical was inhibitory. (44)

p-Phenylazophenol 1689823

E Chemical was inhibitory at 500 mg/L; small degree of biological oxidation was observed after variable lag periods. (44)

Phenylcarbylamine chloride 622446

O May plug filters and exchange beds.

(m-,o-,p-)-Phenylenediamine m = 108452 o = 95545 p = 106503

E At 500 mg/L chemicals were toxic during 24 hours aeration. (45)

Phosphorus 32 14596373

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

E Biochemical oxidation was slightly inhibited in domestic sewage at 10 mci/L. Increase in radioactivity level did not increase inhibition. Stable P^{31} form was favored over P^{32} form during oxidation and removal. (59) (62) (23)

Phosphorus, black 7723140

O Will add to sludge volume.

Phosphorus, white (yellow) 12185103

O Chlorination leads to rapid production of phosphoric acid via phosphorous trichloride. (R-59)

Phosphorus oxychloride 10025873

O May reduce pH and interfere with coagulation.

Phosphorus trichloride 7719122

O May reduce pH and interfere with coagulation.

Picric acid 88891

O 50 ppm causes upset in activated sludge which recovers after ten days of acclimation. 200 ppm has irreversible effects. (R-56)

Plutonium 238 7440075

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Plutonium 239 15117483

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Polonium 13981527

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Polyethoxy fatty ester

E At 100 mg/L the synthetic detergent resisted biodegradation. Resistance to biochemical oxidation increased with size of the polyoxylethylene group. (11)

Polyvinyl chloride 9002862

E Wastewaters containing chemical requires pH adjustment and nutrient addition. Oxygen transfer reduced by surface active agents and dispersants. Latex solids cling to biological flocs and cause stickiness and extreme reduction in organic removal. (10)

Potassium(radio-) 14378213

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Potassium arsenate 7784410

O Not acceptable at municipal sewage treatment plant.

Potassium arsenite 10124502

O Not acceptable at municipal sewage treatment plant.

Potassium bichromate 7778509

O 100 ppm reduces oxygen utilization of sewage by 50%.

Potassium chromate 7789006

O 10.5 ppm reduces oxygen utilization of sewage by 50%.

Potassium cyanide 151508

O Oxygen utilization by synthetic sewage was diminished by 50% in 5 days by 15 ppm KCN.

E At 480 mg/L the chemical completely inhibited oxygen consumption. (52)

Potassium hydroxide 1310583

O Will add significantly to sludge volume.

Praseodymium 142 14191641

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Praseodymium 143 14981794

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Praseodymium 144 14119052

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Promethium 147 14380757

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Propanedinitrile (Malonic dinitrile) 109773

E At 500 mg/L the chemical was toxic for up to 74 hours of oxidation. (43)

Propargite 2312358

O As a sulfite, up to 500 mg/kg can be oxidized if system is acclimated, but increased oxygen is required. (I-62)

Propanenitrile (Propionitrile) 107120

E At 500 mg/L the chemical was toxic for at least 72 hours. (43)

n-Propiolactone 57578

O Toxic to most sewage sludges at 2500 mg/L levels.

E At 500 mg/L the chemical resisted biological oxidation for up to 144 hours. (44)

n-Propylbenzene 103651

E At 37.5 mg/L the chemical could be oxidized biologically but depressed oxygen uptake. One of the more toxic benzene derivatives. (29)

Propylene dichloride 78875

O Can plug filters and exchange beds.

Protactinium 233 13981141

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Protactinium 234 15100284

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Pyrethrin I 121211

O Not amenable to biological treatment at a municipal sewage treatment plant.

Pyrethrin II 121299

0 Not amenable to biological treatment at a municipal sewage treatment plant.

Pyridine 110861

0 0.5 ppm has no effect, but 1 ppm inhibits biochemical oxidation. (C-1)

Radium 226 13982633

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Rhenium 186 14998631

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Rhodium 106 14234345

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Rubidium 86 14932537

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Ruthenium 103 13968531

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Ruthenium 106 13967481

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Salicylaldehyde 90028

O May plug filter and exchange columns.

Salicylic acid 69727

O 110 ppm inhibits oxygen uptake of sewage 50%.

Samarium 151 15715943

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Samarium 153 15766004

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Scandium 46 13967630

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Selenium 75 14265715

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Selenium oxide 7446084

O Not removed by biological treatment at municipal sewage treatment plant.

Silver 7440224

O Dosages of 0.000001 to 0.5 mg/L of silver have been reported as sufficient to sterilize water. At such dosage rates, silver is not an irritant, has no toxic action toward humans, and does not interfere with the taste.

Silver 110 14391765

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Silver 111 15760040

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Silver nitrate 7761888

0 0.3 ppm was toxic to sewage organisms.

Sodium 22 13966320

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Sodium 24 13982042

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Sodium arsenite 7784465

0 Not acceptable at sewage treatment plant.

Sodium bifluoride 1333831

0 Amenable to biological treatment at a municipal sewage treatment plant when diluted.

Sodium borate 1333739

0 A 50% reduction of endogenous respiration for sewage treatment plant organisms occurs from 572 to 1000 ppm boric acid. (R-39)

Sodium chromate 7775113

0 1 ppm inhibited sewage organisms 10%.

Sodium cyanide 143339

O 3.6 ppm inhibited sewage organisms 50%. Resistance builds up with time. (C-1)

Sodium dodecylbenzene sulfonate (ABS) 25155300

O 8 ppm inhibits water softening by coagulation. 300 ppm ABS caused the development of reducing flora, resulting in the formation of sulfides; 60 ppm retarded the development of proteolytic bacteria; 15-60 ppm retarded the growth of aerobic bacteria; 150 ppm retarded the growth of denitrifying bacteria. ABS interferes with the uptake of oxygen; ABS compounds are principal agents causing foam. 1 ppm will cause a light froth. ABS concentration (approx., mg/L) at 50% inhibition of O_2 uptake test (organism/medium): Proteus vulgaris/dextrose-bouillion/2500M/20 Puffers medium/220 & glucose; Staphylococcus aureus/dextrose-bouillion/40 M/20 Puffers medium/200 & glucose; Mycobacterium phlei/dextrose-bouillion/40 M/20 Puffers medium/250 & glucose (sic.). When the "exit coefficient" in the absence of detergents was 30 cm/hr, the addition of ABS reduced the rate of entry of oxygen by about 50%. The effect of 1 mg/L of ABS is to decrease the rate of settling of the mud for any given mud concentration. Causes a marked head loss in the performance of rapid sand filters at concentrations >5 ppm.

Sodium fluoride 7681494

O Can sterilize active biota.

Sodium hydrosulfide 16721805

O Amenable to biological treatment at a municipal sewage treatment plant when reduced.

Sodium hydrosulfite 7775146

O Can lower pH and interfere with coagulation.

Sodium hydroxide 1310732

O Can raise pH and interfere with coagulation.

Sodium hypochlorite 7681529

O When in small amounts or diluted, action similar to that of chlorine in water treatment plants.

Sodium oleate 143191

O 3-4 ppm inhibits nitrification.

Sodium palmitate 408355

O 3-4 ppm inhibits nitrification.

Sodium pentachlorophenol (Sodium pentachlorophenate) 131522

E Slug doses greater than 20 mg/L drastically affected performance of biological systems; chemical was not removed and sludge would not settle. System could be acclimated to chemical. (31) (26)

Sodium phosphate, tribasic 7601549

O Amenable to biological treatment at a municipal sewage treatment plant when diluted.

Sodium selenite 10102188

O 500 ppm inhibitory to unacclimated sewage organisms. (R-45)

Sodium stearate 822162

O 3-4 ppm inhibits nitrification.

Sodium sulphate 7757826

0 4000 ppm stops certain fermentation processes.

Sodium thiocyanate 540727

0 1000 ppm pronounced inhibition of sewage digestion. 563 ppm inhibitory to unacclimated sewage organisms. (R-45)

Strontium 85 13967732

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Strontium 87M 13982644

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Strontium 89 14158271

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Strontium 90 10098972

0 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Strontium chromate 7789062

O Low concentrations produce little effect on sewage organisms. A 500 mg/L dose of 4 hour duration may effect the system for as long as 4 days.

Sulfate 14808798

E At greater than 300 mg/L of sulfate was able to corrode concrete even at neutral pH. (46)

Sulfide 18496258

E Chemical was slightly inhibitory at 25 mg/L. (46)

Sulfur 7704349

O Will add considerably to sludge volume.

Sulfur 35 15117530

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Sulfuric acid 7664939

O 58 ppm caused 50% inhibition of sewage organisms. May drop pH to levels too low for coagulation.

Superphosphate 8011765

O Will add greatly to sludge volume.

Tannic Acid 8828

E A 1/120 N solution inhibited oxygen consumption. (15)

Tantalum 182 13982008

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

TDE 72548

O Not significantly degraded, less than 5% of measured chemical oxygen demand was utilized by DDT. (I-62) Not amenable to biological treatment at a municipal sewage treatment plant. (I-66)

Technetium 99 14133767

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Tellurium 132 14234287

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Terbium 160 13981298

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Terephthalic acid 100210

O Amenable to biological treatment at sewage treatment plant when diluted.

Tetraethyl lead 78002

O May plug filters and exchange beds.

Tetraethyl pyrophosphate (TEPP) 107493

O Not significantly degraded. Less than 5% of COD was utilized. Not amenable to biological treatment at a municipal sewage treatment plant. (I-63)

E Insecticide was not significantly degraded. (53)

Tetramethyl lead 75741

O May plug filters and exchange beds.

1,2,4,5 Tetramethylbenzene (Durene[R]) 95932

E After a 3 hour lag period, the chemical was degraded slightly at a concentration of 500 mg/L. (45)

Thallium 204 13968519

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Thallium sulfate 7446186

O Not amenable to biological treatment at a municipal sewage treatment plant.

Thioacetamide 62555

E Oxygen uptake was completely inhibited at 1000 mg/L concentration. (52)

Thiocyanate 302045

E 1000 mg/L concentration significantly inhibited oxygen consumption. (15)

Thioglycolic acid 68111

E At 650 mg/L the chemical was toxic or resistant to biodegradation. (52)

Thiophosgene 463718

O May lower pH too low for good coagulation.

Thiourea 62566

E At 500 mg/L thiourea inhibited oxygen uptake for up to 144 hours. (44)

Thulium 170 13981301

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Tin 113 13966068

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Tin 119 — 14314353

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Titanium 44 — 15749334

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Toluene — 108883

O >0.05% inhibited sewage sludge digestion.

E Greater than 90% removal was eventually achieved by activated sludge, but at 500 mg/L of toluene, oxidation periods longer than 24 hours were required. (9) (33) (44) (47) (29)

(m-,o-,p-)-Toluidine — o = 95534, m = 108441, p = 106490

O May plug filters and exchange beds.

E At 500 mg/L, m- and p-toluidine were slightly oxidized while o-toluidine was toxic. (45)

Trichlorfon — 52686

O May plug filters and exchange columns.

Trichloroethylene — 79016

O 200-1200 mg/kg dry solids reported to affect anaerobic digestion. 330 mg/kg dry solids (3% solids) thought to be safe. (R-176)

Trichlorofluoromethane 75694

O May plug filters or exchange beds.

Trichlorophenol 25167822

O 60 ppm listed as TLM for sewage bacteria.

2,4,5-Trichlorophenol 95954

E Pesticide was slightly degraded. (53)

2,4,6-Trichlorophenol 88062

E Significant inhibition occurred between 10 and 50 mg/L concentration of chemical. (47)

2,4,5-T Amines 2008460

O Not amenable to biological treatment at a municipal sewage treatment plant.

2,4,5-T Esters 93798

O Not amenable to biological treatment at a municipal sewage treatment plant.

2,4,5-TP Acid esters 32534955

O Not amenable to biological treatment at a municipal sewage treatment plant.

2,4,5-T Salts 13560991

O Not amenable to biological treatment at a municipal sewage treatment plant.

Triethanolamine dodecylbenzene sulfonate 27323417

O Amenable to biological treatment at a municipal sewage treatment plant.

Trimethylamine solution 75503

O Eliminate all ignition sources. May be amenable to biological treatment at a municipal sewer treatment plant when diluted.

1,2,4-Trimethylbenzene (Pseudocumene) 95636

E Toxic at 500 mg/L for at least 18 hours of aeration, after which the material was slightly oxidized. (45)

2,4,6-Trinitrotoluene (TNT) 118967

O Above 1 mg/L retards self-purification of waters.

E Better than 50% removal at concentrations from 5 through 25 mg/L with retention times of 3 to 14 hours. (25)

Tungsten 185 14932413

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Tungsten 187 14983483

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Turpentine 8006642

O Will interfere with settling and floc formation. May plug filters and exchange beds.

Uranium 235 15117961

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Uranium 238 7440611

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Uranium peroxide 19525156

O Not amenable to biological treatment at a municipal sewage treatment plant.

Uranyl nitrate 10102064

O Cannot be processed at municipal sewage treatment facility.

Uranyl sulfate 1314643

O Not amenable to biological treatment at a municipal sewage treatment plant.

Urea 57136

E Oxygen consumption inhibited by urea concentrations up to 720 mg/L. (52)

Urethane 51796

E Chemical completely inhibited oxygen consumption. (44)

Vinylidene chloride 75354

O May plug filters or exchange beds.

Xenon 133 14932424

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

m-Xylylbromide 620133

O Can plug filters and exchange beds.

m-Xylene 108383

O 0.1% seriously retarded sewage digestion.

E At 500 mg/L, m-xylene was toxic during first 24 hours of aeration; median toxicity when compared to o- and p-xylene. (45)

o-Xylene 95476

O 0.1% seriously retarded sewage digestion.

E At 500 mg/L, o-xylene was toxic during first 24 hours of aeration; least toxic when compared to m- and p-xylene. (45)

p-Xylene 106423

O 0.1% seriously retarded sewage digestion.

E At 500 mg/L, p-xylene was toxic during first 24 hours of aeration; most toxic when compared with o- and m-xylene. (45)

Yttrium 90 10098916

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Yttrium 91 14234243

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Zinc 7440666

O 1 ppm inhibited sewage organisms 17%. Concentrations above 20 mg/L were found to have a toxic effect on activated sludge. (R-210) Will increase sludge volume. 62.5 ppm Zn will cause 50% reduction in BOD_5. (C-1) 1 ppm stimulates nitrification while 10 ppm is inhibitory. (C-1)

E The lowest concentration which caused a continuous effect was 10 mg/L. At this concentration 89% zinc removal was achieved, primarily by adsorption of zinc to activated sludge. The lowest 4 hour slug dose to cause a 24 effect was 160 mg/L. (46) (12) (58) (5) (57) (48)

Zinc 65 13982393

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Zinc 69 13982235

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Zinc acetate 557346

O Concentrations above 20 mg/L were found to have a toxic effect on activated sludge. (R-210)

Zinc ammonium chloride 52628258

O Greater than 10 mg/L continuous dose affects sewage organisms. A 160 mg/L, 4 hour dose may cause a 24 hour effect at sewage treatment plant.

Zinc borate 1332076

O Greater than 10 mg/L continuous addition affects sewage organisms.

Zinc bromide 7699458

O Greater than 10 mg/L continuous addition affects sewage organisms. A 160 mg/L, 4 hour slug will produce a 24 hour effect at sewage treatment plant.

Zinc carbonate 3486359

O Little effect on water treatment process since a level of 10 mg/L is required for an effect.

Zinc chloride 7646857

O Concentrations above 20 mg/L were found to have a toxic effect on activated sludge. (R-210)

Zinc chromate 13530659

O 1 ppm zinc inhibits sewage organisms 17%, 1 ppm chromate 10%. Presence of zinc will increase sludge volume. 62.5 ppm zinc will cause 50% reduction in BOD5. (C-1) 1 ppm zinc stimulates nitrification while 10 ppm is inhibitory. (C-1) Concentrations above 20 mg/L were found to have a toxic effect on activated sludge. (R-210)

Zinc cyanide 557211

O The lowest continuous dose which caused an effect was 10 mg/L. At this concentration 89% zinc removal was achieved, primarily by adsorption of zinc to activated sludge. The lowest 4 hour slug dose to cause a 24 hour effect was 160 mg/L. (I-62) Chlorine is commonly used to oxidize strong cyanide solutions to produce carbon dioxide and ammonia. (I-02)

Zinc fluoborate 13826885

O 1 ppm zinc inhibited sewage organisms. 17% will increase sludge volume. 62.5 ppm zinc will cause 50% reduction in BOD_5. (C-1) 1 ppm stimulates nitrification while 10 ppm is inhibitory. (C-1) Concentrations above 20 mg/L were found to have a toxic effect on activated sludge. (R-210)

Zinc fluoride 7783495

O Very toxic to humans. A continuous dose of 10 mg/L adversely affects treatment organisms. A 160 mg/L, 4 hour dose may produce a 24 hour effect at sewage treatment plant.

Zinc formate 557415

O Greater than 10 mg/L continuously affects sewage organisms. A 160 mg/L, 4 hour dose may cause a 24 hour effect at sewage treatment plant.

Zinc hydrosulfite 7779864

O Greater than 10 mg/L continuously affects sewage organisms. A 160 mg/L, 4 hour dose may cause a 24 hour effect at a sewage treatment plant.

Zinc nitrate 7779886

O 62.5 ppm inhibits sewage bacteria 50%. Concentrations above 20 mg/L were found to have a toxic effect on activated sludge.

(R-210)

Zinc phenolsulfonate 127822

O Greater than 10 mg/L continuously affects sewage organisms. A 160 mg/L, 4 hour dose may cause a 24 hour effect at a sewage treatment plant.

Zinc phosphide 1314847

O Toxic. Presents a fire hazard at treatment plant. The zinc reaction products will inhibit growth of sewage organisms at concentrations greater than 10 mg/L.

Zinc silicofluoride 16871719

O Greater than 10 mg/L continuously affects sewage organisms. A 160 mg/L, 4 hour dose may cause a 24 hour effect at a sewage treatment plant.

Zinc sulfate 7733020

O 1000 ppm severely inhibited sewage digestion. Above 20 mg/L were found to have a toxic effect on activated sludge. (R-210)

Zirconium 95 13967710

O 1. Possibility of build-up of radioactivity in water treatment sludge or filters. 2. Possibility of build-up of radioactivity in sewage treatment sludge. 3. Possible toxic effect on sewage treatment bacteria.

Zirconium acetate 5153242

O Not amenable to biological treatment at a municipal sewage treatment plant.

Zirconium nitrate 13746899

O Not amenable to biological treatment at a municipal sewage treatment plant.

Zirconium oxychloride 7699436

O Not amenable to biological treatment at a municipal sewage treatment plant.

Zirconium potassium fluoride 16923958

O Not amenable to biological treatment at a municipal sewage treatment plant.

Zirconium tetrachloride 10026226

O Not amenable to biological treatment at a municipal sewage treatment plant.

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APPENDIX A

DATABASE FOR STRUCTURE - ACTIVITY MODELS OF BIODEGRADABILITY

CATEGORY=BIODEGRADABLE COMPOUNDS

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
50840	191.010	50	52	69	97	137												
50997	261.089	37	45	66	73	102	104	110	134	143								
51285	184.120	3	65	97	137													
51365	191.010	50	52	69	97	137												
52934	308.381	6	10	17	30	41												
55210	121.150	30	67	97	137	181												
55221	152.179	69	77	102	104	110	134	143										
56382	180.159	1	3	10	19	36	63	97	137									
56406	75.080	17	30	41														
56417	180.156	6	17	30	41													
56451	299.346	6	17	30	37	41												
56757	323.150	3	17	22	24	28	38	39	97	137	149	151	315					
56815	92.110	6	18	38														
56848	131.131	6	17	30	42													
56860	289.375	6	19	30	42													
57114	284.540	21	41															
57487	189.221	37	45	66	73	132	104	110	134	143								
57501	257.437	38	46	63	66	75	101	102	107	111	135	144						
58899	290.820	50	52	99	112	134	140											
59676	123.120	69	77	102	104	110	134	143										
61905	131.200	18	30	41	148													
62237	167.130	3	69	97	137													
62533	93.140	58	97	137	310													
64175	46.080	19	37															
64186	46.030	41																
64197	354.100	17	41															
66228	239.322	78	86	102	105	110	134	143	188	334								
67630	63.110	6	18	37														
69727	338.413	65	69	97	137													
70304	239.322	45	50	52	66	97	138											
70473	153.823	6	17	31	39	41	150											
71001	268.359	6	30	41	45	78	101	105	110	134	143							
71238	264.356	20	37															
71363	228.294	20	37															
72186	117.170	18	30	41	148													
72435	345.660	6	7	18	22	24	64	97	138	198	315							
73223	204.250	6	30	41	45	77	97	101	104	118	140	143	331					
73325	131.200	17	19	30	41	148												
74113	214.247	50	51	69	97	137												
75070	373.950	17	39															
75570	109.620	9	18															
77929	192.140	7	18	37	42													
78308	307.195	1	5	46	64	97	139	172										
78319	145.161	1	5	45	64	97	139	172										
78320	190.138	1	5	46	64	97	139	172										
78922	74.140	6	17	19	37													
79094	74.090	19	41															
84662	222.260	19	72	97	137													
84695	59.068	18	19	72	97	137	148											
84742	229.257	20	72	97	137													
84764	418.680	20	72	97	137													

DATABASE FOR STRUCTURE - ACTIVITY MODELS OF BIODEGRADABILITY

--- CATEGORY=BIODEGRADABLE COMPOUNDS ---

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
85416	147.140	77	86	97	101	104	118	134	140	143	189	331						
85472	214.203	4	10	37	97	114	134	141	331									
85687	312.390	45	69	71	97	138												
87592	121.200	46	58	97	137	310												
87650	163.000	50	52	65	97	137												
87694	124.158	38	42	148														
87865	93.129	50	52	65	97	137												
88062	197.440	50	52	65	97	137												
88722	137.150	3	45	97	137													
88755	139.120	3	65	97	137													
88993	166.140	70	97	137														
89781	156.300	6	18	45	65	99	112	134	140									
89838	153.240	6	18	45	65	97	137											
90028	122.123	65	67	97	137													
90153	110.131	65	97	114	134	141	331											
90437	252.101	65	97	130	138													
90960	58.080	18	64	67	97	138	198											
90982	251.110	50	52	67	97	138												
91010	231.255	6	37	97	138													
92875	184.260	59	97	130	134	180	310											
93629	178.190	8	18	19	37	42												
93721	269.510	6	17	41	50	52	63	97	137	172								
93765	255.480	17	41	50	52	63	97	137	172									
94757	221.040	17	41	50	52	63	97	137	172									
95487	108.150	45	65	97	137													
95512	127.580	50	51	58	97	137	310											
95534	107.170	45	58	97	137	310												
95556	109.140	58	65	97	137	310												
95647	121.200	46	58	97	137	310												
95658	122.180	46	65	97	137													
95783	121.200	46	58	97	137	310												
95863	124.160	59	65	97	137	310												
95874	122.180	46	65	97	137													
95954	44.053	50	52	65	97	137												
96413	163.834	65	98	112	134	140												
97187	356.040	10	50	52	66	97	138											
97234	269.130	45	50	52	66	97	138											
97994	102.150	37	45	73	101	104	110	134	143									
98000	98.110	37	45	73	101	104	110	134	143									
98011	96.090	67	73	101	104	110	134	143										
98113	158.180	4	10	37	97	137												
98679	137.025	4	10	37	65	97	137											
98691	112.987	4	10	37	47	97	137											
98953	123.120	3	97	137														
99047	136.160	45	69	97	137													
99058	137.150	58	69	97	137	310												
99081	137.150	3	45	97	137													
99503	267.155	66	69	97	137													
99616	151.130	3	67	97	137													
99990	137.150	3	45	97	137													
100027	139.120	3	65	97	137													

DATABASE FOR STRUCTURE - ACTIVITY MODELS OF BIODEGRADABILITY

CATEGORY=BIODEGRADABLE COMPOUNDS

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
100196	240.214	3	17	67	97	137												
100210	166.140	70	97	137														
101531	295.336	45	65	97	138													
101815	168.250	45	97	138														
103231	399.966	18	19	20	44	148												
103822	344.060	41	45	97	137													
103844	178.234	17	39	56	97	137	182	310										
104018	166.190	17	41	45	63	97	137	198										
104154	172.210	4	10	37	45	97	137											
105602	169.227	77	85	103	104	110	134	143	189	322	325							
105679	122.180	46	65	97	137													
106490	197.170	45	58	97	137	318												
106503	108.160	59	97	137	310													
107153	69.120	19	31															
107211	236.337	19	38															
107642	255.484	2	8	18	21													
107926	88.120	20	41															
107937	197.156	14	17	19	41													
107948	139.530	19	22	23	41	315												
108394	108.150	45	65	97	137													
108429	127.580	50	51	58	97	137	310											
108441	107.170	45	58	97	137	310												
108452	108.160	59	97	137	310													
108463	110.120	66	97	137														
108736	126.120	66	97	137														
108930	100.180	65	99	112	134	140												
108941	98.160	85	99	112	134	140												
109977	67.100	77	101	104	110	134	143											
110156	258.104	19	42															
110270	270.510	6	18	21	43													
110338	183.250	.	44															
110543	86.200	20																
110634	151.165	20	38															
110894	85.170	77	102	104	110	134	143											
111422	105.160	19	28	38														
111466	106.140	19	35	38														
112005	80.514	2	9	18	21	149												
112027	53.064	2	9	18	21	149												
112038	348.130	2	8	18	21													
112538	186.380	21	37															
112618	298.570	17	21	43														
115322	108.144	7	22	24	37	50	52	97	138	315								
115866	326.3)	1	5	64	97	137	172											
117817	390.620	18	19	20	72	97	137	148										
117840	76.099	20	72	97	137													
118923	137.150	58	69	97	137	310												
119368	187.056	17	65	71	97	137												
119619	182.230	67	97	138														
120729	370.490	77	97	101	104	118	134	140	143	331								
120809	119.120	66	97	137														
120832	361.784	50	52	65	97	137												

DATABASE FOR STRUCTURE - ACTIVITY MODELS OF BIODEGRADABILITY

-- CATEGORY=BIODEGRADABLE COMPOUNDS --

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
120923	86.130	85	98	112	134	140												
121573	227.132	4	10	37	58	97	137	310										
121915	166.140	70	97	137														
121926	167.130	3	69	97	137													
122189	330.358	2	9	18	21	45	97	137	149									
122190	424.230	2	9	18	21	45	97	137										
122349	201.661	19	50	51	57	78	102	106	110	134	143							
122429	179.240	6	18	43	56	97	137	310										
122805	150.200	17	39	56	58	97	137	182	310									
123308	109.140	58	65	97	137	310												
123319	110.120	66	97	137														
123728	72.120	20	39															
124185	142.320	21																
126738	202.256	1	5	20	36													
127173	238.246	17	39	41														
131113	239.246	18	72	97	137	167												
131706	289.328	20	69	71	97	137												
134850	291.306	50	51	67	97	138												
135193	144.180	65	97	114	134	141	331											
139082	143.189	2	9	18	21	45	97	137	149									
139139	240.432	8	18	42														
140727	305.802	2	49	77	102	104	110	134	143	149								
142621	116.180	20	41															
142734	133.120	18	28	42														
142916	298.570	6	18	21	43													
143077	200.360	21	41															
144627	90.040	42																
147853	115.132	69	77	101	104	110	134	143										
145675	144.240	6	19	20	41													
149917	173.130	66	69	97	137													
150130	137.150	58	69	97	137	310												
151326	216.241	20	44															
151417	266.440	4	10	31	35	37												
156987	276.338	41	45	65	97	137												
288324	68.090	78	101	105	110	134	143											
301008	216.283	1	15	17	20	43												
309002	364.900	50	52	98	115	127	129	134	142									
334485	172.300	20	41															
445294	149.120	50	54	69	97	137												
452868	233.090	45	66	97	137													
455389	249.097	50	54	69	97	137												
456224	304.349	50	54	69	97	137												
488175	142.029	45	66	97	137													
490799	117.108	66	69	97	137													
499069	239.274	46	69	97	137													
503640	240.350	14	17	19	34	41												
507700	154.280	46	65	98	127	134	141											
526750	122.160	46	65	97	137													
530483	145.162	6	14	17	97	138												
531759	359.573	37	45	61	66	75	85	97	102	107	113	118	135	140	144	331		
535808	73.099	50	51	69	97	137												

-- CATEGORY=BIODEGRADABLE COMPOUNDS --

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
544763	226.231	21																
552169	167.130	3	69	97	137													
552896	151.133	3	67	97	137													
554847	139.120	3	65	97	137													
555168	151.130	3	67	97	137													
563042	265.363	1	5	46	64	97	139											
563122	114.144	1	11	17	19	36												
567180	270.240	4	10	37	65	97	114	134	141	331								
574005	129.159	66	97	114	134	141	331											
576261	122.180	17	22	26	45	65	97	137	315									
585762	112.084	50	53	69	97	137												
586765	328.346	50	53	69	97	137												
589924	307.324	45	85	99	112	134	140											
591275	109.143	58	65	97	137	310												
610355	226.231	65	70	97	137													
611201	145.161	8	62	65	97	137	210	310										
611949	173.171	17	63	67	97	138	172	198										
612000	90.082	6	17	97	138													
618417	256.213	5	10	37	97	137												
618519	199.207	50	55	69	97	137												
619045	182.135	46	69	97	137													
619089	173.563	3	50	51	65	97	137											
629594	143.189	21																
645921	145.161	59	78	85	102	106	110	134	143									
767000	132.119	8	62	65	97	137	210	310										
831812	211.268	45	50	51	97	138												
834128	227.370	6	10	18	19	57	78	102	106	110	134	143						
873621	186.377	8	62	65	97	137	210	310										
931179	213.664	66	99	112	134	140												
947911	196.269	6	39	97	139													
993135	317.322	1	17	35	38													
1002842	242.453	21	41															
1120361	117.108	14	17	21														
1124396	72.063	47	66	97	137													
1137424	171.112	65	67	97	138													
1197553	142.118	41	43	58	97	137	310											
1241947	157.131	1	5	6	17	19	20	35	64	97	138	172						
1610179	211.310	6	18	19	57	63	78	102	106	110	134	143	198					
1698608	221.660	50	51	58	78	95	97	102	105	110	130	134	137	143	310	334		
1817749	302.333	3	45	97	138													
1832548	277.314	1	5	6	19	35	37											
1951128	122.567	6	18	22	23	41	315											
2041147	213.107	1	5	19	30	38	175											
2138229	333.231	50	51	66	97	137												
2212671	187.330	10	19	67	77	103	104	110	134	143	322							
2528361	239.274	1	5	20	36	63	97	137	172									
2620533	312.277	17	28	50	51	71	97	137										
2689432	328.275	8	18	39	50	52	63	67	97	134	193	198	209	310				
2785543	254.183	2	49	77	102	106	110	134	143	149								
3055965	308.375	19	21	36	37													
3055956	46.091	19	21	36	37													

DATABASE FOR STRUCTURE - ACTIVITY MODELS OF BIODEGRADABILITY

-- CATEGORY=BIODEGRADABLE COMPOUNDS --

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
3055967	335.282	19	21	36	37													
3055978	225.182	19	21	36	37													
3055990	217.271	19	21	36	37													
3115284	234.246	6	20	41														
3134121	337.220	8	18	39	50	52	67	97	138	152	310							
3274280	318.543	6	20	41														
3648202	442.800	21	72	97	137													
3648213	331.966	20	72	97	137													
4408644	206.094	8	18	42														
4536236	203.348	6	17	20	41													
4536305	253.753	19	21	35	37													
5254126	248.448	1	5	45	64	97	139	172										
6213907	147.305	6	14	18	22	23	41	315	317									
6214284	377.311	6	14	18	22	23	41	315	317									
6779095	260.124	1	5	19	38	175												
7305615	239.746	1	5	19	35	37												
10374740	290.276	14	20															
13113434	234.299	8	18	39	50	51	67	97	138	152	310							
13138335	555.282	1	5	20	30	38	175											
13673922	310.180	50	52	66	97	137												
14697484	268.276	20	44															
15592742	253.349	4	10	37	48	97	137											
16045924	122.019	6	17	22	23	42	315											
16066356	242.321	4	6	10	18	37	97	137										
17109498	329.374	1	5	11	19	35	97	138										
17345618	193.246	8	62	66	97	137	210	310										
17495497	243.309	8	18	28	39	50	52	97	137	209	310							
18435228	239.274	6	17	19	21													
18521590	207.616	4	10	37	48	97	137											
21964498	109.943	15	18	21														
25354921	282.298	6	17	21	41													
27697514	230.242	2	9	18	19	149												
32815535	354.472	6	20	21	41													
33374286	392.942	19	20	35	72	97	137											
34123596	207.273	6	8	18	39	56	97	137	209	310								
38775223	185.619	4	11	15	38	46	97	130	139	180								
38945276	118.096	6	18	35	42													
39156495	161.121	4	10	37	49	97	137											
52435151	178.187	5	8	11	14	17	19	38	46	57	80	97	102	109	116	139	145	310
55203128	189.175	6	17	35	42													
59957505	339.218	1	5	19	28	30	38	39	151	175								

CATEGORY=NONBIODEGRADABLE COMPOUNDS

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
67663	119.373	6	22	24	315													
67685	123.111	5	10	18														
68122	278.329	8	18	39	152													
72548	320.040	22	24	50	52	97	138	148	315									
72559	318.020	14	22	24	50	52	97	138	148	315								
75014	62.500	14	18	22	23													
78433	430.910	1	5	18	22	24	36	148	315									
83056	183.182	6	41	50	52	97	138											
88744	134.140	3	58	97	137	310												
90971	119.379	6	37	50	52	97	138											
92240	134.122	97	115	134	142	331												
95147	119.149	78	97	101	106	118	134	140	143	331								
99650	168.120	3	97	137														
100254	168.120	3	97	137														
104030	166.223	3	41	45	97	137												
117340	157.015	6	41	97	138													
119562	373.496	6	37	50	51	97	138											
119799	223.260	4	10	37	58	97	114	134	141	310	331							
121471	173.200	4	10	37	58	97	137	310										
121540	448.150	2	7	9	18	19	35	45	63	97	138							
126863	267.240	7	16	18	38	148												
136958	150.210	58	77	81	97	101	105	118	134	140	143	310	331					
149304	167.250	10	77	81	97	101	105	118	134	140	143	331						
194592	267.343	77	97	101	104	115	119	134	142	143	331							
198550	252.316	97	115	129	134	142	331											
217594	228.300	97	115	134	142	331												
329715	184.120	3	65	97	137													
333415	196.209	1	6	10	18	19	36	45	63	78	102	105	110	134	143	334		
366187	364.914	79	102	107	111	130	135	144										
574425	60.100	35	97	139	148													
605027	384.475	97	114	130	134	137	141	331										
609198	197.440	50	52	65	97	137												
609994	323.827	3	65	69	97	137	199											
615214	165.230	30	55	77	81	97	101	105	118	134	140	143	195	310	331			
615225	75.067	10	17	77	81	97	101	105	118	134	140	143	331					
620928	200.250	45	66	97	138													
622479	193.249	41	46	97	137													
728870	193.249	6	18	37	64	97	138	172	198									
751382	159.108	97	114	130	134	139	141	331										
778223	130.191	7	18	97	138													
941571	103.081	4	10	37	77	31	97	101	105	118	134	140	143	331				
1562932	223.319	61	69	97	138	204												
1883325	365.964	6	17	37	97	138												
1926803	244.293	17	20	30	43	149												
2008584	171.156	30	50	52	67	97	137	181										
2051243	213.307	50	52	97	130	138	180	318										
2971224	205.600	6	7	22	24	97	138	315										
3026662	262.308	2	49	77	102	104	110	134	143	149								
3724525	353.282	70	98	112	134	140												
3905644	215.688	7	18	97	114	134	141	331										
4901513	231.880	50	52	65	97	137												

DATABASE FOR STRUCTURE - ACTIVITY MODELS OF BIODEGRADABILITY

CATEGORY=NONBIODEGRADABLE COMPOUNDS

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
5743975	234.299	99	115	134	142													
7508681	367.310	19	61	71	97	138	204											
10275588	257.336	7	18	97	114	134	141	331										
10450698	349.063	2	9	14	18	20	149											
17304620	320.366	45	77	78	81	85	97	101	108	110	118	130	135	140	144	331		
18101581	179.219	4	10	30	58	77	81	97	101	105	118	134	140	143	162	310	331	
19218781	350.583	4	10	17	37	61	63	97	138	190	198							
38380023	497.114	50	52	97	130	133	180	315										
52712046	226.279	50	52	97	130	138	180	318										
65644511	251.665	3	69	77	81	97	101	105	118	130	134	137	140	143	331			

DATABASE FOR STRUCTURE - ACTIVITY MODELS OF BIODEGRADABILITY

CATEGORY=NONBIODEGRADABLE COMPOUNDS/QUALIFIED

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
56893	156.056	11	18	31	42	148												
74840	30.080	19																
74986	44.110	20																
75218	44.060	73	103	104	110	134	143	321										
75285	58.140	6	18															
75854	88.170	7	18	19	37													
78784	72.170	6	18	19														
79298	86.200	13	148															
84866	223.260	4	10	37	58	97	114	134	141	310	331							
89861	154.184	66	69	97	137													
90517	211.114	4	10	37	58	65	97	114	134	141	310	331						
90642	152.160	6	37	41	97	137												
93072	436.907	18	64	69	97	137	167	198										
93583	136.160	17	71	97	137	167												
96731	128.990	6	18	22	24	37	315											
98066	134.240	7	18	97	137													
99627	200.256	19	97	137	148													
100185	240.262	19	97	137	148													
100970	333.274	83	102	109	123	129	134	145										
103742	240.214	37	47	77	102	104	110	134	143									
106923	114.160	14	17	19	35	65	73	103	104	110	134	143	321					
106978	58.140	20																
107028	56.073	16	18	39														
107119	57.110	14	17	19	30													
107197	56.070	16	17	19	37													
107700	130.210	7	18	35	39	167												
107880	90.140	6	17	19	38													
109706	313.149	20	22	23	25	315												
110930	92.525	6	14	18	20	39												

-- CATEGORY=NONBIODEGRADABLE COMPOUNDS/QUALIFIED --

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
111671	98.960	14	19	20														
110321	84.162	4	11	38	65	97	114	134	141	331								
123342	132.193	6	14	18	19	35	38											
124027	97.180	15	18	19	28													
126330	120.180	4	81	101	104	110	134	143										
150765	124.150	17	63	65	97	137	198											
287923	70.150	99	112	134	140													
303388	81.078	66	69	97	137													
513859	90.143	19	38	148														
544252	92.150	100	112	134	140													
565593	137.025	18	19	148														
569642	364.751	2	6	8	9	15	18	69	97	99	112	134	138	140	310			
577559	162.300	18	97	137	148													
584032	90.143	6	17	19	38													
586389	152.160	17	63	69	97	137	198											
589344	376.950	6	17	19	20													
589435	185.249	18	19	148														
589902	112.243	46	99	112	134	140												
591219	211.217	46	99	112	134	140												
611734	150.143	41	67	97	137													
669909	143.189	17	39	39	41	149												
1460168	195.265	69	100	112	134	140												
1678928	158.245	48	99	112	134	140												
2396614	203.348	20	35	38														
2437798	122.142	53	52	97	130	139	180	318										
2461156	165.192	6	17	19	20	35	45	73	103	104	110	134	143	321				
2815589	172.014	46	98	112	134	140												
3033770	294.353	2	9	18	45	71	103	104	110	134	143	149	321					
4316421	229.715	48	78	101	105	110	134	143										
4441638	220.055	41	48	99	112	134	140											
4602840	290.750	15	18	19	20	37	148											
4904614	188.657	100	112	134	140													
5292217	142.229	41	45	99	112	134	140											
5617414	206.267	48	99	112	134	140												
6225101	287.337	17	20	28	39	151												
7098228	229.235	21																
10264296	350.477	20	28	39	151													
15968055	195.221	53	52	97	130	133	180	318										
22352563	282.298	14	18	20	41	148												
32598100	227.267	50	52	97	130	138	180	318										
32598133	435.568	50	52	97	130	138	180	318										
33146451	248.194	50	52	97	130	138	180	318										
37680732	216.195	50	52	97	130	138	180	318										
39485831	195.265	50	52	97	130	138	180	318										
55702459	69.491	50	52	97	130	138	180	318										

APPENDIX B

FRAGMENTS AND THEIR MEANING

The fragment code consists of four parts:

1) the original CROSSBOW fragment code, Keys 1-149
2) additional codes developed especially for Genesee by Fraser-Williams, Keys 150-304
3) keys developed to implement FDA's Animal Health substructures which may be related to carcinogenicity, Keys 305-334 in Appendix B1
4) keys developed from specific features of carcinogens and non-carcinogens, Keys 335-336

APPENDIX B1

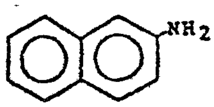
A CATALOGUE OF SUBSTRUCTURAL MOIETIES REQUIRED FOR THE ACTIVITY OF CHEMICAL CARCINOGENS. A GUIDE FOR PREDICTING POTENTIAL NEW CARCINOGENS ON THE BASIS OF MOLECULAR STRUCTURE

1. Aromatic Amino-, Amido-, Hydroxylamino-, Nitroso-, Azo-, Azoxy-, Nitro-

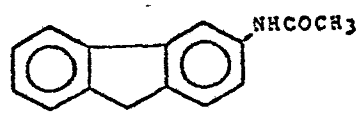
Ar-N(|)-   Ar-N(|)-C(O)-   Ar-N(|)-OH   Ar-N=O

Ar-N=N-   Ar-N(→O)=N-   Ar-N(→O)=O

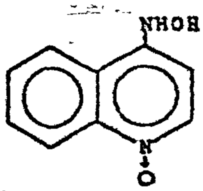
Examples with known activity:



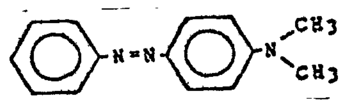
2-Naphthylamine



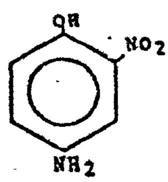
2-Acetylaminofluorene



4-Hydroxylaminoquinoline-1-oxide



4,4-Dimethylaminoazobenzene



4-Amino-2-nitrophenol

MECHANISM: Cellular metabolism is necessary for activity. The best evidence indicates that the hydroxylamino compounds are proximate carcinogenic forms. All of the above functional groups are related by oxidation state and can be converted to hydroxylamines by hydrolases, oxidases or reductases endogenous to most tissues.

COMMENTS: Aromatic nucleus, Ar-, can potentially be any type, including heterocyclic aromatics like furan, quinoline, etc. Carcinogenic potency depends dramatically upon the number of fused or conjugated aromatic rings. Two or more conjugated rings, together with nitrogen substitution at terminal carbon atoms of the longest conjugated chain (para principal), virtually ensure high activity. Monocyclic derivatives usually have lower or no activity. However, they are not exempt from consideration. Recent testing indicates that ring substitution by alkyl-, hydroxyl-, alkoxyl- or amino-groups enhances the potential carcinogenic activity of monocyclic aromatic nitrogen compounds.

2. N-Nitroso-

```
-N-N=O      -N-N=O      -N-N=O
 |           |           |
-CH         -C=O        O=S=O
```

Examples with known activity:

```
CH3                      CH3
|                        |
N-N=O                    N-N=O
|                        |
CH3                      C=NH
                         |
                         NHNO2
```

N-Nitrosodimethylamine (DMN) — N-Methyl-N'-nitro-N-nitrosoguanidine (MNNG)

MECHANISM: For N-nitrosylated secondary amines metabolic activation is necessary. The best evidence indicates that alpha-carbon atom hydroxylation of an alkyl group is a prerequisite to the expression of carcinogenic potential. The fact that N-nitrosodiphenylamine is not carcinogenic is consistent with this model. For N-nitroso compounds derived from ureas, urethanes, carbamates, carboxylic amides and guanidines direct action without prior metabolism is the most likely mode of action.

COMMENTS: There is a relatively high correlation between the presence of an N-nitroso moiety and the capability of a compound to induce cancer. There may be exceptions due to structural prevention of metabolic activation, but these are likely to be few in number. All N-nitroso compounds should be viewed with extreme caution.

3. Organohalogens

a) Mustards

$-N-(CH_2CH_2X)_2$ $-O-S(O)-O-CH_2CH_2X$ $S-(CH_2CH_2X)_2$

b) Di- to polyhalogenated alkanes and cycloalkanes

```
-C-C-     -C-C-X     -CX3
 | |         |
 X X         X
```

c) Alpha-halogenated ethers

-C-O-C-X

d) Halogenated alkenes

```
-C=C-X     -C-C=C-C-X
            |
            X
```

e) Polyhalogenated aromatics

Examples with known activity:

a) CH_3-N-(CH_2CH_2-Cl)$_2$, bis(2-chloroethyl)methylamine, "HN2"

b) CCl_4, carbon tetrachloride

```
-C-C-Br, 1,2-dibromoethane
 |
 Br
```

Mirex

c) Cl-CH_2-O-CH_2-Cl, bis(chloromethyl) ether

d) HC=CH-Cl, vinyl chloride

```
HC=CH-C=CH, chloroprene
      |
      Cl
```

e) Polychlorinated biphenyls, "PCBs"

MECHANISM: Mustards, haloethers and some haloalkanes are alkylating agents. They are thought to be direct acting carcinogens and not need any metabolic alteration for activity. The mechanisms of action for other subclasses of organohalogens have not been well studied. Enzymic epoxidation has been suggested as required for chlorinated alkenes and free radical pathways have been postulated for 1,1,1-trihaloalkanes.

COMMENTS: This is a very diverse group of compounds, none of which, with the possible exception of the mustards, are highly tumorigenic. Prediction of carcinogenic activity is made difficult by the lack of knowledge of metabolism and mechanism of action of these compounds. There appears to be a direct relation between the number of halogens and carcinogenicity, particularly with saturated compounds. But, the fact that methyl iodide is a confirmed carcinogen indicates that this notion is not necessarily reliable. The case for the carcinogenicity of polyhalogenated aromatics is quite weak at this time.

4. Hydrazo-(Hydrazino-), Azoxy- and Azo-

-NHNH- $-NH_2$ $-\overset{O}{\overset{\uparrow}{N}}=N-$ -N=N-

Examples with known activity:

$Ar-CH_2NHNHCH_3$, 1-methyl-2-benzylhydrazine

$n-C_6H_{13}CH=CH-\underset{O}{\underset{\downarrow}{N}}=N-\underset{\underset{CH_3}{|}}{\underset{CH-OH}{|}}{CH}CH_2-O-CH_3$, elaiomycin

$CH_3CH_2-N=N-CH_3$, azoethane

MECHANISM: Metabolic activation is considered to be necessary. The best evidence indicates that N-hydroxylation and a series of other oxidations are prerequisite for activity.

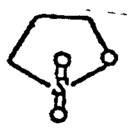
COMMENTS: This class of compounds, particularly the hydrazines, has many members which are carcinogenic. The presence of these substructural moieties gives a compound a high possibility of carcinogenic activity.

5. Alkyl (Aryl) sulfates, sulfonates and sultones

$-S(O_2)-O-$ $-O-S(O_2)-O-$

Examples with known activity:

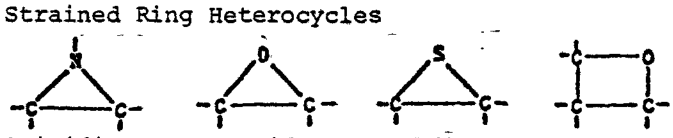
$CH_3CH_2-O-S(O_2)-O-CH_2CH_3$, diethyl sulfate


, 1,3-propanesultone

MECHANISM: Classic alkylating agents, these are direct acting carcinogens requiring no prior metabolism.

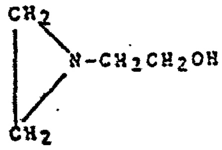
COMMENTS: Carcinogenic activity is greater for gamma-sultones than for delta-sultones, presumably due to more strain, and, hence, higher reactivity of the 5-membered ring compounds.

6. Strained Ring Heterocycles

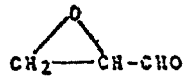


Aziridines Epoxides Sulfides Oxetanes

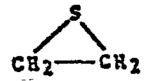
Examples with known activity:



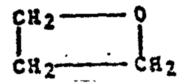
Aziridine ethanol



Glycidaldehyde



Ethylene sulfide

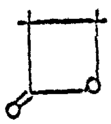


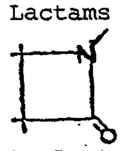
Oxetane

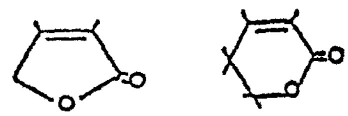
MECHANISM: These are direct acting carcinogens. They are moderately reactive compounds owing to ring strain and are considered to be "alkylating" agents.

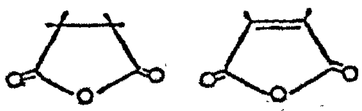
COMMENTS: Compounds containing these moieties are not potent carcinogens. There are many epoxides for which no tumorigenic activity has been found. Thus, the ability to predict activity is somewhat limited with compounds containing these moieties.

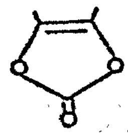
7. Reactive Lactones, Lactams and Anhydrides

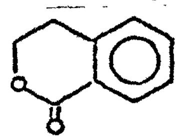

beta-Lactones


beta-Lactams

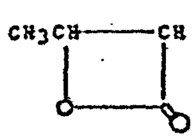

alpha,beta-Unsaturated Lactones


Anhydrides

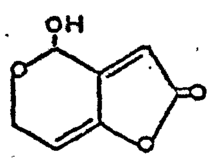

alpha,beta-Unsaturated Carbonates


alpha,beta-Fused Aromatic Lactones

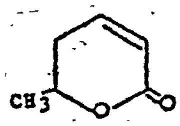
Examples with known activity:



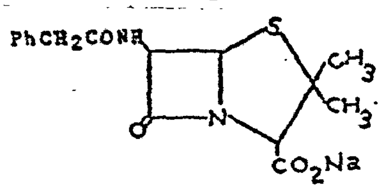
beta-Butyrolactone



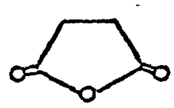
Patulin

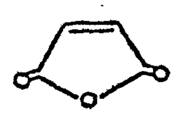


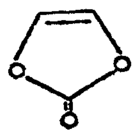
Parasorbic Acid



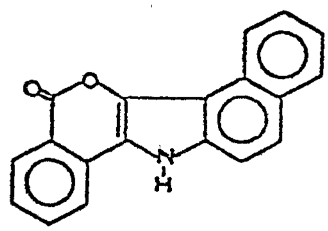
Penicillin G


Succinic Anhydride


Maleic Anhydride



Vinylene Carbonate



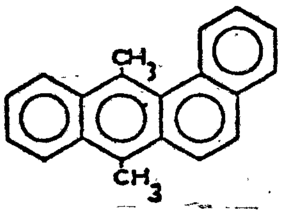
5-Oxo-5H-benzo(e)isochromene-(4,3-b)-indole

MECHANISM: All of these subclasses of compounds are thought to represent direct acting carcinogens.

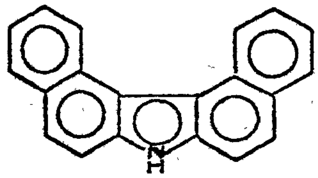
COMMENTS: The aflatoxins and related compounds which could be classified as alpha,beta-unsaturated lactones (6-membered ring) are now thought to need metabolic activation via epoxidation of the furan double bond for their carcinogenic potency. This, however, does not preclude the possibility that the lactone moiety is necessary for their activity.

8. Fused Polynuclear Aromatics

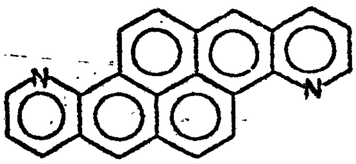
Examples with known activity:



7,12-Dimethylbenz(a)anthracene



7H-Dibenzo(c,g)carbazole



4,11-Diazadibenzo(b,def)chrysene

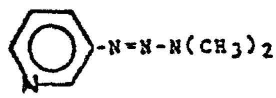
MECHANISM: The best evidence indicates that these aromatic compounds require metabolism for activity. Epoxidation of aromatic ring double bonds is the best candidate for the metabolic pathway leading to ultimate carcinogenic forms.

COMMENTS: Structure-activity is very subtle in this group of compounds. Even slight changes in structure can dramatically change carcinogenic potency. In spite of many years of study no simple reliable models of prediction are available. Any compound that contains three or more fused aromatic rings must be considered suspect, including those with nitrogen and even sulfur containing heterocyclic aromatic residues. Compounds based on the phenanthrene substructure are more often carcinogenic than those containing the linear anthracene moiety. The fact that quinoline has been reported to be carcinogenic, and several derivatives mutagenic, suggests that two fused rings are enough to produce an active compound if N-heterocyclic aromatic rings are involved. Recent epidemiologic data suggest that benzene may be weakly carcinogenic to humans. This notion has not been confirmed in animal studies, however, and the distinct possibility that workers were exposed to impurities (polynuclear hydrocarbons?) has not been ruled out.

9. Aryldialkyltriazenes

Ar-N=N-N-

Example with known activity:

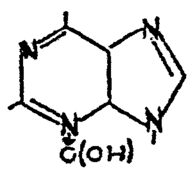


1-(3-Pyridyl)-3,3-dimethyltriazene

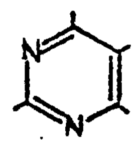
MECHANISM: Both non-metabolic and metabolic pathways have been proposed for the critical reactions responsible for inducing cancer.

COMMENTS: The Ar- can be either substituted phenyl or pyridine rings. Other aromatics may also be active.

10. Purine and Pyrimidine Analogues

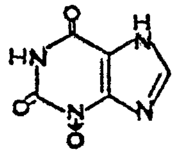


Purine N-Oxides or N-Hydroxides

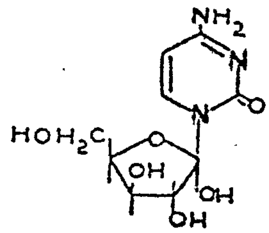


Substituted Pyrimidines

Examples with known activity:



Xanthine-3-oxide



1-beta-p-Arabinofuranosyl-cytosine

MECHANISM: The purine-N-oxides are tautomeric forms of N-hydroxy purines. These hydroxylamines are thought to act similarly to other aromatic hydroxylamines. The mechanism of action of carcinogenic pyrimidine analogues is unknown. Most speculation about their activity centers around their ability to inhibit pyrimidine metabolism or perturb template function.

COMMENTS: The highest potency analogs are the purine-3-oxides. Some purine-1-oxides are also active, but to lesser degrees.

11. Thioamides

$$-\underset{\underset{S}{\|}}{C}-\underset{|}{N}-$$

Examples with known activity:

$CH_3-\underset{\underset{S}{\|}}{C}-NH_2$	$H_2N-\underset{\underset{S}{\|}}{C}-NH_2$
Thioacetamide	Thiourea

12. Carbamates

$$-O-\underset{\underset{O}{\|}}{C}-\underset{|}{N}-$$

Examples with known activity:

$$CH_3CH_2-O-\underset{\underset{O}{\|}}{C}-NH_2$$

Urethane

MECHANISM: N-Hydroxylation has been suggested as required for activity.

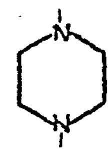
COMMENTS: Esters of carbamic acid other than ethyl have significantly reduced carcinogenic activity. On the other hand, alkyl and aryl substitution on nitrogen does not necessarily reduce or eliminate activity.

13. Amino- and Amido- Compounds Which Can Be Nitrosylated to Active Nitroso- Compounds

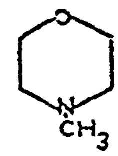
Examples with known activity:

$H_2N-\overset{\displaystyle O}{\overset{\|}{C}}-NHCH_3$

N-Methylurea



Piperazine



N-Methylmorpholine

MECHANISM: N-Nitroso compounds are synthesized from 2° amines, 3° amines and amides in the presence of sodium nitrite, directly in the gut, and in solutions containing animal and human gastric juice. In addition, intestinal bacteria with nitrate reductase activity have been shown to promote the nitrosation of amines in the presence of sodium nitrate, a phenomenon which has been confirmed in vivo in the human gut using diphenylamine and sodium nitrate. Dealkylation of 3° amines followed by nitrosation has been shown to take place in the presence of nitrite in neutral or mildly acidic medium, which indicates that 3° amines and quaternary ammonium salts, in addition to 2° amines, have to be considered as candidates for nitrosation in vivo.

COMMENTS: In some cases chronic feeding of sodium nitrite and amines or amides has lead to the increased incidence of several types of tumors in rodents when the amines or amides used were precursors of known carcinogenic nitroso- compounds. Amines or amides which did not produce cancer under these conditions were claimed to have slow rates of nitrosation. Methylation of liver nucleic acid was found after oral administration of nitrite and dimethylamine, but not with dimethylamine alone, strongly indicating migration of nitrosamines formed in the gut to other organs.

GENERAL COMMENTS: Apart from structural considerations, any chemical compound which displays known reactivity to nucleophilic agents, particularly nucleophilic sites in proteins or nucleic acids, should be considered a possible carcinogen. These direct acting carcinogens, the so-called "alkylating" and "acylating" agents, rarely, however, have potent activity, perhaps because their intrinsic reactivity hinders their reaching appropriate cellular targets. Intracellular metabolism of unreactive procarcinogens to reactive compounds nearer crucial cellular targets is probably why metabolic activation appears to be necessary for most of the more potent carcinogens. Of course, this makes prediction of carcinogenicity of the procarcinogen much more difficult and emphasizes the need for knowledge about metabolism of compounds by tissue.

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APPENDIX B2

CROSSBOW FRAGMENTS AND THEIR MEANING

The CROSSBOW fragment screen is described in "The CROSSBOW Handbook: A Guide for Users and Potential Users of the CROSSBOW System" by P.A. Chubb and D.R. Eakin. This section from that document has been included to give users a brief description of the fragments. In this guide the fragments are divided into groups and the method of identification from the WLN is briefly discussed.

(a) All parts of the Molecule

(1) Atoms other than C,H,O,N,S or halogens.

Character sequence -aa- or the character B (not ▽B) or the character P (not ▽P) found anywhere in the molecule, or the sequence -E-, -F-,-G-,-I- found in a ring.

(2) Positive charge.

Character sequence ▽&Q▽ indicating quarternary salt present, at end of true WLN notation.

(b) All non-cyclic parts of the Molecule

Character sequences must be outside ring signs.

(3) Branching terminal nitro-group - NO2.

The character sequence NW(or WN at the start of the notation).

(4) Dioxo (excluding NO_2).

The character sequence W but not NW or WN. Any substituent W found within ring signs is also included here.

(5) Terminal oxygen (not carbonyl).

The character sequence O& or O▽, or the letter O starting the notation.

(6) One 3-branch carbon atom.

The character Y (but not ▽Y) occurring once only.

Note: More than 1 3-branch carbon is fragment 148.

(7) 4-branch carbon atom.

The character X (but not ▽X).

(8) 3-branch nitrogen atom.

The character N, but not ▽N or NW or WN or NU or UN. This definition also includes unusual conditions of nitrogen, e.g. in cyanide, isocyanide, etc.

(9) Greater than 3-branch nitrogen atom.

The character K but not ∇K.

(10) 1 sulphur atom.

The single occurrence of S, but not ∇S or US∇ or SU or USâ.

(11) More than 1 sulphur atom.

The multiple occurrence of S, but not ∇S or US∇ or SU or USâ.

(12) 1 -C=S group.

The single occurrence of the groups US∇ or USâ (or SU at the start of the notation only).

(13) More than 1 -C=S group.

The multiple occurrence of the groups US∇ or USâ (or SU at the start of the notation only).

(14) 1 double bond, excluding -C=S, -N=, or -C=O.

The single occurrence of the letter U, but not in any of the following groups, ∇U, UU, US∇, USâ, SU, MU, UM, HU, UH.

(15) More than 1 double bond, excluding -C=S, -N=, or -C=O.

The multiple occurrence of the letter U, but not in any of the following groups, ∇U, UU, US∇, USâ, SU, UM, MU, HU or UH.

(16) Triple bond.

The occurrence of the symbol combination UU.

(c) Chain fragments

Character sequences must not be immediately attached to a ring system.

(17) 1 methyl/methylene group.

Single occurrence of the number 1 not followed or preceded by a numeral.

(18) More than 1 methyl/methylene group.

Multiple occurrence of the number 1 not followed or preceded by a numeral.

(19) Ethyl/ethylene group.

Occurrence of the number 2 not followed by or preceded by a numeral.

(20) Alkyl chain $(CH_2)_n$ or $CH_3(CH_2)_{n-1}$ where n = 3-9.

Occurrence of a number in the range 3-9, but not followed by or preceded by a numeral.

(21) Alkyl chain $(CH_2)_n$ or $CH_3(CH_2)_{n-1}$ where n = 10 or more.

Occurrence of the sequence nn or nnn where nn is 10 or more.

(22) Generic halogen.

Occurrence of any of the characters E, F, G, H, I.

(23) One chlorine.

Single occurrence of the character G.

(24) More than one chlorine.

Multiple occurrence of the character G.

(25) Bromine.

Occurrence of one or more E symbols.

(26) Fluorine.

Occurrence of one or more F symbols.

(27) Iodine.

Occurrence of one or more I symbols.

(28) One -NH- group.

Single occurrence of the symbol M, but not UM (or MU at the start of the notation).

(29) More than one -NH- group.

Multiple occurrence of the symbol M, but not UM (or MU at the start of the notation).

(30) One $-NH_2$ group.

Single occurrence of the symbol Z.

(31) More than one $-NH_2$ group.

Multiple occurrence of the symbol Z.

(32) One -N= or HN= group.

Single occurrence of the symbol sequence UN or NU or UM (or MU at the start of the notation).

(33) More than on -N= or HN= group.

Multiple occurrence of the symbol sequence UN or NU or UM (or MU at the start of the notation).

(34) Unusual carbon atom.

One or more occurrences of the symbol C. Usually found in triple bonds, such as cyanides, isocyanides, etc.

(35) One -O- group.

Single occurrence of the symbol O, but not in the sequence OV or VO, or as O∇ or O&.

(36) More than one -O- group.

More than one occurrence of the symbol O, but not in the sequence VO or OV or O& or O∇.

(37) One -OH group.

Single occurrence of the symbol Q, but not in the sequence VQ (or QV at the start of the notation).

(38) More than one -OH group.

Multiple occurrence of the symbol Q, but not in the sequence VQ(or QV at the start of the notation).

(39) One -C=O group.

Single occurrence of the symbol V, but not in the sequence VQ or VO or OV (or QV at the start of the notation).

(40) More than one -C=O group.

Multiple occurrence of the symbol V, but not in the sequence VQ or VO or OV (or QV at the start of the notation).

(41) One -C(=O)-OH (acid) group.

Single occurrence of the symbol combination VQ (or QV at the start of the notation).

(42) More than one -C(=O)-OH (acid) group.

Multiple occurrence of the symbol combination VQ (or QV at the start of the notation).

(43) One -C(=O)-O (ester) group.

Single occurrence of the symbol combination VO or OV.

(44) More than one -C(=O)-O (ester) group.

Multiple occurrence of the symbol combination VO or OV.

(d) Substituent Fragments

The type of fragment in this class is exactly equivalent to the chain class of fragments. The fragments must be directly attached to a ring of some kind, and may be found after a locant in the notation or attached to a trailing ring system.

(45) One methyl/methylene group.

Single occurrence of the number 1 not followed or preceded by a numeral.

(46) More than one methyl/methylene group.

Multiple occurrence of the number 1 not followed or preceded by a numeral.

(47) Ethyl/ethylene group.

Occurrence of the number 2 not followed by or preceded by a numeral.

(48) Alkyl chain $(CH_2)_n$ or $CH_3(CH_2)_{n-1}$ where n = 3-9.

Occurrence of a number in the range 3-9, but not followed by or preceded by a numeral.

(49) Alkyl chain $(CH_2)_n$ or $CH_3(CH_2)_{n-1}$ where n = 10 or more.

Occurrence of the sequence nn or nnn where nn is 10 or more.

(50) Generic halogen.

Occurrence of any of the characters E, F, G, H, I.

(51) One chlorine.

Single occurrence of the character G.

(52) More than one chlorine.

Multiple occurrence of the character G.

(53) Bromine.

Occurrence of one or more E symbols.

(54) Fluorine.

Occurrence of one or more F symbols.

(55) Iodine.

Occurrence of one or more I symbols.

(56) One -NH- group.

Single occurrence of the symbol M, but not UM (or MU at the start of the notation).

(57) More than one -NH- group.

Multiple occurrence of the symbol M, but not UM (or MU at the start of the notation).

(58) One $-NH_2$ group.

Single occurrence of the symbol Z.

(59) More than one $-NH_2$ group.

Multiple occurrence of the symbol Z.

(60) One -N= or HN= group.

Single occurrence of the symbol sequence UN or NU or UM (or MU at the start of the notation).

(61) More than one -N= or HN= group.

Multiple occurrence of the symbol sequence UN or NU or UM (or MU at the start of the notation).

(62) Unusual carbon atom.

One or more occurrences of the symbol C. Usually found in triple bonds, such as cyanides, isocyanides, etc.

(63) One -O- group.

Single occurrence of the symbol O, but not in the sequence OV or VO or O∇ or O&.

(64) More than one -O- group.

More than one occurrence of the symbol O, but not in the sequence VO or OV or O∇ or O&.

(65) One -OH group.

Single occurrence of the symbol Q, but not in the sequence VQ (or QV at the start of the notation).

(66) More than one -OH group.

Multiple occurrence of the symbol Q, but not in the sequence VQ (or QV at the start of the notation).

(67) One -C=O group.

Single occurrence of the symbol V, but not in the sequence VQ or VO or OV (or QV at the start of the notation).

(68) More than one -C=O group.

Multiple occurrence of the symbol V, but not in the sequence VQ or VO or OV (or QV at the start of the notation).

(69) One $-\overset{O}{\overset{\|}{C}}-OH$ (acid) group.

Single occurrence of the symbol combination VQ (or QV at the start of the notation).

(70) More than one $-\overset{O}{\overset{\|}{C}}-OH$ (acid) group.

Multiple occurrence of the symbol combination VQ (or QV at the start of the notation).

(71) <u>One $-\overset{O}{\overset{\|}{C}}-O$ (ester)group.</u>

Single occurrence of the symbol combination VO or OV.

(72) <u>More than one $-\overset{O}{\overset{\|}{C}}-O$ (ester) group.</u>

Multiple occurrence of the symbol combination VO or OV.

(e) <u>Ring Heteroatoms</u>

Each ring system in the molecule is analysed; each ring is isolated and assigned a heteroatomic description. This description lists the heteroatoms present in the ring. The following fragments are set according to the analysis of that ring description.

(73) <u>Single occurrence of oxygen.</u>

A ring description contains only one oxygen (O).

(74) <u>Multiple occurrence of oxygen.</u>

A ring description contains more than one oxygen.

(75) <u>Single occurrence of oxygen in more than one ring.</u>

More than one ring desciption each containing only one oxygen.

(76) <u>Multiple occurrence of oxygen in more than one ring.</u>

More than one ring description containing more than one oxygen.

(77) <u>Single occurrence of nitrogen.</u>

A ring description contains one nitrogen (N, M, K).

(78) <u>Multiple occurrence of nitrogen.</u>

A ring description contains more than one nitrogen.

(79) <u>Single occurrence of nitrogen in more than one ring.</u>

More than one ring description containing one nitrogen.

(80) <u>Multiple occurrence of nitrogen in more than one ring.</u>

More than one ring description containing more than one nitrogen.

(81) <u>Single occurrence of sulphur.</u>

A ring description contains only one sulphur atom (S).

(82) <u>Multiple occurrence of sulphur.</u>

A ring description contains more than one sulphur.

(83) <u>Single occurrence of sulphur in more than one ring.</u>

More than one ring description contains one sulphur.

(84) <u>Multiple occurrence of sulphur in more than one ring.</u>

More than one ring description containing more than one sulphur.

(85) <u>Single occurrence of carbonyl.</u>

A ring description contains one carbonyl (V).

(86) <u>Multiple occurrence of carbonyl.</u>

A ring description contains more than one carbonyl.

(87) <u>Single occurrence of carbonyl in more than one ring.</u>

More than one ring description contains one carbonyl.

(88) Multiple occurrence of carbonyl in more than one ring.

More than one ring description containing more than one carbonyl.

(89) Single occurrence of exocyclic double bond.

A ring description contains one exodouble bond (Y).

(90) Multiple occurrence of exocyclic double bond.

A ring description contains more than one exodouble bond (Y).

(91) Single occurrence of exocyclic double bond in more than one ring.

More than one ring description contains one exodouble bond.

(92) Multiple occurrence of exocyclic double bond in more than one ring.

More than one ring description contains more than one exodouble bond.

(93) Single occurrence of any other heteroatom.

Occurrence of any letter other than H, K, M, N, O, S, T, V, U, X or Y.

(94) Multiple occurrence of any other heteroatom.

Occurrence of any letter other than above more than once in the same ring description.

(95) Single occurrence of any other heteroatom in more than one ring.

More than one ring description contains a letter other than those given above.

(96) Multiple occurrence of any other heteroatom in more than one ring.

More than one ring description contains more than one letter other than those given above.

(f) Ring Types

On analysis of the WLN ring record, a ring type description is set up which gives information on the size of each ring and the saturation/unsaturation value of that ring. The ring descriptor gives the atom types in each ring and this is used to determine whether hetero/carbo.

(97) Aromatic 6-membered ring.

The presence of at least one 6-membered ring, fully unsaturated and no heteroatoms present in the ring description.

(98) Carbocyclic 5-membered ring.

The presence of at least one 5-membered ring saturated or partially saturated and no heteroatoms present in the ring description.

(99) Carbocyclic 6-membered ring.

The presence of at least one 6-membered ring, saturated or partially saturated, and no heteroatoms present in the ring description.

(100) Carbocyclic rings other than 5 and 6-membered.

The presence of at least one ring (not 5 or 6-membered), saturated or partially saturated and no heteroatoms in the ring description.

(101) Heterocyclic 5-membered ring.

The presence of at least one 5-membered ring, saturated or unsaturated, and at least one heteroatom in the ring description.

(102) Heterocyclic 6-membered ring.

The presence of at least one 6-membered ring, saturated or unsaturated, and at least one heteroatom in the ring description.

(103) Heterocyclic rings other than 5 and 6-membered.

The presence of at least one ring (not 5 or 6-membered), saturated or unsaturated, and at least one heteroatom in the ring description.

(g) Heteroatom Count

Count of total number of heteroatoms of any type occurring in one ring.

(104) 1 heteroatom in one ring.

Total of one heteroatom in one ring.

(105) 2 heteroatoms in one ring.

Total of two heteroatoms in one ring.

(106) More than 2 heteroatoms in one ring.

Total of three or more heteroatoms in one ring.

(107) 1 heteroatom in more than one ring.

Total of one heteroatom in more than one ring.

(108) 2 heteroatoms in more than one ring.

Total of two heteroatoms in more than one ring.

(109) More than 2 heteroatoms in more than one ring.

Total of three or more heteroatoms in more than one ring.

(h) Ring Fusions

A set of ring descriptions is set up for each ring system in the order in which they occur. These are compared to find the fusion types.

(110) 1 single heterocyclic ring.

A heterocyclic ring unfused to any other ring.

(111) More than 1 single heterocyclic ring.

More than one heterocyclic ring unfused to any other ring.

(112) 1 single carbocyclic ring.

A carbocyclic ring unfused to any other ring.

(113) More than 1 single carbocyclic ring.

More than one carbocyclic ring unfused to any other ring.

(114) 1 carbo/carbo fusion.

A carbo ring (saturated or unsaturated) fused to a second carbo ring (saturated or unsaturated).

(115) More than 1 carbo/carbo fusion.

More than 1 carbo ring attached to another carbo ring within the same ring system.

(116) <u>1 carbo/carbo fusion in more than 1 ring system.</u>

One carbo ring attached to a second carbo ring occurring in more than one ring system.

(117) <u>More than 1 carbo/carbo fusion in more than 1 ring system.</u>

More than 1 carbo/carbo fusion occurring in more than 1 ring system.

(118) <u>1 carbo/hetero fusion.</u>

A carbo ring (saturated or unsaturated) fused to a hetero ring.

(119) <u>More than 1 carbo/hetero fusion.</u>

More than 1 carbo/hetero fusion occurring in the same ring system.

(120) <u>1 carbo/hetero fusion in more than 1 ring system.</u>

1 carbo/hetero fusion in more than 1 ring system.

(121) <u>More than 1 carbo/hetero fusion in more than 1 ring system.</u>

More than 1 carbo/hetero fusion occurring in more than 1 ring system.

(122) <u>1 hetero/hetero fusion.</u>

Two hetero rings fused to each other.

(123) <u>More than 1 hetero/hetero fusion.</u>

More than 1 hetero/hetero fusion occurring in the same ring system.

(124) <u>1 hetero/hetero fusion in more than 1 ring system.</u>

1 hetero/hetero fusion in more than 1 ring system.

(125) <u>More than 1 hetero/hetero fusion in more than 1 ring system.</u>

More than 1 hetero/hetero fusion occurring in more than 1 ring system.

(I) <u>Ring Linkages</u>

(126) <u>Spiro ring indicator.</u>

Sequence locant-&locant in non-ring part of WLN.

(127) <u>True bridge indicator.</u>

WLN contains a ring notation with cited bridge locants.

(128) <u>1 multi-cyclic point.</u>

Within any ring signs sequence bna where n=1.

(129) <u>More than 1 multi-cyclic point.</u>

Within any ring signs sequence bn where n>1, or sequence bnn.

(130) <u>Bilinkage.</u>

Two ring systems (including benzene) are linked together.

(J) <u>Unusual Conditions</u>

(131) <u>Chelate.</u>

WLN contains the character D. No other reliable fragments are set.

(132) <u>Metallocene.</u>

Ring containing character zero, not within hyphens. Any other fragments set for metallocenes are not reliable.

(133) Inorganics.

Notation begins with a space, but not ∇&&. No other fragments are set.

(k) Total Ring Features

Used to indicate the presence of ring features in the molecule.

(134) 1 ring system.

Occurrence of one ring system (not benzene).

(135) 2 ring systems.

Occurrence of 2 ring systems (not benzene).

(136) More than 2 ring systems.

Occurrence of more than 2 ring systems (not benzene).

(137) 1 benzene ring.

Occurrence of one phenyl group.

(138) 2 benzene rings.

Occurrence of 2 phenyl groups.

(139) More than 2 benzene rings.

Occurrence of more than 2 phenyl groups.

(140) 1 carbocyclic ring.

Occurrence of one individual, fused or aromatic ring (excluding non-fused benzenes) in total molecule.

(141) 2 carbocyclic rings.

Occurrence of two carbocyclic or aromatic rings (excluding non-fused benzenes) in total molecule.

(142) More than 2 carbocyclic rings.

Occurrence of more than 2 carbocyclic or aromatic rings (excluding non-fused benzenes) in total molecule.

(143) 1 heterocyclic ring.

Occurrence of one individual heterocyclic ring in total molecule.

(144) 2 heterocyclic rings.

Occurrence of two heterocyclic rings in total molecule.

(145) More than 2 heterocyclics.

Occurrence of more than 2 heterocyclic rings in total molecule.

(l) Special Compound Types

(146) Polypeptide.

Notation begins with . No other fragments are set.

(147) Polymer.

Notation begins with /. No other fragments are set.

(m) Extensions

(148) More than 1 3-branch carbon atom.

The character Y (but not∇Y) occurring more than once.

Note: See fragment 6.

(149) Presence of suffix

A suffix beginning Ɣ&& is present in the WLN.

ADDITIONAL FRAGMENTS AND THEIR MEANING

Note: the following special symbols have been used in the fragment explanations:

_(underscore)	-	a character string may intervene
(&)	-	a terminal substituent
(C)	-	any Carbon atom eg Y,X,numeric
(N)	-	any Nitrogen atom eg Z,M,N
9	-	any numeric

(a) Additional Chain Fragments

Note: these are set in addition to the simpler fragments described in 1(c) and the character sequences must not be immediately attached to or part of a ring system.

(150) Chain Primary Amide

Char. sequence ZV or VZ bonded to acyclic C only.

(151) Chain secondary amide

Char. seq. VM or MU bonded to acyclic C only.

(152) Chain tertiary amide

Char. seq. N VMM or VN bonded to acyclic C only.

(153) Chain N-unsubstituted acylhydrazide

Char. seq. ZMV or VMZ bonded to acyclic C.

(154) Chain N-substituted acylhydrazides

Char. seq. MMV,VMM,MN_V,VN_M,N_N_V,N_V(&)N,N_MV,VMN, ZN_V,VNZ, with V bonded to acyclic C only.

(155) Chain primary amidine

Char. seq. MUYZ or YZUM bonded to acylic C only and excl. (155).

(156) Chain amidine

Char. seq. (N)_Y_UN,NUY_(N) bonded to acyclic C only and excl. (155).

(159) Chain azo and diazo

Char. seq. NUN,UNN or NNU.

(160) Chain C-nitroso

Char. seq. ON or NO bonded to acyclic C.

(161) Chain N-nitroso

Char. seq. ON(N) or (N)_NO.

(162) Chain sulfonamide

Char. seq. (N)_SW or SW(N), (excl. bit 177).

(163) Chain guanidine

Char. seq. (N)_Y_(N)_(UU),(N)UY_(N)_(UN).

(164) Chain N-N, azoxy

Char. seq. (N)_(N), not part of another bit (e.g. 153, 154), and NUNO& and NO&UN (excl. 305).

(165) Chain thioamide

Char. seq. SUYZ or YZUS.

(166) Chain dialkylamino

Char. seq. 9N9& or N9&9, not bonded to V.

(167) Chain methoxy

Char. seq. O1 or 1O bonded to acyclic C only. (O = letter)

(168) Chain hydroxylamine

Char. seq. Q(N) or (N)_Q.

(169) Chain oxime

Char. seq. QNU or UNQ.

(170) Chain N-nitro

Char. seq. WN(N) or (N)_NW.

(171) Chain phenethyl

Char. seq. R2 or 2R (where R is not further substituted.)

(172) Chain phenoxy

Char. seq. RO or OR (where R is not further substituted).

(173) Chain phenylazo, and phenylhydrazono

Char. seq. RMNU,RNUN,NUNR,UNMR (where R is not further substituted).

(174) Chain phenylureido

Char. seq. RMUM and MUMR(where R is not further substituted).

(175) Chain phosphonyl

Char. seq. QPQO& or PQQO (where O is terminal), but excl. P attached to 4 O atoms.

(176) Chain semicarbazide and semicarbazone

Char. seq. MMVZ,ZVMM,UNMVZ,ZVMNU.

(177) Chain sulfamido

Char. seq. MSWQ or WSQM.

(178) Chain urea

Char. seq. (N)_V(N).

(179) Chain cyano

Char. seq. NC or CN (where N is terminal).

(180) Biphenyl

Char. seq. R locR.

(305) Ar. azoxy

Char. seq. NUNO& or NO&UN on benzene ring.

(306) Chain carbamate

Char. seq. OV(N), (N) VO.

(b) Additional Substituent Fragments

Note: these are set in addition to the simpler fragments described in 1(d) and the character sequences must be immediately attached to a part of a ring system.

(181) Substituent primary amide

Char. sequence ZV or VZ bonded to ring C only.

(182) Substituent secondary amide

Char. seq. VH or HU bonded to ring C only.

(183) Substituent tertiary amide

Char. seq. N_VHH or VN bonded to ring C only.
Note that (N) includes N in a ring.

(184) Substituent N-unsubstituted acylhydrazide

Char. seq. ZHV or VHZ bonded to ring C.

(185) Substituent N-substituted acylhydrazides

Char. seq. HHV,VHH,HN_V,VN_H,N_N_V,N_V(&)N,N_HV,VHN, ZN_V,VNZ, with V bonded to ring C only. Note that (N) includes N in a ring.

(186) Substituent primary amidine

Char. seq. HUYZ or YZUH bonded to ring C only and excl. (166).

(187) Substituent amidine

Char. seq. (N)_Y_UN,HUY_(N) bonded to ring C only and excl. (155). Note that (N) includes N in a ring.

(188) Barbiturate

Char. seq. (N)U(N)V or V(N)V(N) within ring symbols.

(189) Lactam

Char. seq. (N)V or V(N) within ring symbols (excl. bit 188).

(190) Substituent azo and diazo

Char. seq. NUN,UNN or NNU.

(191) Substituent C-nitroso

Char. seq. ON or NO bonded to ring C.

(192) Substituent N-nitroso

Char. seq. ON(N) or (N)_NO. Note that (N) includes N in a ring.

(193) Substituent sulfonamide

Char. seq. (N)_SW or SW(N), (excl. bit 177). Note that (N) includes N in a ring.

(194) Substituent guanidine

Char. seq. (N)_Y_(N)_(UU),(N)UY_(N)_(UN). Note that (N) includes N in a ring.

(195) Substituent N-N

Char. seq. (N)_(N), nor part of another bit (cg 153, 154). Note that (N) includes N in a ring.

(196) Substituent thioamide

Char. seq. SUYZ or YZUS.

(197) Substituent dialkylamino

Char. seq. 9N9& or N9&9, not bonded to V.

(198) Substituent methoxy

Char. seq. O1 or 1O bonded to ring C only. (O = letter)

(199) Substituent hydroxylamine

Char. seq. Q(N) or (N)_Q. Note that (N) includes N in a ring.

(200) Substituent oxime

Char. seq. QNU or UNQ.

(201) Substituent N-nitro

Char. seq. WN(N) or (N)_NW. Note that (N) includes N in a ring.

(202) Substituent phenethyl

Char. seq. R1 or "R (where R is not further substituted).

(203) Substituent phenoxy

Char. seq. RO or OR (where R is not further substituted).

(204) Substituent phenylazo, and phenylhydrazono

Char. seq. RMNU,RNUN,NUNR,UNMR (where R is not further substituted).

(205) Substituent phenylureido

Char. seq. RMUM and MUMR (where R is not further substituted).

(206) Substituent phosphonyl

Char. seq. QPQO& or PQQO (where O is terminal), but excl. P attached to 4 O atoms.

(207) Substituent semicarbazide and semicarbazone

Char. seq. MMVZ,ZVMM,UNMVZ,ZVMNU.

(208) Substituent sulfamido

Char. seq. MSWQ or WSQM.

(209) Substituent ureas

Char. seq. (n)_V(N). Note that (N) includes N in a ring.

(210) Substituent cyano

Char. seq. NC or cn (where N is terminal).

(309) Substituent carbamate

Char. seq. OV(N), (N)_VO.

(c) Additional Metal Fragments

These are found by locating the character seq -AA- where AA is the metal WLN atomic symbol anywhere in the notation. Note: KA (potassium), WO (Tungsten), UR (uranium), VA (vanadium) and YT (yttrium) are not standard atomic symbols.

Metal	Fragment	Metal	Fragment	Metal	Fragment
Ac	211	He	242	Re	275
Al	212	Ho	243	Rh	276
Am	213	In	244	Rb	277
Sb	214	Ir	245	Ru	278
Ar	215	Fe	246	Sm	279
As	216	Kr	247	Sc	280
At	217	La	248	Se	281
Ba	218	Lr	249	Si	282
Bk	219	Pb	250	Ag	283
Be	220	Li	251	Na	284
Bi	221	Lu	252	Sr	285
Cd	222	Mg	253	Ta	286
Ca	223	Mn	254	Tc	287
Cf	224	Md	255	Te	288
Ce	225	Hg	256	Tb	289
Cs	226	Mo	257	Tl	290
Cr	227	Nd	258	Th	291
Co	228	Ne	259	Tm	292
Cu	229	Np	260	Sn	293
Cm	230	Ni	261	Ti	294
Dy	231	Nb	262	W	295
Es	232	No	263	U	296
Er	233	Os	264	V	297
Eu	234	Pd	265	Xe	298
Fm	235	Pt	266	Yb	299
Fr	236	Pu	267	Y	300
Gs	237	Po	268	Zn	301
Ga	238	K	269	Zr	302
Ge	239	Pr	270		
Hu	240	Pm	271		
Hf	241	Pa	272		
		Ra	273		
		Ru	274		

APPENDIX B3

DESCRIPTION OF THE PROGRAMMED CARCINOGENESIS KEYS

Key 310 Aromatic amino:

[Key 97 (aromatic 6-membered ring] AND [Key 8 (3-branch nitrogen) OR Key 56 (substituent N-H bond) OR Key 58 (amino group) OR Key 59 (> 2 amino group)]

Key 311 N-nitroso, sulfonyl:

[Key 161 (chain N-nitroso)] AND [Key 162 (chain sulfonamide)]

Keys 312 thru 314 Organohalogen mustards:

Key 312

[Key 8 (3-branch nitrogen) OR Key 28 (chain N-H bond) OR Key 56 (substituent N-H bond)] AND [Key 19 (ethyl or ethylene group)] AND [Key 22 (generic halogen)]

Key 313

[Key 10 (sulfur atom)] AND [Key 19 (ethyl or ethylene group)] AND [Key 22 (generic halogen)]

Key 314

[Key 313] AND [Key 36 (>1 chain oxygen)]

Key 315 Halo alkanes:

[Key 6 (3-branch carbon) OR Key 7 (4-branch carbon) OR Key 17 (methyl or methylene group) OR Key 19 (ethyl or ethylene group) OR Key 20 (alkyl chain $(CH_2)_n$,n=3-9) OR Key 148 (>1 3-branch carbon)] AND [Key 22 (generic halogen)]

Key 316 Haloethers:

[Key 6 (3-branch carbon) OR Key 7 (4-branch carbon) OR Key 17 (methyl or methylene group) OR Key 19 (ethyl or ethylene group) OR Key 148 (>1 3-branch carbon)] AND [Key 35 (1 chain oxygen)] AND [Key 22 (generic halogen)]

Key 317 Haloalkenes:

[Key 6 (3-branch carbon) OR Key 17 (methyl/methylene group)] AND [Key 14 (carbon double bond, not c=oh,c=N,c=S] AND [Key 22 (generic halogen)]

Key 318 Halogenated aromatics:

[Key 50 (substituent halogen)] AND [Key 97 (aromatic 6-membered ring)] AND [Key 180 (biphenyl) OR Keys 114 thru 125 (any one or more) various types and amount of ring fusions in overall compound]

Key 319 Alkyl sulfates:

[Key 4 (dioxo group) OR Key 36 (>1 oxygen)] AND [Key 10 (sulfur)]

Key 320 Sultones:

[Key 4 (dioxo group)] AND [Key 73 (oxygen as ring heteroatom)] AND [Key 81 (sulfur as ring heteroatom)] AND [Keys 104 or 107 (1 heteroatom in 1 or >1 ring)]

Key 321 Epoxides:

[Key 103 (heterocyclic ring, not 5- or 6-membered)] AND [Key 73 (oxygen as ring heteroatom)] AND [Keys 104 or 107 (1 heteroatom in 1 or >1 ring)]

Key 322 Aziridines:

[Key 103 (heterocyclic ring, not 5- or 6-membered)] AND [Key 77 (nitrogen as ring heteroatom)] AND [Keys 104 or 107 (1 heteroatom in 1 or >1 ring)]

Key 323 Sulfides:

[Key 103 (heterocyclic ring, not 5- or 6-membered)] AND [Key 81 (sulfur as ring heteroatom)] AND [Keys 104 or 107]

Key 324 β-Lactones:

[Key 321 (epoxides)] AND [Key 85 (carbonyl in ring)]

Key 326 β-Unsaturated lactones:

[Key 101. (heterocyclic 5-membered ring)] AND [Key 73 (oxygen as ring heteroatom)] AND [Key 85 (carbonyl in ring)] AND [Keys 104 or 107 (1 heteroatom in 1 or >1 ring)]

Key 327 Anhydrides:

[Key 101 (heterocyclic 5-membered ring)] AND [Key 73 (oxygen as ring heteroatom)] AND [Key 86 (>1 carbonyl in ring)] AND [Keys 104 or 107 (1 heteroatom in 1 or >1 ring)]

Key 328 α-β Unsaturated carbonates:

[Key 101 (heterocyclic 5-membered ring)] AND [Key 24 (>1 oxygen as ring heteroatom)] AND [Key 85 (carbonyl in ring)] AND [Keys 105 or 108 (2 heteroatoms in one or >1 ring)]

Key 329 α-β Unsaturated lactones:
[Key 102 (heterocyclic 6-membered ring)] AND [Key 73 (oxygen as ring heteroatom)] AND [Key 85 (carbonyl in ring)] AND [Keys 104 or 107 (1 heteroatom in 1 or >1 ring)]

Key 330 Fused aromatic α-β unsaturated lactones:
[Key 329] AND [Key 97 (aromatic 6-membered ring)] AND [Key 118 (1 carbo/hetero fusion)]

Key 331 Fused polynuclear aromatics:
[Keys 114 thru 125 (any one)] AND [Key 97 (aromatic 6-membered ring)]

Key 332 Aryldialkatriazenes:
[Key 97 (aromatic 6-membered ring)] AND [Key 204 (substituent phenylazo)] AND [Key 8 (3-branch nitrogen)]

Key 333 Purine analog:
[Key 80 (>1 nitrogen as heteratom in >1 ring)] AND [Key 101 (heterocyclic 5-membered ring)] AND [Key 102 (heterocyclic 6-membered ring)] AND [Key 108 (2 heteroatoms in >1 ring)] AND [Key 122 (1 hetero/hetero fusion)]

Key 334 Pyrimidine analogs:
[Key 78 (>1 nitrogen as heteroatom in 1 ring)] AND [Key 102 (heterocyclic 6-membered ring)] AND [Key 105 (2 heteroatoms in 1 ring)]

Key 335 Any one or more of the following keys: 100,207,223,285,314,330,332.

Key 336 Any one or more of the following keys: 21,42,94,176,281,309.

APPENDIX C

DATABASE FOR FINAL STRUCTURE - ACTIVITY MODEL OF BIODEGRADABILITY

---------- CATEGORY=BIODEGRADABLE COMPOUNDS ----------

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
50840	191.010	50	52	69	97	137												
50997	261.089	37	45	66	73	102	104	110	134	143								
51285	184.120	3	65	97	137													
51365	191.010	50	52	69	97	137												
52904	308.391	6	10	17	30	41												
55210	121.150	30	67	97	137	181												
55221	152.179	69	77	102	104	110	134	143										
56382	180.159	1	3	10	19	36	63	97	137									
56406	75.080	17	30	41														
56417	190.156	6	17	30	41													
56451	298.346	6	17	30	37	41												
56757	323.150	3	17	22	24	28	38	39	97	137	148	151	315					
56815	92.110	6	18	38														
56848	131.131	6	17	30	42													
56860	299.375	6	19	30	42													
57116	284.540	21	41															
57487	189.221	37	45	66	73	102	104	110	134	143								
57501	257.437	38	46	63	66	75	101	102	107	111	135	144						
58899	290.820	50	52	99	112	134	140											
59676	123.120	69	77	102	104	110	134	143										
61905	131.200	18	30	41	148													
62237	167.130	3	69	97	137													
62533	93.140	58	97	137	310													
64175	46.080	19	37															
64186	46.030	41																
64197	354.100	17	41															
66228	239.322	78	86	102	105	110	134	143	188	334								
67630	60.110	6	18	37														
69727	338.413	65	69	97	137													
70304	239.322	45	50	52	66	97	138											
70473	153.823	6	17	31	39	41	150											
71001	268.359	6	30	41	45	78	101	105	110	134	143							
71238	268.356	20	37															
71363	228.294	20	37															
72184	117.170	18	30	41	148													
72435	345.660	6	7	18	22	24	64	97	138	198	315							
73223	204.250	6	30	41	45	77	97	101	104	118	140	143	331					
73325	131.200	17	19	30	41	148												
74113	214.247	50	51	69	97	137												
75070	373.950	17	39															
75570	109.620	9	18															
77929	192.140	7	18	37	42													
78308	307.105	1	5	46	64	97	139	172										
78319	145.161	1	5	45	64	97	139	172										
78320	198.138	1	5	46	64	97	139	172										
78922	74.140	6	17	19	37													
79094	74.090	19	41															
84662	222.260	19	72	97	137													
84695	59.068	18	19	72	97	137	148											
84742	229.257	20	72	97	137													
84764	418.690	20	72	97	137													

DATABASE FOR FINAL STRUCTURE - ACTIVITY MODEL OF BIODEGRADABILITY

CATEGORY=BIODEGRADABLE COMPOUNDS

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
85416	147.140	77	86	97	101	104	118	134	140	143	189	331						
85472	214.203	4	10	37	97	114	134	141	331									
85687	312.390	45	69	71	97	138												
87592	121.200	46	58	97	137	310												
87650	163.000	50	52	65	97	137												
87694	124.158	38	42	148														
87865	93.129	50	52	65	97	137												
88062	197.440	50	52	65	97	137												
88722	137.150	3	45	97	137													
88755	139.120	3	65	97	137													
88993	166.140	70	97	137														
89781	156.300	6	18	45	65	97	112	134	140									
89838	150.240	6	18	45	65	97	137											
90029	122.123	65	67	97	137													
90153	110.131	65	97	114	134	141	331											
90437	252.101	65	97	130	138													
90960	58.080	18	64	67	97	138	198											
90982	251.110	50	52	67	97	138												
91010	231.255	6	37	97	138													
92875	184.260	59	97	130	138	188	310											
93629	178.190	8	18	19	37	42												
93721	269.510	6	17	41	50	52	63	97	137	172								
93765	255.480	17	41	50	52	63	97	137	172									
94757	221.040	17	41	50	52	63	97	137	172									
95437	108.150	45	65	97	137													
95512	127.580	50	51	58	97	137	310											
95534	107.170	45	58	97	137	310												
95556	109.140	58	65	97	137	310												
95647	121.200	46	58	97	137	310												
95658	122.180	46	65	97	137													
95783	121.200	46	58	97	137	310												
95863	124.160	59	65	97	137	310												
95874	122.180	46	65	97	137													
95954	46.053	50	52	65	97	137												
96413	163.834	65	98	112	134	140												
97187	356.040	10	50	52	66	97	138											
97234	269.130	45	50	52	66	97	138											
97994	102.150	37	45	73	101	104	110	134	143									
98000	98.110	37	45	73	101	104	110	134	143									
98011	96.090	67	73	101	104	110	134	143										
98113	158.180	4	10	37	97	137												
98679	137.025	4	10	37	65	97	137											
98691	112.987	4	10	37	47	97	137											
98953	123.120	3	97	137														
99047	136.160	45	69	97	137													
99059	137.150	58	69	97	137	310												
99081	137.150	3	45	97	137													
99503	267.155	66	69	97	137													
99616	151.130	3	67	97	137													
99990	137.150	3	45	97	137													
100027	139.120	3	65	97	137													

DATABASE FOR FINAL STRUCTURE - ACTIVITY MODEL OF BIODEGRADABILITY

--- CATEGORY=BIODEGRADABLE COMPOUNDS ---

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
100196	240.214	3	17	67	97	137												
100210	166.140	70	97	137														
101531	295.336	45	65	97	138													
101815	168.250	45	97	138														
103231	399.966	18	19	20	44	148												
103822	344.060	41	45	97	137													
103844	178.234	17	39	56	97	137	182	310										
104018	166.190	17	41	45	63	97	137	198										
104154	172.210	4	10	37	45	97	137											
105602	169.227	77	85	103	104	110	134	143	189	322	325							
105679	122.180	44	65	97	137													
106490	107.170	45	58	97	137	310												
106503	108.160	59	97	137	310													
107153	60.120	19	31															
107211	236.337	19	38															
107642	255.494	2	8	18	21													
107926	88.120	20	41															
107937	107.156	14	17	19	41													
107948	108.530	19	22	23	41	315												
108394	108.150	45	65	97	137													
108429	127.580	50	51	58	97	137	310											
108441	107.170	45	58	97	137	310												
108452	108.160	59	97	137	310													
108463	110.120	66	97	137														
108736	126.120	66	97	137														
108930	100.180	65	99	112	134	140												
108941	98.160	85	99	112	134	140												
109977	67.100	77	101	104	110	134	143											
110156	258.104	19	42															
110270	270.510	6	18	21	43													
110338	180.250	20	44															
110543	86.200	20																
110634	151.165	20	38															
110894	85.170	77	102	104	110	134	143											
111422	105.160	19	28	38														
111466	106.140	19	35	38														
112005	80.514	2	9	18	21	149												
112027	53.064	2	9	18	21	149												
112038	349.130	2	8	18	21													
112538	184.390	21	37															
112618	298.570	17	21	43														
115322	198.144	7	22	24	37	50	52	97	138	315								
115866	326.300	1	5	64	97	139	172											
117817	390.620	18	19	20	72	97	137	148										
117840	76.099	20	72	97	137													
118923	137.150	58	69	97	137	310												
119368	187.066	17	65	71	97	137												
119619	182.230	67	97	138														
120729	370.490	77	97	101	104	118	134	140	143	331								
120809	110.120	66	97	137														
120832	361.784	50	52	65	97	137												

DATABASE FOR FINAL STRUCTURE - ACTIVITY MODEL OF BIODEGRADABILITY

-- CATEGORY=BIODEGRADABLE COMPOUNDS --

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
120923	84.130	85	98	112	134	140												
121573	227.132	4	10	37	58	97	137	310										
121915	166.140	70	97	137														
121926	167.130	3	69	97	137													
122189	330.358	2	9	18	21	45	97	137	149									
122190	424.230	2	9	18	21	45	97	137										
122349	201.661	19	50	51	57	78	102	106	110	134	143							
122429	179.240	6	18	43	56	97	137	310										
122805	130.200	17	39	56	58	77	137	182	310									
123308	109.140	58	65	97	137	310												
123319	110.120	66	97	137														
123728	72.120	20	39															
124185	147.320	21																
126738	202.256	1	5	20	36													
127173	238.246	17	39	41														
131113	239.246	18	72	77	137	167												
131704	289.328	20	69	71	97	137												
134850	291.306	50	51	67	97	138												
135193	144.180	65	97	114	134	141	331											
139082	143.189	2	9	18	21	45	97	137	149									
139139	240.432	8	18	42														
140727	305.802	2	49	77	102	104	110	134	143	149								
142621	116.180	20	41															
142734	133.120	18	28	42														
142916	298.570	6	18	21	43													
143077	200.360	21	41															
144627	90.040	42																
147853	115.132	69	77	101	104	110	134	143										
149575	144.240	6	19	20	41													
149917	170.130	66	69	77	137													
150130	137.150	58	69	97	137	310												
151326	216.241	29	44															
151417	266.440	4	10	21	35	37												
156387	276.338	41	45	65	97	137												
288324	68.090	78	101	105	110	134	143											
301008	216.283	1	15	17	20	43												
309002	364.900	50	52	98	115	127	129	134	142									
334485	172.300	20	41															
445294	140.120	50	54	69	97	137												
452868	233.098	45	66	97	137													
455389	249.077	50	54	69	97	137												
456224	304.349	50	54	69	97	137												
488175	142.029	45	66	97	137													
490799	117.108	66	69	97	137													
499069	239.274	46	69	97	137													
503640	240.350	14	17	19	34	41												
507700	154.280	46	65	78	127	134	141											
526750	122.180	46	65	97	137													
531759	359.573	37	45	63	66	75	85	97	102	107	110	118	135	140	144	331		
535808	73.099	50	51	69	97	137												
544763	226.231	21																

DATABASE FOR FINAL STRUCTURE — ACTIVITY MODEL OF BIODEGRADABILITY

CATEGORY=BIODEGRADABLE COMPOUNDS

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
552169	167.130	3	69	97	137													
552896	151.139	3	67	97	137													
554847	139.129	3	65	97	137													
555168	151.139	3	67	97	137													
563042	265.360	1	5	46	64	97	139											
563122	114.144	1	11	17	19	36												
567180	270.240	4	10	37	65	97	114	134	141	331								
576261	122.180	17	22	26	45	65	97	137	315									
585762	112.080	50	53	69	97	137												
586765	328.346	50	53	69	97	137												
589924	307.328	45	85	99	112	134	140											
591275	199.140	58	65	97	137	310												
610353	226.231	65	70	97	137													
611201	145.161	8	62	65	97	137	210	310										
611949	173.171	17	63	67	97	138	172	198										
612000	90.082	6	17	97	138													
618417	256.213	5	10	37	97	137												
618519	199.209	50	55	69	97	137												
619045	182.135	46	69	97	137													
619089	173.560	3	50	51	65	97	137											
629594	143.189	21																
645921	145.161	59	78	85	102	106	110	134	143									
767000	132.119	8	62	65	97	137	210	310										
831812	211.269	45	50	51	97	138												
834128	227.370	6	10	19	19	57	78	102	106	110	134	143						
873621	186.377	8	62	65	97	137	210	310										
947911	196.260	6	39	97	138													
993135	317.322	1	17	35	38													
1002842	242.450	21	41															
1120361	117.109	14	17	21														
1124396	72.063	47	66	97	137													
1137424	171.112	65	67	97	138													
1197553	142.118	41	45	58	97	137	310											
1241947	157.133	1	5	6	17	19	20	35	64	97	138	172						
1610179	211.310	6	18	19	57	53	78	102	106	110	134	143	198					
1698609	221.460	50	51	58	78	95	97	102	105	110	130	134	137	143	310	334		
1832548	239.319	1	5	6	19	35	37											
1951128	122.569	6	18	22	23	41	315											
2041147	213.307	1	5	19	30	38	175											
2138229	333.231	50	51	66	97	137												
2212671	187.330	10	19	67	77	133	104	110	134	143	322							
2528361	239.274	1	5	20	36	53	97	137	172									
2620533	312.277	17	28	50	51	71	97	137										
2689432	329.276	8	18	39	50	52	63	67	97	138	183	198	209	310				
2785548	254.103	2	49	77	102	104	110	134	143	149								
3055945	308.375	19	21	36	37													
3055956	96.099	19	21	36	37													
3055967	315.282	19	21	36	37													
3055978	225.182	19	21	36	37													
3055990	217.271	19	21	36	37													
3115284	239.244	6	20	41														

DATABASE FOR FINAL STRUCTURE - ACTIVITY MODEL OF BIODEGRADABILITY

CATEGORY=BIODEGRADABLE COMPOUNDS

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
3134121	337.220	8	18	39	50	52	67	97	138	152	310							
3274280	318.543	6	20	41														
3648202	442.900	21	72	97	137													
3648213	331.766	20	72	97	137													
4408644	206.094	8	18	42														
4536236	203.348	6	17	20	41													
4536305	253.750	19	21	35	37													
5254126	248.448	1	5	45	64	97	139	172										
6213907	187.305	6	14	18	22	23	41	315	317									
6214284	377.311	6	14	19	22	23	41	315	317									
6779095	266.124	1	5	19	38	175												
7305615	239.746	1	5	19	35	37												
10374740	290.275	14	20															
13113434	234.299	8	18	39	50	51	67	97	138	152	310							
13138335	555.282	1	5	20	30	38	175											
13673922	310.180	50	52	66	97	137												
14697404	268.274	20	44															
15592742	253.349	4	10	37	48	97	137											
16045924	122.019	6	17	22	23	42	315											
16066356	242.321	4	6	10	18	37	97	137										
17109498	329.374	1	5	11	19	35	97	138										
17345618	193.246	8	62	66	97	137	210	310										
17495497	243.309	8	18	28	39	50	52	97	137	209	310							
18435228	239.274	6	17	19	21													
18521590	207.616	4	10	37	48	97	137											
21964498	109.943	15	18	21														
25354921	292.298	6	17	21	41													
27697514	230.242	2	9	19	19	149												
32815535	354.472	6	20	21	41													
33374286	392.942	19	20	35	72	97	137											
34123596	207.273	6	8	18	39	56	97	137	209	310								
38775223	185.610	4	11	15	38	46	97	130	139	180								
38945276	118.095	6	18	35	42													
39156495	161.121	4	10	37	49	97	137											
52435151	178.197	5	8	11	14	17	19	38	46	57	80	97	102	109	136	139	145	310
55203128	189.175	6	17	35	42													
59457505	339.219	1	5	19	28	30	38	39	151	175								

DATABASE FOR FINAL STRUCTURE - ACTIVITY MODEL OF BIODEGRADABILITY

CATEGORY=NONBIODEGRADABLE COMPOUNDS

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
67685	123.111	5	10	18														
68122	278.329	8	18	39	152													
72548	320.040	22	24	50	52	97	138	148	315									
72559	319.020	14	22	24	50	52	97	138	148	315								
75014	62.500	14	18	22	23													
78433	430.910	1	5	18	22	24	36	148	315									
83056	193.192	6	41	50	52	97	138											
88744	138.140	3	55	97	137	310												
90971	119.379	6	37	50	52	97	138											
92240	138.122	97	115	134	142	331												
95147	117.140	78	97	101	106	118	134	140	143	331								
99650	168.120	3	97	137														
100254	168.123	3	97	137														
104830	156.223	3	41	45	97	137												
117340	157.015	6	41	97	139													
119562	373.496	6	37	50	51	97	138											
119799	223.269	4	10	37	58	97	114	134	141	310	331							
121471	173.200	4	10	37	58	97	137	310										
121540	449.159	2	7	9	18	19	35	45	63	97	138							
126863	267.240	7	16	18	38	149												
136958	150.210	58	77	81	97	101	105	118	134	140	143	310	331					
149304	167.250	10	77	81	97	101	105	118	134	140	143	331						
194592	267.340	77	97	101	104	115	119	134	142	143	331							
198550	252.316	97	115	129	134	142	331											
217594	228.303	97	115	134	142	331												
333415	196.209	1	6	10	18	19	36	45	63	78	102	105	110	134	143	334		
366187	364.914	79	102	107	111	130	135	144										
574425	60.100	35	97	139	148													
605827	384.475	97	114	130	134	137	141	331										
609994	323.827	3	65	69	97	137	199											
615214	165.230	30	56	77	81	97	101	105	118	134	140	143	195	310	331			
615225	75.067	10	17	77	81	97	101	105	118	134	140	143	331					
620928	200.250	45	66	97	138													
622479	193.249	41	46	97	137													
728870	193.249	6	18	37	64	97	138	172	198									
751382	159.188	97	114	130	134	139	141	331										
778223	139.191	7	18	97	138													
941571	103.081	4	10	37	77	81	97	101	105	118	134	140	143	331				
1562932	223.319	61	69	97	138	204												
1883325	365.964	6	17	37	97	138												
1926803	244.293	17	20	30	43	149												
2008584	171.156	30	50	52	67	97	137	181										
2051243	213.307	50	52	97	130	138	150	318										
2971224	285.600	6	7	22	24	97	138	315										
3026662	262.308	2	49	77	102	104	110	134	143	149								
3724525	335.282	70	98	112	134	140												
3905644	215.688	7	18	97	114	134	141	331										
5743975	234.299	99	115	134	142													
7508681	367.910	19	61	71	97	138	204											
10275588	257.336	7	19	97	114	134	141	331										
10450698	349.063	2	9	14	18	20	149											

DATABASE FOR FINAL STRUCTURE - ACTIVITY MODEL OF BIODEGRADABILITY

CATEGORY=NONBIODEGRADABLE COMPOUNDS

CAS	MWT	KEY1	KEY2	KEY3	KEY4	KEY5	KEY6	KEY7	KEY8	KEY9	KEY10	KEY11	KEY12	KEY13	KEY14	KEY15	KEY16	KEY17
17304620	320.366	45	77	78	81	85	97	101	108	110	118	130	135	140	144	331		
18101581	177.219	4	10	30	58	77	81	97	101	105	118	134	140	143	162	310	331	
19218781	350.588	4	10	17	37	61	63	97	138	190	198							
38380028	497.114	50	52	97	130	138	180	318										
52712046	226.279	50	52	97	139	138	180	318										
65644511	251.665	3	69	77	81	97	101	105	118	130	134	137	140	143	331			

APPENDIX D

CLASSIFICATION FUNCTIONS

Variable		Group: Degr	Group: Nondegr
1	MW	0.02302	0.02802
4	K1	2.73695	-2.27090
5	K3	0.11129	3.30623
6	K7	-0.03238	4.26684
7	K16	-0.80634	7.44804
9	K19	3.93332	1.36762
10	K20	3.76515	1.47810
11	K21	5.49241	0.46134
13	K35	-1.64318	1.33443
14	K36	-1.91663	3.52740
15	K38	4.25407	1.46794
16	K39	2.69657	-0.35391
17	K42	7.46411	3.61787
18	K43	0.78917	3.24463
20	K57	-1.97048	-6.80428
21	K61	-3.57630	8.52544
22	K65	3.17291	0.14256
23	K66	1.52237	-0.07360
24	K67	1.96106	-2.74657
25	K69	1.58738	-0.51867
27	K81	-4.82418	9.06071
28	K85	4.17258	-1.98354
29	K97	4.25909	6.61427
30	K98	4.64651	9.73883
33	K106	-1.43059	5.91972
34	K114	0.61680	4.01281
35	K127	0.38637	-12.45826
36	K130	-0.99169	1.10736
37	K137	1.76695	-2.17223
38	K142	-0.22826	10.24929
39	K143	6.33623	3.99009
40	K148	0.18197	3.54732
41	K149	-0.05331	4.75073
42	K152	-1.79415	4.41078

	Group	
Variable	Degr	Nondegr
43 K175	-6.98254	-0.37777
44 K181	-0.23633	11.19320
45 K188	7.64662	-4.99037
46 K199	-8.60300	7.77257
48 K318	-0.70588	7.74792
50 K334	-7.01111	4.04462
Constant	-6.33960	-9.75803

APPENDIX E

EXAMPLES OF CALCULATION OF PROBABILITY OF BIODEGRADATION

The following three examples demonstrate the simplicity of the prediction once a compound has been converted into its proper substructural fragments, or Keys. Until additional work is done, the results of this feasibility study may only be applied to compounds containing any of the 39 Keys listed in Appendix D plus the following nonquantified Keys, which were eliminated from the final model for lack of sufficient influence on it: 17, 33, 45, 75, 101, 102. As previously indicated the presence of Keys 22, 138, 139, 141, 145, or 315 has been shown to have an unacceptably variable influence on the model, so that compounds containing one of these as the only "guess" Key should be exempted from the inevitable attempts at extrapolation.

Examples 1 and 2 are drawn from Appendix C - Biodegradable, and 3 from Appendix C - Nonbiodegradable.

Example 1.

Registry Number: 51-28-5
Name: 2,4-Dinitrophenol
Keys: Constant, MW, 3, 65, 97, 137

Step 1. Sum values for each Key from Degr(adable) column in Appendix D:

Constant + (MW + 3 + 65 + 97 + 137)

(-)6.340 + (0.023 + 0.111 + 3.173 + 4.259 + 1.767)

(-)6.340 + (+)9.333 = (+)2.993

Step 2. Repeat Step 1 using values from Nondegr(adable) column:

(-)9.758 + (0.028 + 3.306 + 0.143 + 6.614 + (-)2.172)

(-)9.758 + (10.091 + (-)2.172)

(-)9.758 + (+)7.919 = (-)1.839

Step 3. Insert values from Steps 1 and 2 in the Probability Equation:

P = exp(Step 1)/(exp(Step 1) + exp(Step 2))

P = exp2.993/(exp2.993 + exp(-)1.839)

Step 4. By inspection, the denominator is only slightly larger than the numerator, indicating P is 0.9 - 0.99, i.e., a high probability of degradation

Example 2.

Registry Number: 490-79-9
Name: 2,5-Dihydroxybenzoic Acid
Keys: Constant, MW, 66, 69, 97, 137

Step 1.

(-)6.340 + (0.023 + 1.522 + 1.587 + 4.259 + 1.767)

(-)6.340 + (+)9.158 = 2.818

Step 2.

(-)9.758 + (0.028 + (-)0.074 + (-)0.519 + 6.614 + (-)2.172)

(-)9.758 + (+)3.877 = (-)5.881

Step 3.

P = exp2.818/(exp2.818 + exp(-)5.881)

Step 4. By inspection, again, the denominator is only slightly larger than the numerator, so the compound should be highly degradable.

Example 3.

Registry Number: 609-99-4
Name: 3,5-Dinitro-2-hydroxybenzoic Acid
Keys: Constant, MW, 3, 65, 69, 97, 137, 199

Step 1.

(-)6.340 + (0.023 + 0.111 + 3.173 + 1.587 + 4.259 + 1.767 + (-)8.603)

(-)6.340 + (10.920 + (-)8.603)

(-)6.340 + (+)2.317 = (-)4.023

Step 2.

(-)9.758 + (0.028 + 3.306 + 0.143 + (-)0.519 + 6.614 + (-)2.172 + 7.773)

(-)9.758 + (17.864 + (-)2.691)

(-)9.758 + (+)15.173 = 5.415

Step 3.

P = exp(-)4.023/(exp(-)4.023 + exp5.415)

Step 4. By inspection, the denominator is much larger than the numerator, indicating P is closer to 0.1 than to 0.9, i.e., a low probability of degradation.

In some cases the inspection method of handling Step 3 will not work and calculation of the exponential terms will have to be carried out.

APPENDIX F

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable Compounds

Name	CAS
Acetaldehyde	75-07-0
Acetamide, N-(4-aminophenyl)-	122-80-5
Acetamide, 2,2-dichloro-N-(2-hydroxy-1-(hydroxymethyl)-2-(4-nitrophenyl)ethyl)-, (R-R*,R*))-	56-75-7
Acetamide, N-phenyl-	103-84-4
Acetanilide	103-84-4
Acetic acid	64-19-7
Acetic acid, (2,4-dichlorophenoxy)-	94-75-7
Acetic acid, (2,4,5-trichlorophenoxy)-	93-76-5
Adipic acid, diheptyl ester	14697-48-4
Adipic acid, dinonyl ester	151-32-6
Adipic ketone	120-92-3
L-Alanine	56-41-7
Aldrin	309-00-2
4-Aminoacetanilide	122-80-5
2-Aminoacetic acid	56-40-6
2-Aminobenzoic acid	118-92-3
3-Aminobenzoic acid	99-05-8

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category -Biodegradable Compounds

Name	CAS
4-Aminobenzoic acid	150-13-0
Aminodiacetic acid	142-73-4
2-Aminoethanephosphonic acid	2041-14-7
2-Amino-3-hydroxypropanoic acid	56-45-1
2-Aminopentanedioic acid	56-86-0
2-Aminophenol	95-55-6
3-Aminophenol	591-27-5
p-Aminophenylacetic acid	1197-55-3
(3-Aminopropyl)phosphonic acid	13138-33-5
L-Aminosuccinic acid	56-84-8
Amphenicol	56-75-7
Aniline	62-53-3
L-Asparagine	70-47-3
L-Aspartic acid	56-84-8
2H-Azepin-2-one, hexahydro-	105-60-2
1H-Azepine-1-carbothioic acid, hexahydro-, S-ethyl ester	2212-67-1
Azole	109-97-7
Benzaldehyde, 2-hydroxy-	90-02-8
Benzaldehyde, 2-nitro-	552-89-6
Benzaldehyde, 3-nitro-	99-61-6
Benzaldehyde, 4-nitro-	555-16-8
Benzamide	55-21-0

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category- Biodegradable Compounds

Name	CAS
Benzamide, N-(4-chlorophenyl)-N-[(dimethylamino)carbonyl]-	13113-43-4
Benzamide,N-(3,4-dichlorophenyl)-N-[(dimethylamino)carbonyl]-	3134-12-1
Benzamide, N-(3,4-dichlorophenyl)-N-[(dimethylamino)carbonyl] -4-methoxy-	2689-43-2
Benzenamine	62-53-3
Benzenamine, 2-chloro-	95-51-2
Benzenamine, 3-chloro-	108-42-9
Benzenamine, 2,3-dimethyl-	87-59-2
Benzenamine, 2,5-dimethyl-	95-78-3
Benzenamine, 3,4-dimethyl-	95-64-7
Benzenamine, 2-methyl-	95-53-4
Benzenamine, 3-methyl-	108-44-1
Benzenamine, 4-methyl-	106-49-0
Benzene, 1-chloro-4-(phenylmethyl)-	831-81-2
Benzene, 1,1'-ethenylidenebis-	530-48-3
Benzene, 1,1'-ethylidenebis-	612-00-0
gamma-Benzene hexachloride	58-89-9
Benzene, 1-methyl-2-nitro-	88-72-2
Benzene, 1-methyl-3-nitro-	99-08-1
Benzene, 1-methyl-4-nitro-	99-99-0
Benzene, 1,1'-methylenebis-	101-81-5
Benzene, 1,1'-methylenebis(4-nitro-	1817-74-9

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable Compounds

Name	CAS
Benzene, nitro-	98-95-3
Benzene, 1,1'-(2,2,2-trichloroethylidene)bis(4-methoxy-	72-43-5
Benzeneacetaldehyde, alpha-phenyl-	947-91-1
Benzeneacetic acid	103-82-2
Benzeneacetic acid, 4-amino-	1197-55-3
Benzeneacetic acid, 4-hydroxy-	156-38-7
Benzeneacetic acid, 4-methoxy-	104-01-8
1,3-Benzenediamine	108-45-2
1,4-Benzenediamine	106-50-3
1,2-Benzenedicarboxylic acid	88-99-3
1,3-Benzenedicarboxylic acid	121-91-5
1,4-Benzenedicarboxylic acid	100-21-0
1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl)ester	117-81-7
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	84-69-5
1,2-Benzenedicarboxylic acid, 2-butoxyethyl butyl ester	33374-28-6
1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	85-68-7
1,2-Benzenedicarboxylic acid, dibutyl ester	84-74-2
1,2-Benzenedicarboxylic acid, diethyl ester	84-66-2
1,2-Benzenedicarboxylic acid, diheptyl ester	3648-21-3
1,2-Benzenedicarboxylic acid, dimethyl ester	131-11-3
1,2-Benzenedicarboxylic acid, dinonyl ester	84-76-4
1,2-Benzenedicarboxylic acid, dioctyl ester	117-84-0

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable Compounds

Name	CAS
1,2-Benzenedicarboxylic acid, diundecyl ester	3648-20-2
1,2-Benzenedicarboxylic acid, 4-hydroxy-	610-35-5
1,2-Benzenedicarboxylic acid, monobutyl ester	131-70-4
1,2-Benzenediol	120-80-9
1,3-Benzenediol	108-46-3
1,4-Benzenediol	123-31-9
1,2-Benzenediol, 4-chloro-	2138-22-9
1,2-Benzenediol, 3,5-dichloro-	13673-92-2
1,2-Benzenediol, 4-ethyl-	1124-39-6
1,2-Benzenediol, 3-methyl-	488-17-5
1,2-Benzenediol, 4-methyl-	451-86-8
Benzenemethanaminium, N-hexadecyl-N,N-dimethyl-, chloride	122-18-9
Benzenemethanaminium, N,N-dimethyl-N-octadecyl-, chloride	122-19-0
Benzenemethanaminium, N,N-dimethyl-N-tetradecyl-, chloride	139-08-2
Benzenemethanol, alpha-phenyl-	91-01-0
Benzenemethanol, 4-chloro-alpha-(4-chlorophenyl-alpha-(trichloromethyl)-	115-32-2
Benzenesulfinic acid	618-41-7
Benzenesulfonic acid	98-11-3
Benzenesulfonic acid, 4-amino-	121-57-3
Benzenesulfonic acid, 2,2'-(biphenyl)4,4'-diyldi-2,1-ethenediyl)bis-	38775-22-3
Benzenesulfonic acid, 4-butyl-	18521-59-0

APPENDIX F (Continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable Compounds

Name	CAS
Benzenesulfonic acid, 2,2'-(1,2 ethenediyl)bis(5-((4-((2-hydroxyethyl)methylamino 6-(phenylamino)-1,3,5-triazin-2-yl)amino)-	52435-15-1
Benzenesulfonic acid, 4-ethyl-	98-69-1
Benzenesulfonic acid, 4-hydroxy-	98-67-9
Benzenesulfonic acid, 4-methyl-	104-15-4
Benzenesulfonic acid, 4-(1-methylethyl)-	16066-35-6
Benzenesulfonic acid, 4-propyl-	15592-74-2
Benzenesulfonic acid, 4-undecyl-	39156-49-5
Benzenetriol	108-73-6
Benzidine	92-87-5
Benzoic acid, 2-amino-	118-92-3
Benzoic acid, 3-amino-	99-05-8
Benzoic acid, 4-amino-	150-13-0
Benzoic acid, 3-bromo-	585-76-2
Benzoic acid, 4-bromo-	586-76-5
Benzoic acid, 3-chloro-	535-80-8
Benzoic acid, 4-chloro-	74-11-3
Benzoic acid, 2,4-dichloro-	50-84-0
Benzoic acid, 3,5-dichloro-	51-36-5
Benzoic acid, 2,5-dihydroxy-	490-79-9
Benzoic acid, 3,4-dihydroxy-	99-50-3
Benzoic acid, 3,4-dimethyl-	619-04-5

APPENDIX F (Continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable Compounds

Name	CAS
Benzoic acid, 3,5-dimethyl-	499-06-9
Benzoic acid, 2-fluoro-	445-29-4
Benzoic acid, 3-fluoro-	455-38-9
Benzoic acid, 4-fluoro-	456-22-4
Benzoic acid, 2-hydroxy-	69-72-7
Benzoic acid, 2-hydroxy-, methyl ester	119-36-8
Benzoic acid, 3-iodo-	618-51-9
Benzoic acid, 3-methyl-	99-04-7
Benzoic acid, 2-nitro-	552-16-9
Benzoic acid, 3-nitro-	121-92-6
Benzoic acid, 4-nitro	62-23-7
Benzoic acid, 3,4,5-trihydroxy-	149-91-7
Benzonitrile, 3,4-dihydroxy-	17345-61-8
Benzonitrile, 2-hydroxy-	611-20-1
Benzonitrile, 3-hydroxy-	873-62-1
Benzonitrile, 4-hydroxy-	767-00-0
Benzophenone	119-61-9
2H-1-Benzopyran-2-one, 6-(beta-D-glucopyranosyloxy)-7-hydroxy-	531-75-9
2,3-Benzopyrrole	120-72-9
Benzuron	3134-12-1
4-Benzylphenol	101-53-1
Besylic acid	98-11-3

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable Compounds

Name	CAS
Bicyclo(2.2.1)heptan-2-ol, 1,7,7-trimethyl-, endo	507-70-5
(1,1'-Biphenyl)-4,4'-diamine	92-87-5
(1,1'-Biphenyl-2-ol	90-43-7
Bis(2-ethylhexyl) adipate	103-23-1
Bis(2-ethylhexyl) 1,2-benzenedicarboxylate	117-81-7
4,4'-Bis(2-sulfostyrl)biphenyl	38775-22-3
Borneol	507-70-0
3-Bromobenzoic acid	585-76-2
Butanal	123-72-8
Butanoic acid	107-92-6
Butanoic acid, 3-chloro-	1951-12-8
Butanedioic acid	110-15-6
Butanedioic acid, (carboxymethoxy)-	38945-27-6
Butanedioic acid, chloro-	16045-92-4
Butanedioic acid, 2,3-dihydroxy-	87-69-4
1,4-Butanediol	110-63-4
1-Butanol	71-36-3
2-Butanol	78-92-2
2-Butenoic acid, (E)-	107-93-7
2-Butenoic acid, (Z)-	503-64-0
Butoxyethyl butyl phthalate	33374-28-6
Butyl alcohol	71-36-3

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable Compounds

Name	CAS
Butyl benzyl phthalate	85-68-7
Butyl hydrogen phthalate	131-70-4
Butyl phthalate	84-74-2
4-Butylbenzenesulfonic acid	18521-59-0
Butyraldehyde	123-72-8
Butyric acid	107-92-6
Carbamic acid, methyl-, 4-chlorophenyl ester	2620-53-3
Carbamic acid, phenyl-, 1-methylethyl ester	122-42-9
Capric acid	334-48-5
Caproic acid	142-62-1
Caprolactam	105-60-2
3-Carboxylpyridine	59-67-6
(Carboxymethoxy)malonic acid	55203-12-8
Carboxymethyloxysuccinic acid	38945-27-6
4-Carboxypyridine	55-22-1
Cetane	544-76-3
Cetyltrimethylammonium chloride	112-02-7
Chloramphenicol	56-75-7
Chloridazon	1698-60-8
2-Chloroaniline	95-51-2
3-Chloroaniline	108-42-9
3-Chlorobenzoic acid	535-80-8

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable Compounds

Name	CAS
4-Chlorobenzoic acid	74-11-3
4-Chlorobenzophenone	134-85-0
3-Chlorobutyric acid	1951-12-8
3-Chlorocrotonic acid	6214-28-4
cis-3-Chlorocrotonic acid	6213-90-7
p-Chlorodiphenylmethane	831-81-2
2-Chloro-4-nitrophenol	619-08-9
4-Chlorophenyl methylcarbamate	2620-53-3
Chloromycetin	56-75-7
3-Chloropropionic acid	107-94-8
4-Chloropyrocatechol	2138-22-9
2-Chlorosuccinic acid	16045-92-4
Citric acid	77-92-9
3-Cresol	108-39-4
Crotonic acid, (E)	107-93-7
Crotonic acid, (Z)	503-64-0
Crotonic acid, 3-chloro- (E)	6214-28-4
Crotonic acid, 3-chloro-, (Z)	6213-90-7
Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1alpha,2alpha,3beta,4alpha,5alpha,6beta)-	58-89-9
1,2-Cyclohexanediol	931-17-9
Cyclohexanol	108-93-0

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1alpha,2beta,5alpha)-	89-78-1
Cyclohexanone	108-94-1
Cyclohexanone, 4-methyl-	589-92-4
Cyclopentanol	96-41-3
Cyclopentanone	120-92-3
Cysteine	52-90-4
Decane	124-18-5
Decanoic acid	334-48-5
Dextrose	50-99-7
1,4-Diaminobenzene	106-5--3
2,4-Diaminophenol	95-86-3
2,4-Diamino-1,3,5-triazin-6-one	645-92-1
1,3-Diazole	288-32-4
Dibutylacetic acid	3115-28-4
2,4-Dichlorobenzoic acid	50-84-0
3,5-Dichlorobenzoic acid	51-36-5
4,4'-Dichlorobenzophenone	90-98-2
2,4-Dichlorophenol	120-83-2
2,6-Dichlorophenol	87-65-0
(2,4-Dichlorophenoxy)acetic acid	94-75-7
Dichloropyrocatechol	13673-92-2

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Diethanolamine	111-42-2
Diethion	563-12-2
Diethylene glycol	111-46-6
Diheptyl adipate	14697-48-4
Diheptyl phthalate	3648-21-3
Dihexyl adipate	110-33-8
3,4-Dihydroxybenzoic acid	99-50-3
2.5-Dihydroxybenzoic acid	490-79-9
3,4-Dihydroxybenzonitrile	17345-61-8
1,4-Dihydroxybutane	110-63-4
1,2-Dihydroxynaphthalene	574-00-5
Diisobutyl phthalate	84-69-5
1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a,-hexahydro-, (1alpha,4alpha,4abeta,5alpha,8alpha,8abeta)-	309-00-2
4,4'-Dimethoxybenzophenone	90-96-0
2,3-Dimethylanilihe	87-59-2
2,5-Dimethylaniline	95-87-3
3,4-Dimethylaniline	95-64-7
3,4-Dimethylbenzoic acid	619-04-5
3,5-Dimethylbenzoic acid	499-06-9
Dimethylbenzyloctadecylammonium chloride	122-19-0
Dimethyldistearylammonium chloride	107-64-2

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
2,3-Dimethylphenol	526-75-0
2,4-Dimethylphenol	105-67-9
2,5-Dimethylphenol	95-87-4
2,6-Dimethylphenol	576-26-1
3,4-Dimethylphenol	95-65-8
Dimethyl phthalate	131-11-3
4,4'-Dinitrodiphenylmethane	1817-74-9
2,4-Dinitrophenol	51-28-5
Di-n-octyl phthalate	117-84-0
2,2-Diphenylacetaldehyde	947-91-1
1,1-Diphenylethane	612-00-0
1,1-Diphenylethylene	530-48-3
Diphenyl 2-ethylhexyl phosphate	1241-94-7
Diphenylmethane	101-81-5
Diphenyl p-tolyl phosphate	78-31-9
Diundecyl phthalate	3648-20-2
1-Dodecanaminium, N,N,N-trimethyl-, chloride	112-00-5
Dodecanoic acid	143-07-7
1-dodecanol	112-53-8
Dodecyl hexaethylene glycol	3055-96-7
Dodecyl sulfate	151-41-7
Dodecyl triethylene glycol	3055-94-5

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Dodecyltrimethylammonium chloride	112-00-5
Esculin	531-75-9
Ethanaminium, N,N,N-trimethyl-, chloride	27697-51-4
1,2-Ethanediamine	107-15-3
Ethanedioic acid	144-62-7
1,2-Ethanediol	107-21-1
Ethanoic acid	64-19-7
Ethanol	64-17-5
Ethanol, 2-(dodecyloxy)-	4536-30-5
Ethanol, 2-(2-(2-(dodecyloxy)ethoxy)ethoxy)-	3055-94-5
Ethanol, 2,2'-iminobis-	111-42-2
Ethanol, 2,2'-oxybis-	111-46-6
Ethanone, 1-(4-nitrophenyl)-	100-19-6
Ethyl alcohol	64-17-5
Ethyl aldehyde	75-07-0
O-Ethyl S,S-diphenyl phosphorodithioate	17109-49-8
O-Ethyl ethylphosphonate	7305-61-5
Ethyl parathion	56-38-2
2-Ethylamino-4-isopropylamino-6-methylthio-s-triazine	834-12-8
4-Ethylbenzenesulfonic acid	98-69-1
Ethylene glycol	107-21-1
Ethylene glycol dodecyl ether	4536-30-5

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Ethylenediamine	107-15-3
Ethylphosphonic acid	6779-09-5
4-Ethylpyrocatechol	1124-39-6
2-Fluorobenzoic acid	445-29-4
3-Fluorobenzoic acid	455-38-9
4-Fluorobenzoic acid	456-22-4
Formic acid	64-18-6
D-Fructose	57-48-7
2-Furancarboxaldehyde	98-01-1
2-Furanmethanol	98-00-0
2-Furanmethanol, tetrahydro-	97-99-4
2-Furfuraldehyde	98-01-1
Furfuryl alcohol	98-00-0
Gallic acid	149-91-7
alpha-D-Glucopyranoside, beta-D-fructofuranosyl	57-50-1
D-Glucose	50-99-7
L-Glutamic acid	56-86-0
Glycerol	56-81-5
Glycine	56-40-6
Glycine, N-(carboxymethyl)-	142-73-4
Glycine, N-(carboxymethyl)-N-(2-hydroxyethyl)-	93-62-9
Glycine, N-(carboxymethyl)-N-methyl-	4408-64-4

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Glycine, N, N-bis(carboxymethyl)-	139-13-9
Heptaethylene glycol dodecyl ether	3055-97-8
3,6,9,12,15,18,21-Heptaoxatritriacontan-1-ol	3055-97-8
Hexachlorophene	70-30-4
1-Hexadecanaminium, N,N,N-trimethyl-, chloride	112-02-7
Hexadecane	544-76-3
Hexadecanoic acid, 1-methylethyl ester	142-91-6
Hexadecyldimethylbenzylammonium chloride	122-18-9
Hexadecylpyridinium bromide	140-72-7
Hexahydropyridine	110-89-4
Hexane	110-54-3
Hexanedioic acid, dinonyl ester	151-32-6
Hexanedioic acid, dihexyl ester	110-33-8
Hexanedioic acid, bis(2-ethylhexyl) ester	103-23-1
Hexanoic acid	142-62-1
Hexanoic acid 2-butyl-	3115-28-4
Hexanoic acid, 2-ethyl-	149-57-5
Hexanoic acid, 2-methyl-	4536-23-6
Hexanoic acid, 2-propyl-	3274-28-0
Hexanon	108-94-1
3,6,9,12,15,18-Hexaoxatriacontan-1-ol	3055-96-7

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Histidine	71-00-1
Hydroquinone	123-31-9
4-Hydroxyaniline	123-30-8
4-Hydroxybenzenesulfonic acid	98-67-9
2-Hydroxybenzoic acid	69-72-7
2-Hydroxybenzonitrile	611-20-1
3-Hydroxybenzonitrile	873-62-1
4-Hydroxybenzonitrile	767-00-0
4-Hydroxybenzophenone	1137-42-4
2-Hydroxybiphenyl	90-43-7
2-Hydroxybutane	78-92-2
Hydroxycyclohexane	108-93-0
Hydroxycyclopentane	96-41-3
Hydroxydiphenylmethane	91-01-0
Hydroxyethylaminodiacetic acid	93-62-9
Hydroxynaphthalene	90-15-3
2-Hydroxynaphthalene	135-19-3
2-Hydroxyphenol	120-80-9
(4-Hydroxyphenyl)acetic acid	156-38-7
4-Hydroxyphthalic acid	610-35-5
1H-Imidazole	288-32-4
1H-Indole	120-72-9

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
3-Iodobenzoic acid	618-51-9
1H-Isoindole-1,3(2H)-dione	85-41-6
L-Isoleucine	73-32-5
Isophthalic acid	121-91-5
Isopropanol	67-63-0
Isopropyl carbanilate	122-42-9
Isopropyl palmitate	142-91-6
4-Isopropylbenzenesulfonic acid	16066-35-6
Kelthane	115-32-2
Lauryl alcohol	112-53-8
L-Leucine	61-90-5
Lindane	58-89-9
Menthol	89-78-1
Methanaminium, N.N,N-trimethyl-, chloride	75-57-0
Methanoic acid	64-18-6
Methanone, bis(4-chlorophenyl)-	90-98-2
Methanone, (4-chlorophenyl)phenyl-	134-85-0
Methanone, diphenyl-	119-61-9
Methanone, (4-hydroxyphenyl)phenyl-	1137-42-4
Methanone, bis(4-methoxyphenyl)-	90-96-0
Methanone, (4-methoxyphenyl)phenyl-	611-94-9
4-Methoxybenzophenone	611-94-9

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Methoxychlor	72-43-5
(4-Methoxyphenyl)acetic acid	104-01-8
Methyl linolenate	301-00-8
Methyl salicylate	119-36-8
Methyl stearate	112-61-8
2-Methylaniline	95-53-4
3-Methylaniline	108-44-1
4-Methylaniline	106-49-0
3-Methylbenzoic acid	99-04-7
3-Methylcatechol	488-17-5
4-Methylcatechol	452-86-8
4-Methylcyclohexanone	589-92-4
2,2'-Methylenebis(4-chlorophenol)	97-23-4
2-Methylhexanoic acid	4536-23-6
Methylimidodiacetic acid	4408-64-4
2-Methylnitrobenzene	88-72-2
2-Methylpentadecanoic acid	25354-92-1
2-Methylphenol	95-48-7
3-Methylphenol	108-39-4
2-Methylphenyl diphenyl phosphate	5254-12-6
Methylphosphonic acid	993-13-5
3-Methyltetradecane	18435-22-8

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Myristic acid, isopropyl ester	110-27-0
N-(4-Isopropylphenyl)-N',N'-dimethylurea	34123-59-6
1,2-Naphthalenediol	574-00-5
1-Naphthalenesulfonic acid	85-47-2
2-Naphthalenesulfonic acid, 1-hydroxy-	567-18-0
1-Naphthalenol	90-15-3
2-Naphthalenol	135-19-3
1-Naphthol-2-sulfonic acid	567-18-0
Nicotinic acid	59-67-6
Nitrilotriacetic acid	139-13-9
4'-Nitroacetophenone	100-19-6
2-Nitrobenzaldehyde	552-89-6
3-Nitrobenzaldehyde	99-61-6
4-Nitrobenzaldehyde	555-16-8
Nitrobenzene	98-95-3
2-Nitrobenzoic acid	552-16-9
3-Nitrobenzoic acid	121-92-6
4-Nitrobenzoic acid	62-23-7
2-Nitrophenol	88-75-5
3-Nitrophenol	554-84-7
4-Nitrophenol	100-02-7
2-Nitrotoluene	88-72-2

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
3-Nitrotoluene	99-08-1
4-Nitrotoluene	99-99-0
Nonaethylene glycol monododecyl ether	3055-99-0
3,6,9,12,15,18,21,24,27-Nonaoxanonatriacontan-1-ol	3055-99-0
Nonyl phthalate	84-76-4
1-Octadecanaminium, N,N-dimethyl-N-octadecyl-, chloride	107-64-2
1-Octadecanaminium, N,N,N-trimethyl-, chloride	112-03-8
Octadecanoic acid	57-11-4
Octadecanoic acid, methyl ester	112-61-8
9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-	301-00-8
Octadecyltrimethylammonium chloride	112-03-8
Oxalic acid	144-62-7
Parathion	56-38-2
Pentachlorophenol	87-86-5
Pentadecanoic acid	1002-84-2
Pentadecanoic acid, 2-methyl-	25354-92-1
Pentadecanoic acid, 2-propyl-	32815-53-5
Pentadecylic acid	1002-84-2
Pentaethylene glycol dodecyl ether	3055-95-6
3,6,9,12,15-Pentaoxaheptacosan-1-ol	3055-95-6
Phenol, 2-amino-	95-55-6
Phenol, 3-amino-	591-27-5

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Phenol, 4-amino-	123-30-8
Phenol, 2-chloro-4-nitro-	619-08-9
Phenol, 2,4-diamino-	95-86-3
Phenol, 2,4-dichloro-	120-83-2
Phenol, 2,6-dichloro-	87-65-0
Phenol, 2,3-dimethyl-	526-75-0
Phenol, 2,4-dimethyl-	105-67-9
Phenol, 2,5-dimethyl-	95-87-4
Phenol, 2,6-dimethyl-	576-26-1
Phenol, 3,4-dimethyl-	95-65-8
Phenol, 2,4-dinitro-	51-28-5
Phenol, 2-methyl-	95-48-7
Phenol, 3-methyl-	108-39-4
Phenol, 5-methyl-2-(1-methylethyl)-	89-83-8
Phenol, 2,2'-methylenebis(3,4,6-trichloro-	70-30-4
Phenol, 2,2'-methylenebis(4-chloro-	97-23-4
Phenol, 2-nitro-	88-75-5
Phenol, 3-nitro-	554-84-7
Phenol, 4-nitro-	100-02-7
Phenol, pentachloro-	87-86-5
Phenol, 4-(phenylmethyl)-	101-53-1
Phenol, 2,2'-thiobis(4,6-dichloro-	97-18-7

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Phenol, 2,4,5-trichloro-	95-95-4
Phenol, 2,4,6-trichloro-	88-06-2
Phenylacetic acid	103-82-2
Phenylcarboxyamide	55-21-0
1,3-Phenylenediamine	108-45-2
Phenylsulfinic acid	618-41-7
Phloroglucinol	108-73-6
Phosphonic acid, (2-aminoethyl)-	2041-14-7
Phosphonic acid, (2-((3-amino-1-oxopropyl)amino)ethyl)-	59957-50-5
Phosponic acid, (3-aminopropyl)-	13138-33-5
Phosphonic acid, ethyl-	6779-09-5
Phosphonic acid, ethyl-, monoethyl ester	7305-61-5
Phosphonic acid, methyl-	993-13-5
Phosphonic acid, methyl-, mono(1-methylethyl)ester	1832-54-8
Phosphoric acid, dibutyl phenyl ester	2528-36-1
Phosphoric acid, 2-ethylhexyl diphenyl ester	1241-94-7
Phosphoric acid, 2-methylphenyl diphenyl ester	5254-12-6
Phosphoric acid, 4-methylphenyl diphenyl ester	78-31-9
Phosphoric acid, tributyl ester	126-73-8
Phosphoric acid, triphenyl ester	115-86-6
Phosphoric acid, tris(2-methylphenyl) ester	78-30-8
Phosphoric acid, tris(3-methylphenyl) ester	563-04-2

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Phosphoric acid, tris(4-methylphenyl) ester	78-32-0
Phosphorothioic acid, O,O-diethyl O-(4-nitrophenyl) ester	56-38-2
Phosphorodithioic acid, O-ethyl S,S-diphenyl ester	17109-49-8
Phosphorodithioic acid, S,S'-methylene O,O,O',O'-tetraethyl ester	563-12-2
Phthalic acid	88-99-3
Phthalimide	85-41-6
Piperidine	110-89-4
L-Proline	147-85-3
Propanedioic acid, (carboxymethoxy)-	55203-12-8
1,2,3-Propanetricarboxylic acid, 2-hydroxy-	77-92-9
1,2,3-Propanetriol	56-81-5
Propanoic acid	79-09-4
Propanoic acid, 3-chloro-	107-94-8
Propanoic acid, 2-oxo-	127-17-3
Propanoic acid, 2-(2,4,5-trichlorophenoxy)-	93-72-1
1-Propanol	71-23-8
2-Propanol	67-63-0
Propionic acid	79-09-4
Propyl alcohol	71-23-8
2-Propylpentadecanoic acid	32815-53-5
3(2H)-Pyridazinone, 5-amino-4-chloro-2-phenyl-	1698-60-8

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
3-Pyridinecarboxylic acid	59-67-6
4-Pyridinecarboxylic acid	55-22-1
Pyridinium, 1-hexadecyl-, bromide	140-72-7
Pyridinium, 1-tetradecyl-, chloride	2785-54-8
2,4(1H,3H)-Pyrimidinedione	66-22-8
Procatechitol	931-17-9
1H-Pyrrole	109-97-7
2-Pyrrolidinecarboxylic acid	147-85-3
Pyruvic acid	127-17-3
Resorcinol	108-46-3
L-Serine	56-45-1
Silvex	93-72-1
Simazine	122-34-9
Stearic acid	57-11-4
Succinic acid	110-15-6
Sucrose	57-50-1
Sulfanilic acid	121-57-3
Sulfuric acid, monododecyl ester	151-41-7
Terephthalic acid	100-21-0
1,13-Tetradecadiene	21964-49-8
Tetradecane	629-59-4
Tetradecane, 3-methyl-	18435-22-8

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Tetradecanoic acid, 1-methylethyl ester	110-27-0
1-Tetradecene	1120-36-1
7-Tetradecene	10374-74-0
Tetradecyldimethylbenzylammonium chloride	139-08-2
Tetrahydrofurfuryl alcohol	97-99-4
Tetramethylammonium chloride	75-57-0
2,2'-Thiobis(4,6-dichlorophenol)	97-18-7
Thymol	89-83-8
o-Toluidine	95-53-4
2,4,5-TP	93-72-1
1,3,5-Triazin-2(1H)-one, 4,6-diamino-	645-92-1
1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-diethyl-	122-34-9
1,3,5-Triazine-2,4-diamine, N-ethyl-6-methoxy-N'-(1-methylethyl)-	1610-17-9
1,3,5-Triazine-2,4-diamine, N-ethyl-N'-(methylethyl)-6-(methylthio)-	834-12-8
s-Triazine, 2-(ethylamino)-4-(isopropylamino)-6-methoxy-	1610-17-9
Tributyl phosphate	126-73-8
2,4,5-Trichlorophenol	95-95-4
2,4,6-Trichlorophenol	88-06-2
(2,4,5-Trichlorophenoxy)acetic acid	93-76-5
2,4,5-Trichlorophenoxypropionic acid	93-72-1
Tri-m-cresyl phosphate	563-04-2

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Biodegradable

Name	CAS
Trimethylethylammonium chloride	27697-51-4
Triphenyl phosphate	115-86-6
Tris(o-cresyl) phosphate	78-30-8
Tris(p-cresyl) phosphate	78-32-0
L-Tryptophan	73-22-3
p-Undecylbenzenesulfonic acid	39156-49-5
Uracil	66-22-8
Urea, 1-p-anisoyl-1-(3,4-4dichlorophenyl)-3,3-dimethyl-	2689-43-2
Urea, N-(3,4-dichlorophenyl)-N,N'-dimethyl-	17495-49-7
Urea, N,N-dimethyl-N'-(4-(1-methylethyl)phenyl)-	34123-59-6
L-Valine	72-18-4

APPENDIX F (Continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable Compounds

Name	CAS
1,2-Aminoazophenylene	95-14-7
2-Aminobenzothiazole	136-95-8
1-Amino-6-naphthalenesulfonic acid	119-79-9
Ammonium, trimethyl-9-octadecenyl-, chloride,(Z)	10450-69-8
7-Aza-7H-dibenzo(c,g)fluorene	194-59-2
Azoic acid	1562-93-2
Benzamide, 2,6-dichloro-	2008-58-4
2,3-Benzanthracene	92-24-0
Benzenamine, 2-nitro-	88-74-4
Benzene, 1,1'-(dichloroethenylidene)bis(4-chloro-	72-55-9
Benzene, 1,1'-(2,2-dichloroethylidene)bis(4-chloro-	72-54-8
Benzene, 1,3-dinitro-	99-65-0
Benzene, 1,4-dinitro-	100-25-4
Benzene, 1,1',1'',1'''-(oxydimethylidyne)tetrakis-	574-42-5
Benzene, 1,1'-(2,2,2-trichloroethylidene)bis-	2971-22-4
Benzeneacetic acid, alpha-phenyl-	117-34-0
Benzeneacetic acid, 4-chloro-alpha-(4-chlorophenyl)-	83-05-6
Benzeneacetic acid, 4-methyl-	622-47-9

APPENDIX F (Continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable Compounds

Name	CAS
Benzeneacetic acid, 4-nitro-	104-03-0
Benzenemethanaminium, N,N-dimethyl-N-(2-(4-(1,1,3,3-tetramethylbutyl)phenoxy)ethoxy)-ethyl)-, chloride	121-54-0
Benzenemethanol, 4-chloro-alpha-(4-chlorophenyl)-	90-97-1
Benzenemethanol, 4-chloro-alpha-phenyl-	119-56-2
Benzenemethanol, 4-methoxy-alpha-(4-methoxyphenyl)-	728-87-0
Benzenesulfonic acid, 3-amino-	121-47-1
Benzenesulfonic acid, p-((p-methoxyphenyl)azo)-,sodium salt	19218-78-1
Benzethonium chloride	121-54-0
Benzoic acid, 2-hydroxy-3,5-dinitro-	609-99-4
Benzoic acid, 4-(phenylazo)-	1562-93-2
Benzoic acid, p-(phenylazo)-, ethyl ester	7508-68-1
Benzo(1)phenanthrene	217-59-4
2-Benzothiazolamine	136-95-8
Benzothiazole, 2-(methylthio)-	615-22-5
6-Benzothiazolecarboxylic acid, 2-(4-nitrophenyl)-	65644-51-1
6-Benzothiazolesulfonamide, 2-amino-	18101-58-1
2-Benzothiazolesulfonic acid	941-57-1
2(3H)-Benzothiazolethione	149-30-4
2(3H)-Benzothiazolone, hydrazone	615-21-4
1H-Benzotriazole	95-14-7

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable Compounds

Name	CAS
1,1'-Biphenyl, 2,2',3,3',4,4',5,5',6,6'-decachloro-	2051-24-3
1,1'-Biphenyl, 2,2',3,4,4,4'-hexachloro-	52712-04-6
1,1'-Biphenyl,2,2',3,4,5'-pentachloro-	38380-02-8
2,2'-Bipyridine	366-18-7
Bis(4-chlorophenyl)hydroxymethane	90-97-1
Bis(diphenylmethyl) ether	574-42-5
Bis(p-hydroxyphenyl)methane	620-92-8
Bis(p-methoxyphenyl)carbinol	728-87-0
4-Chlorobenzhydrol	119-56-2
Chloroform	67-66-3
1,2,3,4-Cyclopentanetetracarboxylic acid	3724-52-5
DDD	72-54-8
DDE	72-55-9
Decachlorobiphenyl	2051-24-3
5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-	126-86-3
Diazinon	333-41-5
Dibenz(de,kl)anthracene	198-55-0
7H-Dibenzo(c,g)carbazole	194-59-2
2,6-Dichlorobenzamide	2008-58-4
Dichlorodiphenylacetic acid	83-05-6
1,4-Diisobutyl-1,4-dimethylbutynediol	126-86-3

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable Compounds

Name	CAS
Dimethyl sulfoxide	67-68-5
Dimethylformamide	68-12-2
1,3-Dinitrobenzene	99-65-0
1.4-Dinitrobenzene	100-25-4
3,5-Dinitro-2-hydroxybenzoic acid	609-99-4
2,5-Dinitrophenol	329-71-5
Diphenylacetic acid	117-34-0
2,2-Diphenylethanol	1883-32-5
2,2-Diphenylpropane	778-22-3
Diphenyltrichloroethane	2971-22-4
2,2'-Dipyridine	366-18-7
2,6-Di-tert-butylnaphthalene	3905-64-4
2,7-Di-tert-butylnaphthalene	10275-58-8
Dodecylpyridinium iodide	3026-66-2
Ethanol, 2,2-diphenyl-	1883-32-5
Ethene, chloro-	75-01-4
Ethyl 4-(phenylazo) benzoate	7508-68-1
Formamide, N,N-dimethyl-	68-12-2
2,2', 3,4,5,5'-Hexachlorobiphenyl	52712-04-6
Hexanoic acid, 6-amino-, methyl ester, hydrochloride	1926-80-3
2-Hydrazinobenzothiazole	615-21-4

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable Compounds

Name	CAS
2-Mercaptobenzothiazole	149-30-4
Methane, sulfinylbis-	67-68-5
Methane, trichloro-	67-66-3
Methyl 6-aminohexanoate monohydrochloride	1926-80-3
(4-Methylphenyl)acetic acid	622-47-9
2-(Methylthio)benzothiazole	615-22-5
Naphthacene	92-24-0
Naphthalene, 2,6-di-tert-butyl-	3905-64-4
Naphthalene, 2,7-di-tert-butyl-	10275-58-8
Naphthalene, 1-phenyl-	605-02-7
Naphthalene, 1,2,3,4-tetraphenyl-	751-38-2
2-Naphthalenesulfonic acid, 5-amino-	119-79-9
2-Nitroaniline	88-74-4
(4-Nitrophenyl)acetic acid	104-03-0
9-Octadecen-1-aminium, N,N,N-trimethyl-,chloride	10450-69-8
Perylene	198-55-0
Phenanthrene, tetradecahydro-	5743-97-5
Phenol, 2,5-dinitro-	329-71-5
Phenol, 4,4'-methylenebis-	620-92-8
Phenol, 2,3,4,5-tetrachloro-	4901-51-3

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable Compounds

Name	CAS
Phenol, 3,4,5-trichloro-	609-19-8
1-Phenylnaphthalene	605-02-7
Phosphorothioic acid, O,O-diethyl O-(6-methyl-2-(1-methylethyl)-4-pyrimidinyl) ester	333-41-5
Propane, 2,2-diphenyl-	778-22-3
1-Propanol, 2,3-dichloro-, phosphate (3·1)	78-43-3
3H-Pyrazol-3-one, 2-(2-benzothiazolyl)-2,4-dihydro-5-methyl-	17304-62-0
Pyridinium, 1-dodecyl-, iodide	3026-66-2
m-Sulfanilic acid	121-47-1
1,2,3,4-Tetracarboxycyclopentane	3724-52-5
2,3,4,5-Tetrachlorophenol	4901-51-3
1,2,3,4-Tetraphenylnaphthalene	751-38-2
3,4,5-Trichlorophenol	609-19-8
Triphenylene	217-59-4
tris(2,3-dichloropropyl) phosphate	78-43-3
Vinyl chloride	75-01-4

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable/Qualified

Name	CAS
Acrolein	107-02-8
Allylamine	107-11-9
3-(Allyloxy)propanediol	123-34-2
1-Amino-4-naphthalenesulfonic acid	84-86-6
Aminonaphthol sulfonic acid gamma	90-51-7
D-arabino-2-Hexulosonic acid	669-90-9
Benzene, 1,2-bis(1-methylethyl)-	577-55-9
Benzene, 1,3-bis(1-methylethyl)-	99-62-7
Benzene, 1,4-bis(1-methylethyl)-	100-18-5
Benzene, (1,1-dimethylethyl)-	98-06-6
Benzeneacetic acid, alpha-hydroxy-	90-64-2
Benzeneacetic acid, alpha-oxo-	611-73-4
Benzoic acid, 2,3-dihydroxy-	303-38-8
Benzoic acid, 2,4-dihydroxy-	89-86-1
Benzoic acid, 3,4-dimethoxy-	93-07-2
Benzoic acid, 3-methoxy-	586-38-9
Benzoic acid, methyl ester	93-58-3
1,1'-Biphenyl, 2,6-dichloro-	33146-45
1,1'-Biphenyl, 2,2',4,5,5'-pentachloro-	37680-73-2
1,1'-Biphenyl, 2,2',4,4',6-pentachloro-	39485-83-1
1,1'-Biphenyl, 2,2',6,6-tetrachloro-	15968-05-5
1,1'-Biphenyl, 2,2',4,4'-tetrachloro-	2437-79-8

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable/Qualified

Name	CAS
1,1'-Biphenyl, 2,3',4,4'-tetrachloro-	32598-10-0
1,1'-Biphenyl, 3,3',4,4'-tetrachloro-	32598-13-3
1,1'-Biphenyl, 3,2,6-trichloro-	55702-45-9
Butane	106-97-8
Butane, 2,3-dimethyl-	79-29-8
Butane, 2-methyl-	75-85-4
1,2-Butanediol	584-03-2
1,3-Butanediol	107-88-0
2,3-Butanediol	513-85-9
2-Butanol, 2-methyl	75-85-4
t-Butylbenzene	98-06-6
1,2-Butylene glycol	584-03-2
1-Butylimidazole	4316-42-1
1-Chloro-3-bromopropane	109-70-6
1,5,9-Cyclododecatriene	4904-61-4
Cycloheptanecarboxylic acid	1460-16-8
1,3,5-Cycloheptatriene	544-25-2
Cyclohexane, 1,3-dimethyl-	591-21-9
Cyclohexane, 1,4-dimethyl-	589-90-2
Cyclohexane, propyl-	1678-92-8
Cyclohexane, heptyl-	5617-41-4
Cyclohexaneacetic acid	5292-21-7

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable/Qualified

Name	CAS
Cyclohexanebutanoic acid	4441-63-8
Cyclopentane	287-92-3
Cyclopentane, 1,2,4-trimethyl-	2815-58-9
L-Cystine	56-89-3
Diallylamine	124-02-7
2,6-Dichlorobiphenyl	33146-45-1
1,3-Dichloroisopropanol	96-23-1
2,3-Dihydroxbenzoic acid	303-38-8
2,4-Dihydroxbenzoic acid	89-86-1
1,3-Dihydroxybutane	107-88-0
2,3-Dihydroxybutane	513-85-9
1,2-Diisopropylbenzene	577-55-9
1,3-Diisopropylbenzene	99-62-7
1,4-Diisoproylbenzene	100-18-5
3,4-Dimethoxybenzoic acid	93-07-2
1,3-Dimethylcyclohexane	591-21-9
1,4-Dimethylcyclohexane	589-90-2
2,4-Dimethylhexane	589-43-5
2,3-Dimethylpentane	565-59-3
2,6,10-Dodecatrien-1-01, 3,7,11-trimethyl-	4602-84-0
Ethane	74-84-0
Ethylene oxide	75-21-8

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable/Qualified

Name	CAS
Ethynylcarbinol	107-19-7
Farnesyl alcohol	4602-84-0
D-Glucosonic acid	669-90-9
5-Hepten-2-one, 6-methyl-	110-93-0
Heptane, 1-cyclohexyl-	5617-41-4
2-Hexadecenoic acid, 3,7,11,15-tetramethyl-, (R-(R*,R*-(E)))-	22352-56-3
Hexamethylenetetramine	100-97-0
Hexanamide, N-hexyl-	10264-29-6
Hexane, 2,4-dimethyl-	589-43-5
Hexane, 3-methyl-	589-34-4
2-(2-Hydroxyethyl)pyridine	103-74-2
2-Hydroxy-6,8-naphthalenedisulfonic acid	118-32-1
1H-Imidazole, 1-butyl-	4316-42-1
Isobutane	75-28-5
Malachite green	569-64-2
Methanaminium, N-(4-((4-dimethylamino)phenyl)phenylmethylene)-2,5-cyclohexadien-1-ylidene)-N-methyl-, chloride	569-64-2
3-Methoxybenzoic acid	586-38-9
4-Methoxyphenol	150-76-5
Methyl benzoate	93-58-3
2-Methyl-2-hepten-6-one	110-93-0
4-Methyl-4-methoxy-2-pentanone	107-70-0

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable/Qualified

Name	CAS
3-Methylhexane	589-34-4
N-Methylpentanamide	6225-10-1
1,3-Naphthalenedisulfonic acid, 7-hydroxy-	118-32-1
1-Naphthalenesulfonic acid, 4-amino-	84-86-6
2-Naphthalenesulfonic acid, 6-amino-4-hydroxy-	90-51-7
2-Octene	111-67-1
Oxirane	75-21-8
Oxirane, [[(2-ethylhexyl)oxy]methyl]-	2641-15-6
Oxiranemethanaminium, N,N,N-trimethyl-, chloride	3033-77-0
Oxirane, [(2-propenyloxy)methyl]-	106-92-3
1,1'-Biphenyl, 2,2',4,5,5'-pentachloro-	37680-73-2
2,2',4,4',6-Pentachlorobiphenyl	39485-83-1
Pentamethylene	287-92-3
Pentanamide, N-methyl-	6225-10-1
2-Pentanone, 4-methoxy-4-methyl-	107-70-0
Pentane, 2,3-dimethyl-	565-59-3
Phenol, 4-methoxy-	150-76-5
Phenylglyoxylic acid	611-73-4
Phenylhydroxyacetic acid	90-64-2
Propane	74-98-6
Propane, 1-bromo-3-chloro-	109-70-6
Propane, 2-methyl-	75-28-5

APPENDIX F (continued)

ALPHABETICAL LIST OF COMPOUNDS FROM APPENDIX A

Category - Nonbiodegradable/Qualified

Name	CAS
1,2-Propanediol, 3-(2-propenyloxy)-	123-34-2
2-Propanol, 1,3-dichloro-	96-23-1
1-Propanol, 3,3'-oxydi-	2396-61-4
2-Propen-1-amine	107-11-9
2-Propen-1-amine, N-2-propenyl-	124-02-7
2-Propenal	107-02-8
Propylcyclohexane	1678-92-8
2-Propyn-1-ol	107-19-7
2-Pyridineethanol	103-74-2
tert-Amyl alcohol	75-85-4
1,3,5,7-Tetraazatricyclo(3.3.1.1(3,7))decane	100-97-0
2,2',4,4'-Tetrachlorobiphenyl	2437-79-8
2,2',6,6'-Tetrachlorobiphenyl	15968-05-5
2,3',4,4'-Tetrachlorobiphenyl	32598-10-0
3,3',4,4'-Tetrachlorobiphenyl	32598-13-3
Tetrahydrothiophene dioxide	126-33-0
1,1,2,2-Tetramethylethane	79-29-8
Tetratetracontane	7098-22-8
Thiophene, tetrahydro-, 1,1-dioxide	126-33-0
2,3,6-Trichlorobiphenyl	55702-45-9
Trimethylglycidylammonium chloride	3033-77-0