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PRELIMINARY SCORING OF SELECTED ORGANIC AIR POLLUTANTS

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Waste Management
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

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by

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Office of Air and Waste Management
Office of Air Quality Planning and Standards
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Preface

This report presents a preliminary evaluation of the relative hazard to humans from air emissions from production of certain synthetic organic chemicals. Numerical scores establishing a relative ranking have been assigned to 326 of these chemicals based on production, volatility, and toxicity data.

EPA's Office of Air Quality Planning and Standards will use this report as an aid to identifying significant organic chemical processes. However, EPA's strategy for controlling organic air emissions will be based on other information in addition to this report. Therefore, the relative ranking contained herein should not be construed to establish EPA standard setting priorities.

ABSTRACT

In a four-week project for the Emissions Standards and Engineering Division of the U.S. Environmental Protection Agency funded by the Standards and Air Strategies Division, chemical properties of 637 organic compounds were analyzed and a scheme developed for ranking them based on production, fraction lost during production, volatility, and toxicity. A discussion of this methodology and other possible ranking schemes was included in addition to a discussion of possible follow-on work.

This revision includes additional production, chemical, and toxicity data gathered in an intensive effort to complete as many of the dossiers for the original 637 compounds as was possible. The completed dossiers then served as the framework for ranking these compounds in the same manner as was done initially.

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1.0 INTRODUCTION

The Emissions Standards and Engineering Division of the U.S. Environmental Protection Agency is embarking on a major program to control industrial air emissions of synthetic organic compounds. The need for such a program becomes apparent when one considers that total emissions of volatile organic compounds from all stationary industrial sources are believed to exceed 11.35 million tons per year (High Volume Industrial Organic Chemical Study Final Report, EPA, 1976).

The number of organic chemicals synthesized commercially in the United States and used for industrial purposes is enormous, with hundreds of new compounds entering the market annually. Dealing with such a large number of individual compounds is difficult and inefficient unless they can be grouped in a meaningful fashion. It is therefore desirable to approach the problem of control of industrial organic emissions through a system of classification in which all chemicals deriving from a given source or utilized by a given industry or sharing a set of common characteristics, and so forth, are studied as a group and ranked according to their capacity to inflict adversity upon man and his environment relative to the other members of the group.

The compounds addressed in the present effort are those potentially released to the atmosphere from chemical manufacturing plants. In order to assist the U.S. Environmental Protection Agency in determining which of these compounds are most likely to cause adverse health and environmental effects, The MITRE Corporation, in an initial four-week effort, compiled a preliminary list of 637 industrial organic chemicals. In addition to assembling this list, the first two weeks of MITRE's initial effort were devoted to obtaining information on production levels, toxicity potential, and chemical and physical properties of these compounds and to developing a suitable system for "weighting" or "scoring" each compound for each pertinent parameter. The last two weeks were spent in analyzing the information, scoring the compounds for production-release, volatility and toxicity, mathematically determining the individual scores to obtain a final score for each compound when possible, and documenting the findings. The results of this effort were published in June 1976 as MTR-7248 entitled "Scoring of Organic Air Pollutants." Due to the limited time allowed for the initial task, difficulties were encountered in procuring the required information, duplications went undetected, and printing errors proved unavoidable. The present document represents a revision of the original report in which considerable effort has been expended to exhaust all readily available secondary sources of information and to correct errors and duplications. Use of the Chemical Abstracts Service Registry Number (referred to herein as the CAS number) to ascertain the chemical name for each compound further aided in clarifying ambiguities and in avoiding repetition. When no information was available for a compound, or when a compound was not presently manufactured in the United States the compound was deleted from the document. Where sufficient data were available, compounds previously grouped together as a single entry were separated and described individually. Final scores were determined for additional compounds when the acquision of new information rendered this possible. The total number of compounds reviewed in this final version of the document is 637. However, many of these compounds could not be fully evaluated due either to the fact that their production statistics are considered proprietary information or to a lack of suitable toxicological studies reported in the literature.

The purpose of this project, once again, is to provide information which will enable the Environmental Protection Agency to assess the relative potential threat to human health and to the environment of chemicals or groups of chemicals released to the atmosphere from chemical manufacturing plants only. The document does not address those threats occurring as a result of losses from vehicle loading, pipeline transfer or transportation of the compounds or losses due to their utilization as precursors in industrial synthesis. Neither does the document provide sufficient information to ascertain the relative threat posed by losses incurred as a result of or subsequent to industrial and nonindustrial applications.

A detailed description of the approach and methodology used for this effort is presented in Sections 2.0 and 3.0, and the scores for each of the-637 chemicals analyzed are presented in Section 4.0. The dossiers containing all the available information on each compound are presented in a series of appendices to this report. Various chemical, industrial, and biological criteria have been suggested as suitable for an environmentally relevant organic chemical classification scheme. These criteria, as well as some indication of appropriate applications for each, are presented in Section 5.0.

This effort was designed to assess the feasibility of evaluating the relative potential for adverse environmental effects of a large number of organic compounds entering the atmosphere from a specific type of industrial source (namely, a production facility) by use of chemical, toxicological, and industrial data. Such an analysis appears practicable provided that sufficient information is available. To insure a truly valid scoring, a more precise mathematical analysis of the variables must be performed. Computerization seems advisable due to the number of compounds involved and the number of possible variables for each compound. Additional variables, such as dispersion, adsorption, and solubility should be included in any accurate analysis as should data on photoreactivity and photodegradation. Such information is, however, generally obtainable only directly from the research literature and would require considerable time and effort to compile. These and other possible follow-on projects are discussed in more detail in Section 6.0 of this report.

The data and conclusions included here represent only an initial attempt to score organic chemicals based on their production, volatility, and toxicity. Far more work is required before this sort of a ranking scheme can be finalized.

2.0 APPROACH

Any attempt to rank organic compounds according to their relative capacity for inflicting adversity upon man and his environment as a result of production losses to the atmosphere, must commence with the compilation of a comprehensive list of those compounds of possible concern. An initial listing of 350 compounds was prepared by The Radian Corporation under contract to the U.S. Environmental Protection Agency and submitted to The MITRE Corporation as a preliminary guide. Seven prominent listings were also utilized as supplementary material. These eight references are presented in Table 2-1. A total of 1,521 entries were included in these sources; however, elimination of duplications and of those compounds for which little or no information was available narrowed the final list to 637 compounds.

The second stage of this effort involved the elucidation of those properties and characteristics of the compounds in question which must be assembled in order to perform the desired type of ranking. The required information appeared to fall into one of four categories: (1) measures of abundance; (2) measures of tendency to enter the atmosphere; (3) measures of tendency to persist in the atmosphere, and (4) measures of harmfulness. The best sources of information relating to the abundance of a chemical are production statistics. Production data relevant to release from industrial sources include the annual U.S. production and the fraction of

TABLE 2-1

LISTS OF SYNTHETIC ORGANICS

Radian - 350 raw materials, intermediates, products
NSF/Rann - Research Program on Hazard Priority Ranking of Manufactured Organic Chemicals (278)
NIOSH Priority List of Criteria Development for Toxic Substances and Physical Agents (471)
IARC Monographs on the Evaluation of Carcinogenic Risk (150)
OSHA Standards for Carcinogens (14)
EPA - High Volume Industrial Organic Chemicals (22)
Chemical Engineering - "The Industrially Significant Organic Chemicals" (100)
Chemical Week, "Pesticides '72" (81)

production lost. This information was readily available for many of the compounds under consideration but not for all. The sources consulted for production statistics are presented in Table 2-2.

The tendencies to enter and persist in the atmosphere may best be estimated from consideration of certain physical and chemical properties. Included among these are vapor pressure and boiling point (measures of volatility); reactivity towards alkoxy, alkyl peroxy, or hydroxide radicals; and other reactions of note (for example, photodegradability) which bear upon the atmospheric stability of the compounds. Physical data sufficient for categorizing each compound with respect to volatility was available for the majority of the 637 compounds; information concerning atmospheric stability can only be found through an extensive literature search. An effort of this nature was beyond the scope of this task.

The only measure of harmfulness for which abundant data could consistently be found was toxicity. Consequently, toxicity was the only measure of harmfulness considered for the ranking scheme. The major toxicological data sought for each compound included the range of LD_{50}'s and/or LC_{50}'s in experimental animals; the non-lethal effects resulting from acute exposure; and the carcinogenic, mutagenic, and teratogenic potential, where applicable. Effects of chronic exposure other than those mentioned above were not summarized in any of the indexes or other reference materials available for this study. However, the extent to which a compound may adversely affect human health following prolonged or repeated exposure is

TABLE 2-2

SOURCES REVIEWED FOR PRODUCTION STATISTICS

A. PERIODICALS

TITLE	PUBLISHER
American Chemical Society Journal	American Chemical Society
Chemical Abstracts	American Chemical Society
Chemicals	U.S. Department of Commerce
Chemical Engineering	McGraw-Hill, Inc.
Chemical and Engineering News	American Chemical Society
Chemical Engineering Progress	American Institute of Chemical Engineers
Chemical Marketing Reporter	Schnell Publishing Co.
Chemical Week	McGraw-Hill, Inc.
Chemistry and Industry	The Society of the Chemical Industry
Journal of Applied Physics	Argonne National Laboratory
Modern Plastics	McGraw-Hill, Inc.
Pesticide Review	U.S. Department of Agriculture

B. BOOKS, MONOGRAPHS AND REPORTS

TITLE	PUBLISHER OR AUTHOR
Assessment of Industrial Hazardous Waste Practices, Organic Chemicals, Pesticides and Explosives Industries	NTIS
Chemical Economics Handbook	Stanford Research Institute
Chemical Forecasts by Computer	Hull and Company
Chemical Technology and Economics in Environmental Perspectives	U.S. EPA
Dangerous Properties of Industrial Materials	N.I. Sax

TABLE 2-2 (CONTINUED)

B. BOOKS, MONOGRAPHS AND REPORTS (Continued)

TITLE	PUBLISHER OR AUTHOR
Directory of Chemical Producers-U.S.A.	Stanford Research Institute
Facts and Figures of the Plastics Industry	The Society of the Plastics Industry, Inc.
Final Report of the NSF Workshop Panel to Select Organic Compounds Hazardous to the Environment; Raw Data Sheets prepared for the Panel on 289 Chemicals	National Science Foundation and Stanford Research Institute
High Volume Industrial Organic Chemical Study (HVIOC) Final Report	U.S. EPA
IARC Monographs on the Evaluation of Carcinogenic Risk of Chemicals to Man	International Agency for Research on Cancer
The Kline Guide to the Chemical Industry	Kline and Company, Inc.
The Manufacture and Use of Selected Aryl and Alkyl Aryl Phosphate Esters	U.S. EPA
Production, Distribution, Use and Environmental Impact of Selected Pesticides	NTIS
Standard and Poor's Industry Surveys. Chemicals-Basic Analysis	Standard and Poor's Corp.
Synthetic Organic Chemicals, U.S. Production and Sales	U.S. Tariff Commission
System Analysis of Air Pollutant Emissions from the Chemical/Plastics Industry	U.S. EPA
Vapor-Phase Organic Pollutants-Volatile Hydrocarbons and Oxidation Products	U.S. EPA

TABLE 2-2 (CONCLUDED)

C. DATA BANKS, AGENICES, COMPANIES AND OTHER ORGANIZATIONS
The American Chemical Society
The Bureau of the Census
The Dow Chemical Company
The Eastman-Kodak Company
The Manufacturing Chemists Association
The National Agricultural Library
Scisearch (Multidiciplinary Index to the Literature of Science and Technology)
The Shell Chemical Company
The Union-Carbide Corporation
The U.S. Department of Agriculture

often reflected in the occupational ambient air standards set for the compound. These standards (or in their absence, the established threshold limit values) were therefore utilized as supplementary indicators of toxicity. Although some measure of toxicological potential was available for almost every compound, in no instance was data available for each of the designated categories.

Dossiers containing the relevant data for each compound were prepared in the third stage of the project. Several parameters, not directly related to air pollution via volatilization from industrial sources, were included in the dossiers under the categories of production and chemical and physical properties since the information in many cases was readily available and might prove useful at some future date. Examples of such parameters are water solubility and fraction of production dispersed through use. The dossiers for the 637 compounds are presented in the Appendices. While the chemical and physical properties of many of these compounds render it unlikely that they would constitute a serious air pollution hazard (e.g, compounds which are nonsubliming solids), they were included in the evaluation since all compounds have a finite vapor pressure and it was believed that low volatility would be reflected in the ranking procedure.

3.0 METHODOLOGY FOR PRIORITY RANKING

The determination of numerical values by which the organic chemicals under consideration could be rated for their comparative potential to enter the atmosphere from industrial sources and pose a toxicological threat, was accomplished in two phases. The first phase was the designation of a score for each parameter (and sub-parameter) selected as relevant to the nature of the rankings. As was stated in Section 2.0, of the four parameters chosen (plant release, volatility, atmospheric stability, and toxicity) little information was available on atmospheric stability and this category was subsequently eliminated from the input. The scoring systems for each of the parameters included in the ranking are presented in Table 3-1. With few exceptions, the scoring system is self-explanatory.

The first exception concerns the category of production. Where actual production figures were unavailable, 80 percent capacity was used (Chemical Week, May 12, 1976); where a fraction of production lost was unknown, a value of 0.015 was assumed. The second exception deals with volatility. In those cases where vapor pressure was not obtainable, the boiling point was used as an index of volatility. Liquids boiling at or above the boiling point of water (100°C) were given scores of 2; those boiling between 80°C and 100°C were scored as 3. Finally, those with boiling points below 80°C were considered as highly volatile liquids and were given scores of 4. The next set of exceptions concerns the occupational standards. Where no

TABLE 3-1

SCORING SYSTEM FOR PRIORITY RANKING OF INDUSTRIAL ORGANIC CHEMICALS

Annual U.S. Production (10^6 lbs)

Range	Score
<1	0
>1≤10	1
>10≤25	2
>25≤50	3
>50≤100	4
>100	5

Fraction of Production Lost

Range	Score
<0.01	1
≥0.01<0.015	2
≥0.015<0.02	3
≥0.02<0.03	4
≥0.03	5

Volatility (vapor pressure in mmHg at normal temperatures)

State	Range	Score
Solid	-	1
Liquid	≤24	2
Liquid	>24≤100	3
Liquid	>100	4
Gas	-	5

Acute Toxicity I: (LD_{50} in mg/kg)

Range	Score
<50	5
≥50<250	4
≥250<1000	3
≥1000<5000	2
≥5000<10,000	1
>10,000	0

Acute Toxicity II: (LC_{50} in ppm)

Range	Score
<100	5
≥100<200	4
≥200<1000	3
≥1000<3000	2
≥3000<5000	1
>5000	0

Nonlethal Acute Effects

Type of effect	Score
Mild	1
Severe	2

TABLE 3-1 (CONCLUDED)

Carcinogenicity		Mutagenicity		Teratogenicity		Occupational Standard (TWA* in ppm)	
Effects noted or status	Score	Status	Score	Status	Score	Range	Score
Carcinogenic	5	Mutagenic	5	Teratogenic	5	≤5 or carcinogen	5
Produces neoplasm	4	Not tested	0	Not tested	0	>5≤10	4
Under test	3	Negative	0_T**	Negative	0_T**	>10≤25	3
Not tested	0					>25≤100	2
Negative	0_T**					>100≤200	1
						>200	0

*TWA - time weighted average concentration in the air over an 8-hour work day assuming a 40-hour work week.

**0_T - indicates a negative result following testing of the compound for carcinogenicity, mutagenicity or teratogenicity.

standard was established or when the standard was not readily obtainable, the threshold limit value, when available, was substituted. The justification for this substitution lies in the fact that in the majority of cases where both values are known, the values are identical. In addition, the occupational standards, usually given in ppm, are sometimes presented in mg/m^3. These units are usually employed when the corresponding ppm would be less than 1. Consequantly, a value of "5," indicative of a reasonably toxic compound, was assigned to the majority of compounds in which the standards were expressed in the units of mg/m^3. In the summarization of data in Section 4.0, values for occupational standards are presented in ppm unless otherwise noted.

The final set of exceptions concerns the scoring for acute toxicity. When the range of LD_{50}'s or LC_{50}'s, following internal exposure in mammalian species, did not fall into one of the arbitrarily designated categories, the score was assigned based on the median value. Furthermore, in a few cases where LD_{Lo}'s or LC_{Lo}'s were available but LD_{50}'s or LC_{50}'s were not, scoring was based on the highest LD_{Lo} or LC_{Lo} recorded in a mammal.

The final phase of the task consisted of the development of a suitable mathematical procedure for combining the individual scores to produce a final score for each compound which would place that compound in its appropriate position in the hierarchy. Simple addition of the scores was ruled out since this operation would not permit a wide enough spread in the scores. Multiplication of scores seemed a better alternative, provided that provisions were made for mathematical compensation where data gaps existed. The following formula was decided upon:

$$P \times F_{PL} \times V \times \frac{T\ (\text{total})}{T\ (\text{possible})} = S_F$$

where P is the score for annual production, F_{PL} is the score for fraction of production lost, V is the score for volatility, T (total) is the sum of the scores for the various categories of toxicity, T (possible) is the total toxicity score possible for the compound (based on available data), and S_F is the final score. While T (total) was determined by simple addition of the constituent scores, T (possible) was modified so as not to penalize those compounds for which LD_{50}'s, occupational standards or nonlethal acute effects data were not available. In addition, an effort was made to give heavier weight to those compounds known to be carcinogenic, mutagenic, or teratogenic. Specifically, scores for acute toxicity, nonlethal acute effects, occupational standards or any combination of these were omitted from T (possible) when the respective data were not available; however, when data concerning mutagenicity, carcinogenicity, or teratogenicity were not available, negative results were assumed, a score of "0" was assigned to the compound, and a full value of "5" for each category was included in T(possible). Those compounds receiving scores of 0 due to negative results following laboratory testing are differentiated from untested compounds by the symbol 0_T in the appropriate column of the data summary and scoring sheets in Section 4.0. Thus, the highest score for T (total)/T (possible) could only be achieved if a compound were highly mutagenic, highly carcinogenic, and highly teratogenic. Information was, in all cases, insufficient to place any compound in this category.

Where production and/or toxicity data were unavailable, the compound received no final score. In addition, annual production of less than 1 million pounds per year was scored as zero, thus eliminating compounds produced in small quantities from the final analysis. The number of compounds receiving final scores was, therefore, limited to 326.

4.0 CHEMICAL RANKING

The scores calculated for each of the 637 organic compounds and the data utilized to obtain these scores are presented in Table 4-1. A dash indicates that a given variable could not be computed, this being different from a score of zero or an N.A. when data was not available. The maximum possible score is 125 (5 x 5 x 5 x 1).

TABLE 4-1
CHEMICAL RANKING

COMPOUND	PLANT RELEASE: Production X Actual	Production Score	Production Loss Fraction	Production Loss Score	= Product	VOLATILITY: Vapor Pressure	Volatility Score	TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcinogenicity Score	Mutagenicity Score	Teratogenicity Score	Total / Total Possible	FINAL SCORE
Acenaphthene	na	–	na	–	–	Solid	1	na	–	na	–	–	3	0	0	3/15	–
Acetal	56.8	4	0.03	5	20	28.8 mm at 25 C	3	na	–	4570	2	1	0	0	0	3/22	8
Acetaldehyde	1500	5	0.015	3	15	923 mm at 25 C	4	200	1	560-1930	3	1	5	0	0	10/27	22
Acetaldol	226.5	5	0.015	3	15	10 mm at 25 C	2	na	–	2180-140	2	–	0	0	0	2/20	3
Acetamide	na	–	na	–	–	Solid	1	na	–	8300-10,000	1	1	5	0	0	7/22	–
Acetamido fluorene	na	–	na	–	–	Solid	1	na	–	1020	2	–	5	0	5	12/20	–
Acetanilide	5.5	1	0.015	3	3	Solid	1	na	–	800 - 1210	3	1	0	0	0	4/27	<1
Acetic acid	2097	5	0.015	3	15	11.4 mm at 20 C	2	10	4	525-4960 5620*	2 0*	2	0	0	0	8/27	9
Acetic anhydride	1633.1	5	0.015	3	15	5.09 mm at 25 C	2	5	5	1780	2	2	0	0	0	9/27	10
Acetone	1980.3	5	0.015	3	15	227.3 at 25 C	4	1000	0	1295-5300	2	2	3	0	0	7/27	16
Acetone cyanohydrin	537.9	5	0.015	3	15	na (BP=82 C at 23 mm	3	na	–	3-17 575*	5 3*	–	0	0	0	5/20	11
Acetonitrile	135	5	0.015	3	15	92.8 mm at 25 C	3	40	2	1920-3800	2	2	3	0	5	14/27	23
Acetophenone	2.68	1	0.015	3	3	1 mm at 37.1 C	2	na	–	900	3	2	0	0	0	5/22	1
Acetylene	538	5	0.015	3	15	gas	5	na	–	90,000**	0	1	0	0	0	1/22	3
Acetylene tetrabromide	na	–	na	–	–	1 mm at 65 C	2	1	5	400	3	1	0	0	0	9/27	–
Acetylene tetrachloride	na	–	na	–	–	6.75 mm at 25 C	2	5	5	700†	3	2	0	0	0	10/27	–
Acrolein	61.73	4	0.015	3	12	288.2 mm at 25 C	4	0.1	5	7-562	5	2	0	0	0	12/27	21

†LD_{LO}
**LC_{LO}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X (Actual)	Production (Score)	Production Loss (Fraction)	Production Loss (Score)	= Product	X VOLATILITY: Vapor Pressure	Volatility Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Acrylamide	35	3	0.015	3	9	Solid	1	0.3mg/m^3	5	170	4	2	0	0	0	11/27	4
Acrylic acid	233	5	0.015	3	15	4.61 mm at 25 C	2	na	-	60-340	3	1	0	0	0	4/22	5
Acrylonitrile	1411.8	5	0.015	3	15	113.8 mm at 25 C	4	20	3	93-280 576*	4 3*	2	0	0	0	9/27	20
Adipic acid	1478.4	5	0.015	3	15	Solid	1	na	-	1900	2	-	0	0	0	2/20	2
Alachlor	20	2	0.01	2	4	na (BP=100 C)	2	na	-	1200-3000	2	-	0	0	0	2/20	1
Aldrin	25	3	0.01	2	6	Solid	1	0.25 mg/m^3	5	7-200	5	2	4	0	0	16/27	4
Allyl alcohol	na	-	na	-	-	25.6 mm at 25 C	3	2	5	42-96 165*	5 4*	2	0	0	0	12/27	-
Allyl chloride	295	5	0.015	3	15	359 mm at 25 C	4	1	5	155-7150	2	2	0	0	0	9/27	20
Allylene	na	-	na	-	-	Gas	5	na	-	na	-	1	0	0	0	1/17	-
Allyl naphthalene	na	-	na	-	-	Solid	1	na	-	na	-	-	0	0	0	-	-
Amiben	20	2	0.01	2	4	Solid	1	na	-	5620	1	-	3	0	0	4/20	<1
p-Aminobenzoic acid	na	-	na	-	-	Solid	1	na	-	1830-6000	2	2	3	0	0	7/22	-
p-Aminobiphenyl	na	-	na	-	-	Solid	1	car.§	5	500	3	-	5	0	0	13/25	-
Aminoethylethanolamine	13.5	2	0.015	3	6	<.01 mm at 20 C	2	na	-	1800-3000	2	-	0	0	0	2/20	1

§ carcinogen

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Score	Production Loss Fraction	Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	Score	Acute Toxicity LD_{50} or LC^{*}_{50} Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	= Total / Total Possible	FINAL SCORE
Amyl acetate	7.6	1	0.015	3	3	9.43 mm at 25 C	2	125	2	7400	1	1	0	0	0	4/27	<1
Amyl alcohol	na	-	na	-	-	3.16 mm at 25 C	2	100	2	200-3030	2	2	0	0	0	6/27	-
Amylamine	na	-	na	-	-	na (BP= 104.4 C)	2	na	-	470-1120	3	1	0	0	0	4/22	-
Amyl chloride	na	-	na	-	-	10 mm at 25 C	2	na	-	na	-	1	0	0	0	1/17	-
n-Amylene	na	-	na	-	-	858.0 mm at 25 C	4	na	-	na	-	2	0	0	0	2/17	-
Amyl ether	na	-	na	-	-	na (BP= 190 C)	2	na	-	na	-	-	0	0	0	-	-
Amyl mercaptan	na	-	na	-	-	13.8 mm at 25 C	2	na	-	na	-	1	0	0	0	1/17	-
Aniline	551.2	5	0.015	3	15	0.67 mm at 25 C	2	5	5	64-1400 175*	3 4*	2	4	0	0	15/27	17
Aniline hydrochloride	na	-	na	-	-	Solid	1	na	-	750-1072	3	2	0	0	0	5/22	-
Anisidine (o and p)	2.3	1	0.015	3	3	1 mm at 61 C	2	0.05mg/m3	5	1400	2	1	0	0	0	8/27	3
Anisole	na	-	na	-	-	10 mm at 42.2 C	2	na	-	2800-3700	2	-	0	0	0	2/20	-
Anthranilic acid	na	-	na	-	-	Solid	1	na	-	4620	2	-	4	0	0	6/20	-
Anthraquinone	na	-	na	-	-	Solid	1	na	-	na	-	1	4	0	0	5/17	-
Auramine	na	-	na	-	-	Solid	1	na	-	na	-	1	5	0	0	6/17	-
Azodrin	5	1	0.015	3	3	Solid	1	na	-	2-107	5	-	0	0	0	5/20	<1
Banvel D	2	1	0.015	3	3	Solid	1	na	-	1000-3000	2	-	0	0	0	2/20	<1
Banvel T	na	-	na	-	-	Solid	1	na	-	300	3	-	0	0	0	3/20	-

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Benzaldehyde	3.4	1	0.015	3	3	1 mm at 26.2 C	2	na	–	1000-1300	2	1	0	0	0	3/22	1
Benzamide	na	–	na	–	–	Solid	1	na	–	1160	2	–	0	0	0	2/20	–
Benzene	11,120	5	0.01	2	10	95.9 mm at 25 C	3	10	4	468-4700	2	2	5	5	0	18/27	20
Benzenedisulfonic acid	na	–	na	–	–	Solid	1	na	–	na	–	1	0	0	0	1/17	–
Benzenesulfonic acid	na	–	na	–	–	Solid	1	na	–	2050	2	1	0	0	0	3/22	–
Benzidine	10.4	2	0.015	3	6	Solid	1	na	–	214-309	3	2	5	0	0	10/22	3
Benzil	na	–	0.015	3	–	Solid	1	na	–	2710	2	–	0	0	0	2/20	–
Benzilic acid	na	–	0.015	3	–	Solid	1	na	–	na	–	–	0	0	0	–	–
Benzoic acid	79	4	0.015	3	12	Solid	1	na	–	1460-3040	2	1	0	0	0	3/22	2
Benzoin	na	–	na	–	–	Solid	1	na	–	na	–	–	3	0	0	3/15	–
Benzonitrile	na	–	na	–	–	1 mm at 28 C	2	na	–	1200	2	1	0	0	0	3/22	–
Benzophenone	na	–	na	–	–	Solid	1	na	–	na	–	–	3	0	0	3/15	–
Benzoquinone	na	–	na	–	–	Solid	1	0.1 mg/m^3	5	25-8500	4	2	5	0	0	16/27	–
Benzotrichloride	na	–	na	–	–	1 mm at 45.8 C	2	na	–	2150†	2	1	0	0	0	3/22	–
Benzoyl chloride	16.8	2	0.015	3	6	1 mm at 32.1 C	2	na	–	790-2460	2	1	0	0	0	3/22	2
Benzyl alcohol	10.4	2	0.015	3	6	1 mm at 58.0 C	2	na	–	64-1940 1000*	3 3*	1	0	0	0	4/22	2
Benzyl amine	na	–	na	–	–	1 mm at 29 C	2	na	–	na	–	–	0	0	0	–	–
Benzyl benzene	na	–	na	–	–	1 mm at 76 C	2	na	–	5000†	1	–	0	0	0	1/20	–

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC^*_{50} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total/Total Possible	= FINAL SCORE
Benzyl benzoate	na	-	na	-	-	<10 mm at 25 C	2	na	-	1000-2240	2	-	0	0	0	2/20	-
Benzyl chloride	66.4	4	0.015	3	12	1.4 mm at 25 C	2	na	-	1000-1624	2	2	4	0	0	8/22	9
Benzyl dichloride	na	-	na	-	-	<10 mm at 25 C	2	na	-	467-3249 200*	2 3*	1	0	0	0	4/22	-
Bis (chloromethyl) ether	na	-	na	-	-	na	-	na	-	210-280	4	-	5	0	0	9/20	-
Bisphenol A	370.4	5	0.015	3	15	Solid	1	0.5	5	150	4	-	0	0	0	9/25	5
Bromacil	8	1	0.015	3	3	Solid	1	na	-	3400	2	-	0	0	0	2/20	<1
Bromobenzene	na	-	na	-	-	48 mm at 25 C	3	na	-	na	-	2	0	0	0	2/17	-
Bromonaphthalene	na	-	na	-	-	Solid	1	na	-	na	-	-	0	0	0	-	-
1, 3 Butadiene	3682.1	5	0.015	3	15	Gas	5	1000	0	250,000	0	1	0	0	0	1/27	3
Butane	2331.1	5	0.01	2	10	Gas	5	500	0	658*	3*	1	0	0	0	4/27	7
1-Butene 2-Butene (cis & trans)	2478	5	0.015	3	15	Gas	5	na	-	na	-	1	0	0	0	1/17	4
2-Butoxyethanol	133.3	5	0.015	3	15	0.88 mm at 25 C	2	na	-	230-1480 700*	3 3*	1	0	0	0	4/22	5
n-Butyl acetate	77.2	4	0.015	3	12	15 mm at 25 C	2	150	1	1230	3	1	0	0	0	5/27	4
sec-Butyl acetate	na	-	na	-	-	na (BP= 112.2 C)	2	200	1	na	-	1	0	0	0	2/22	-
tert-Butyl acetate	na	-	na	-	-	na (BP=98 C)	3	200	1	na	-	1	0	0	0	2/22	-

TABLE 4-1 (CONTINUED)

	PLANT RELEASE			X		VOLATILITY		X		TOXICITY					=		FINAL SCORE
	Production X		Production Loss		= Product	Vapor Pressure	Score	OSHA Standard (air)		Acute Toxicity LD_{50} or LC^*_{50}		Non-lethal Acute Effects	Carcino-genicity	Muta-genicity	Terato-genicity	Total / Total Possible	
COMPOUND	Actual	Score	Fraction	Score				TWA	Score	Range	Score	Score	Score	Score	Score		
n-Butylacrylate	na	-	na	-	-	5.63 mm at 25 C	2	na	-	2000-3730	2	-	0	0	0	2/20	-
n-Butyl alcohol	557.6	5	0.015	3	15	7.69 mm at 25 C	2	100	2	790	3	2	0	0	0	7/27	8
sec-Butyl alcohol	417	5	0.015	3	15	17.5 mm at 25 C	2	150	1	771	3	-	0	0	0	4/25	5
tert-Butyl alcohol	1000	5	0.015	3	15	41.54 mm at 25 C	3	100	2	933-3500	2	1	0	0	0	5/27	8
n-Butyl aldehyde	na	-	na	-	-	<10 mm at 25 C	1	na	-	2490-2700	2	1	0	0	0	3/22	-
sec-Butylamine	na	-	na	-	-	169.8 mm at 25 C	4	na	-	380	3	1	0	0	0	4/22	-
tert-Butylamine	na	-	na	-	-	169.8 mm at 25 C	4	na	-	180-900	3	1	0	0	0	4/22	-
Butylbenzoic acid	na	-	na	-	-	Solid	1	na	-	735	3	1	0	0	0	4/22	-
Butylenes (α, β, γ)	3200	5	0.015	-	15	Gas	5	na	-	na	-	1	0	0	0	1/17	4
1, 3 Butylene glycol	na	-	na	-	-	0.06 mm at 20 C	2	na	-	na	-	-	0	0	0	-	-
n-Butyl-glycidyl ether	na	-	na	-	-	na (BP=164 C)	2	50	2	700-2520	2	1	0	0	0	5/27	-
Butyl mercaptan	na	-	na	-	-	<10 mm at 25 C	2	10	4	399-1500 2500-4020*	3 2*	1	0	0	0	8/27	-
tert-Butyl phenol	na	-	na	-	-	Solid	1	na	-	2520-3250	2	1	0	0	0	3/22	-
tert-Butyl toluene	na	-	na	-	-	<10 mm at 25 C	2	10	4	900-2000 248-1500*	2 3*	2	0	0	0	9/27	-
n-Butyric acid	na	-	na	-	-	1 mm at 25.5 C	2	na	-	800-3180	2	1	0	0	0	3/22	-

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Production Score	Production Loss Fraction	Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
n-Butyric anhydride	na	–	na	–	–	<10 mm at 25 C	2	na	–	na	–	–	0	0	0	–	–
n-Butyronitrile	na	–	na	–	–	20 mm at 25.7 C	2	na	–	500	3	–	0	0	0	3/20	–
Buxten	6	1	0.015	3	3	Solid	1	na	–	1050	2	–	0	0	0	2/20	<1
Cacodylic acid	2	1	0.015	3	3	Solid	1	na	–	185–1350	3	–	5	0	0	8/20	1
Calcium propionate	21.4	2	0.03	5	10	Solid	1	na	–	na	–	–	0	0	0	–	–
Calcium stearate	37.8	3	0.03	5	15	na	–	na	–	na	–	–	0	0	0	–	–
Camphor	na	–	na	–	–	Solid	1	2	5	900	3	2	4	0	0	14/27	–
Caprolactam	950	5	0.015	3	15	Solid	1	na	–	2140	2	1	0	0	0	3/22	2
Captan	18	2	0.01	2	4	Solid	1	5mg/m^3	5	480	3	–	0	0	5	13/25	2
Carbaryl	55	4	0.015	3	12	Solid	1	5mg/m^3	5	48–710	4	1	5	0	5	20/27	9
Carbofuran	8	1	0.015	3	3	Solid	1	.05mg/m^3	5	2–11 32–85*	5 5*	–	0	0	0	10/25	1
Carbon disulfide	767.8	5	0.015	3	15	na BP=46.3 C	4	20	3	400†	3	2	0	0	0	8/27	18
Carbon tetrabromide	1000	5	0.015	3	15	Solid	1	100 ppb	5	298	3	1	0	0	0	9/27	5
Carbon tetrachloride	1047	5	0.015	3	15	115.2 mm at 25 C	4	10	4	1770–6380	2	2	5	5	0	18/27	40
Castor oil	100	5	0.03	5	25	na (BP= 313 C)	2	na	–	na	–	–	0	0	0	–	–
Cellulose acetate	807.1	5	0.03	5	25	Solid	1	na	–	na	–	–	0	0	0	–	–
Chloranil	na	–	na	–	–	Solid	1	na	–	500–4000	2	–	0	0	0	2/20	–
Chlordane	25	3	0.01	2	6	<1 mm at 25 C	2	0.5 mg/m^3	5	100–700	3	2	0	0	0	10/27	4

†LD_{LO}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Volatility Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}^{*} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcinogenicity Score	Mutagenicity Score	Teratogenicity Score	Total / Total Possible	= FINAL SCORE
Chloroacetaldehyde	na	–	na	–	–	100 mm at 45 C	3	1	5	2-1390	5	1	0	0	0	11/27	–
Chloroacetic acid	84	4	0.015	3	12	Solid	1	na	–	5-76	4	1	0	0	0	5/22	3
2-Chloroacetophenone	na	–	na	–	–	1 mm at 48 C	2	0.05	5	na	–	1	0	0	0	6/22	–
m-Chloroaniline	na	–	na	–	–	1 mm at 63.5 C	2	na	–	880	3	–	0	0	0	3/20	–
o-Chloroaniline	na	–	na	–	–	1 mm at 63.5 C	2	na	–	256	3	–	0	0	0	3/20	–
p-Chloroaniline	na	–	na	–	–	1 mm at 63.5 C	2	na	–	100-420	4	–	0	0	0	4/20	–
o-Chlorobenzaldehyde	na	–	na	–	–	10 mm at 25 C	2	na	–	10†	5	1	0	0	0	6/22	–
p-Chlorobenzaldehyde	na	–	na	–	–	Solid	1	na	–	na	–	–	0	0	0	–	–
Chlorobenzene	690	5	0.015	3	15	12.14 mm at 25 C	2	75	2	2830-2910	2	2	0	0	0	6/27	7
Chlorobenzilate	2	1	0.015	3	3	na (BP=148 C)	2	na	–	700-724	3	–	5	0	0	8/20	2
Chlorobenzoic acid	na	–	na	–	–	Solid	1	na	–	na	–	–	0	0	0	–	–
o-Chlorobenzoyl chloride	na	–	na	–	–	na (BP=238 C)	2	na	–	na	–	–	0	0	0	–	–
o-Chlorobenzylidene malonitrile	na	–	na	–	–	Solid	1	0.05	5	35-178	5	2	0	0	0	12/27	–
Chlorodifluoroethane	0.2	0	0.015	3	0	Gas	5	na	–	na	–	1	0	0	0	1/17	0
Chlorodifluoromethane	80	3	0.015	3	9	Gas	5	na	–	na	–	1	0	0	0	1/17	3
2-Chloro-4-ethylamino-6-isopropylamino-s-triazine	110	5	0.01	2	10	Solid	1	na	–	1750-3080	2	–	0	0	0	2/20	1

†LD_{LO}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC^*_{50} Range	Acute Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Chloroform	234.7	5	0.015	3	15	200 mm at 25.9 C	4	50	5	704-800 28-100*	3 4*	2	5	0	0	16/27	36
Chloronaphthalene	5	1	0.015	3	3	1 mm at 80.6 C	2	2 mg/m³	5	1091-1540	2	1	0	0	0	8/27	2
m-Chloronitrobenzene	142	5	0.015	3	15	< 10 mm at 25 C	2	1	5	135-288	4	2	0	0	0	11/27	12
o-Chloronitrobenzene	142	5	0.015	3	15	na (BP= 245 C)	2	1	5	135-288	4	2	4	0	0	15/27	17
p-Chloronitrobenzene	142	5	0.015	3	15	10 mm at 25 C	2	1 mg/m³	5	420-1414	3	–	0	0	0	8/25	10
1-Chloro-1-nitropropane	na	–	na	–	–	na (BP= 139.5 C)	2	20	3	165-510	3	2	0	0	0	8/27	–
m-Chlorophenol	na	–	na	–	–	Solid	1	1	5	355-1390	3	1	0	0	0	9/27	–
o-Chlorophencl	na	–	na	–	–	2.97 mm at 25 C	2	1	5	230-950	3	2	4	0	0	14/27	–
p-Chlorophenol	na	–	na	–	–	Solid	1	1	5	281-1030	3	1	0	0	0	9/27	–
Chloroprene	396	5	0.015	3	15	215.4 mm at 25 C	4	25	3	1600†	2	2	0	5	0	12/27	27
Chloropropham	2	1	0.015	3	3	Solid	1	na	–	1200-5000	2	–	4	0	0	6/20	1
m-Chlorotoluene	na	–	na	–	–	4.17 mm at 25 C	2	na	–	na	–	–	0	0	0	–	–
o-Chlorotoluene	66	4	0015	3	–	4.11 mm at 25 C	2	na	–	na	–	–	0	0	0	–	–
p-Chlorotoluene	76	4	0.015	3	12	4.06 mm at 25 C	2	na	–	na	–	–	0	0	0	–	–
Citric acid	163	5	0.03	5	25	Solid	1	na	–	42-961	3	1	0	0	0	4/22	5
Crag herbicide 1	na	–	na	–	–	Solid	1	15 mg/m³	5	730	3	–	0	0	0	8/25	–
m-cresol	31.4 (P+M)	–	0.015	3	–	1 mm at 52.0 C	2	5	5	242-2050	2	2	0	0	0	9/27	–
o-cresol	49.7	3	0.015	3	9	1 mm at 38.2 C	2	5	5	121-1380	3	1	4	3	0	16/27	11
p-cresol	31.4 (P+M)	–	0.015	3	–	Solid	1	5	5	207-750	3	2	0	0	5	15/27	–
Crotonaldehyde	226	5	0.015	3	15	<10 mm at 25 C	2	2	5	6-300 1510-4000*	4 2*	2	0	0	0	11/27	12

† LD_{LO}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	Score	Acute Toxicity LD_{50} or LC^*_{50} Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	= Total / Total Possible	FINAL SCORE
Crotonic acid	na	–	na	–	–	Solid	1	na	–	600-1000	3	–	0	0	0	3/20	–
Cumene	2292.9	5	0.01	2	10	6.56 mm at 25 C	2	50	2	1400 8000*	2 0*	2	0	0	0	6/27	4
Cumene hydroperoxide	2000	5	0.015	3	15	1 mm at 70 C	2	na	–	95-400 200-220*	3 3*	1	4	0	0	8/22	11
Cyanoacetic acid	200	5	0.015	3	15	Solid	1	na	–	200	4	–	0	0	0	4/20	3
Cyanogen chloride	na	–	na	–	–	Gas	5	na	–	118-207*	4	1	0	0	0	5/22	–
Cyanuric acid	na	–	na	–	–	Solid	1	na	–	na	–	–	0	0	0	–	–
Cyanuric chloride	na	–	na	–	–	Solid	1	na	–	485	3	2	4	0	0	9/22	–
Cyclohexane	416	5	0.015	3	15	98.14 mm at 25 C	3	300	0	1297	2	1	0	0	0	3/27	5
Cyclohexanol	716.9	5	0.015	3	15	1.7 mm at 25 C	2	50	2	2060	2	2	0	0	0	6/27	7
Cyclohexanone	784.4	5	0.015	3	15	4.77 mm at 25 C	2	50	2	1350-1620	2	1	0	0	0	5/27	6
Cyclohexene	2298.4	5	0.01	2	10	160 mm at 38 C	4	300	0	na	–	–	0	0	0	–	–
Cyclohexylamine	12	2	0.015	3	6	Na (BP=134.5)[2]	2	10	4	320-710	3	1	0	0	0	8/27	4
Cyclopentadiene	80	4	0.015	3	12	10 mm at 25 C	2	75	2	na	–	2	0	0	0	4/22	4
Cyprex	2.0	1	0.01	2	2	Solid	1	na	–	566-1000	3	–	0	0	0	3/20	<1
Dacthal	2.0	1	0.015	3	3	Solid	1	na	–	3000	2	–	0	0	0	3/20	<1
Dalapon	5	1	0.015	3	3	Solid	1	na	–	3860-9300	1	–	0	0	0	1/20	<1

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity, LD_{50} or LC_{50}* Range	Acute Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Dasanit	4	1	0.015	3	3	<10 mm at 25 C	2	na	-	2-10	5	-	0	0	0	5/20	2
DBDC	10	1	0.015	3	3	na	2	na	-	173-275	4	1	0	0	0	5/22	1
DDT	45	3	0.015	3	9	Solid	1	1mg/m^3	5	113-1500	3	1	4	0	0	13/27	4
Decahydronaphthalenes	na	-	na	-	-	<10 mm at 25 C	2	na	-	4170	2	1	0	0	0	3/22	-
Decyl alcohol	152.5	5	0.015	3	15	1 mm at 69.5	2	na	-	4720 4000*	2 1*	-	0	0	0	2/20	3
DEET	10	1	0.015	3	3	<10 mm at 25 C	2	na	-	200-2000	2	1	0	0	0	3/22	1
DEF	5	1	0.015	3	3	<10 mm at 25 C	2	na	-	150	4	2	0	0	0	6/22	2
Diacetone alcohol	na	-	na	-	-	1.1 mm at 20 C	2	50	2	93-4000	2	2	0	0	0	6/27	-
Diaminobenzoic acid	na	-	na	-	-	Solid	1	na	-	na	-	-	0	0	0	-	-
Diazinon	10	1	0.015	3	3	<10 mm at 25 C	2	0.1 mg/m^3	5	2-85	5	-	0	0	0	10/25	2
Diazomethane	na	-	na	-	-	Gas	5	0.2	5	175**	4	2	5	0	0	16/27	-
Dibromodifluoromethane	na	-	na	-	-	<10 mm at 25 C	2	100	2	2300**	1	1	0	0	0	4/27	-
Di-tert-butyl-p-cresol	36	3	0.015	3	9	Solid	1	na	-	1040-3510	2	-	0	0	5	7/20	3
Dibutyl phthalate	35.5	3	0.015	3	9	<10 mm at 25 C	2	5 mg/m^3	5	na	-	-	0	0	5	10/20	9
24-Dichloroaniline	na	-	na	-	-	Solid	1	na	-	157	4	1	0	0	0	5/22	-
34-Dichloroaniline	na	-	na	-	-	Solid	1	na	-	648-740	3	-	0	0	0	3/20	-
o-Dichlorobenzene	62.4	4	0.015	3	12	Solid	1	50	2	330-2000† 700-800**	†3† 3**	2	5	0	0	12/27	5
p-Dichlorobenzene	77.3	4	0.015	3	12	Solid	1	75	2	500-2950	2	2	5	0	0	11/27	5

** LC_{Lo}
† LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	X Score	Production Loss Fraction	Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	Score	Acute Toxicity LD_{50} or LC_{50}* Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	= Total / Total Possible	FINAL SCORE
Dichlorobenzidine	4.6	1	0.015	3	3	Solid	1	50	2	4740†	2	1	5	0	0	10/27	1
Dichlorodifluoromethane	488.4	5	0.015	3	15	Gas	5	1000	0	324 mg/ℓ†	3†	1	0	3	0	7/27	19
1,3-Dichloro-5, 5-dimethyl-hydantoin	na	-	na	-	-	Solid	1	0.2 mg/m³	5	600	3	2	0	0	0	10/27	-
Dichloroethylene	na	-	na	-	-	204.88 mm at 25 C	4	200	1	770	3	2	0	0	0	6/27	-
Dichloroethyl ether	na	-	na	-	-	1.23 mm at 25 C	2	15	4	105	4	1	5	0	0	14/27	-
Dichlorofluoromethane	487	5	0.015	3	15	Gas	5	1000	0	10,000** ppm	0	1	0	0	0	1/27	3
Dichlorohydrin	na	-	na	-	-	1 mm at 28 C	2	na	-	93-490	4	2	0	0	0	6/22	-
Dichloropentane	na	-	na	-	-	<20 mm at 25 C	2	na	-	64†	4	-	0	0	0	4/20	-
2, 4-Dichlorophenoxy-acetic acid	43	3	0.01	2	6	Solid	1	10 mg/m³	5	80-541	3	2	0	0	5	15/27	3
Dichloropropane	60	4	0.1	5	20	53.02 mm at 25 C	3	75	2	860-1900	2	2	0	0	0	6/27	13
Dichloropropene	60	4	0.01	2	8	35 mm at 25 C	3	na	-	250	4	2	3	0	0	9/22	10
Dichlorotetrafluoroethane	21.7	2	0.015	3	6	Gas	5	1000	0	na	-	1	0	0	0	1/22	1
Dicofol	4.0	1	0.015	3	3	Solid	1	na	-	575-1810	2	-	0	0	0	2/20	<1
Dicumyl peroxide	15	2	0.02	4	8	Solid	1	na	-	4100	2	-	0	0	0	2/20	1
Dicyclohexylamine	na	-	na	-	-	<10 mm at 25 C	2	na	-	373	3	1	4	0	0	8/22	-
Dieldrin	<1	0	0.015	3	0	Solid	1	0.250 mg/m³	5	10.5 - 46	5	1	4	0	0	15/27	0

**LC_{Lo} †LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Loss Score	= Product	X VOLATILITY: Vapor Pressure	Volatility Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}^* Range	Acute Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Diethanolamine	101.1	5	0.015	3	15	5 mm at 138 C	2	na	-	710-3553	2	1	0	0	0	3/22	4
Diethylamine	8.8	1	0.015	3	3	247.1 mm at 25 C	4	25	3	540-649 4000*	3 1*	2	0	0	0	8/27	4
Diethylaminoethanol	na	-	na	-	-	21 mm at 20 C	2	10	4	1220-1561	2	1	0	0	0	7/27	-
Diethylene glycol	350	5	0.015	3	15	1 mm at 91.8 C	2	na	-	1000-9000	2	1	0	0	0	3/22	4
Diethylene glycol, dibutyl ether	na	-	na	-	-	0.02 mm at 20 C	2	na	-	3900	2	-	0	0	0	2/20	-
Diethylene glycol, diethyl ether	na	-	na	-	-	<10 mm at 25 C	2	na	-	1850	2	-	0	0	0	2/20	-
Diethylene glycol, dimethyl ether	na	-	na	-	-	2.95 mm at 25 C	2	na	-	na	-	-	0	0	0	-	-
Diethylene glycol, monobutyl ether	41.2	3	0.015	3	9	<1 mm at 20 C	2	na	-	850-2000	2	-	0	0	0	2/20	2
Diethylene glycol, monobutyl ether acetate	na	-	na	-	-	<0.01 mm at 20 C	2	na	-	2340-5000	2	-	0	0	0	2/20	-
Diethylene glycol, monoethyl ether	24.8	2	0.015	3	6	<1 mm at 20 C	2	na	-	900-5638	2	1	0	0	0	3/22	2
Diethylene glycol, monoethyl ether acetate	na	-	na	-	-	0.05 mm at 20 C	2	na	-	3930	3	-	0	0	0	3/20	-
Diethylene glycol, monohexyl ether	na	-	na	-	-	0.01 mm at 20 C	2	na	-	2920	2	-	0	0	0	2/20	-

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X: Actual	Score	Production Loss: Fraction	Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air): TWA	Score	Acute Toxicity LD_{50} or LC_{50}^{*}: Range	Score	Non-lethal Acute Effects: Score	Carcino-genicity: Score	Muta-genicity: Score	Terato-genicity: Score	Total / Total Possible	= FINAL SCORE
Diethylene glycol, monomethyl ether	12.7	2	0.03	5	10	0.2 mm at 20 C	2	na	-	4160	2	-	0	0	0	2/20	2
Diethylene glycol, monomethyl ether acetate	na	-	na	-	-	0.12 mm at 20 C	2	na	-	3460	2	-	0	0	0	2/20	-
Diethylenetriamine	32.4	3	0.015	3	9	0.22 mm at 20 C	2	1	5	71-1080	3	1	0	0	0	9/27	6
Di (2-ethyl hexyl) adipate	na	-	na	-	-	<0.01 mm at 20 C	2	na	-	540-900	3	-	0	0	0	3/20	-
Di (2-ethylhexyl) phthalate	389.7	5	0.015	3	15	1.3 mm at 200 C	2	5 mg/m^3	5	143	4	2	4	5	5	25/27	28
Diethylstilbesterol	<1	0	0.015	3	0	Solid	1	na	-	34-67	5	2	5	0	5	17/22	0
Diethyl sulfate	na	-	na	-	-	1 mm at 47 C	2	na	-	340-647	3	-	5	5	5	18/20	-
Difluoroethane	na	-	na	-	-	Gas	5	na	-	na	-	1	0	0	0	1/17	-
Difolatan	2	1	0.015	3	3	Solid	1	na	-	2500	2	-	0	0	5	7/20	1
Dihydrotri-methylquinoline	30	3	0.3	5	15	Solid	1	na	-	1450-2000	2	-	0	0	0	2/20	2
Diisobutylene	na	-	na	-	-	na	2	na	-	na	-	2	0	0	0	2/17	-
Diisobutyl ketone	na	-	na	-	-	na	-	25	3	1416	2	2	0	0	0	7/27	-
Diisodecyl phthalate	153.3	5	0.015	3	15	<10 mm at 25 C	2	na	-	na	-	-	0	0	0	-	-
Diisooctyl phthalate	43.2	3	0.015	3	9	<10 mm at 25 C	2	na	-	na	-	-	0	0	0	-	-
Diisopropylamine	2	1	0.015	3	3	na	4	5	5	700	3	1	0	0	0	9/27	4
Diketene	na	-	na	-	-	na	-	na	-	560	3	1	0	0	0	4/22	-

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Production Loss = Product — Actual	Production Score	Production Loss Fraction	Production Loss Score	Product	VOLATILITY: Vapor Pressure	Volatility Score	TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcinogenicity Score	Mutagenicity Score	Teratogenicity Score	Total / Total Possible	FINAL SCORE
Dimethoate	2.0	1	0.015	3	3	Solid	1	na	-	30-350	3	2	0	0	0	5/22	1
Dimethoxy benzidine	< 1	0	0.015	3	0	Solid	1	na	-	1920-3000	2	-	4	0	0	6/20	0
N.N-dimethyl acetamide	na	-	na	-	-	1.3 mm at 25 C	2	10	4	2240	2	1	0	0	5	12/27	-
Dimethylamine	95.9	4	0.015	3	12	Gas	5	10	4	240-698	3	1	0	3	0	11/27	24
Dimethylaminoazobenzene	na	-	na	-	-	1 mm at 52.6 C	2	carcinogen	5	280-850	3	2	5	0	0	15/27	-
Dimethylaniline	15	2	0.015	3	6	1 mm at 29.5 C	2	5	5	1770	2	1	0	0	0	8/27	4
Dimethyl butyl acetate	na	-	na	-	-	na	-	50	2	1000**	1	1	0	0	0	4/27	-
Dimethyl ether	na	-	na	-	-	Gas	5	na	-	na	-	1	0	0	0	1/17	-
N, N-dimethyl formamide	na	-	na	-	-	3.7 mm at 25 C	2	10	4	400-4200	2	2	0	0	0	8/27	-
Sym-dimethylhydrazine	na	-	na	-	-	na	-	na	-	95-220	4	-	0	0	0	4/20	0
Asym-dimethylhydrazine	<1.1	1	0.015	3	3	1.57 mm at 25 C	4	1 mg/m^3	5	60-1329 172-3578**	4 3*	1	5	0	0	15/27	7
N-(1, 4-dimethylpentyl)-N' phenyl-p-phenylenediamine	20	3	0.03	5	15	na	-	na	-	na	-	-	0	0	0	-	-
Dimethylphthalate	10	1	0.015	3	3	0.01 mm at 20 C	2	5 mg/m^3	5	1580-8500	2	-	0	0	5	12/25	3
Dimethyl sulfate	na	-	na	-	-	<20 mm at 25 C	2	1	5	100-440	4	-	5	0	5	19/25	-
Dimethyl sulfide	na	-	na	-	-	530.8 mm at 25 C	4	na	-	535-3700	2	-	0	0	0	2/20	-
Dimethyl sulfoxide	na	-	na	-	-	0.37 mm at 20 C	2	na	-	20-2050	2	2	0	0	5	9/22	-
Dimethyl terphthalate	2714	5	0.015	3	15	1 mm at 100 C	2	na	-	4390	2	-	0	0	0_T	2/17	3
Dinitrobenzenes (M,O,P) combined	na	-	na	-	-	Solid	1	1	5	na	5	2	0	0	0	12/27	-

**LC_{Lo}

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TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Production Score	Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	Score	Acute Toxicity* LD_{50} or LC_{50} Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Dinitrobenzoic acid	na	-	na	-	-	Solid	1	na	-	na	-	-	0	0	0	-	-
Dinitro-o-cresol	na	-	na	-	-	Solid	1	0.200 mg/m^3	5	19-25	5	2	0	0	0	12/27	-
2, 4-dinitrophenol	na	-	na	-	-	Solid	1	na	-	20-81	5	2	0	0	0	7/22	-
Dinitrotoluene	na	-	na	-	-	Solid	1	1.5	5	268-1625	3	2	0	0	0	10/27	-
Dinoseb	3	1	0.015	3	3	Liquid	2	na	-	8-60	5	1	0	0	5	11/22	3
Dioxane	13.8	2	0.015	3	6	39.7 mm at 25 C	3	100	2	790-3150	2	2	5	0	0	11/27	7
Dioxolane	na	-	na	-	-	70 mm at 20 C	3	na	-	729-3000	2	1	0	0	0	3/22	-
Diphenamid	3.0	1	0.015	3	3	Solid	1	na	-	293-600	3	-	0	0	0	3/20	0.5
Diphenyl	na	-	na	-	-	Solid	1	0.2	5	2400-3280	2	2	0	0	0	9/27	
Diphenylamine	na	-	na	-	-	Solid	1	1 mg/m^3	5	250-3000†	2	2	5	0	5	19/27	-
Diphenyl oxide	na	-	na	-	-	1 mm at 66 C	2	1	5	3370	2	1	0	0	0	9/27	-
Diphenylthiourea	na	-	na	-	-	Solid	1	na	-	600-720	3	-	0	0	0	3/20	-
Dipropylene glycol	67	4	0.015	3	12	0.01 mm at 20 C	2	na	-	na	-	1	0	0	0	1/17	1
Dipropylene glycol monomethyl ether	na	-	na	-	-	Liquid	2	100	2	7500	1	-	0	0	0	3/25	-
Disodium methanearsonate	35.0	3	0.015	3	9	Solid	1	na	-	600-1800	2	-	5	0	0	7/20	3
Disulfoton	8	1	0.015	3	3	Liquid	2	.10 mg/m^3	5	2.6-7	5	-	0	0	0	10/25	2

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Production Loss = Product — Production Actual	Production Score	Production Loss Fraction	Production Loss Score	Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Standard (air) Score	Acute Toxicity LD_{50} or LC^*_{50} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Ditridecylphthalate	27.2	2	0.015	3	6	na	-	na	-	na	-	-	0	0	0	-	-
Diuron	6	1	0.015	3	3	Solid	1	na	-	437-3400	2	-	0	0	0	2/20	<1
Dodecane	na	-	na	-	-	1 mm at 478 C	2	na	-	na	-	-	0	0	0	-	-
Dodecylbenzene	553.2	5	0.015	3	15	<10 mm at 75 C	2	na	-	na	-	-	0	0	0	-	-
Dodecylbenzenesulfonic acid, sodium salt	364.1	5	0.015	3	15	Liquid	2	na	-	105-2000	2	1	0_T	0	0	3/17	5
Dodecyl mercaptan	15	2	0.02	4	8	Liquid	2	na	-	309	3	-	0	0	0	3/20	2
Dodecylphenol	17.4	2	0.03	5	10	<10 mm at 25 C	2	na	-	2140	2	2	0	0	0	4/22	4
Dodecyl sulfate, sodium salt	26.8	3	0.03	5	15	Solid	1	na	-	1300	2	-	0	0	0	2/20	1
Dodecyl sulfate, tri-ethanolamine salt	16.1	2	0.03	5	10	Liquid	2	na	-	na	-	-	0	0	0	-	-
Dursban	5	1	0.015	3	3	Solid	1	na	-	145-500	4	-	0	0	0	4/20	<1
Dyfonate	2	1	0.015	3	3	10 mm at 25 C	2	na	-	3	5	-	0	0	0	5/20	2
Endosulfan	2.0	1	0.015	3	3.	Solid	1	.1 mg/m^3	5	18-40	5	-	0	0	0	10/25	1

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Standard (air) Score	Acute Toxicity LD_{50} or LC^*_{50} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	= Total / Total Possible	FINAL SCORE
Endothal	2	1	0.015	3	3	Solid	1	na	-	51	4	-	0	0	0	4/20	<1
Epichlorohydrin	495	5	0.015	3	15	16.8 mm at 25 C	2	5	5	90-238	4	1	4	0	0	14/27	16
Eptam	5	1	0.015	3	3	<10 mm at 25 C	2	na	-	112 1630	4	-	4	0	0	8/20	2
Ethane	5485	5	0.01	1	5	Gas	5	na	-	1000*	2*	2	0	0	0	4/22	5
Ethanolamine	293	5	0.015	3	15	6 mm at 60 C	2	3	5	305-2537	2	1	0	0	0	8/27	9
Ethion	2	1	0.015	3	3	<10 mm at 25 C	2	na	-	26-55	5	2	0	0	0	7/22	2
Ethyl acetate	212.0	5	0.015	3	15	92.5 mm at 25 C	3	400	-	709-5000 1600*	2 2*	2	0	0	0	4/22	8
Ethyl acetoacetate	na	-	na	-	-	1 mm at 28.5 C	2	na	-	3980	2	1	0	0	0	3/22	-
Ethyl acrylate	na	-	0.015	3	-	38.5 mm at 25 C	3	25	3	830-1950 420†	2 3†	2	0	0	0	8/27	-
Ethyl alcohol	1850.6	5	0.015	3	15	54.3 mm at 25 C	3	na	-	1440-8285	2	1	5	0	0	8/22	16
Ethylamine	45.9	3	0.015	3	9	1094.2 mm at 25 C	4	10	4	400†	3	1	0	0	0	8/27	11
Ethyl sec-amyl ketone	na	-	na	-	-	na	-	25	3	2500-3800	2	-	0	0	0	5/25	-
Ethylbenzene	6920	5	0.01	2	10	9.63 mm at 25 C	2	100	2	3500	2	2	0	0	0	6/27	4
Ethyl bromide	na	-	na	-	-	482.76 mm at 25 C	4	200	1	2200**	2	2	0	0	0	5/27	-
Ethyl butyl ketone	na	-	na	-	-	<1 mm at 20 C	2	50	2	2760	2	-	0	0	0	4/25	-
Ethyl chloride	660	5	0.01	2	10	Gas	5	1000	0	na	-	2	0	0	0	2/22	5

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Ethyl chloroacetate	na	–	na	–	–	4.93 mm at 25 C	2	na	–	na	–	1	0	0	0	1/17	–
Ethyl cyanoacetate	na	–	na	–	–	1 mm at 67.8 C	2	na	–	750	3	–	0	0	0	3/20	–
Ethylene	20,852.1	5	0.015	3	15	Gas	5	na	–	na	–	2	0	0	0	2/17	9
Ethylene carbonate	na	–	na	–	–	0.01 mm at 20 C	2	na	–	na	–	–	0	0	0	–	–
Ethylene chlorohydrin	na	–	na	–	–	7.65 mm at 25 C	2	5	5	67-580 385*	4 3*	1	0	0	0	10/27	–
Ethylenediamine	54.4	4	0.015	3	12	13.04 mm at 25 C	2	10	4	424-760 4000*	3 1*	1	0	0	0	8/27	7
Ethylene dibromide	315.5	5	0.015	3	15	14.54 mm at 25 C	2	20	3	55-250	4	–	0	0	0	7/25	8
Ethylene dichloride	9293	5	0.015	3	15	84.42 mm at 25 C	3	50	2	680-860	3	1	0	0	0	6/27	10
Ethylene glycol	3761.1	5	0.015	3	15	0.05 mm at 20 C	2	na	–	2000-6610	2	2	4	0	0	8/22	11
Ethylene glycol, diacetate	na	–	na	–	–	1 mm 38.3 C	2	na	–	1070-4940	2	–	0	0	0	2/20	–
Ethylene glycol, diethyl ether	na	–	na	–	–	9.4 mm at 20 C	2	na	–	2440-4390	2	–	0	0	0	2/20	–
Ethylene glycol, dimethyl ether	na	–	na	–	–	77.52 mm at 25 C	3	na	–	na	–	–	0	0	0	–	–
Ethylene glycol, monoacetate	na	–	na	–	–	(BP 181-182 C)	2	na	–	1310-3800	2	–	0	0	0	2/20	–

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Production Score	Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcinogenicity Score	Mutagenicity Score	Teratogenicity Score	Total / Total Possible	= FINAL SCORE
Ethylene glycol, monobutyl ether	na	-	na	-	-	0.76 mm at 20 C	2	50	2	280-1480	3	1	0	0	0	6/27	-
Ethylene glycol, monoethyl ether	205.4	5	0.015	3	15	3.8 mm at 20 C	2	200	1	1400-4300	2	2	0	0	0	5/27	6
Ethylene glycol, monoethyl ether acetate	na	-	na	-	-	1.2 mm at 20 C	2	100	2	1420-1910	2	1	0	0	0	5/27	-
Ethylene glycol, monohexyl ether	na	-	na	-	-	0.05 mm at 20 C	2	na	-	1480	2	-	0	0	0	2/20	-
Ethylene glycol, monomethyl ether	137.4	5	0.015	3	15	6.2 mm at 20 C	2	25	3	950-2460 1340*	2 2*	2	0	0	0	7/27	8
Ethylene glycol, monomethyl ether acetate	na	-	na	-	-	1.2 mm at 20 C	2	25	3	1250-3390	2	1	0	0	0	6/27	-
Ethylene glycol monooctyl ether	na	-	na	-	-	0.02 mm at 20 C	2	na	-	na	-	-	0	0	0	-	-
Ethylene glycol, monophenyl ether	na	-	na	-	-	<0.01 mm at 20 C	2	na	-	1260	2	-	0	0	0	2/20	-
Ethylene glycol, monopropyl ether	na	-	na	-	na	(BP 150 C at 743 mm)	2	na	-	4890	2	-	0	0	0	2/20	-
Ethyleneimine	5	1	0.015	3	3	160 mm at 20 C	4	1 mg/m^3	5	3.8-15	5	2	5	5	0	22/27	10
Ethylene oxide	3961.8	5	0.015	3	15	Gas	5	50	2	270-330 836-1462*	3 3*	2	5	5	0	17/27	47
Ethyl ether	103.2	5	0.015	3	15	442 mm at 20 C	4	400	0	1700	2	1	0	0	0	3/27	5
Ethyl formate	na	-	na	-	-	258.48 mm at 25 C	4	100	2	1100-2070	2	1	0	0	0	5/27	-

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X		Production Loss =		Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air)		Acute Toxicity LD_{50} or LC_{50}*		Non-lethal Acute Effects	Carcino-genicity	Muta-genicity	Terato-genicity	= Total / Total Possible	FINAL SCORE
	Actual	Score	Fraction	Score				TWA	Score	Range	Score	Score	Score	Score	Score		
Ethylhexanol	264.7	5	0.015	3	15	1 mm at 50 C	2	na	–	3200	2	–	0	0	0	2/20	3
Ethylidene chloride	na	–	na	–	–	230 mm at 25 C	4	100	2	725	3	2	0	0	0	7/27	–
Ethyl mercaptan	na	–	na	–	–	551.91 mm at 25 C	4	10	4	450–682	3	–	0	0	0	7/25	–
Ethyl methansulfonate	0	0	na	–	0	(BP 159 C)	2	na	–	200†	4	–	5	5	5	19/20	0
N-Ethylmorpholine	na	–	na	–	–	(BP 138 C)	2	20	4	1780	2	1	0	0	0	7/27	–
Ethyl naphthalene	na	–	na	–	–	1 mm at 20 C	2	na	–	5000†	1	1	0	0	0	2/22	–
Ethyl oxalate	na	–	na	–	–	1 mm 47.4 C	2	na	–	400	3	2	0	0	0	5/22	–
Ethyl parathion	15	2	0.01	2	4	<10 mm at 25 C	2	.11 mg/m^3	5	2–1500	5	–	0	0	0	10/25	3
Ethyl silicate	na	–	na	–	–	1 mm at 20 C	2	100	2	1000†	2	2	0	0	0	6/27	–
Ferbam	2.3	1	0.015	3	3	Solid	1	15 mg/m^3	5	2700–4000	2	1	5	0	0	13/27	1
Ferrocene	na	–	na	–	–	Solid	1	na	–	335–1550	3	–	0	0	0	3/20	–
Fluometuron	4	1	0.015	3	3	Solid	1	na	–	89–900	3	2	0	0	0	5/22	1
Folex	3	1	0.015	3	3	Liquid	2	na	–	76–910	3	–	0	0	0	3/20	<1
Folpet	2	1	0.015	3	3	Solid	1	na	–	10,000	1	1	0	0	5	7/22	1
Formaldehyde	5651.8	5	0.015	3	15	Gas	5	3	5	260–420	3	1	5	0	0	14/27	39

† LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X — Actual	Production X — Score	Production Loss — Fraction	Production Loss — Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) — TWA	OSHA Standard (air) — Score	Acute Toxicity LD_{50} or LC_{50}* — Range	Acute Toxicity — Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Formamide	na	–	na	–	–	1 mm at 70.5 C	2	20	3	2539	2	1	0	0	5	11/27	–
Formic acid	46.9	3	0.015	3	9	42.38 mm at 25 C	3	5	5	145–1210	2	1	0	0	0	8/27	8
Fumaric acid	42	3	0.015	3	9	Solid	1	na	–	na	–	–	0	0	0	–	–
Furfural	149.6	5	0.015	3	15	2.08 mm at 25 C	2	5	5	127–2300	3	1	0	0	0	9/27	10
Furfuryl alcohol	70	4	0.015	3	12	1 mm 31.8 C	2	50	2	40–650	3	1	0	0	0	6/27	5
Glycerol	199.2	5	0.015	3	15	<1 mm at 25 C	2	na	–	7750	1	2	0	0	0	3/22	4
Glycerol monostearate	27.2	2	0.030	5	10	Solid	1	na	–	200	4	–	0	0	0	4/20	2
Glycidol	160	5	0.015	3	15	Liquid	2	50	2	450–850	3	1	0	0	0	6/27	7
Glycine	na	–	na	–	–	Solid	1	na	–	na	–	–	0	0	0	–	–
Glyoxal	na	–	na	–	–	<10 mm at 25 C	2	na	–	100–760	3	1	0	0	0	4/22	–
Guanidine	na	–	na	–	–	Solid	1	na	–	100–1500†	3	–	0	0	0	3/20	–
Guthion	4	1	0.015	3	3	Solid	1	0.2 mg/m^3	5	4–16	5	1	0	0	0	11/27	1
Heptachlor	6	1	0.01	2	2	Solid	1	0.5 mg/m^3	5	27–116	4	2	0	0	0	11/27	1
Heptenes (mixed)	114	5	0.015	3	15	48.24 mm at 25 C	3	na	–	na	–	1	0	0	0	1/17	3

† LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Score	Production Loss Fraction	Score	= Product	VOLATILITY: Vapor Pressure	Score	TOXICITY: OSHA Standard (air) TWA	Score	Acute Toxicity LD_{50} or LC_{50}^{*} Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	FINAL SCORE
Herban	2.0	1	0.015	3	3	Solid	1	na	-	1470-4600	2	-	0	0	0	2/20	<1
Hexachloroethane	na	-	na	-	-	Solid	1	1	5	325-4000	2	2	0	0	0	9/27	-
Hexachloronaphthalene	na	-	na	-	-	Solid	1	0.2 mg/m^3	5	11†	5	2	0	0	0	12/27	-
Hexalene glycol	na	-	na	-	-	<10 mm at 25 C	2	na	-	3730	2	-	0	0	0	2/20	-
Hexamethylenetetramine	101	5	0.015	3	15	Solid	1	na	-	200-9200	2	2	5	5	0	14/22	10
Hexanediamine	613.4	5	0.015	3	15	Solid	1	na	-	na	-	2	0	0	0	2/17	2
Hydrogen cyanide	141.6	5	0.015	3	15	Liquid	4	10	4	3700-820 169-544*	2 3*	1	0	0	0	8/27	22
Hydroquinone	29.7	2	0.015	3	6	Solid	1	2 mg/m^3	5	70-550	4	1	4	0	0	14/27	3
Indene	na	-	na	-	-	2.23 mm at 25 C	2	10	4	na	-	1	0	0	0	5/22	-
Isoamyl alcohol	na	-	na	-	-	<10 mm at 25 C	2	100	2	1300	2	1	0	0	0	5/27	-
Isobutyl acetate	na	-	na	-	-	19.61 mm at 25 C	2	150	1	4760	2	-	0	0	0	3/25	-
Isobutyl alcohol	96.4	4	0.015	3	12	12.6 mm at 25 C	2	100	2	2460	2	1	0	0	0	5/27	4
Isobutyl aldehyde	na	-	na	-	-	210 mm at 25 C	4	na	-	2810	2	-	0	0	0	2/20	-
Isobutylene	na	-	na	-	-	Gas	5	na	-	na	-	-	0	0	0	-	-

†LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC^*_{50} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total/Total Possible	= FINAL SCORE
Isobutyric acid	na	–	na		–	2.67 mm at 25 C	2	na	–	280	3	–	0	0	0	3/20	–
Isodecyl alcohol	147	5	0.015	3	15	<0.01 mm at 20 C	2	na	–	na	–	–	0	0	0	–	–
Isoctyl alcohol	na	–	na		–	0.2 mm at 20 C	2	na	–	1490	2	–	0	0	0	2/20	–
Isooctylphenol, ethoxylated	20	2	0.030	5	10	Liquid	2	na	–	900-4000	2	–	0	0	0	2/20	1
Isophorone	na	–	na	–	–	1 mm at 38 C	2	25	3	2330	2	2	0	0	0	7/27	–
Isophthalic acid	100	4	0.015	3	12	Solid	1	na	–	4200	2	–	0	0	0	2/20	1
Isoprene	467	5	0.015	3	15	600.93 mm at 25 C	4	na	–	144-180**	4	1	0	0	0	5/22	14
Isopropyl acetate	41.9	3	0.015	3	9	58.8 mm at 25 C	3	250	0	3000	2	2	0	0	0	4/27	4
Isopropyl alcohol	1790	5	0.015	3	15	44.29 mm at 25 C	3	400	0	933-6000	2	2	0	0	0	4/27	7
Isopropylamine	18	2	0.015	3	6	321.2 mm at 25 C	4	5	5	820	3	2	0	0	0	10/27	9
Isopropyl chloride	na	–	na	–	–	534.5 mm at 25 C	4	na	–	na	–	1	0	0	0	1/17	–
Isopropyl ether	14	2	0.015	3	6	150 mm at 25 C	2	500	0	812	3	1	0	0	0	4/27	2
o-isopropylphenol	2084	5	0.015	3	15	1 mm at 56.6 C	2	na	–	na	–	–	0	0	0	–	–
p-isopropyl phenol	na	–	na	–	–	1 mm at 67 C	2	na	–	na	–	–	0	0	0	–	–

** LC_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Volatility Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	= Total / Total Possible	FINAL SCORE
Ketene	na	-	ma	-	-	Gas	5	0.5	5	1300	2	1	0	0	0	8/27	-
Ligninsulfonic acid, ammonium salt	40	3	0.030	5	15	Solid	1	na	-	na	-	-	0	0	0	-	-
Ligninsulfonic acid, calcium salt	326.6	5	0.030	5	25	Solid	1	na	-	na	-	-	0	0	0	-	-
Ligninsulfonic acid, ferrochrome salt	60	4	0.030	5	20	Solid	1	na	-	na	-	-	0	0	0	-	-
Ligninsulfonic acid, sodium salt	58.7	4	0.030	5	20	Solid	1	na	-	na	-	-	0	0	0	-	-
Lindane	<1	0	0.015	3	0	Solid	1	500 mg/m^3	0	60-840	4	2	0	5	0	16/27	0
Linuron	2	1	0.015	3	3	Solid	1	na	-	500-3300	2	-	0	0	0	2/20	<1
Magenta	.116	0	0.015	3	0	Solid	1	na	-	150†	4	-	5	0	0	9/15	0
Malathion	30	3	0.010	2	6	<1 mm at 25 C	2	15	3	50-599	3	1	0	0	0	7/27	3
Maleic acid	283.2	5	0.015	3	15	Solid	1	na	-	708	3	1	0	0	0	4/22	3
Maleic anhydride	211.8	5	0.015	3	15	Solid	1	0.25	5	60	4	2	5	0	0	16/27	9
Maleic hydrazide	3.0	1	0.015	3	3	Solid	1	na	-	3800	2	-	5	0	0	7/20	1
Malic acid	na	-	na	-	-	Solid	1	na	-	1600†	2	-	0	0	0	2/20	-
Melamine	170	5	0.015	3	15	Solid	1	na	-	1600†	2	-	0	0	0	2/20	2
Mesityl oxide	na	-	na	-	-	9.16 mm at 25 C	2	25	3	354-1120	3	2	0	0	0	8/27	-

† TD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Production Score	Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Volatility Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC^*_{50} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Mesitylene	na	–	na	–	–	Liquid	2	25	3	2400** 303-1500†	2** 2*†	1	0	0	0	6/27	–
Methacrylic acid	na	–	na	–	–	1 mm at 25.5 C	2	na	–	49	5	1	0	0	0	6/22	–
Methacrylonitrile	10	1	0.015	3	3	72.38 mm at 25 C	3	1	5	250- 37-328*	4 4*	1	0	0	0	10/27	3
Methallyl alcohol	na	–	na	–	–	Liquid	2	na	–	500†	3	–	0	0	0	3/20	–
Methallyl chloride	na	–	na	–	–	101.7 mm at 20 C	4	na	–	2000*	2	–	0	0	0	2/20	–
Methane	12,400	5	0.015	3	15	Gas	5	na	–	400*	3	1	0	0	0	4/22	14
Methanearsonic acid	30.7	3	0.010	2	6	Solid	1	na	–	3350	2	–	0	0	0	2/20	1
Methomyl	2.0	1	0.015	3	3	Solid	1	na	–	17-24	5	–	0	0	0	5/20	1
Methoxychlor	10	2	0.015	3	6	Solid	1	15 mg/m^3	5	5000-6430	1	1	4	0	0	11/27	2
Methoxyethanol	119.1	5	0.015	3	15	6.2 mm at 20 C	2	25	3	890-2460	2	–	0	0	0	5/25	6
2-[2-(2-methoxyethoxy) ethoxy] ethanol	31.7	3	0.015	3	9	na	–	na	–	na	–	–	0	0	0	–	–
Methyl acetate	8.8	1	0.015	3	3	212.5 mm at 25 C	4	200	1	3700	2	1	0	0	0	4/27	2
Methylal	na	–	na	–	–	330 mm at 20 C	4	1000	0	3013†	2	1	0	0	0	1/22	–
Methyl alcohol	5103.5	5	0.015	3	15	127.9 mm at 25 C	4	200	1	9800 1000*	1 3*	1	0	0	0	5/27	11
Methylamine	319	5	0.015	3	15	Gas	5	na	–	3000	2	–	0	0	0	2/20	8
Methylamylacetate	na	–	na	–	–	3.8 mm at 20 C	2	50	2	4000†	1	1	0	0	0	4/27	–
Methylamyl alcohol	50	3	0.015	3	9	2.8 mm at 20 C	2	25	3	812-2600	2	2	0	0	0	7/27	5
Methylaniline	na	–	na	–	–	1 mm at 36 C	2	2	5	24-1200	3	2	5	0	0	15/27	–

$^{**}LC_{Lo}$ $^{\dagger}LD_{Lo}$

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Volatility Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Methylbenzyl alcohol	na	-	na	-	-	0.25 mm at 25 C	2	na	-	400		-	0	0	0	2/20	-
Methyl bromide	24.6	2	0.010	2	4	Gas	5	20	3	21*	5	2	0	0	0	10/27	7
Methylbutyl ketone	na	-	na	-	-	10 mm at 38.8 C	2	100	2	2590	2	1	0	0	0	5/27	-
Methylbutynol	na	-	na	-	-	(BP 104 C)	2	na	-	3600	2	-	0	0	0	2/20	-
Methyl cellulose	20	2	0.03	5	10	Solid	1	na	-	na	-	-	0	0	0	-	-
Methyl chloride	458	5	0.010	2	10	Gas	5	100	2	1800	2	2	0	0	0	6/27	11
Methylcholanthrene	na	-	na	-	-	Solid	1	na	-	100†	4	-	5	0	0	9/20	-
Methyl cyclohexane	na	-	na	-	-	47.06 mm at 25 C	3	500	0	7500* 4000†	0* 2†	1	0	0	0	2/27	-
Methylcyclohexanol	na	-	na	-	-	<10 mm at 25 C	2	100	2	1750†	2	1	0	0	0	5/27	-
Methylcyclohexanone	na	-	na	-	-	<5 mm at 25 C	2	100	2	2140	2	2	0	0	0	6/27	-
Methyldioxolane	na	-	na	-	-	na (BP 81-82C)	3	na	-	3000	2	-	0	0	0	2/20	-
4, 4'-methylene bis (2-chloroaniline)	7.716	1	0.015	3	3	Solid	1	na	-	na	-	-	5	0	0	5/15	1
Methylene chloride	591	5	0.015	3	15	435.8 mm at 25 C	4	500	0	1500-6460	2	2	0	0	0	4/27	9
Methylenedianiline	2.2	1	0.015	3	3	Solid	1	na	-	280-347	3	-	5	0	0	8/20	1
Methyl ethyl ketone	509	5	0.015	3	15	96.4 mm at 25 C	3	200	1	616-3400	2	1	0	0	0	4/27	7

† LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Loss Score	= Product	X VOLATILITY: Vapor Pressure	Volatility Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Methyl formate	na	-	na	-	-	602.5 mm at 25 C	4	100	2	1620	2	1	0	0	0	5/27	-
Methylhydrazine	na	-	na	-	-	49.6 mm at 25 C	3	0.35 mg/m^3	5	12-33	5	2	5	0	5	22/27	-
Methyl iodide	na	-	na	-	-	400 mm at 25.3 C	4	5	5	110-	4	1	4	0	0	14/27	-
Methyl isoamyl ketone	na	-	na	-	-	BP 144 C	2	100	2	4760	2	-	0	0	0	4/25	-
Methyl isobutyl ketone	208.3	5	0.015	3	15	7.1 mm at 25 C	2	100	2	268-2080	2	-	0	0	0	4/25	5
Methyl isocyanate	na	-	na	-	-	(BP 59.6C)	4	0.02	5	8-14*	5	2	0	0	0	12/27	-
Methyl mercaptan	na	-	na	-	-	Gas	5	10	4	2.4	5	-	0	0	0	9/25	-
Methyl methacrylate	718.8	5	0.015	3	15	40 mm at 25.5 C	3	100	2	1000-7500 3750*	1 1*	1	0	0	0	4/27	7
Methylnaphthalene	na	-	na	-	-	<10 mm at 25 C	2	na	-	5000	1	-	0	0	0	1/20	-
N-methyl-N'-nitro-N-nitrosoguanidine	na	-	na	-	-	na	-	na	-	400	4	-	5	0	0	9/20	-
Methyl parathion	51.1	4	0.010	2	8	Solid	1	0.2 mg/m^3	5	9-9300	5	-	0	0	0	10/25	3
Methylpentanediol	50	3	0.015	3	9	<0.1 mm at 20 C	2	na	-	1299-3860	2	-	0	0	0	2/20	2
Methylpentynol	na	-	na	-	-	(BP 120-121 C)	2	na	-	300-750	3	2	0	0	0	5/22	-
Methylphenylcarbinol	na	-	na	-	-	Liquid	2	na	-	na	-	-	0	0	0	-	-
a-methyl styrene	65	4	0.015	3	12	1 mm at 7.4 C	2	100	2	4900	2	1	0	0	0	5/27	4
Mevinphos	<1	0	0.015	3	0	0.0029 mm at 21 C	2	0.4 mg/m^3	5	0.89-4	5	-	0	0	0	10.25	0

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Volatility Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}^{*} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Mirex	<1	0	0.015	3	0	Solid	1	na	-	300-600	3	-	5	0	0	8/20	0
Monosodium glutamate	47.3	3	0.030	5	15	Solid	1	na	-	4253-8000	1	2	0	0	5	8/22	5
Morpholine	23.3	2	0.030	5	10	10 mm at 23 C	2	20	3	1050	2	2	4	0	0	11/27	8
MSMA	35.0	2	0.015	3	6	Solid	1	na	-	50-1800	3	-	0	0	0	3/20	1
Nabam	1.4	1	0.015	3	3	Solid	1	na	-	395-580	3	-	0	0	0	3/20	<1
Naled	2.0	1	0.015	3	3	Solid	1	3 mg/m^3	5	250	3	-	0	0	0	8/25	1
Naptalam	2.0	1	0.015	3	3	Solid	1	na	-	1700-5000	2	-	0	0	0	2/20	<1
Naphtha (solvent)	8288.4	5	0.010	2	10	(BP 160-220 C)	2	100	2	1600†	2	2	5	0	0	9/22	8
Naphthalene	143	5	0.010	2	10	Solid	1	10	4	1780	2	2	4	0	0	12/27	4
α-Naphthalene sulfonic acid	na	-	na	-	-	Solid	1	na	-	na	-	-	0	0	0	-	-
β-Naphthalenesulfonic acid	39.0	3	0.015	3	9	Solid	1	na	-	400	3	-	0	0	0	3/20	1
α-Naphthol	na	-	na	-	-	Solid	1	na	-	2590	2	2	0	0	0	4/22	-
β-Naphthol	0	0	na	-	0	Solid	1	na	-	2420	2	2	0	0	0	4/22	0
1-Naphthylamine	1.1	1	0.015	3	3	Solid	1	na	-	779	3	-	5	0	0	8/20	1
2-Naphthylamine	1.28	1	0.015	3	3	Solid	1	car-cin-ogen	5	727	3	-	5	0	0	13/22	2
Neopentanoic acid	5	1	0.015	3	3	Solid	1	na	-	5000†	1	-	0	0	0	1/20	<1
Nitrilotriacetic acid, trisodium salt	85	4	0.015	3	12	Solid	1	na	-	254-1100	3	-	0	0	0	3/20	2

$^{\dagger}LD_{Lo}$

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X		Production Loss =		Product	X VOLATILITY: Vapor Pressure		X TOXICITY: OSHA Standard (air)		Acute Toxicity LD_{50} or LC_{50}^{*}		Non-lethal Acute Effects	Carcino-genicity	Muta-genicity	Terato-genicity	= Total / Total Possible	FINAL SCORE
	Actual	Score	Fraction	Score		Vapor Pressure	Score	TWA	Score	Range	Score	Score	Score	Score	Score	Total / Total Possible	
p-nitro-aniline	8.17	1	0.015	3	3	Solid	1	1	5	250-3249	2	2	0	0	0	9/27	1
Nitroanisole	na	-	na	-	-	Solid	1	na	-	1400-4700	2	-	0	0	0	2/20	-
Nitrobenzene	551.2	5	0.015	3	15	0.284 mm at 25 C	2	5	5	150-2000	3	2	0	0	5	15/27	17
p-nitrobenzoic acid	na	-	na	-	-	Solid	1	na	-	770-1960	2	-	0	0	0	2/20	-
Nitrocellulose	50	3	0.030	5	15	Solid	1	na	-	na	-	-	0	0	0	-	-
Nitroethane	na	-	na	-	-	20.3 mm at 25 C	2	100	2	860-1100	3	1	0	0	0	6/27	-
Nitroglycerine	na	-	na	-	-	1 mm at 127 C	2	2 mg/m^3	5	40-450†	4	1	0	0	0	10/27	-
Nitromethane	na	-	na	-	-	36.27 mm at 25 C	3	100	2	940-950	3	2	0	0	0	7/27	-
m-nitrophenol	14.8	2	0.015	3	6	Solid	1	na	-	447-1414	3	-	0	0	0	3/20	1
o-nitrophenol	14.8	2	0.015	3	6	Solid	1	na	-	1297-2828	2	2	0	0	0	4/22	1
p-nitrophenol	52	4	0.015	3	12	Solid	1	na	-	75-467	4	2	0	0	0	6/22	3
1-nitropropane	na	-	na	-	-	9.87 mm at 25 C	2	25	3	800	3	1	0	0	0	7/27	-
2-nitropropane	na	-	na	-	-	17.42 mm at 25 C	2	25	3	75-500† 74-462**	3† 2**	1	0	0	0	7/27	-
N-nitrosodiethylamine	na	-	na	-	-	Liquid	2	na	-	11-246	4	-	5	5	5	19/20	-
N-nitroso dimethylamine	na	-	na	-	-	Liquid	2	na	-	26-45 57-78	5 5*	2	5	0	5	17/22	-
Nitrosoethylurea	na	-	na	-	-	Solid	1	na	-	240-300	3	1	5	0	5	14/22	-
Nitrosomethylurea	na	-	na	-	-	Solid	1	na	-	110-180	4	-	5	0	5	14/20	-
m-nitrotoluene	na	-	na	-	-	1 mm at 50 C	2	5	5	330-3600	2	-	0	0	0	7/25	-

† LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Score	Production Loss Fraction	Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	Score	Acute Toxicity LD_{50} or LC^{*}_{50} Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
o-nitrotoluene	na	–	na	–	–	1 mm at 50C	3	5	5	891-2462	2	–	0	0	0	7/25	–
p-nitrotoluene	na	–	na	–	–	Solid	1	5	5	940-2144	2	–	0	0	0	7/25	–
Nonene	na	–	na	–	–	(BP 149.9C)	2	na	–	na	–	–	0	0	0	–	–
Nonyl phenol	191	5	.007	1	5	10 mm at 25 C	2	na	–	1620–2140	2	–	0	0	0	2/25	1
Octyl alcohol	na	–	na	–	–	0.2 mm at 20C	2	na	–	1480	2	–	0	0	0	2/20	–
m-octyl M-decyl phthalate	200	5	0.015	3	15	<10 mm at 25 C	2	na	–	na	–	–	0	0	0	–	–
Octyl phenol	na	–	na	–	–	Solid	1	na	–	25†	5	–	0	0	0	5/20	–
Oxalic acid	18	2	0.015	3	6	Solid	1	1 mg/m^3	5	700–1000†	2	2	0	0	0	9/22	2
Paraldehyde	na	–	na	–	–	25.3 mm at 20 C	3	na	–	3500	2	1	4	0	0	7/22	–
Paraquat	0	0	na	–	0	Solid	1	na	–	22–80	4	2	0	0	5	11/22	0
PCNB	3	1	0.01	2	2	Solid	1	na	–	1650	2	–	5	0	0	7/20	<1
PCP (and salts)	46	2	0.015	3	6	Solid	1	500 $\mu g/m^3$	5	27–100	4	1	3	5	0	18/27	3
Pentaerythritol	100.4	5	0.015	3	15	Solid	1	na	–	na	–	–	0	0	0	–	–
n-Pentane	478	5	0.015	3	15	400 mm at 18.5	4	1000	0	na	–	1	5	0	0	6/22	16
Pentylenes	na	–	na	–	–	na	4	na	–	na	–	1	0	0	0	1/17	–

† LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Score	Production Loss Fraction	Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	Score	Acute Toxicity LD_{50} or LC_{50}^* Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	= Total / Total Possible	FINAL SCORE
Perchloroethylene	673.7	5	0.015	3	15	18.47 mm at 25 C	2	100	2	85-5000†	1	1	0_T	0	0	3/22	4
Perchloromethyl mercaptan	na	-	na	-	-	Liquid	2	800	-	83	4	1	0	5	0	10/22	-
o-phenetidine	na	-	na	-	-	1 mm at 67 C	2	na	-	na	-	2	5	0	0	7/17	-
p-phenetidine	na	-	na	-	-	<10 mm at 25 C	2	na	-	na	-	-	5	0	0	5/15	-
Phenol	2399	5	0.015	3	15	Solid	1	5	5	250-414	3	2	5	0	0	15/27	8
Phenothiazine	na	-	na	-	-	Solid	1	5 mg/m^3	5	5000	2	2	0	0	0	9/27	-
o-phenylenediamine	na	-	na	-	-	Solid	1	100 µg/m^3	5	na	3	2	0	0	0	10/27	-
p-phenylenediamine	48	3	0.015	3	9	Solid	1	100 µg/m^3	5	17-200†	4	2	0	0	0	11/27	4
Phenylhydrazine	na	-	na	-	-	Solid	1	5	5	80-188	4	2	0	0	0	11/27	-
Phosgene	728.2	5	0.015	3	15	Gas	5	0.1	5	75-3211*	3*	1	0	0	0	9/27	25
Phthalic anhydride	933	5	0.015	3	15	Solid	1	2	5	800-4020	2	2	0	0	0	9/27	5
Phthalimide	na	-	na	-	-	Solid	1	na	-	na	-	-	0	0	0	-	-
Phthalonitrile	na	-	na	-	-	Solid	1	na	-	35-1860	4	-	0	0	0	4/20	-
Picloram	na	-	na	-	-	Solid	1	10 mg/m^3	5	1500-3750	2	-	0	0	0	7/25	-
β-picoline	>60	4	0.015	3	12	10.46 mm at 25 C	2	na	-	na	-	-	0	0	0	-	-
α- and β-pinene	120.7	5	0.015	3	15	1 mm at 37.3 C	2	na	-	na	-	1	0	0	0	1/17	2

†LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Production X Score	Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC^*_{50} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Piperazine	4.6	1	0.015	3	3	Solid	1	na	-	1100	2	1	0	0	0	3/22	<1
Piperonyl butoxide	1.0	1	0.015	3	3	na	2	na	-	3800-11500	1	-	0	0	0	1/20	<1
Planavin	2	1	0.015	3	3	Solid	1	na	-	2000	2	-	0	0	0	2/20	1
Polyacrylamide	12.8	2	0.030	5	10	Solid	1	na	-	na	-	-	0	0	0	-	-
Polybutenes	335.0	5	0.015	3	15	<10 mm at 25 C	2	na	-	na	-	-	0	0	0	-	-
PCBS (polychlorinated biphenyls)	5.495	1	0.01	2	2	<1 mm at 25 C	2	.5-1 mg/m^3	5	2000-10,000	1	2	5	0	5	13/22	5
Polyethylene and co-polymers	2295.9	5	0.030	5	25	Solid	1	na	-	na	-	-	4	0	0	4/15	7
Polyethylene glycol	52.4	4	0.015	3	12	<10 mm at 25 C	2	na	-	na	-	-	5	0	0	5/15	8
Polyethylene glycol chloride	na	-	na	-	-	na	2	na	-	1070	2	-	0	0	0	2/20	-
Polyethylene tetra-phthalate	2500	5	0.015	3	15	Solid	1	na	-	na	-	-	4	0	0	4/15	-
Polypropylene	2162	5	0.030	5	25	Solid	1	na	-	na	-	-	0	0	0	-	-
Polypropylene glycol	359.2	5	0.015	3	15	Liquid	2	na	-	419	3	-	0	0	0	3/20	5
Polystyrene	3322	5	0.030	5	25	Solid	1	na	-	na	-	-	4	0	0	4/15	7
Polystyrene, thermo-plastic resins	1647	5	0.030	5	25	Solid	1	na	-	na	-	-	4	0	0	4/15	7
Polytetrafluoroethylene	13.2	2	0.030	5	10	Solid	1	na	-	na	-	2	4	0	0	6/17	3
Polyvinyl alcohol	100-141	5	0.030	5	25	Solid	1	na	-	na	-	-	5	0	0	5/15	8
Polyvinyl chloride	4562	5	0.030	5	25	Solid	1	na	-	na	-	1	5	0	5	11/17	16
Princep	5	1	0.015	3	3	<10 mm at 25 C	2	na	-	5000	1	-	0	0	0	1/20	<1

TABLE 4-1 (CONTINUED)

PLANT RELEASE X VOLATILITY X TOXICITY = FINAL SCORE

COMPOUND	Production X: Actual	Production X: Score	Production Loss: Fraction	Production Loss: Score	= Product	Vapor Pressure	Score
Propachlor	23	2	0.010	2	4	Solid	1
Propane	9608.3	5	0.010	2	10	Gas	5
Propanil	6	1	0.015	3	3	Solid	1
Propargyl alcohol	na	-	na	-	-	Volatile Liquid	3
Propazine	4	1	0.015	3	3	Solid	1
β-propiolactone	na	-	na	-	-	na	2
Propionaldehyde	na	-	na	-	-	<10 mm at 25 C	2
Propionic acid	60.4	4	0.015	3	12	4.49 mm at 25 C	2
n-propyl acetate	32.4	3	0.015	3	9	40 mm at 28.8 C	3
n-propyl alcohol	83.1	4	0.015	3	12	19.8 mm at 25 C	2
n-propylamine	0.2	0	0.015	3	0	248 mm at 20 C	4
n-propyl chloride	na	-	na	-	-	348.8 mm at 25 C	4
Propylene	23000	5	0.015	3	15	Gas	5
Propylene chlorohydrin	na	-	na	-	-	4.9 mm at 20 C	2
Propylene glycol	562.6	5	0.015	3	15	1 mm at 45.5 C	2
Propylene imine	na	-	na	-	-	na	4

COMPOUND	OSHA Standard (air): TWA	OSHA Standard (air): Score	Acute Toxicity LD_{50} or LC_{50}*: Range	Acute Toxicity: Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	FINAL SCORE
Propachlor	na	-	800-1200	3	-	0	0	0	3/20	1
Propane	1000	0	na	-	2	0	0	0	2/22	5
Propanil	na	-	500-1500	2	-	0	0	0	2/20	<1
Propargyl alcohol	1	5	0.07	5	1	0	0	0	11/27	-
Propazine	na	-	485	3	-	4	0	0	7/20	1
β-propiolactone	na	-	345	3	-	5	0	0	8/20	-
Propionaldehyde	na	-	680-820	3	1	0	0	0	4/22	-
Propionic acid	na	-	625-1900	2	1	0	0	0	3/22	3
n-propyl acetate	200	1	6630	1	1	0	0	0	3/27	3
n-propyl alcohol	200	1	1870-3230	2	1	0	0	0	4/27	4
n-propylamine	na	-	2310*	2*	1	0	0	0	3/22	0
n-propyl chloride	na	-	na	-	1	0	0	0	1/17	-
Propylene	na	-	na	-	1	0	0	0	1/17	4
Propylene chlorohydrin	na	-	220-720	3	-	0	0	0	3/20	-
Propylene glycol	na	-	195-945	3	-	0	0	0	3/20	5
Propylene imine	2	5	19-43	4	-	5	0	0	14/25	-

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Production Score	Production Loss Fraction	Production Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity* LD_{50} or LC_{50} Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcinogenicity Score	Mutagenicity Score	Teratogenicity Score	Total / Total Possible	= FINAL SCORE
Propylene oxide	1640	5	0.015	3	15	596 mm at 25 C	4	100	2	690–930	3	1	3	0	0	9/27	20
Pyridine	>60	4	0.015	3	12	20.3 mm at 25 C	2	5	5	891–1000 4000*	3 1*	2	0	0	0	10/27	9
Randox	10	1	0.015	3	3	<20 mm at 25 C	2	na	–	700	3	–	0	0	0	3/20	2
Resorcinol	35	3	0.015	3	9	Solid	1	na	–	301–340	3	2	0	0	0	5/22	2
Ronnel	2	1	0.015	3	3	Solid	1	10	4	118–2823	2	2	0	0	0	8/27	1
Ruelene	2	1	0.015	3	3	Solid	1	5 mg/m^3	5	100–1000	3	–	0	0	0	8/25	1
Salicylic acid	35	3	0.03	5	15	Solid	1	na	–	891	3	1	0	0	0	4/22	3
Silvex	3	1	0.015	3	3	Solid	1	na	–	375–1200	3	–	0	0	0	3/20	<1
Sodium acetate	16.5	2	0.015	3	6	Solid	1	na	–	335–8000	2	–	0	0	0	2/20	<1
Sodium benzoate	6	1	0.015	3	3	Solid	1	na	–	2000–4100	2	–	0	0	0	2/20	<1
Sodium carboxymethyl cellulose	69	4	0.03	5	20	Solid	1	na	–	na	–	–	4	0	0	4/15	5
Sodium chloroacetate	na	–	na	–	–	Solid	1	na	–	76–165	4	–	0	0	0	4/20	–
Sodium formate	32	3	0.015	3	9	Solid	1	na	–	807–2500	2	–	0	0	0	2/20	1
Sorbic acid	40	3	0.015	3	9	Solid	1	na	–	7400	1	–	5	0	0	6/20	3
Sorbitol	84.1	4	0.015	3	12	Solid	1	na	–	na	–	–	0	0	0	–	–

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X — Actual	Score	Production Loss = Product — Fraction	Score	Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) — TWA	Score	Acute Toxicity LD_{50} or LC_{50}* — Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
Styrene	4394	5	0.015	3	15	6.05 mm at 25 C	2	100	2	216-5000	2	2	0	0	0	6/27	7
Succinic acid	na	-	na	-	-	Solid	1	na	-	2000†	2	-	0	0	0	2/20	-
Succinonitrile	na	-	na	-	-	Solid	1	na	-	100	4	-	0	0	0	4/20	-
Sulfanilic acid	na	-	na	-	-	Solid	1	na	-	na	-	1	0	0	0	1/17	-
Sulfolane	35	3	0.015	3	9	.01 mm at 20 C	2	na	-	1540-3180	2	-	0	0	0	2/20	2
Sulfosuccinic acid, bis (2-ethyl hexyl) ester, ~~sodium salt~~	12.4	2	0.03	5	10	Solid	1	na	-	60-4800	2	-	0	0	0	2/20	1
Sutan	6	1	0.015	3	3	<10 mm at 25 C	2	na	-	4000-5366	2	-	0	0	0	2/20	1
2, 3, 6-TBA	2.0	1	0.015	3	3	Solid	1	na	-	615-1644	3	-	0	0	0	3/20	<1
TCA	1.0	1	0.015	3	3	Solid	1	na	-	3320	2	1	0	0	0	3/22	<1
Terephthalic acid	4644.1	5	0.015	3	15	Solid	1	na	-	1430	2	-	0	0	0	2/20	2
Termik	2.0	1	0.015	3	3	Solid	1	na	-	0.93-2.5	5	-	0	0	0	5/20	1
1, 1, 2, 2-tetrachloro-1, 2-difluoroethane	na	-	na	-	-	na	3	na	-			-	0	0	0	-	-
1, 1, 1, 2-tetrachloro-2, 2-difluoroethane	na	-	na	-	-	52.53 mm at 25 C	3	na	-	10,000*	0	1	0	0	0	1/22	-
Tetrachloronaphthalene	na	-	na	-	-	Solid	1	2 mg/m^3	5	na	-	1	0	0	0	6/22	-

†LD_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production X Actual	Score	Production Loss Fraction	Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	Score	Acute Toxicity LD50 or LC50* Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	= Total / Total Possible	FINAL SCORE
Tetrachlorophthalic anhydride	na	-	na	-	-	Solid	1	na	-	na	-	-	0	0	0	-	-
Tetraethyl lead	353	5	0.015	3	15	1 mm at 38.4 C	2	.0117 mg/m^3	5	15	5	2	5	0	5	22/27	24
Tetrahydrofuran	59.0	4	0.015	3	12	143 mm at 20 C	4	200	1	500-3000†	2	1	0	0	0	4/27	7
1, 2, 3, 4-Tetrahydrophthalene	na	-	na	-	-	1 mm at 38.0 C	2	na	-	2860	2	2	0	0	0	4/22	-
Tetrahydrophthalic anhydride	na	-	na	-	-	Solid	1	na	-	500†	3	-	0	0	0	3/20	-
Tetramethylethylenediamine	na	-	na	-	-	na	2	na	-	1580†	2	-	0	0	0	2/20	-
Tetramethyl lead	972.5	5	0.015	3	15	6.0 mm at 10 C	2	.09 mg/m^3	5	105-109	4	2	0	0	0	11/27	12
Tetramethyl Succinonitrile	na	-	na	-	-	Solid	1	3 mg/m^3	5	60**	4	-	0	0	0	9/25	-
Tetranitromethane	na	-	na	-	-	1 mm at 22.7 C	2	1	5	33** 500†	5** 3†	1	0	0	0	11/27	-
Tetrapropylene	na	-	na	-	-	na	2	na	-	na	-	-	0	0	0	-	-
Tetryl	na	-	na	-	-	Solid	1	1.5 mg/m^3	5	500	3	1	0	0	0	9/27	-
Thiuram	15.7	2	0.015	3	6	Solid	1	5 mg/m^3	5	210-1350	3	2	0	0	5	15/27	3
o-tolidine	na	-	na	-	-	Solid	1	na	-	404	4	-	5	0	0	9/20	-
Toluene	6937.9	5	0.010	2	10	28.4 mm at 25 C	3	200	1	1640-5000 5300*	2 0*	2		0	0	5/27	6
Toluene-2, 4-diamine	63	4	0.015	3	12	Solid	1	na	-	50-500†	3	2	4	0	0	9/22	5
Toluene diisocyanate	420	4	0.015	3	12	<0.01 mm at 20 C	2	.14 mg/m^3	5	10-14*	5*	2	0	0	0	12/27	11

†LD_{Lo} **LC_{Lo}

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Loss Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity, LD_{50} or LC_{50}* Range	Acute Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	= FINAL SCORE
p-Toluene sulfonamide	na	–	na	–	–	Solid	1	na	–	75-250	4	–	0	0	0	4/20	–
o-Toluenesulfonic acid	na	–	na	–	–	Solid	1	na	–	na	–	1	0	0	0	1/17	–
p-Toluenesulfonic acid	na	–	na	–	–	Solid	1	na	–	400	3	2	0	0	0	5/22	–
p-Toluenesulfonyl chloride	na	–	na	–	–	Solid	1	na	–	na	–	2	0	0	0	2/17	–
m-Toluidene	na	–	na	–	–	1 mm at 41 C	2	na	–	150-974	3	2	4	0	0	9/22	–
o-Toluidene	na	–	na	–	–	1 mm at 41 C	2	5	5	150-3250	3	2	4	0	0	14/27	–
p-Toluidene	na	–	na	–	–	Solid	1	na	–	42-50	5	2	5	0	0	12/22	–
Toxaphene	48	3	0.010	2	6	Solid	1	0.5 mg/m^3	5	60	4	1	0	0	0	10/27	2
Tributyl phosphate	na	–	na	–	–	20 mm at 20 C	2	5	5	3000	2	–	0	0	0	7/25	–
Trichloroaniline	na	–	na	–	–	Solid	1	na	–	na	–	–	0	0	0	–	–
Trichlorobenzene	10	1	0.015	3	3	1 mm at 40 C	2	na	–	756-766	3	1	0	0	0	4/22	1
1, 1, 1-trichloroethane	591	5	0.015	3	15	130.86 mm at 25 C	4	350	0	5660-9470	1	2	0	0	0	3/27	7
1, 1, 2-trichloroethane	na	–	na	–	–	25 mm at 25 C	3	10	4	227-580	3	2	0_T	0	0	9/27	–
Trichloroethylene	285.2	5	0.015	3	15	77.5 mm at 25 C	3	100	2	34-4920	2	2	5	0	0	11/27	18
Trichlorofluoromethane	299.6	5	0.015	3	15	717.5 mm at 25 C	4	1000	0	na	–	1	0	0	0	1/22	3
Trichloroisocyanuric acid	40.0	3	0.03	5	15	Solid	1	100	1	750	4	1	0	0	0	6/27	2
Trichloronaphthalene	na	–	na	–	–	Solid	1	na	–	na	–	–	0	0	0	–	–
2,4,5-Trichlorophenoxy acetic acid	6	1	0.015	3	3	Solid	1	10 mg/m^3	5	100-500	3	–	0	0	5	13/25	2

TABLE 4-1 (CONTINUED)

COMPOUND	PLANT RELEASE: Production Actual	Production Score	X Production Loss Fraction	Production Loss Score	= Product	VOLATILITY: Vapor Pressure	Score	TOXICITY: OSHA Standard (air) TWA	OSHA Score	Acute Toxicity LD_{50} or LC_{50}* Range	Acute Toxicity Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total / Total Possible	FINAL SCORE
1, 2, 3-trichloropropane	na	-	na	-	-	3.59 mm at 25 C	2	50	2	320	3	2	0	0	0	7/27	-
1, 1, 2-trichloro-1, 2, 2-trifluoroethane	na	-	na	-	-	Gas	5	1000	0	na	-	-	5	0	0	5/20	-
Tricresyl phosphate	50.2	4	0.015	3	12	0.29 mm at 20 C	2	0.1 mg/m^3	5	100-4680†	2	1	0_T	0	0	8/27	7
Tridecyl benzene sulfonic acid, sodium salt	149.9	5	0.015	3	15	<10 mm at 25 C	1	na	-	na	-	-	0	0	0	-	-
Triethanolamine	100.7	5	0.015	3	15	<0.01 mm at 20 C	2	na	-	8000	1	-	0	0	0	1/20	2
Triethylamine	22.8	2	0.015	3	6	na	3	25	3	460-546	3	2	0	0	0	8/27	5
Triethylene glycol	113	5	0.015	3	15	1mm at 14 C	2	na	-	9739	1	-	0	0	0	1/20	2
Triethylene glycol, diethyl ether	na	-	na	-	-	0.9 mm at 20 C	2	na	-	na	-	-	0	0	0	-	-
Triethylene glycol, monomethyl ether	31.7	3	0.015	3	9	<0.01 mm at 20 C	2	na	-	na	-	-	0	0	0	-	-
Trifluralin	20	2	0.01	2	4	Solid	1	na	-	500-500,000	2	-	0	0	0	2/20	<1
Triisobutylene	na	-	na	-	-	2.08 mm at 25 C	2	na	-	na	-	-	0	0	0	-	-
Trimethylamine	28.8	3	0.015	3	9	Gas	5	na	-	90	4	1	0	0	0	5/22	10
2, 2, 4-trimethyl-1, 3-pentanediol	20	2	0.015	3	6	Solid	1	na	-	na	-	-	0	0	0	-	-
Trinitrotoluene	na	-	na	-	-	Solid	1	na	-	na	-	-	0	0	0	-	-
Trithion	2	1	0.015	3	3	<10 mm at 25 C	2	na	-	6-218	5	1	0	0	0	6/22	2
Urea	8390	5	0.15	5	25	Solid	1	na	-	511-2000	2	-	0	0	0	2/20	3
Vernam	2	1	0.015	3	3	<10 mm at 25 C	2	na	-	1470-1800	2	-	0	0	0	2/20	1

†LD_{Lo}

TABLE 4-1 (CONCLUDED)

COMPOUND	PLANT RELEASE: Production Actual	X Score	Production Loss Fraction	Score	= Product	X VOLATILITY: Vapor Pressure	Score	X TOXICITY: OSHA Standard (air) TWA	Score	Acute Toxicity LD_{50} or LC_{50}^{*} Range	Score	Non-lethal Acute Effects Score	Carcino-genicity Score	Muta-genicity Score	Terato-genicity Score	Total/Total Possible	= FINAL SCORE
Vinyl acetate	1210.7	5	0.015	3	15	107.5 mm at 25 C	4	10	4	2920	2	1	0	0	0	7/27	16
Vinyl chloride	4174.6	5	0.02	4	20	Gas	5	1	5	na	–	2	5	5	0	15/20	75
Vinylidine chloride	260	5	0.03	5	25	617.4 mm at 25 C	4	25	3	225–5750†	2	1	3	5	0	14/27	52
Vinyltöluene	40	3	0.015	3	9	1.15 mm at 25 C	2	100	2	4000	2	2	0	0	0	6/27	4
Warfarin	12.0	2	0.015	3	6	Solid	1	0.1 mg/m^3	5	3–800	4	–	0	0	0	9/25	2
m-Xylene	1710	5	0.01	2	10	8.56 mm at 25 C	2	100	2	5000	2	2	4	0	0	10/27	7
o-Xylene	679.7	5	0.01	2	10	10 mm at 32.1 C	2	100	2	1500–5000	2	–	4	0	0	8/25	6
p-Xylene	2419.3	5	0.01	2	10	10 mm at 273 C	2	100	2	5000	2	2	4	0	0	10/27	7
Xylenesulfonic acid sodium salt	37.4	3	0.03	5	15	<10 mm at 25 C	1	na	–	500	4	–	0	0	0	4/20	3
2, 6- ylenol	na	–	na	–	–	Solid	1	100	2	150–980	3	–	4	0	0	7/20	–
3, 5-Xylenol	na	–	na	–	–	Solid	1	100	2	1070	2	–	0	0	0	2/20	–
Zinc stearate	19.4	2	0.03	5	10	Solid	1	na	–	na	–	2	0	0	0	2/17	1

† LD_{Lo}

5.0 CLASSIFICATION AND RANKING OF INDUSTRIAL ORGANIC CHEMICALS

5.1 Chemical Classifications

Prior to classification, each chemical should be identified by IUPAC chemical name, synonyms, Chemical Abstracts Service (CAS) registry number, and structure. This will uniquely identify each specific compound and overcome difficulties posed by the ambiguous nomenclature often associated with industrial organic compounds. The use of CAS numbers will facilitate computerization.

5.1.1 Traditional Chemical Classes

Organizing industrial organic chemicals into traditional chemical classes based on molecular structure and functional groups is highly recommended. This should usually be done as a prerequisite to further classifications. Some chemicals (e.g., fluorocarbons or polychlorinated biphenyls) are almost always considered by regulatory agencies as classes rather than as individual compounds.

A typical chemical classification scheme is presented in Table 5-1. Once compounds are grouped in chemical classes, chemical, physical, and biological properties of individual compounds can often be predicted. Members of a chemical class often behave in a qualitatively similar fashion. In addition, some properties increase or decrease systematically along homologous series.

Chemical classification of compounds with several types of functional groups can be complicated. Computerized chemical classification schemes have been developed and are particularly

TABLE 5-1

TRADITIONAL CHEMICAL CLASSES

ALIPHATIC COMPOUNDS

- Hydrocarbons
- Halides
- Alcohols
- Ethers
- Sulfur Compounds
- Esters of Inorganic Acids
- Nitro and Nitroso Compounds
- Amines
- Alkylhydrazines
- Aldehydes & Ketones
- Monobasic Acids
- Derivatives of Acids
- Polyhydric Alcohols
- Alkamines & Diamines
- Hydroxyaldehydes & Hydroxyketones
- Hydroxyacids
- Dicarbonyl Compounds
- Aldehyde and Ketone Acids
- Dibasic Acids
- Polybasic Acids
- Cyanogen and Related Compounds
- Purines and Derivatives
- Carbohydrates
- Amino Acids/Proteins

ALICYCLIC COMPOUNDS

- Cyclopropane
- Cyclobutane
- Cyclopentane
- Cyclohexane
- Bicyclic Terpenes
- Tricyclic Terpenes
- Sesquiterpenes
- Carotenoids
- Chlorane

TABLE 5-1 (CONCLUDED)

AROMATIC COMPOUNDS

- Benzene
- Homologs of Benzene
- Unsaturated Benzene Hydrocarbons
- Aromatic Halogens
- Aromatic Sulfonic Acids
- Nitro Compounds of Benzene Hydrocarbons
- Arylamines
- Phenol
- Aromatic Alcohols
- Aromatic Aldehydes
- Aromatic Ketones
- Phenolic Alcohols, Adlehydes, Ketones
- Quinones and Related Compounds
- Aromatic Carboxylic Acids
- Polynuclear Hydrocarbons
- Condensed Rings

HETEROCYCLIC COMPOUNDS

- 5-Membered Rings
- 6-Membered Rings
- Alkaloids

ORGANOPHOSPHOROUS AND ORGANOMETALLIC

- Aliphatic Compounds
- Aromatic Compounds

useful in these cases (Flinn et al., 1974). A computerized system would allow all chemical compounds with a specific functional group to be retrieved regardless of the presence or absence of other groups.

5.1.2 Partition Coefficient

The partition coefficient is a measure of the distribution of a solute between two immiscible liquid phases in which it is soluble. For a single molecular species, the partition coefficient is a constant and does not depend on relative volumes of solutions used. The most commonly used system is the octanol-water system. The octanol-water partition coefficient indicates relative solubility in aqueous and organic phases, providing information on the hydrophobic or hydrophilic nature of the compound (Leo et al., 1971).

Partitioning between aqueous and organic phases can serve as a model of how a solute passes through membranes in a living tissue. The absorption and accumulation of toxic pollutants are related to their partition coefficients. The octanol-water partition coefficient has been shown to be useful in predicting the binding of solutes to serum albumin and purified enzymes (Leo et al., 1971).

A "bonding" parameter based on partition coefficients from a single reference system is very useful when these values can be calculated so that not every value need be determined experimentally. Increments in partition coefficients along a homologous series have been found to be additive for CH_2, OH, NH_2, halogens, and other functional groups (Leo et al., 1971).

5.1.3 Vapor Pressure

Volatilization from water, soil, plants, and other surfaces is an important route of atmospheric dispersion for organic pollutants. Vapor pressure of a chemical compound is an indicator of its potential volatility. When a substance evaporates into air, its rate of evaporation will be determined by its vapor pressure and its rate of diffusion through the air. All liquids and solids exhibit definite vapor pressures of greater or smaller degree at all temperatures. In general, among liquids in the same chemical class, the vapor pressure at any specified temperature decreases with increasing molecular weight (Stull, 1947). The vapor pressures of solids are generally small.

5.1.4 Physical State

Compounds can be classified by the physical state in which they are most likely to be found under any given conditions of temperature and pressure. At a constant pressure (atmospheric pressure for most regulatory applications) boiling points and melting points define temperatures at which changes of state occur.

Classifying chemicals as primarily gases, liquids, or solids indicates in which phases of the atmosphere they are most likely to be found (the continuous gaseous phase, dispersed liquid droplets, or solid particulates). This information is important in designing monitoring and control strategy.

5.1.5 Adsorption Affinity

Organic chemicals in the atmosphere are often found to be adsorbed on fine particulates. The forces responsible for adsorption appear to be primarily electrical in nature. These forces are usually characterized as either physical or chemical. The forces responsible for physical adsorption are similar to Van der Waals forces between molecules. The much stronger binding forces responsible for chemical adsorption are comparable to those leading to the formation of chemical compounds (National Academy of Science, 1975).

Physical adsorption increases with the partial pressure of a chemical compound (National Academy of Sciences, 1975). At low partial pressures, the extent of physical adsorption is small, although a great deal of chemical adsorption can occur. The partial pressure of a chemical compound in the atmosphere is a function of the atmospheric concentration of that compound.

Unlike chemical adsorption, physical adsorption is a readily reversible process. A gas is desorbed when its vapor pressure in the adsorbed phase exceeds its partial pressure in the gas phase. It is an experimentally observed fact that, in general, for physical adsorption, a gas of high molecular weight and low volatility is adsorbed in preference to a gas of low molecular weight and high volatility. Such a preferentially adsorbed gas or vapor will displace other gases which have already been adsorbed.

Adsorption affinities of organic compounds are particularly influenced by the polarity of the molecule. Some common chemical classes ranked in order of decreasing adsorption affinity of their functional groups are:

1. acids and bases
2. hydroxy, amino, thio, and nitro compounds
3. aldehydes, ketones, and esters
4. halogen compounds
5. unsaturated hydrocarbons
6. saturated hydrocarbons

The adsorption sequence will also be influenced by the position of functional groups and the size of the molecule.

The atmospheric persistence of those chemicals which exist primarily adsorbed on fine particulates will be affected by the chemical's affinity for the particulate relative to water, the size of the particulate, and the chemical's water solubility. Water, a relatively polar compound, can displace less strongly adsorbed solutes. The adsorption affinity of a compound relative to water will determine the extent to which it is "washed out" of suspended particulates by rain. The size of the particulate will also affect its atmospheric stability. If a compound is water soluble, it is more likely to be "washed out" than one which is hydrophobic.

Both adsorption affinity and vapor pressure should be considered when ranking chemicals with respect to their likelihood of being found in the atmosphere. Vapor pressure will indicate their likelihood of being found in the gaseous phase. Adsorption affinity is a factor in determining their likelihood of being adsorbed on atmospheric particulates.

5.1.6 Persistence in the Environment

This information can be categorized by media since different factors would be primary determinants of persistance in the atmosphere, hydrosphere, and lithosphere. For example, microbial degradation is more important in the hydrosphere and lithosphere than it is in the atmosphere (National Academy of Sciences, 1975). All media should be considered, even when focusing on air pollution problems since pollutants are transported between media. A dynamic equilibrium exists between concentrations of a chemical in each compartment of the environment. A compound which is emitted into the atmosphere or distributed by airborne transport may accumulate primarily in the lithosphere or hydrosphere.

A system used by Abrams *et al*. (1975) for ranking organic chemicals with respect to persistence in the environment is shown in Table 5-2. Because this system emphasizes biodegradation rather than chemical reactivity, it is more appropriate for describing persistence in soil or water than persistence in the atmosphere.

The suggested parameter for persistence in the atmosphere is half life, the time required for removal of half of the molecules of a given compound from the atmosphere. The half life in the atmosphere will be a function of such properties as photoreactivity, reactivity towards active forms of oxygen, water solubility,

TABLE 5-2

BIODEGRADABILITY (PERSISTENCE) CATEGORIES

Category	Biodegradability	Persistence in Unadapted Soil	Success of Biological Treatment of Point Source	Typical Chemical
1	Easily degraded	1-3 weeks	Susceptible to normal waste treatment	Acetic acid
2	Degraded without much difficulty	1-3 months	Susceptible to normal waste treatment	Benzoic acid
3	Difficult to degrade	3 months to 1 year	Prolonged treatment needed.	e-caprolactam
4	Very difficult to degrade	1-2 years	Leakage possible even with prolonged treatment	Chlorobenzene
5	Refractory	2 years	Cannot be treated biologically	Hexachlorobenzene

Source: Abrams, E. F., "Identification of Organic Compounds in Effluents from Industrial Sources," Office of Toxic Substances, U.S. Environmental Protection Agency PB 241 641, 1975.

volatility, and adsorption to fine particulates (National Academy of Science, 1975). All of these factors should be considered when ranking chemicals as to their persistence in the atmosphere.

5.2 Industrial Classifications

5.2.1 Production Level and Release to the Environment

Ranking of industrial organic chemicals by production level and/or by the rate at which they are released to the environment would be useful in establishing priorities for selection of chemicals for control or further investigation.

Production levels, production capacity, transport volumes, imports, exports, net sales, and levels of consumption are all relevant parameters that can be used for classifying organic chemicals.

The release rate is an interesting index recently developed by the National Science Foundation Workshop Panel to Select Organic Compounds Hazardous to the Environment. The release rate, R, is defined as follows:

$$]R = (P)L + (P + 1)D[$$

where P = overall annual U.S. production

I = annual quantity imported

L = fraction of the production which is lost at the plant site during manufacturing, conversion, and formulation

D = fraction of the material which goes to nonintermediate dispersive uses.

Other parameters of interest are losses in transportation and storage, the location of production facilities, and impurities and contaminants of the product.

Data on production and production losses will often be difficult to obtain because of the proprietary nature of industrial processes.

5.2.2 Standard Industrial Classifications

Chemicals can be classified by the manufacturing industries from which they are likely to be discharged. The Standard Industrial Classification (SIC) system has been developed to promote comparability of statistics describing various facets of the national economy. The structure of the SIC classification system makes it possible to tabulate and analyze data on a 2-digit, 3-digit, or 4-digit industry code basis, according to the level of industrial detail considered appropriate (Office of Management and Budget, 1972).

SIC code numbers can be assigned to both producers and users of industrial organic materials. An input-output matrix can be developed showing the portions of a chemical from a specific source going to each of several consumers.

Some organic chemicals which have already been classified by industry in the SIC manual are shown in Table 5-3. Other chemicals have also been assigned SIC codes and additional chemicals can be classified by industry according to this scheme. Such a classification scheme would indicate which industries to focus on when attempting to reduce environmental levels of an industrial chemical pollutant.

TABLE 5-3

MAJOR GROUP 28- CHEMICALS AND ALLIED PRODUCTS

GROUP NO.	INDUSTRY NO.	
286		INDUSTRIAL ORGANIC CHEMICALS
	2861	Gum and Wood Chemicals
		Acetate of lime, natural
		Acetone, natural
		Annato extract
		Brazilwood extract
		Brewers' pitch, product of softwood distillation
		Calcium acetate, product of hardwood distillation
		Charcoal, except activated
		Chestnut extract
		Dragons' blood
		Dyeing materials, natural
		Dyestuffs, natural
		Ethyl acetate, natural
		Extracts, dyeing and tanning: natural
		Fustic wood extract
		Gambler extract
		Gum naval stores, processing but not gathering or warehousing
		Hardwood distillates
		Hemlock extract
		Logwood extract
		Mangrove extract
		Methanol, natural (wood alcohol)
		Methyl acetone
		Methyl alcohol, natural (wood alcohol)
		Myrobalans extract
		Naval stores, bum: processing but not gathering or warehousing
		Naval stores, wood
	2865	Cyclic (Coal Tar) Crudes, and Cyclic Intermediates, Dyes, and Organic Pigments (Lakes and Toners)
		Acid dyes, synthetic
		Acids, coal tar: derived from coal tar distillation
		Alkylated diphenylamines, mixed
		Alkylated phenol, mixed

TABLE 5-3 (CONTINUED)

GROUP NO.	INDUSTRY NO.	
286	2865	(Continued)
		Aminoanthraquinone
		Aminoazobenzene
		Aminoazotoluene
		Aminophenol
		Aniline
		Aniline oil
		Anthracene
		Anthraquinone dyes
		Azine dyes
		Azo dyes
		Azobenzene
		Azoic dyes
		Benzaldehyde
		Benzene hexachloride (BHC)
		Benzene, product of coal tar distillation
		Benzoic acid
		Benzol, product of coal tar distillation
		Biological stains
		Chemical indicators
		Chlorobenzene
		Chloronaphthalene
		Chlorophenol
		Chlorotoluene
		Coal tar crudes, derived from coal tar distillation
		Coal tar distillates
		Coar tar intermediates
		Color lakes and toners
		Color pigments, organic: except animal black and bone black
		Colors, dry: lakes, toners, or full strength organic colors
		Colors, extended (color lakes)
		Cosmetic dyes, synthetic
		Creosote oil, product of coal tar distillation
		Cresols, product of coal tar distillation
		Cresylic acid, product of coal tar distillation
		Cyclic crudes, coal tar: product of coal tar distillation
		Cyclic intermediates

TABLE 5-3 (CONTINUED)

GROUP NO.	INDUSTRY NO.	
286	2865	<u>(Continued)</u>
		Cyclohexane
		Diphenylamine
		Drug dyes, synthetic
		Dye (cyclic) intermediates
		Dyes, food: synthetic
		Dyes, synthetic organic
		Eosine toners
		Ethylbenzene
		Hydroquinone
		Isocyanates
		Lake red C toners
		Leather dyes and stains, synthetic
		Lithol rubine lakes and toners
		Maleic anhydride
		Methyl violet toners
		Naphtha, solvent: product of coal tar distillation
		Naphthalene chips and flakes
		Naphthalene, product of coal tar distillation
		Naphthol, alpha and beta
		Nitro dyes
		Nitroaniline
		Nitrobenzene
		Nitrophenol
		Nitroso dyes
		Oil, aniline
		Oils: light, medium, and heavy-product of coal tar distillation
		Organic pigments (lakes and toners)
		Orthodichlorobenzene
		Paint pigments, organic
		Peacock blue lake
		Pentachlorophenol
		Persian orange lake
		Phenol
		Phloxine toners
		Phosphomolybdic acid lakes and toners
		Phosphotungstic acid lakes and toners
		Phthalic anhydride

TABLE 5-3 (CONTINUED)

GROUP NO.	INDUSTRY NO.	
286	2865	(Concluded)
		Phthalocyanine toners
		Pigment scarlet lake
		Pitch, product of coal tar distillation
		Pulp colors, organic
		Quinoline dyes
		Resorcinol
		Scarlet 2 R lake
	2869	Industrial Organic Chemicals, Not Elsewhere Classified
		Accelerators, rubber processing: cyclic and acyclic
		Acetaldehyde
		Acetates, except natural acetate of lime
		Acetic acid, synthetic
		Acetic anhydride
		Acetin
		Acetone, synthetic
		Acid esters, amines, etc.
		Acids, organic
		Acrolein
		Acrylonitrile
		Adipic acid
		Adipic acid esters
		Adiponitrile
		Alcohol, aromatic
		Alcohol, fatty: powdered
		Alcohol, methyl: synthetic (methanol)
		Alcohols, industrial: denatured (non-beverage)
		Algin products
		Amyl acetate and alcohol
		Antioxidants, rubber processing: cyclic and acylic
		Bromochloromethane
		Butadiene, from alcohol
		Butyl acetate, alcohol, and propionate
		Butyl ester solution of 2,4-D
		Calcium oxalate
		Camphor, synthetic

TABLE 5-3 (CONTINUED)

GROUP NO.	INDUSTRY NO.	
286	2869	(Continued)
		Carbon bisulfide (disulfide)
		Carbon tetrachloride
		Casing fluids, for curing fruits, spices, tobacco, etc.
		Cellulose acetate, unplasticized
		Chemical warfare gases
		Chloral
		Chlorinated solvents
		Chloroacetic acid and metallic salts
		Chloroform
		Chloropicrin
		Citral
		Citrates
		Citric acid
		Citronellal
		Coumarin
		Cream of tartar
		Cyclopropane
		DDT, technical
		Decahydronaphthalene
		Dichlorodifluoromethane
		Diethylcyclohexane (mixed isomers)
		Diethylene glycol ether
		Dimethyl divinyl acetylene (di-isopropenyl acetylene)
		Dimethylhydrazine, unsymmetrical
		Embalming fluids
287		AGRICULTURAL CHEMICALS
	2873	Nitrogenous Fertilizers
		Ammonia liquor
		Ammonium nitrate and sulfate
		Anhydrous ammonia
		Aqua ammonia, made in ammonia plants
		Fertilizers: natural (organic), except compost
		Nitric acid
		Nitrogen solutions (fertilizer)

TABLE 5-3 (CONCLUDED)

GROUP NO.	INDUSTRY NO.	
287	2873	(Continued)
		Plant foods, mixed: made in plants producing nitrogenous fertilizer
		Urea
	2874	Phosphatic Fertilizers
		Ammonium phosphate
		Calcium meta-phosphate
		Defluorinated phosphate
		Diammonium phosphate
		Fertilizers, mixed: made in plants producing phosphatic fertilizer materials
		Phosphoric acid
		Plant foods, mixed: made in plants producing phosphatic fertilizer
		Superphosphates, ammoniated and not ammoniated

Source: Office of Management and Budget, Standard Industrial Classification Manual, GPO, 1972.

5.2.3 Process Classifications

While the SIC codes provide a system of classifying organic chemicals at the industrial level, they do little to describe the organic chemical industry at the manufacturing plant level.

Industrial organic chemicals can be classified according to the processes by which they are manufactured. Each commercial synthesis process will be characterized by specific effluents and emissions since quantities of byproducts and other chemicals associated with the process are often discharged at the point of production.

The Stanford Research Institute "Chemical Economics Handbook" used in conjunction with the "Directory of Chemical Products" provides a main source of process information. The Handbook briefly explains all the manufacturing processes for a given product and often gives a process breakdown.

A system for classifying chemicals by manufacturing method was developed by Abrams, 1975. Those chemicals with several methods of manufacture were listed under each appropriate category. The categories they used are shown in Table 5-4.

A process classification system has been developed by Catalytic, Inc., 1975, to code organic chemicals by manufacturer, plant, and manufacturing process. The code number would refer to the combination of the chemical product and the process by which it was manufactured. For example, one code number could be assigned to the production of vinyl chloride by addition of hydrochloric acid to acetylene and a

TABLE 5-4

CATEGORIZATION BY MANUFACTURING METHOD

Petroleum distillates
Constituents in Petroleum Refining and Coal Processing Wastes
Phthalic Anhydride Reactions
Esterification of Acids
Recovered from Natural Materials
Oxidation of Alcohols
Oxidation of Other Compounds
Dehydrogenation or Dehydrohalogenation
Alkylation of Aromatics
Halogenation of Aromatics
Halogenation of Nonaromatics
Hydrogenations
Condensations
Miscellaneous

Source: Abrams, E. F., "Identification of Organic Compounds in the Effluents from Industrial Sources," Office of Toxic Substances, U.S. Environmental Protection Agency PB241-641, 1975.

second code number to production of vinyl chloride by cracking of ethylene dichloride.

The U.S. Environmental Protection Agency investigated 55 product/process segments of the organic chemicals manufacturing industry and developed water effluent limitations guidelines for 28 product/process segments (Catalytic, Inc., 1975). For these studies, product/process groups were classified into four main subcategories shown in Table 5-5.

Since specific organic chemical effluents will be found associated with production of a chemical product by a particular process, any plant producing the chemical by that process could be monitored for those effluents. If the effluents to the atmosphere have been determined at one plant producing an organic chemical by a coded process, results of that analysis can be applied to other plants producing a chemical with the same product/process code. The product/process code for every chemical produced at each plant can be compiled and computerized allowing easy retrieval of information for control purposes.

5.2.4 Source of Emissions

Stationary sources of pollutant emissions can be divided into the broad general categories of "point sources" and "non-point sources." Most industrial and municipal discharges would be classified as point sources. Natural and consumer related sources would usually be classified as non-point sources.

TABLE 5-5

MAJOR PROCESS CATEGORIES

Continuous nonaqueous processes
Continuous vapor phase processes where contact process water is used as diluent, quench, or vent gas absorbent
Continuous aqueous liquid phase reaction systems
Batch and semi-continuous processes

Source: Abrams, E. F., "Identification of Organic Compounds in the Effluents from Industrial Sources," Office of Toxic Substances, U.S. Environmental Protection Agency PB241-641, 1975.

Abrams et al., 1975, categorized industrial point sources discharging organic chemicals to the environment by SIC codes. Chemicals can then be assigned to the point source categories from which they are likely to be emitted. A sample classification of organic chemicals by SIC point source is shown in Table 5-6. This classification is useful in identifying point sources which would be appropriate for regulation and control of specific compounds.

Within an industrial plant, chemicals can be classified by the specific point or type of emission. A sample list of point-of-emission categories is shown in Table 5-7.

5.2.5 Raw Materials

Manufactured organic chemicals can be classified by tracing the manufacturing process back to basic raw materials. A class derived from the same raw material would tend to be accompanied by characteristic effluents and emissions. Petrochemical manufacturing plants might be monitored for polycyclic aromatic hydrocarbons. Plants manufacturing chlorinated chemicals might be more likely than other plants to have the characteristic toxic emissions shown in Table 5-8.

5.2.6 Use

Chemicals can be classified by ultimate use. Classification by use provides information concerning the level of exposure, a major factor in estimation of health risk. A greater exposure risk is usually associated with dispersive uses than contained. Contained uses are those in which the chemical is not systematically released

TABLE 5-6

CATEGORIZATION BY PROBABLE MANUFACTURING SIC INDUSTRY POINT SOURCE

EXTRACTION OF PINE GUM SIC 0843	
1-terpineol	limonene
borneol	methanol
camphor	o-cresol
isoborneol	guaiacol
BOTTLED AND CANNED SOFT DRINKS AND CARBONATED WATERS SIC 2086	
n-docosane	pentadecane
eicosane	octadecane
n-tridecane	hexadecane
tetradecane	
BROAD WOVEN FABRIC MILLS, MAN-MADE FIBER AND SILK SIC 2221	
e-caprolactam	cis-2-methyl-4-ethyl dioxolane
2,4,6-trichlorophenol	trans-2-methy-4-ethyl dioxolane
trichloroethylene	dieldrin
trichlorobenzene	trichlorobiphenyl
tetrachloroethylene	tetrachlorobiphenyl
propylbenzene	pentachlorobiphenyl
propylamine	tridecane
propanol	ethylene dichloride
methyl benzoate	vinyl benzene
dibutyl phthalate	chloroform

TABLE 5-6 (CONTINUED)

BROAD WOVEN FABRIC MILLS, MAN-MADE FIBER AND SILK SIC 2221 (Continued)	
tetradecane	acetophenone
2-hydroxyadiponitrile	chlorobenzene
methylpropanal	dichlorobenzene
borneol	toluene
dichloroethyl ether	ethyl benzene
bis-chloroisopropyl ether	naphthalene
diethyl phthalate	dodecane
methyl naphthalene	

SYNTHETIC RUBBER (VULCANIZABLE ELASTOMERS) SIC 2822	
vinyl benzene	acetaldehyde
n-tridecane	acetic acid
1,1,2-trichloroethane	acetophenone
tetradecane	acetylene dichloride
tetrachloroethylene	benzene
tetrachloroethane	benzothiazole
propylamine	carbon disulfide
pentadecane	carbon tetrachloride
octadecane	hexachloro-1,3-butadiene
nitrobenzene	n-docosane
2-methylpropanal	eicosane
methyl chloride	ethanol
isopropyl benzene	hexachloroethane
hexadecane	isophorone
pentachlorophenol	methyl naphthalene
pentanol	o-cresol

TABLE 5-6 (CONTINUED)

PETROLEUM REFINING SIC 2911	
docosane	pentane
n-dodecane	propylbenzene
eicosane	tetradecane
ethyl benzene	toluene
2-ethyl-n-hexane	n-tridecane
hexadecane	undecane
indene	xylene
isodecane	bromobenzene
1-isopropenyl-4-isopropylbenzene	triphenyl phosphate
isopropyl benzene (cumene)	methyl phenyl carbinol
methane	methyl biphenyl
methyl napththalene	di(2-ethyl hexyl)phthalate
dimethyl phenol	dioctyl phthalate
1-terpineol	pentanol

LUBRICATING OILS AND GREASES SIC 2992	
limonene	pentachlorobiphenyl
2-methyl propanal	methyl stearate
trichlorobiphenyl	naphthalene
tetrachlorobiphenyl	methyl ethyl ketone

TABLE 5-6 (CONCLUDED)

LEATHER TANNING AND FINISHING SIC 3111	
propylamine	2-methylpropanal
methylene chloride	
GYPSUM PRODUCTS SIC 3275	
acetone	propanol
methylene chloride	

Source: Abrams, E. F., "Identification of Organic Compounds in Effluents from Industrial Sources," Office of Toxic Substances, U.S. Environmental Protection Agency PB 241 641, 1975.

TABLE 5-7

CATEGORIES OF EMISSION FROM INDUSTRIAL FACILITIES

Fugitive emissions
Tank vent emissions
Pump emissions
Batch loading of reactor emissions
Duct emissions
Stack emissions
Incinerator emissions
Evaporation of volatile solvents
Spills and accidents

TABLE 5-8

COMPOUNDS WHICH MAY BE FORMED BY CHLORINATION

acetylene dichloride	1,4-dichlorobenzene
bromobenzene	dichlorodifluoroethane
bromochlorobenzene	1,2-dichloroethane
bromodichloromethane	dichloroethyl ether
bromoform	hexachloro-1,3-butadiene
bromoform butanal	hexachloroethane
bromophenyl phenyl ether	methyl chloride
butyl bromide	methylene chloride
1,2-bis-chloroethoxy ethane	octyl chloride
b-chloroethyl methyl ether	pentachlorobiphenyl
chloroform	1,1,3,3-tetrachloroacetone
chlorohydroxy benzophenone	tetrachlorobiphenyl
bis-chloroisopropyl ether	tetrachloroethane
chloromethyl ether	tetrachloroethylene
chloromethyl ethyl ether	trichlorobenzene
m-chloronitrobenzene	trichlorobiphenyl
3-chloropyridine	1,1,2-trichloroethane
dibromobenzene	1,1,2-trichloroethylene
dibromochloromethane	trichlorofluoromethane
dibromodichloroethane	2,4,6-trichlorophenol

Source: Abrams, E. F., "Identification of Organic Compounds in Effluents from Industrial Sources," Office of Toxic Substances, U.S. Environmental Protection Agency PB 241 641, 1975.

to the environment as a direct result of use (e.g., PCBs in transformers). In dispersive uses, chemicals are released to the environment as a direct consequence of use (e.g., pesticides, aerosols, and solvents). The size of the population at risk is usually greater for consumer uses than for commercial or industrial uses. The use (e.g., food additive, pesticide, drug) would often determine which Federal agency has regulatory responsibility for that chemical.

5.2.7 Disposal

For many chemicals, especially those with nondispersive uses, disposal is the main route of entry into the environment. Classification of these chemicals by means of disposal will provide information concerning the compartments of the environment in which they are most likely to be found. The chemical nature of materials can often be altered during disposal. Incineration of halogenated and nitrogenated compounds will result in emissions of the corresponding halogen acids and oxides of nitrogen (National Academy of Sciences, 1975). Open-burning can lead to emission of the products of partial combustion. Effluents and sludge from sewage treatment plants as well as drainage from dumps or landfills, can contaminate ground and surface water.

5.3 Biological Classification

5.3.1 Population at Risk

Toxic chemicals can be classified by size or type of population exposed. Typical categories for type of population exposed are listea in Table 5-9. Population groups can be further classified according to whether their exposure is voluntary or involuntary.

Priority considerations should be given to chemicals to which there is extensive involuntary public exposure or to which susceptible segments of the population are exposed. Some ranking schemes consider certain segments of the population more "valuable" than others (e.g., the young more valuable than the old) (National Academy of Sciences, 1975). This approach is highly subjective and ethically questionable.

5.3.2 Target Organ

Toxic chemicals can be classified by the organ or system which they attack. A possible classification scheme of this type is shown in Table 5-10.

5.3.3 Route of Exposure

Chemicals can be classified by the most likely route of human exposure: inhalation, oral, or dermal. The categories give an indication of potential health hazard from environmental exposure. Toxic substances to which people are exposed by inhalation would often be the most difficult to avoid.

5.3.4 Structure-Activity Correlations

Relationships between molecular structure and biological activity of chemical substances can provide an indication of a potential for hazardous effects. Although predictions cannot currently be based solely on structure-activity correlations, some decisions can be made on the basis of analogies with other known chemicals. These

TABLE 5-9

CLASSIFICATION BY POPULATION AT RISK

General human population
Regional
Neighborhood
Industrial vicinity
Occupational groups
Highly susceptible groups

TABLE 5-10

CHEMICALS CLASSIFIED BY BIOLOGICAL SYSTEM ON WHICH THEY ACT

Central Nervous System
Synaptic and Neuroeffecter Junctional Sites
Cardiovascular System
Blood and Blood-forming Organs
Immunological System
Renal System and Electrolyte Balance
Hormone Balance
Hepatic Function
Microsomal Enzymes and Biological Oxidation
Reaction with DNA

correlations can be useful in selection of chemicals for testing and for determining the sequence of testing.

Structure-activity relationships are reasonably well understood for certain chemical series and certain toxic effects (e.g., polycyclic aromatic hydrocarbons and carcinogenicity) (Valkenburg, 1972). Some other types of biological activity for which structure-activity relations have been developed are central nervous system activity, enhancement or inhibition of enzymatic activity, cytotoxicity, hallucinogenesis, and mutagenicity (Valkenburg, 1972).

One method often used for defining structure-activity relationships is the Hansch multiple parameter method. In a homologous series of biologically active compounds, the biological activity of a reference compound is considered a constant. The Hansch equation defines increments in biological activity (of a homolog relative to the reference compound) as a function of increments in electronic components, hydrophobic components, and steric components of the molecule:

$$\Delta BA = f(\Delta E, \Delta H, \Delta S)$$

where ΔH = the hydrophobic substituent constant derived from octanol-water partition coefficient

ΔE = the Hammet constant for polar factors

ΔS = the steric constant

ΔBA = magnitude of the biological effect

Computer storage and retrieval methods are useful in developing structure-activity correlations. Wiswesser Line Notation can be used for computerizing organic chemical structures.

5.3.5 Acute Toxicity Dosage

The biological effect of a chemical depends on the quantity with which the organism must deal. Chemicals having adverse effects at low dosage would be considered more toxic than chemicals having similar effects only at much higher dose levels. It is difficult to perform this ranking at low effect levels. The effects of low dosages are often subtle. Direct experimental estimation of the level affecting one percent of the population may require several hundred animals to obtain adequate statistical precision. For these reasons, lethal dosage levels are usually used in ranking chemicals for acute toxicity.

A common parameter of acute toxicity is the LD_{50}, the dose of a substance at which half the test animals would die. To be comparable, results should be based on animals of the same species or strain, sex, and age. The same route of administration should be used.

Other commonly used parameters of acute toxicity based on lethal doses are:

LC_{50} - the concentration which is lethal to half the test population. The duration of exposure should be specified. LC_{50} is usually used for concentration in air, but can also be used for concentration in the ambient water to which aquatic organisms are exposed.

LD_{Lo} - the lowest reported lethal dose

LC_{Lo} - the lowest reported lethal concentration

Available data based on these parameters for 16,500 different chemicals is summarized in the Registry of Toxic Effects of Chemical Substances published by NIOSH.

5.3.6 Cancer Risk

It would be useful to categorize chemicals as highly carcinogenic, moderately carcinogenic, weakly carcinogenic, co-carcinogenic, tumorigenic, or having no neoplastic effects. There is usually not enough information available, however, to do this. Dose-response curves are rarely determined for carcinogens. Negative results in carcinogenicity tests are often not accepted as proof of noncarcinogenicity. Comparisons between strength of carcinogenicity have been made on the basis of percentage of a test population developing malignant tumors, lowest dosage causing malignancy, or lag time between administration of chemical and observation of tumors.

Chemicals are sometimes classified with respect to certainty of their carcinogenicity (e.g., known carcinogen or suspected carcinogen). EPA has recently attempted to order the NIOSH suspected carcinogens list according to the relative degree of concern that might be warranted regarding possible human carcinogenic potential. A four-digit code was used. The first digit represented the species in which carcinogenic response was reported. The second digit designated the number of different species for which a carcinogenic response was reported. The third digit was assigned on the basis of route of administration. The last digit was a count of the number of different species/route combinations (Letkiewicz, 1976).

The most complete source of data and references related to chemical carcinogenesis is the National Cancer Institute "Survey of Compounds Which Have Been Tested for Carcinogenic Activity." A master index of the series is maintained on tape at National Cancer Institute headquarters.

Evaluations of carcinogenic risk are made by the International Agency for Research on Cancer under the auspices of the World Health Organization. They do not use a formal ranking system.

6.0 PROPOSED FOLLOW-ON PROJECTS

Prioritization of organic chemicals according to their relative potential for adversely affecting the environment may be accomplished through a careful and critical analysis of appropriate data. The results presented herein represent a preliminary effort at applying such an approach to synthetic organic chemicals released to the atmosphere from production facilities. Much additional labor is, however, necessary in order to maximize both the validity and usefulness of this work. The recommended additions to the present endeavor as well as other significant and worthwhile projects arising as logical extensions to this effort are presented below.

6.1 Acquisition of Additional Information

Although all available secondary sources of production and toxicity data have been exhausted, other means of procuring this data may be available for selected compounds. An in-depth search of the primary research literature may, for instance, reveal studies on the acute and/or chronic toxicity of many compounds which have not to date been included in review articles or toxicological anthologies. Information on compounds just recently tested for carcinogenicity, mutagenicity and teratogenicity can only be found through an intensive review of current journal articles. When evidence indicates that a compound may be of particular concern as an atmospheric pollutant, a serious effort may be undertaken to circumvent the proprietary status of production statistics and obtain the data necessary to complete the scoring for that compound. In addition, information concerning the number of companies producing a particular chemical and their locations would help to modify the production-release parameter in such a way as to allow the determination of the release-rate at a given site. This type of modification would provide a more accurate means of assessing the health and environmental effects of production site emissions than does production level alone. Any facilities at production plant sites which limit or control the level of pollutant emissions should also be noted and the production-release score modified accordingly.

The validity of the ranking system could be maximized by the incorporation of additional parameters into the formula for determining a final score. An extremely important variable, for example, is the tendency or lack thereof of a compound to persist in the atmosphere. Measures of this tendency include the rate and extent of biodegradation, photodegradation and any other chemical reactions likely to occur following release to the atmosphere. Since interest in studies relating to atmospheric persistance is only of fairly recent origin, few review articles exist and most information must be obtained from primary sources. Where information is available on biodegradation and photoreactivity, the byproducts of these reactions should also be considered to determine their health and environmental effects.

A second important variable is the degree to which a compound adsorbs to various types of particulate matter. This variable is of particular importance for compounds which are nonsubliming solids under ordinary conditions and are thus not likely to be emitted from production facilities in the vapor phase. Many pesticides fall into this category and studies of adsorbtive tendency are not uncommon for this class of compounds.

6.2 Periodic Updating of Dossiers

Procedures should be established for periodically updating the dossiers as additional production information and the results of toxicological and chemical studies become available. For example, a large number of compounds are currently being screened for carcinogenic or mutagenic activity and definitive results may not be available for quite some time. Many of these compounds have received scores indicative of the fact that they are "under test." However, these scores are substantially lower than the scores these same compounds would recieve should test results prove positive. The scoring must continuously undergo revision and modification if the validity of the position of any given compound in the prioritization hierarchy is to be maintained.

6.3 Inclusion of Additional Compounds

More compounds may also be added to the study to increase its scope. Those compounds which are highly toxic but which are produced in quantities of less than 1 million pounds per year could be scored. In general, the initial choice of compounds was limited to those with production rates of over a million pounds per year. Compounds derived from fuels and petrochemicals and compounds derived from natural sources could be added. For the most part, organometallics have also been excluded from the initial effort. Finally, any compound known or suspected to be a contaminant of a commercial-grade or impure preparation of any of the compounds considered in this study should be thoroughly investigated using the same criteria as were used for the parent compound.

6.4 Data Analysis and Evaluation

Once these data have been amassed, they are only useful if analytical procedures are applied to determine the importance of each piece of information, to determine the relationships among the various data and to derive a final prioritization scheme. Without this statistical analysis, the lists of data are only minimally useful and their sheer volume becomes a hindrance.

Many possibilities exist for evaluation of the chemicals with respect to their potential health and environmental effects. In order to facilitate data manipulation, it will be necessary to computerize the data. As a part of this computerization, a cross index of synonyms could be easily prepared. This would prevent duplication and increase the usefulness of the data. Following this initial effort, analyses of the data using statistical methods should be performed. Possibilities include the development of discriminant functions related to factor analysis using toxicity as the independent variable. This would show the degree of correlation of the variables used and indicate which could be ignored in future efforts. Various weighting schemes for the dependent variables should be stochastically determined, applied, and tested. It may additionally be possible to apply a Hansch approach to the correlations existent in these data. From these analyses, it should be possible to develop a more sophisticated ranking scheme for evaluating the present data and any future organic compounds requiring ranking.

6.5 Accessibility of Data Files

Once these data have been collected, the results will represent a substantial library of information. Plans should be initiated so that these data could be rapidly accessed in response to queries from EPA on a given chemical or chemical class.

6.6 Structure-Function Analyses

Since those reactions which effect atmospheric persistence are gaining increasing importance as measures of pollution potential, a study of how the structures and properties of compounds relate to their reactions in the atmosphere would be extremely useful. Following this analysis, it would then be possible to define existing data gaps and suggest areas where laboratory research should be performed. This type of analysis has, to date, been attempted only for a few common chemicals. The expansion of this body of knowledge would be useful not only in evaluating the pollution resulting from organic chemical production but also that from dispersive uses. Another area where future research is needed concerns the relationship of structure and activity of organic compounds to various observed health effects.

Such a series of relationships would be very useful tools for predicting the probability of adverse environmental consequences following release of a compound whose health effects have not been fully characterized. For example, it may be possible to deduce the biological effect of the addition of a chlorine atom or a nitro group to an existing structure, by modeling its effect in other similar configurations. Predictions such as these would be especially useful in light of the number of new organic compounds being produced each year which are impossible to test fully prior to marketing.

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15. SUPPLEMENTARY NOTES

16. ABSTRACT

This report presents a scheme for evaluating the relative hazard to humans resulting from air emissions of synthetic organic chemicals. Data on production, fraction lost during production, volatility, and toxicity have been compiled for 637 organic chemicals. Numerical scores were then assigned based on these data.

Four appendices were published with this report. The appendices are dossiers containing chemistry, production, and toxicity data for the 637 synthetic organic chemicals.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
organic air pollutants organic chemical toxicity ranking of organic air pollutants chemistry data for organic chemicals		

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