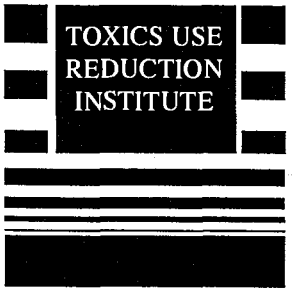


THE MASSACHUSETTS
TOXICS USE REDUCTION INSTITUTE

Categorization of the Toxics Use Reduction List of Toxic and Hazardous Substances

Methods and Policy Report No. 18 **1999**

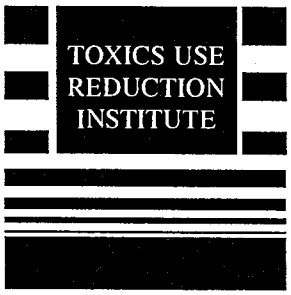
University of Massachusetts Lowell

Categorization of the Toxics Use Reduction List of Toxic and Hazardous Substances

Report on the work of the
Toxics Use Reduction Science Advisory Board

The Toxics Use Reduction Institute
University of Massachusetts Lowell

March 1999



The Toxics Use Reduction Institute is a multi-disciplinary research, education, and policy center established by the Massachusetts Toxics Use Reduction Act of 1989. The Institute sponsors and conducts research, organizes education and training programs, and provides technical support to promote the reduction in the use of toxic chemicals or the generation of toxic chemical byproducts in industry and commerce. Further information can be obtained by writing the Toxics Use Reduction Institute, University of Massachusetts Lowell, One University Avenue, Lowell, Massachusetts 01854.

QUINCY
COLLEGE

34 Coddington Street, Quincy, Massachusetts 02169 617-984-1600

Dr. Michael Ellenbecker
Acting Director
Toxics Use Reduction Institute
One University Avenue
Lowell, MA 01854-2866

Dear Dr. Ellenbecker,

Attached is a report by the Toxics Use Reduction Science Advisory Board on its "Categorization of the Toxics Use Reduction List of Toxic and Hazardous Substances" project. The Board has been working on this project for the past 18 months and is very pleased to submit this work product. It represents a concerted effort on the part of the Board to categorize 258 chemicals into three categories, high hazard, low hazard and uncategorized chemicals.

Many Board members contributed their time and expertise to this project. Those Board members are: James J. Ahearn Jr., Ph.D. from Polaroid Corporation, Andrew F. Beliveau of the U. S. Environmental Protection Agency, Richard Clapp, Sc.D. of B.U. School of Public Health, George M. Gray, Ph.D. of the Harvard School of Public Health, Center for Risk Analysis, Thomas Trayers from the Division of Occupational Safety's Occupational Hygiene Program, and Lawrence H. Boise from the Gloucester Co., Inc.; and two former Board members, Halina Brown, Ph.D. from Clark University and Christine Oliver, M. D. from Mass. General Hospital.

The Board realizes that this work will never be complete as new data on existing chemicals are generated and as new chemicals are reported in the Commonwealth. Adjustments to the list will be made based on new information in these areas. We trust that the list will aid the decisions made concerning TURA Program priorities. In addition, the Board respectfully requests to be informed of any policy decisions resulting from the use of these lists. Thank you.

Sincerely,

David T. Williams

David T. Williams
Executive Director
Quincy College
Center for Technology & Health
and Chair, Toxic Use Reduction SAB

Summary
For the past eighteen months, the Toxics Use Reduction Science Advisory Board has been working on a project to categorize the 258 chemicals which have ever been reported under the Massachusetts Toxics Use Reduction Act (TURA). The resulting lists of more hazardous[1], less hazardous and uncategorized chemicals will be used by the Toxics Use Reduction Program to aid in setting priorities and will serve as guidance for companies making chemical substitution decisions. The lists of more hazardous (Category 1) and less hazardous (Category 2) substances follow. The specific chemicals in the categories may change based on new data becoming available or new chemicals being used above TUR reportable threshold quantities in the Commonwealth.

Table 1: Category 1 Chemicals[2]

Acrylamide	Diethylsulfate	Nickel compounds
Acrylonitrile	Dimethylformamide	Nitrobenzene
Arsenic compounds	Dioxane	Phosgene
Arsenic	Epichlorohydrin	Propyleneimine
Cadmium compounds	Ethylene oxide	Propyleneoxide
Cadmium	Formaldehyde	Selenium and selenium compounds
Carbon tetrachloride	Hydrazine	
Chlorine	Hydrogen cyanide	Silver chromate
Chloroform	Hydrogen fluoride	Sulfuric acid
Chromic acid	Lead	Sulfuric acid (fuming)
Chromium compounds (+6)	Lead compounds	Tetrachloroethylene
Cyanide compounds	Methylene bisphenyl isocyanate	Toluenediisocyanate
Dibromochloropropane		Trichloroethylene
Dichloroethane		

[1] For this work,"hazard" includes inherent toxicity, potential for exposure through dispersal in the workplace (based on the physico-chemical properties of the chemicals, e.g., vapor pressure) and indicators of safety of use (e.g., flammability). Potential for exposure and indicators of safety do not include site-specific conditions.

[2] Chemical names with CAS numbers can be found in Table 4 of this report.

Table 2: Category 2 Chemicals[3]	
Acetic acid	Ferrous chloride
Acetone	Ferrous sulfate
Ammonium bicarbonate	Isobutyl alcohol
n-Butyl alcohol	Methylethylketone
sec-Butyl alcohol	Methanol
Chromium compounds (+3)	Silver in alloy form
Ethyl acetate	Sodium phosphate, dibasic
Ethylene glycol	Sodium phosphate, tribasic
Ferric chloride	Zinc in alloy form
Ferric sulfate	Zinc borate
Ferrous ammonium sulfate	Zinc sulfate

Introduction

As required under the Toxics Use Reduction Act (M.G.L. c.21I) the Toxic Use Reduction Science Advisory Board serves in an advisory capacity to the Toxics Use Reduction Institute (the Institute) in the following three areas, 1) adding chemicals to or deleting chemicals from the reporting list, 2) establishing priority user segments, and 3) general advice to the Institute on other related matters. In December 1994, the Institute organized the first meeting of the TUR Science Advisory Board. The full Board is composed of eleven members with expertise in the areas of toxicology, epidemiology, medicine, worker issues, industry issues, environmental chemistry and risk assessment. A list of the members who worked on the Chemical Categorization Project is included in Appendix A.

For the past three years, the Toxics Use Reduction Science Advisory Board has assisted the Institute in preparing recommendations for the Administrative Council for delisting chemicals from the TURA Toxic and Hazardous Substance List[4]. Fourteen industry petitions requesting delisting were submitted. The Board recommended delisting in ten cases. Appendix B provides a summary of the recommendations. Throughout this petitioning process the Board has struggled with decisions which seemed to require, at least implicitly, a ranking of the relative hazards of chemicals. Delisting (or refusal to delist) particular chemicals was seen as having the potential to effect the use of one material in preference to another. Therefore, the Board has spent the last eighteen months discussing the categorization of chemicals on the list into one of the following three groups:

[3]Chemical names with CAS numbers can be found in Table 5 of this report.

[4]Massachusetts Department of Environmental Protection, Bureau of Waste Prevention, Toxics Use Reduction 1995 Reporting Package.

- Category 1 - more hazardous chemicals
- Category 2 - less hazardous chemicals
- Category 3 - uncategorized chemicals - which includes chemicals not reported under TURA since 1990 and chemicals reported under TURA but not categorized as more or less hazardous due to insufficient information or because the chemical was deemed to be of medium hazard.

The resulting categorized list is intended to provide guidance to companies and technical assistance providers making chemical substitution decisions, to aid in targeting technical assistance and research efforts and, ultimately, to aid in reducing overall risk to workers and the environment. It is also intended to provide information to the Institute and the other entities created under TURA, for their use in guiding the implementation of the TURA program. Categorization will not address the issue of varying risk associated with the same chemical used in different processes; this issue has been discussed frequently by the Board during the petition review processes.

Approach

To begin the Categorization project, the Board reviewed many existing models for chemical prioritization which are briefly described in Appendix C. All models, with the exception of the Swedish National Chemicals Inspectorate's system, rely entirely on a scoring system based on health and environmental data. Only one model used by the Indiana Clean Manufacturing Technology and Safe Materials Institute considers occupational safety issues which are of particular concern to the Board. In the initial stages the Board assumed that they, like the other groups, would create a model based on an algorithm using environmental, health and safety data. The Board was concerned, however, that the necessary data might not be available to accurately assess chemical hazard.

Using the criteria from existing models as a starting point, the Board chose their own set of criteria. In choosing criteria for categorizing the list, the following three items were discussed:

- the data should be generally available
- the data should be reliable
- the scheme should be defensible and understandable

Data points were discussed in the following four major areas:

- human health
- environmental
- safety
- persistence/bioaccumulation

After lengthy discussions, the Board choose the following eight criteria:

- Carcinogenicity (IARC Classification)
- Oral LD_{50}
- Reference dose (RfD)
- Threshold limit value (TLV) / time weighted average (TWA)
- Aquatic LC_{50}
- Flash point (FP)
- pH (used pKa and pKb)
- Bioconcentration factor (BCF)

These criteria are defined in Appendix D. The Board requested that the data for each chemical be provided to them for further discussion. In order to make the task less daunting, the Board decided to categorize only the 258 chemicals that had ever been reported under the Toxics Use Reduction Act[5].

It was necessary to choose surrogate compounds for chemicals listed as groups (e.g., lead compounds). Using the surrogate choices from other chemical ranking schemes as a guide, the criteria used for this selection were as follows: most toxic member of a group, most data available, most widely used. A list of the chemical group name, the surrogate used and an explanation of the choice can be found in Appendix E. In addition, the listings for individual metals and metal compounds were defined based on similar toxicity. These definitions can be found in Appendix F.

The Institute contracted with the Tellus Institute to collect the available data. The data for each chemical, which was provided to each Board member on computer disk, is in Appendix G along with data sources and General Comments authored by the Tellus Institute concerning the collection of data. Table 3 shows the availability of data for the 258 chemicals.

Other models for chemical prioritization reviewed and considered by the Board, rely completely on algorithms which assign either a value of zero to a missing datum point, or use quantitative or qualitative structure-activity relationships[6] to derive an estimate of the value. The Board rejected these ideas due to the lack of available data for many compounds and the crude assumptions used in algorithms to complete data sets. Instead of developing an algorithm that might be difficult to understand or could ignore known risks, the Board chose to use an expert judgment method

---

[5]The list of substances reportable under TURA contains the approximately 1500 substances reportable under the federal laws, EPCRA and CERCLA, with the exception of a few federally listed substances that have been delisted by the TURA Administrative Council. Only those chemicals which a TURA filer uses or processes in quantities of 25,000 pounds or more per year, or otherwise uses in the amount of 10,000 pounds or more per year at any one facility are reportable.

[6]Quantitative Structure Activity Relationship software is available (e.g., Ecosar and MicroQSAR can be obtained from the U.S. EPA).

(based on the principles of the Delphi Method). This approach was used by Polaroid in developing their chemical ranking system[7], and it allows for incorporation of the Board members' professional experiences which is especially important for chemicals that have little or no data available. The Board members supported the expert judgment method and found it to be more satisfactory than the algorithm method

Table 3: Percent Data Available for each Criterion	
Criterion	Percent data available
IARC Classification	40%
LD_{50}	55%
RfD	38%
TLV (TWA)	70%
TLV (STEL)	19%
LC_{50}	41%
FP	41%
pKa	8%
pKb	6%
BCF	54%

The Delphi Method and the Expert Judgement Method

The term Delphi Method came from a study concerning the use of expert opinion called Project Delphi performed by the Rand Corporation in the 1950s for the U. S. Air Force. This study aimed to "obtain the most reliable consensus of opinion of a group of experts."[8] The Delphi method is appropriate when "accurate information is unavailable or expensive to obtain or evaluation models require subjective inputs to the point where they become the dominating parameters."[9] The rationale behind the method is that "if the opinion of one expert on an uncertain point is useful, the opinion of many experts - when boiled down to a single group opinion - should be even better."[10]

---

[7]Ahearn, J., Fatkin, H., and Schwalm, W., "Polaroid Corporation's Systematic Approach to Waste Minimization," Pollution Prevention Review, Summer 1991, pp. 257-271.

[8]Linstone, H.A., and Turoff, M., "The Delphi Method: Techniques and Applications," Addison-Wesley, Reading, Mass., 1975, pp. 3-12.

[9]Ibid.

[10]Gautschi, T.F., "Delphi Method Predicts the Future," Design News, Feb. 1990, p. 414.

The original method uses a series of questionnaires to solicit the opinions of the experts. The results of the questionnaires are summarized by an investigator who provides feedback to the experts. A modified questionnaire is then used to obtain a second round of opinions and the process continues until consensus is reached.

The Science Advisory Board's Expert Judgement Method began with each expert choosing fifty "more hazardous chemicals" and fifty "less hazardous chemicals", subsequently named Category 1 and Category 2 respectively. Each member used their own ranking scheme based on the data, their area of expertise and personal experiences. The votes from each expert were tabulated and the chemicals were ranked by the number of expert votes received for the category.

When asked to describe the criteria used to categorize the chemicals, the following statements were made by Board members for the more hazardous list of chemicals: "data revealed at least two criteria of concern and toxicity was rated higher than flammability", "aquatic toxicity ranked highest", "focused on carcinogenicity", "looked at potential for exposure to workers", "ratio of TLV/LD_{50}". These comments illustrate the diversity of expert opinion that contributed to the creation of these categories. Commonly, the criteria used for the less hazardous list were simply opposite of the more hazardous list or "didn't raise any concerns".

Refinement

Following the initial vote, two lists were prepared of chemicals that received a number of votes for each Category. The number cutoff was determined in order to produce lists of 25-30 chemicals each for further discussion. This ended up being 4 votes for Category 2 and 5 votes for Category 1 as there was considerable consensus for many of the chemicals on the Category 1 list. Each list was then discussed chemical by chemical. In some cases, additional data were requested. In some cases, chemicals receiving one vote less than the cuttoff were discussed. For the more hazardous chemical list, the Board decided to discuss every chemical that had an IARC classification of 1, 2a or 2b. As each chemical was discussed, consensus decisions were made to put the chemical in Category 1, 2 or 3.

For chemicals that received more than one vote for each list, the Board reviewed the data that were available and discussed the chemicals at length. In all cases the discrepancy was due to either conflicting data (e.g., low TLV and high LC_{50}), the lack of data or, in the case of metals, different definitions being used by members. This exercise resulted in a complete review of all metals and metal categories to be certain that all Board members were making the same assumptions. (See Appendix F, mentioned previously.)

The Board also compared its list to other lists of hazardous chemicals such as EPA's list of Extremely Hazardous Substances, the list created by EPA's Waste Minimization Prioritization Tool, and the Swedish National Chemicals Inspectorate list of Chemical Substances Which Require Particular Attention. In each case, the Board discussed similarities and discrepancies, and concluded that their process and resulting categories were more appropriate for the purposes of the project.

The Resulting Categories

Following are the Category 1 and 2 chemicals with CAS numbers as defined by the TUR Science Advisory Board. For chemicals in Category 1, along with the chemical name are a few phrases summarizing the discussion that resulted in the chemical's placement in this category. The list of Category 3 chemicals can be found in Appendix H. It is important to note that these three categories represent only the 258 chemicals that have been reported under TURA at the time of this project. For a complete list of the approximately 1200 chemicals on the TURA List of Toxic and Hazardous Substances, please refer to the Massachusetts Department of Environmental Protection, Bureau of Waste Prevention, Toxics Use Reduction Reporting Package.

Table 4: Category 1 Chemicals with CAS Numbers		
CAS Number(s)	Chemical Name	Summary
79-06-1	Acrylamide	IARC 2a, potential worker exposure problem
107-13-1	Acrylonitrile	IARC 2a, evidence of human carcinogenicity
01-00-1, 7440-38-2	Arsenic and arsenic compounds	IARC 1, acutely toxic
01-00-4, 7440-43-9	Cadmium and cadmium compounds	IARC 1
56-23-5	Carbon tetrachloride	Montreal Protocol chemical, liver toxin, suspect human carcinogen, IARC 2b
7782-50-5	Chlorine	low RfD, gas, toxic, corrosive to skin, heavier than air, stable in air, used in large quantities, toxic to aquatic organisms
67-66-3	Chloroform	low RfD, acute effects to the liver, medium bioaccumulation factor, IARC 2b
7738-94-5, 11115-74-5	Chromic acid	hexavalent chromium
01-01-2, 7440-47-3	Chromium compounds (+6 valence)	IARC 1, confirmed carcinogens
01-01-6, 143-33-9	Cyanide compounds and sodium cyanide	acutely toxic
96-12-8	Dibromodichloropropane (DBCP)	banned as a fumigant in 1977, PEL 1 ppb, IARC 2b
107-06-2	1,2-Dichloroethane (Ethylene dichloride)	acute toxicity, IARC 2b
64-67-5	Diethyl sulfate	IARC 2a, incompatible with water, highly irritating, reactive alkylating agent
68-12-2	Dimethylformamide	limited evidence of testicular cancer in humans, inadequate in animals, very soluble in water, PEL 10 ppm, easily absorbed into skin, exposures are likely to be high because of its large use, occupational hazard, highly mobile in soil
123-91-1	1,4-Dioxane	acute effects, strong skin absorber, IARC 2b

Table 4: Category 1 Chemicals with CAS Numbers		
CAS Number(s)	Chemical Name	Summary
106-89-8	Epichlorohydrin	IARC 2a, reportable quantity 10 pounds
75-21-8	Ethylene oxide	IARC 2a, mutagenic, reactive, eye and skin irritant, carcinogenic, and highly flammable
50-00-0	Formaldehyde	reactive, irritating, IARC 2a, acutely toxic
302-01-2	Hydrazine	eye and skin irritant, flammable, IARC 2b, TLV 10 ppb
01-02-6, 7439-92-1, 10099-74-8	Lead and lead compounds	neuro-toxic and impairs reproduction, IARC 2b
101-68-8	Methylenebis(phenylisocyanate)	
01-02-9	Nickel compounds	IARC 1 classification for nickel and nickel compounds (1990)
98-95-3	Nitrobenzene	carcinogen, causes liver damage, eye and skin irritant, smells foul, very low RFD and TLV=1 ppm
75-44-5	Phosgene	Leukocyte, severe eye, skin, mucous membrane irritant, TLV=0.1 ppm
75-55-8	Propyleneimine	very reactive, PEL=2ppm, skin absorbing, sufficient carcinogenic evidence in humans, IARC 2b
75-56-9	Propyleneoxide	TLV 20 ppm, evidence of mutagenicity, carcinogenicity, acute hazard
01-03-6, 7782-49-2	Selenium and selenium compounds	
7664-93-9, 8014-95-7	Sulfuric acid and fuming sulfuric acid	IARC 1, fuming is the actual toxic factor (due to its vapor pressure), corrosive, carcinogenic, reactive, causes lung damage
127-18-4	Tetrachloroethylene	IARC 2b, suspected carcinogen
584-84-9, 91-08-7, 26471-62-5	Toluenediisocyanate (2,4 and 2,6 and mixed isomers)	irritating to eyes, nose, skin and TLV 5 ppb, IARC 2b
79-01-6	Trichloroethylene	causes eye, skin, liver and central nervous system damage and low TLV

Table 5: Category 2 Chemicals with CAS Numbers	
64-19-7	Acetic Acid
67-64-1	Acetone
1066-33-7	Ammonium bicarbonate
71-36-3	n-Butyl Alcohol
78-92-2	sec-Butyl Alcohol
- - -	$Chromium^{3+}$ compounds
141-78-6	Ethyl Acetate
107-21-1	Ethylene Glycol
7705-08-0	Ferric chloride
10028-22-5	Ferric Sulfate
10045-89-3	Ferrous Ammonium Sulfate
7758-94-3	Ferrous Chloride
7720-78-7, 7782-63-0	Ferrous Sulfate
78-83-1	Isobutyl Alcohol
78-93-3	Methylethylketone
67-56-1	Methanol
7558-79-4, 10039-32-4, 10140-65-5	Sodium Phosphate, dibasic
7601-54-9, 7758-29-4, 7785-84-4, 10101-89-0, 10124-56-8, 10361-89-4	Sodium Phosphate, tribasic
1332-07-6	Zinc Borate
7733-02-0	Zinc Sulfate

Maintenance and Further Work

The Board realizes that the chemicals in the specific categories may change based on new data becoming available or new chemicals being used above TUR reportable threshold quantities in the Commonwealth. The Board will establish a review process whereby the Category 1 and Category 2 lists will be reviewed annually and new chemicals reported in Massachusetts will be evaluated. This review process will begin at the Board meeting following the release of Toxics Use Réduction data by the Department of Environmental Protection.

Appendix A: List of Members

David T. Williams
Director, Center for Technology and Health
Quincy College

James J. Ahearn Jr., Ph.D.
Polaroid Corporation

Andrew F. Beliveau
Environmental Protection Agency

Richard Clapp, Sc.D.
Boston University School of Public Health

George M. Gray, Ph.D.
Harvard School of Public Health
Center for Risk Analysis

Thomas Trayers
Division of Occupational Safety
Occupational Hygiene Program

Lawrence H. Boise
Gloucester Co., Inc.

Halina Brown, Ph. D. (ex officio)
Clark University

Christine Oliver, M. D. (ex officio)
Public Health Resource Group
Mass. General Hospital

Appendix B: Summary of Toxics Use Reduction Science Advisory Board Recommendations

Chemical Name	Recommendation	Supplemental Information	Status or Outcome
Nickel in alloy form	delist except for aerosols (less than 50 um)	Unanimous vote to accept recommendation. Aerosols should be reported under TURA because planning for efficient use is beneficial.	Delisting petition request accepted by Admin Council per SAB recommendation.
Chromium in alloy form	delist except for aerosols (less than 50 um)	Unanimous vote to accept recommendation. Aerosols should be reported under TURA because planning for efficient use is beneficial.	Delisting petition request accepted by Admin Council per SAB recommendation.
Copper in alloy form	delist except for aerosols (less than 50 um)	Unanimous vote to accept recommendation. Aerosols should be reported under TURA because planning for efficient use is beneficial.	Delisting petition request accepted by Admin Council per SAB recommendation.
Manganese in alloy form	delist except for aerosols (less than 50 um)	Unanimous vote to accept recommendation. Aerosols should be reported under TURA because planning for efficient use is beneficial.	Delisting petition request accepted by Admin Council per SAB recommendation.
Cobalt in alloy form	delist except for aerosols (less than 50 um)	Unanimous vote to accept recommendation. Aerosols should be reported under TURA because planning for efficient use is beneficial.	Delisting petition request accepted by Admin Council per SAB recommendation.
Chromium (III) oxide	delist	Unanimous vote to accept recommendation. Chromium (III) oxide is not known to cause significant human health effects, is not known to cause significant adverse effects on the env., does not bioaccumulate and the oxidation of chromium (III) to chromium (VI) is not likely to occur.	Delisting petition request accepted by Admin Council per SAB recommendation.
Sodium hydroxide	not delist	Majority decision to accept recommendation. Decision based primarily on its potential for acute toxicity to workers. For specific applications, there may be uses of sodium hydroxide for which there is scientific justification to determine that sodium hydroxide is the least hazardous material and presents the least risk; this should be considered by the Administrative Council	Delisting petition request denied by Admin Council per SAB recommendation.
Hydroquinone	delist, except for manufacture	Unanimous vote to accept recommendation. Material has moderate to low toxicity. Recommendation to delist was made because material did not satisfy the criteria of "significant health effects"	Delisting petition request accepted by Admin Council per SAB recommendation.

Prepared 12/3/96, Updated 10/29/97

Chemical Name	Recommendation	Supplemental Information	Status or Outcome
Butyl benzyl phthalate	delist	Unanimous vote to accept recommendation. The Board recommended delisting in the absence of science to prove that butyl benzyl phthalate is estrogenic despite emerging science that suggests that this potential exists.	From a policy perspective, the Institute questioned whether the absence of knowledge is a sufficient basis to support a delisting at this time. The Admin Council denied the delisting petition.
Ethyl Acetate	not delist	Unanimous vote to accept recommendation. Recommendation based primarily on its potential for acute toxicity to workers.	Delisting petition request denied by Admin Council per SAB recommendation.
Acetic Acid	delist at conc. below 12%	Unanimous vote to accept recommendation.	Delisting petition request accepted by Admin Council per SAB recommendation.
Sodium Hypochlorite	not delist	Majority decision to accept recommendation.	Delisting petition request denied by Admin Council per SAB recommendation.
Acetone	no recommendation	Board vote was split.	Delisting request denied. Acetone will be reviewed again in one year and categorization of the list of chemicals will be evaluated.
Zinc oxide	delist	Unanimous vote to accept recommendation.	Delisting petition request accepted by Admin Council per SAB recommendation.

Appendix C: Bibliography of Categorization/Prioritization Schemes

Davis, Gary et al., Center for Clean Products and Clean Technologies, University of Tennessee, "Chemical Hazard Evaluation for Management Strategies: A Method for Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts", EPA Document EPA/600/R-94/177, June 1994. *This model uses risk-based chemical ranking and scoring combining the toxic effects of chemicals and the potential for exposure to those chemicals. The report ranks 140 TRI chemicals based on 99% of total releases. The method does not include secondary global impacts such as ozone depleting and global warming, nor does it include worker safety. Potential uses of the methodology are: priority setting for regulatory action, for business decisions and to set priorities for pollution prevention.*

Davis, Gary et al., Center for Clean Products and Clean Technologies, University of Tennessee, "Comparative Evaluation of Chemical Ranking and Scoring Methodologies", April 7, 1994.

Gray, George and Jennifer Hartwell, Harvard Center for Risk Analysis, Harvard School of Public Health, "The Role of Risk in Chemical Substitution Decisions," prepared for the Massachusetts Toxics Use Reduction Institute, July 1994. *Outlines a risk-based substitution decision-making framework, the chemical substitution tree (CST). Suggests looking at both the application exposure and the disposal exposure for potential effects on the environment, workers and the public. Gives some ideas of chemical characteristics to consider and where to find relevant information. The model seeks to identify areas of potentially high risk so that companies can make informed decisions on how to reduce the risk.*

Grimsted, Bradley, et al., "A Multimedia Assessment Scheme to Evaluate Chemical Effects on the Environment and Human Health" Pollution Prevention Review, Summer 1994, pp. 259-268. *This article presents a model for calculating a common unit of measure - the Pollution Unit - that allows comparisons of potential relative effects of chemicals on different environmental media. The scheme incorporates environmental and human health factors (using ambient standards and regulatory criteria) but can be adjusted to stress one over the other or may be developed to incorporate occupational standards if worker health is of primary concern. Authors boast "easy to use", "technically defensible" and "versatile" as words to describe the model.*

Indiana Clean Manufacturing Technology and Sage Materials Institute, Pollution Prevention Progress Measurement Method (3P2M), Purdue University, February 1998. *This work builds on the Center for Clean Products and Clean Technologies algorithm to include factors for worker exposure and atmospheric hazards. This model does not include releases to the environment as did the Clean Products work. It has an option for inputting number of pounds of a chemical used in the workplace. The worker exposure component has three parts: health effects (chronic and acute), routes of exposure (vapor pressure, oral, skin, dust/mist) and safety (flammability, reactivity, corrosivity). For carcinogenicity, the most protective rating of EPA, ACGIH and IARC was used. The acute hazard value is based on the short term exposure limit (STEL); if an STEL does not exist, the score is 0. For oral exposure, the only compounds with scores other than zero are lead compounds.*

Massachusetts Toxics Use Reduction Institute,"Blanket Wash Technology Study: An Evaluation of Commercially Available Blanket Washes," Technical Report No. 16, 1994. *This study gives comparative information on the performance, environmental, health and safety characteristics of blanket washes commonly used in sheetfed offset lithography. Each attribute was given a good, fair or poor score. The non-performance attributes scored included VOC content, flash point, health hazard and potential regulatory impact. For determining a score for the health hazard, mixtures were given the highest score of any ingredient and data were obtained from REPROTEXT. For determining the potential regulatory impact, chemicals were given scores based on how many times they appeared on nineteen regulated chemical lists.*

Swedish National Chemicals Inspectorate, "Observation List of Chemical Substances Which Require Particular Attention," Printgraf AB, Stockholm, Sweden, January 997. *This work was done to guide users of chemicals to pay particular attention to the use of chemicals on the Observation List which contains 199 chemicals. A substance was placed on the list if it met any of an established list of criteria indicating environmental or health hazards. These criteria include bioaccumulation, aquatic toxicity, ozone depletion, acute toxicity, sensitizer, chronic toxicity, neurotoxicity, reproductive toxicity and carcinogenicity.*

Swedish National Chemicals Inspectorate, "Selecting Multiproblem Chemicals for Risk Reduction." *This work began with 7000 chemicals which was a combination of 70 national and international lists of chemicals hazardous to human health or the environment. In Step I, the list was narrowed to 500 chemicals that appeared on several lists. In Step II, the list was narrowed to 100 chemicals using 18 criteria of equal weight in the categories of environmental properties, health properties, and exposure potential. If no data was available, the criteria was not used. From this list of 100 chemicals, 45 were chosen based on additional data and use patterns in Sweden. Finally, 27 chemicals were chosen as candidates for risk reduction by a panel of experts who used the available data and member's experience and knowledge.*

Tiley, Jaimie, "Solvent Substitution Methodology using Multiattribute Utility Theory and the Analytical Hierarchical Process", Department of the Air Force, Air Force Institute of Technology, Wright-Patterson Air Force Base, OH. *This thesis presents a multicriteria decision making methodology for ranking alternatives to solvent cleaning. It compares Multiattribute Utility Theory and the Analytical Hierarchical Process. The cleaning situation studied is general cleaning of aircraft engine components. There were problems associated with both decision models including independence constraints and scaling issues. The author used group decision making scoring (1-7) in four areas: environmental impact, health/safety, process compatibility, cleaning effectiveness. Important attributes within each category were chosen by survey. Interesting to note which attributes were chosen in the environmental impact and health/safety categories (p 46.)*

US Environmental Protection Agency, "Waste Minimization Prioritization Tool," EPA 530-R-97-019, June 1997. *This work began with the adoption and modification of earlier work on the Use Cluster Scoring System. The Tool uses persistence, bioaccumulation and toxicity (human cancer, human non-cancer and ecological) characteristics for chemical risk screening. The mass of a chemical can be input into the tool's software. 900 chemicals were scored due to the*

availability of data. Partial chemical data is available for an additional 3800 chemicals which were not scored. If data did not exist, the chemical is not scored. The tool ignores acute effects, including those to workers.

Wolf, Katy, "The Generic Classification System: A Simplified Approach to Selecting Alternatives to Chlorinated Solvents" Pollution Prevention Review, Winter 1993-94, p 15-29. *The author sets up a generic classification system for choosing alternative to a chlorinated solvents. The properties/classifications of PEL, VOC, HAP, flash point, evaporation rate, solvent strength, ozone depleting potential, global warming potential and toxicity are covered. Good reference for data on the available solvent alternatives. Methodology is practical but very specific to solvents alternatives.*

Working Group of Accelerated Reduction/Elimination of Toxics (ARET), "Environmental Leaders - Voluntary Commitments to Action on Toxics through ARET," Ontario, March 1995. *This work began with 2000 substances from the Chemical Evaluation Search and Retrieval System. Approximately 500 of these substance had sufficient information to screen them for the ARET list. The criteria were chosen in the areas of toxicity, persistence and bioaccumulation. The toxicity criteria were in the following seven groups: acute lethality, chronic toxicity non-mammals, chronic toxicity plants, chronic toxicity mammals, teratogenicity, carcinogenicity, genotoxicity.*

Appendix D: Criterion Definitions

Oral LD_{50}: A single calculated dose of a substance administered through food or gavage (tube feeding) in mg per kg of body weight, which kills 50% of a group of test animals within 14 days. A lower LD_{50} indicates a more toxic substance.

Reference Dose (RfD): An estimate of the daily exposure level for the human population that is likely to be without an appreciable risk of adverse effects over a lifetime. RfDs are often estimated from the highest dose at which no adverse effects are observed in animals, the No Observed Adverse Effects Level (NOAEL). The Environmental Protection Agency has defined RfD's for a number of chemicals.

Carcinogen: International Agency for Research on Cancer (IARC) uses the term "carcinogen to denote an agent that is capable of increasing the incidence of malignant meoplasms; the induction of benign neoplasms may in some circumstances contribute to the judgement that an agent is carcinogenic..."

> IARC Classification. Carcinogens are rated in 1 of 5 groups: (1) Group 1 - the agent is carcinogenic to humans; (2) Group 2A - the agent is probably carcinogenic to humans; (3) Group 2B - the agent is possible carcinogenic to humans; (4) Group 3 - the agent is not classifiable as to its carcinogenicity to humans (when agents cannot be placed in any other group); and (5) Group 4 - the agent is probably not carcinogenic to humans.

TLV (Threshold Limit Value): Published by the American Conference of Governmental Industrial Hygienists (ACGIH), defined as airborne concentrations under which it is believed that nearly all workers may be repeatedly exposed day after day without adverse effects. TLV's are generally established on a consensus basis; as such, some workers may be affected at or below these limits due to unusual susceptibility or pre-existing conditions. A lower TLV indicates a more toxic substance.

Aquatic LC_{50}: The concentration of a chemical, in water, that causes death in 50% of the fish tested. Aquatic LC_{50} can be calculated for both freshwater and saltwater fish (and sometimes for other aquatic organisms).

Bioconcentration: Describes the tendency for a chemical to accumulate in biological systems, and more specifically the ability of a substance to accumulate in the tissues of organisms. Bioconcentration is a function of the physicochemical properties of a chemical, especially the chemical's lipid solubility (solubility in fat). Two parameters most frequently used to express bioconcentration are the octanol-water partition coefficient (K_{ow}) and the Bioconcentration factor (BCF).

- Bioconcentration factor is the ratio of the concentration of a chemical in an organism to its concentration in the test medium or environment, typically water, at steady-state conditions. This factor is a measure of the chemical's ability to bioaccumulate

K_{ow} is defined as the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase 1-octanol/water system at equilibrium. In other words, it represents the distribution tendency of organic chemicals between organic and aqueous phases. As lipid soluble chemicals are generally also soluble in solvents such as octanol and are relatively insoluble in water, K_{ow} can be used to predict the bioconcentration factor. A low log K_{ow} value is considered hydrophilic and has a low fat solubility and high water solubility. K_{ow} is generally expressed in log units.

Flash point: The temperature at which material gives off sufficient vapor to form an ignitable mixture with the air near the surface of the material. The lower the flash point, the more probability an explosion could occur under normal working conditions.

pH: A logarithmic index for the hydrogen ion concentration in an aqueous solution. A pH below 7 indicates acidity, and one above 7 alkalinity (at 25C). The pH scale ranges from 0-14, with extreme values representing a more corrosive aqueous solution. Values closest to 7 represent the lowest hazard.

Appendix E: Surrogate Chemicals

Mass. #	CAS #	Chemical Group Name	Suggested Surrogate	Notes
01-00-0	1309-64-4	Antimony compounds	Diantimony trioxide	Tennessee surrogate
01-00-1	1303-28-2	Arsenic compounds	Arsenic pentoxide	Tennessee surrogate
01-00-2	10361-37-2	Barium compounds	Barium chloride	Tennessee surrogate
01-00-4	10108-64-2	Cadmium compounds	Cadmium chloride	Tennessee surrogate
01-01-2	1333-82-0	Chromium Compounds	Chromium oxide	Tennessee surrogate
01-01-3	7646-79-9	Cobalt compounds	Cobalt chloride	Tennessee surrogate
01-01-5	7758-98-7	Copper compounds	Copper sulfate	Tennessee surrogate
01-01-6	143-33-9	Cyanide compounds	Sodium cyanide	Most widely used, most toxic, most data available
01-02-2	110-80-5	Glycol ethers	Glycolmonoethylether	Most common, most data available
01-02-6	7758-95-4	Lead compounds	Lead chloride	Tennessee surrogate
01-02-7	1344-43-0	Manganese compounds	Manganese oxide	Tennessee surrogate
01-02-9	37211-05-5 373-02-4 6018-89-9	Nickel and compounds	Nickel chloride Nickel acetate Nickel acetate tetrahydrate	Tennessee surrogate for all except mammalian oral toxicity For mammalian oral toxicity due to availability of data Choose specific Nickel acetate with the most data
01-03-3	117-81-7	Phthalate esters	Diethylhexylphthalate	Most common, most data available
01-03-6	7446-08-4 7783-00-8 7488-56-4 7783-79-1 12033-59-9 14832-90-7 57-12-5	Selenium and compounds	Selenium IV dioxide Selenium IV disulfide Selenium hexaflouride Selenium nitride Selenium oxide Selenium	Tellus choose chemical in this group that has the most data

Mass. #	CAS #	Chemical Group Name	Suggested Surrogate	Notes
01-03-7	7783-90-6 7761-88-8 7783-91-7 7784-01-2 506-64-9	Silver and compounds	Silver chloride Silver nitrate Silver chlorite Silver chromate Silver cyanide	Tellus choose chemical in this group that has the most data
01-03-9	1314-13-2 7733-02-0	Zinc and compounds	Zinc oxide Zinc sulfate	Tennessee surrogate for all except fish toxicity For fish toxicity b/c Zinc oxide not soluble in water
01-09-0	7761-88-8	Nitrate compounds	Zinc nitrate	Note: water dissociable nitrate compounds reportable only in aqueous solutions on SARA 313. Silver nitrate most soluble.
Notes: For Nickel acetate, Selenium compounds and Silver compounds, choose the specific chemical based on the availability for the most data. Glycomonoethyl and Diethylhexylphthalate are listed separately also.				

Appendix F: Metals

At the November, 1997 meeting of the Science Advisory Board, members proposed groupings for metals and metal compounds to represent similarities in metal toxicities. If the base metal is a category by itself (e.g., copper), that particular category represents the toxicity of the metal itself (e.g., metallic copper). If the base metal is in a category with other metal compounds (e.g., lead and lead compounds), it was the opinion of the group that the metal toxicities of the base metal and the metal compounds were basically similar. For categories that are comprised of more than one compound, the CAS number for the group is given.

Base Metal	Metal Categories		CAS #
Aluminum	1	Aluminum, Aluminum oxide	7429-90-5
	2	Aluminum sulfate	
Antimony	1	Antimony, Antimony cmpds, Antimony trioxide	1309-64-4
Arsenic	1	Arsenic, Arsenic compounds	1303-28-2
Barium	1	Barium	
	2	Barium compounds	
Cadmium	1	Cadmium, Cadmium compounds	10108-64-
Chromium	1	Chromium, Chromium and cmpds [valence 0 and 3]	7440-47-3
	2	Hexavalent chromium [valence 6]	1333-82-0
Cobalt	1	Cobalt	
	2	Cobalt compounds	
Copper	1	Copper	
	2	Copper compounds	
Iron	1	Ferric chloride, Ferric sulfate, Ferrous ammonium sulfate, Ferrous chloride, Ferrous sulfate	7705-08-0

Base Metal	Metal Categories		CAS #
Lead	1	Lead, Lead chromate, Lead compounds, Lead nitrate	7758-97-6
Manganese	1	Manganese, Manganese cmpds, Potassium permanganate	7439-96-5
Nickel	1	Nickel	
	2	Nickel acetate, Nickel acetate tetrahydrate, Nickel and compounds	37211-05-
Potassium	1	Potassium hydroxide	
Selenium	1	Selenium, Selenium & cmpds, Selenium cmpd, Selenium dioxide, Selenium hexaflouride, Selenium nitride, Selenium oxide	7488-56-4
Silver*	1	Silver	
	2	Silver and compounds	
	3	Silver chlorite	
	4	Silver chromate	
	5	Silver cyanide	
	6	Silver nitrate	
*For the Silver compounds, it was noted that the Silver chloride is not very soluble and that the Chromate and Cyanide compounds are more toxic due to the presence of those components, not the silver.			
Sodium	1	Sodium	
	2	Sodium bichromate	
	3	Sodium bisulfite	
	4	Sodium cyanide	
	5	Sodium dimethyldithiocarbamate	
	6	Sodium dodecylbenzenesulfonate	

Base Metal	Metal Categories		CAS #
	7	Sodium fluoride	
	8	Sodium hydrosulfide	
	9	Sodium hydroxide	
	10	Sodium hypochlorite	
	11	Sodium methylate	
	12	Sodium nitrite	
	13	Sodium phosphate, dibasic	
	14	Sodium phosphate, tribasic	
	15	Sodium phosphate, tribasic dodecahydrate	
	16	Sodium phosphate, tribasic anhydrous	
Zinc	1	Zinc	
	2	Zinc and compounds	
	3	Zinc oxide fume	
	4	Zinc sulfate	
	5	Zinc ammonium chloride	
	6	Zinc borate	
	7	Zinc sulfate	

Appendix G: Data, Collection and Sources

MASTER DATA FILE

CAS Number	Chemical Name	IARC	RFD	TLV(TWA in mg/m^3)	FP (C)	BCF	pKa	pKa (ca)	pK notes	LD50, pT	c LC50 , pT	Aquatic LC50 notes	LD50 notes	TLV Notes
0001717-00-6	1,1-DICHLORO - 1 FLUOROETHANE													
0000872-50-4	1-METHYL-2-PYRROLIDONE					0.0738								
0000540-84-1	2,2,4-TRIMETHYLPENTANE				-7	848.7								
0000612-83-9	3,3'DICHLOROBENZIDINE									-1.07			Rat, TerraTox	
0055406-53-6	3-IODO-2-PROPYNYL													
0000075-07-0	ACETALDEHYDE	2B		no TWA	-40	0.4202				-1.64	0.15	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000064-19-7	ACETIC ACID			25	40	0.1146	4.75			-0.94	-0.12	96hr, FHM, Static, TerraTox	Mouse,	
0000108-24-7	ACETIC ANHYDRIDE			21	54	0.0486				-1.24			Rat, TerraTox	
0000067-64-1	ACETONE		0.1	1188	-17	0.099				-1.71	-2.15	96hr, FHM, Static, TerraTox	Mouse,	
0000075-05-8	ACETONITRILE		0.01	67	5	0.0803				-0.82	-1.61	96hr, FHM, Static, TerraTox	Mouse,	
0000098-86-2	ACETOPHENONE		0.1	49	82	4.9805				-0.79	-0.13	96hr, FHM, Static, TerraTox	Mouse,	
0000079-06-1	ACRYLAMIDE ←	2A	0	0.03		0.0319				-0.18	-0.19	96hr, FHM, Static, TerraTox	Mouse,	skin
0000079-10-7	ACRYLICACID		0.5	5.9	54					0.33			Rat, TerraTox	skin
0000107-13-1	ACRYLONITRILE	2A	0	4.3	0	0.2764				0.29	0.47	96hr, FHM, Static, TerraTox	Mouse,	skin
0000124-04-9	ADIPIC ACID			5	196	0.1936	4.42							
0000107-05-1	ALLYLCHLORIDE			3	-28	4.6771				-0.74	0.5	96hr, FHM, Static, TerraTox	Mouse,	
0007429-90-5	ALUMINUM			5									multiple TLVs, welding fumes and pyro powders	
0001344-28-1	ALUMINUMOXIDE			10										
0010043-01-3	ALUMINUMSULFATE			2						-1.26			Mouse,	luminum soluble salts
0007664-41-7	AMMONIA			17		0.265		4.75	CRC		0.98	96hr, FHM, Static, TerraTox		
0001066-33-7	AMMONIUMBICARBONATE													
0001341-49-7	AMMONIUMBIFLUORIDE													
0012125-02-9	AMMONIUMCHLORIDE			10										fume
0012125-01-8	AMMONIUMFLUORIDE										-0.99	96hr, FHM, Static, TerraTox		
0001336-21-6	AMMONIUMHYDROXIDE													
0007773-06-0	AMMONIUMSULFAMATE			10						-1.24			Rat, TerraTox	
0000062-53-3	ANILINE			7.6	70	2.5704		4.69		-0.67	0	96hr, FHM, Static, TerraTox	Rat, TerraTox	LV incl. homologues
0007440-36-0	ANTIMONY		0	0.5										and compounds
0001309-64-4	ANTIMONY COMPOUNDS	2B	0	0.5										Antimony TLV
0001309-64-4	ANTIMONYTRIOXIDE	2B	0	0.5										Antimony TLV
0007440-38-2	ARSENIC		0	0.01										and inorg. cmpds, not Arsine
0001303-28-2	ARSENIC COMPOUNDS			0.01										Arsenic TLV
0007440-39-3	BARIUM		0.07	0.5										and soluble cmpds
0010361-37-2	BARIUM COMPOUNDS			0.5										Barium TLV
0000094-36-0	BENZOYLPEROXIDE			5						-1.37			Mouse,	
0000092-52-4	BIPHENYL			1.3		436.52				-1.09	1.9	96hr, FHM, Static, TerraTox	Mouse,	
0000103-23-1	BISETHYLHEXYL		0.6		205	546.36								
0007726-95-6	BROMINE			0.66	none									
0000353-59-3	BROMOCHLORODIFLUOROMETHANE													
0000074-83-9	BROMOMETHANE		0	3.9		1.981				-0.35			Rat, TerraTox	skin
0000110-19-0	BUTYL ACETATE-I			713	21	6.8197								
0000540-88-5	BUTYL ACETATE-T			200	16	7.7332					-0.45	96hr, FHM, Static, TerraTox		
0000123-86-4	BUTYLACETATE			713	22	7.4159				-1.78	0.81	96hr, FHM, Static, TerraTox	Mouse,	
0000141-32-2	BUTYLACRYLATE			52	39	22.986				-0.85			Rat, TerraTox	
0000071-36-3	BUTYLALCOHOLA		0.1	no TWA	35	1.0347				-1.03	-1.37	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000078-92-2	BUTYLALCOHOLB			303	26									
0000075-65-0	BUTYLALCOHOLC			303	4	0.3408				-1.67	-1.94	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000085-68-7	BUTYLBENZYLPHTHALA		0.2		213	776.25				-0.87	2.13	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000084-74-2	BUTYLPHTHALATE		0.1		171	3013.9				-1.28	2.4	96hr, FHM, Static, TerraTox	Mouse,	
0000123-72-8	BUTYRALDEHYDE				-11	1.0347				-1.54	0.65	96hr, FHM, Static, TerraTox	Rat, TerraTox	

CAS Number	Chemical Name	IARC	RFD	TLV(TWA in mg/m^3)	FP (C)	BCF	pKa	pKa (ca)	pK notes	LD50, pT	c LC50 , pT	Aquatic LC50 notes	LD50 notes	TLV Notes
0007440-43-9	CADMIUM	1	0	0.01										and compounds
0010108-64-2	CADMIUM COMPOUNDS	1		0.01						0.49	2.08	96hr, FHM, Static, TerraTox	Mouse,	Cadmium TLV
0000075-20-7	CALCIUM CARBIDE													
0007778-54-3	CALCIUM HYPOCHLORITE													
0000105-60-2	CAPROLACTAM DUST AND VAPOR		0.5	1		0.6525								Dust TLV=1, Vapor TLV=23
0000056-23-5	CARBONTETRACHLORIDE	2B	0	31	none	17.378				-1.06	0.55	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0007782-50-5	CHLORINE		0.1	1.5										
0000108-90-7	CHLOROBENZENE		0.02	46	24	446.68				-1.31	0.7	96hr, FHM, Static, TerraTox	Mouse,	
0000075-45-6	CHLORODIFLUOROMETHANE			3540		1.5732								
0000067-66-3	CHLOROFORM	2B	0.01	49	none	6.0256				0.52	0.23	96hr, FHM, Static, TerraTox	Mouse,	
0000074-87-3	CHLOROMETHANE			103	-40	1.1018				-1.55	-1.04	96hr, bgill, static, TerraTox	Rat, TerraTox	skin
0000095-57-8	CHLOROPHENOL		0.01		64	213.8	8.56			-0.43	1.02	96hr, FHM, Static, TerraTox	Mouse,	
0007790-94-5	CHLOROSULFONIC ACID				none									
0001897-45-6	CHLOROTHALONIL		0.02			41.319				-1.14	2.83	96hr, bgill, static, TerraTox	Mouse,	
0007738-94-5	CHROMIC ACID			0.01			0.74		CRC					Insol Cr (VI) cmpds
0010101-53-8	CHROMIC SULFATE			0.5										TLV for Cr metal & Cr(III) cmpds
0007440-47-3	CHROMIUM	1	0.01	0.5										Cr metal & Cr(III) cmpds
0001333-82-0	CHROMIUM AND COMPOUNDS	1		0.01			0.74		CRC					Insol Cr (VI) cmpds
0028407-37-6	CI DIRECT BLUE 218													
0002832-40-8	CIDISPERSEYELLOW													
0000081-88-9	CIFOODRED15									-0.27			Mouse,	
0000097-56-3	CISOLVENTYELLOWA					1278.2								
0007440-48-4	COBALT	2B		0.02										and inorganic cmpds
0007646-79-9	COBALT COMPOUNDS	2B		0.02										TLV for Cobalt
0007440-50-8	COPPER			0.05								& inorg cmpds; TLV for fume and respirable particles		
0007758-98-7	COPPER COMPOUNDS			0.05						-0.27			Rat, TerraTox	TLV for Copper
0008001-58-9	CREOSOTE ←	2A												
0000108-39-4	CRESOLA		0.05	22	86	10.369	10.1			-0.35	0.29	96hr, FHM, Static, TerraTox	Rat, TerraTox	Cresol mixed isomer
0000095-48-7	CRESOLB		0.05	22	81	10.715	10.3			-0.05	0.77	96hr, FHM, Static, TerraTox	Rat, TerraTox	Cresol mixed isomer
0001319-77-3	CRESOLMIXEDISOMER		0	22										skin; all isomers
0000098-82-8	CUMENE		0.04	246	46	348.29				-1.07	1.28	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0003251-23-8	CUPRIC NITRATE			0.05										TLV for Copper
0007758-98-7	CUPRIC SULFATE			0.05						-0.27			Rat, TerraTox	TLV for Copper
0000143-33-9	CYANIDE COMPOUNDS		0.04	no TWA		0.0047				0.88	2.46	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000110-82-7	CYCLOHEXANE			1030	-18	220.19				-0.98	0.38	96hr, bgill, static, TerraTox	Mouse,	
0000108-94-1	CYCLOHEXANONE		5	100	47	0.8935				-1.22	-0.81	96hr, FHM, Static, TerraTox	Mouse,	skin
0000096-12-8	DBCP	2B				80.736				0.14			Rat, TerraTox	
0001163-19-5	DECABROMODIPHENYLOX		0.01			0.0315								
0000095-50-1	DICHLOROBENZENEA		0.09	150	66	89.125				-0.53	1.4	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000106-46-7	DICHLOROBENZENEC	2B		60	66	60.256				-0.53	1.62	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0025321-22-6	DICHLOROBENZENEMIX			60	64									TLV for p-dichlorobenze
0000075-27-4	DICHLOROBROMOMETHANE	2B	0.02		none	10.813				-0.44			Mouse,	
0000075-71-8	DICHLORODIFLUOROMETHANE		0.2	4950		15.119								
0000107-06-2	DICHLOROETHANE	2B		40	16	1.9953				-0.69	-0.14	96hr, FHM, Static, TerraTox	Mouse,	
0000156-60-5	DICHLOROETHYLENE		0.02		6	13.057				-1.1			Rat, TerraTox	
0000075-09-2	DICHLOROMETHANE	2B	0.06	174	none	2.2464				-1.39	-0.56	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000076-14-2	DICHLOROTETRAFLUOROETHANE			6990		60.23								
0000111-42-2	DIETHANOLAMINE			2	138	0.0082		8.88		-0.83	-1.65	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0000109-89-7	DIETHYLAMINE			15	-28	0.5518		11.09		-0.83	-1.07	96hr, FHM, Static, TerraTox	Mouse,	skin
0000117-81-7	DIETHYLHEXYLPHT	2B	0.02	5	207	851.14				-1.89	1.8	96hr, goldf, static, TerraTox	Rat, TerraTox	

CAS Number	Chemical Name	IARC	RFD	TLV(TWA in mg/m^3)	FP (C)	BCF	pKa	pKa (ca)	pK notes	LD50, pT	c LC50 , pT	Aquatic LC50 notes	LD50 notes	TLV Notes
0000084-66-2	DIETHYLPHTHALATE		0.8	5	162	117.49				-1.44	0.84	96hr, FHM, Static, TerraTox	Mouse,	
0000064-67-5	DIETHYLSULFATE	2A			78	1.784				-0.62			Mouse,	
0000822-06-0	DIISOCYANATES			0.034	140	133.38				-0.32			Mouse,	
0000124-40-3	DIMETHYLAMINE			9.2	15	0.0738		10.78		-0.85	-0.67	96hr, guppy, static, TerraTox	Mouse,	
0000121-69-7	DIMETHYLANILINE		0	25	63	20.701				-1.07	0.19	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000068-12-2	DIMETHYLFORMAMIDE	2B	0.1	30	58	0.0197				-1.58	-2.16	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000131-11-3	DIMETHYLPHTALATE		10	5	156	57.544				-1.54	0.21	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000117-84-0	DIOCTYLPHTHALATE		0.02		219	7455.7				-2.08			Rat, TerraTox	
0000123-91-1	DIOXANE	2B		90	12	0.0679				-1.68	-2.05	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0027176-87-0	DODECYLBENZENESULFONIC ACID									-0.3			Rat, TerraTox	
0000106-89-8	EPICHLOROHYDRIN	2A	0	1.9	33	0.4202				0.01	0.86	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0000110-80-5	ETHOXYETHANOL		0.4	18	44	0.0528				-1.43	-2.05	96hr, bgill, static, TerraTox	Mouse,	skin
0000141-78-6	ETHYLACETATE		0.9	1440	-3	0.7556				-1.67	-0.42	96hr, FHM, Static, TerraTox	Mouse,	
0000140-88-5	ETHYLACRYLATE	2B		20	16	2.6013				-1.25	1.6	96hr, FHM, Static, TerraTox	Mouse,	
0000100-41-4	ETHYLBENZENE		0.1	434	22	120.14				-1.52	0.4	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000074-85-1	ETHYLENE			listed, no TLV		1.747								
0000142-59-6	ETHYLENE BIS DITHIOCARBAMATE					0.0017				-0.19	1.65	96hr, guppy, static, TerraTox	Rat, TerraTox	
0000107-15-3	ETHYLENEDIAMINE		0.02	25	34	0.0112		9.93		-0.91	-0.28	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0000060-00-4	ETHYLENEDIAMINE-TETRAACETIC				33	5E-05				-0.01	0.69	96hr, FHM, Static, TerraTox	Mouse,	
0000107-21-1	ETHYLENEGLYCOL		2	no TWA		0.0029				-2.08	-2.93	96hr, FHM, Static, TerraTox	Mouse,	aerosol
0000075-21-8	ETHYLENEOXIDE	2A		1.8	>110	0.0873				-0.88	-0.28	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000096-45-7	ETHYLENETHIOUREA	2B	0			0.0411				-1.25	-2.87	96hr, guppy, static, TerraTox	Rat, TerraTox	
0000060-29-7	ETHYLETHER		0.2	1210	-40	1.0347				-1.22	-1.54	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0007705-08-0	FERRICCHLORIDE			1										soluble iron salts
0010028-22-5	FERRICSULFATE			1										soluble iron salts
0010045-89-3	FERROUSAMMONIUM SULFATE			1										soluble iron salts
0007758-94-3	FERROUSCHLORIDE			1										soluble iron salts
0007720-78-7	FERROUSSULFATE			1										soluble iron salts
0007782-63-0	FERROUSSULFATE			1										soluble iron salts
0000133-07-3	FOLPET		0.1			327.2				-0.72	3	96hr, FHM, Static, TerraTox	Mouse,	
0000050-00-0	FORMALDEHYDE	2A	0.2	no TWA	56	0.3408	13.29			-0.15	0.1	96hr, FHM, Static, TerraTox	Mouse,	
0000064-18-6	FORMIC ACID		2	9.4	69	0.0528	3.75			-1.18			Mouse,	
0000076-13-1	FREON113		30			122.68								
0000110-17-8	FUMARIC ACID						3.03		CRC	-1.9			Rat, TerraTox	
0000109-99-9	FURAN, TETRAHYDRO-			590	-17	0.4291		-2.1		-1.5	-1.48	96hr, FHM, Static, TerraTox	Mouse,	
0000098-01-1	FURFURAL		0	7.9	73	538.75				0.17	0.67	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0000110-80-5	GLYCOL ETHERS		0.4	18	44	0.0528				-1.43	-2.05	96hr, bgill, static, TerraTox	Mouse,	skin
0000110-54-3	HEXANE (N-HEXANE)		0.06	176	-23	705				-2.52	1.54	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000302-01-2	HYDRAZINE	2B		0.013	52	0.0021				-0.26	1.51	96hr, bgill, static, TerraTox	Mouse,	skin
0007647-01-0	HYDROCHLORICACID			no TWA		0.5075								
0007664-39-3	HYDROGENFLUORIDE			no TWA	none									
0000078-83-1	ISOBUTYL ALCOHOL		0.3	152	37	0.8046				-1.52	-1.3	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000078-59-1	ISOPHORONE		0.2	no TWA	84	7.0795				-1.23	-0.22	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0004098-71-9	ISOPHORONE DIISOCYANATE			0.045	84									
0000067-63-0	ISOPROPYLALCOHOL			983	22	0.1818				-1.78	-2.21	96hr, FHM, Static, TerraTox	Mouse,	
0000080-05-7	ISOPROPYLIDENED		0.05							-1.02			Mouse,	
0007439-92-1	LEAD	2B		0.05										and inorganic compounds
0007758-97-6	LEAD CHROMATE	1		0.012										as Cr, .05 as Lead
0007758-95-4	LEAD COMPOUNDS			0.05										TLV for Lead
0010099-74-8	LEADNITRATE			0.05										TLV for Lead

CAS Number	Chemical Name	IARC	RFD	TLV(TWA in mg/m^3)	FP (C)	BCF	pKa	pKa (ca)	pK notes	LD50, pT	c LC50 , pT	Aquatic LC50 notes	LD50 notes	TLV Notes
0014307-35-8	LITHIUM CHROMATE			0.05										water sol Cr (VI) cmpds
0000110-16-7	MALEICACID						1.83		CRC					
0000108-31-6	MALEICANHYDRIDE		0.1	1	103	4.8773				-0.61			Rat, TerraTox	
0007439-96-5	MANGANESE		0.14	0.2										and inorganic compounds
0001344-43-0	MANGANESE COMPOUNDS			0.2										TLV for Manganese
0000126-98-7	METHACRYLONITRILE		0	2.7	12	0.6805				0.6			Mouse,	skin
0000067-56-1	METHANOL		0.5	262	11	0.0326	15.5			-2.25	-2.95	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0000109-86-4	METHOXYETHANOL			16	46	0.0326				-1.49			Rat, TerraTox	skin
0000096-33-3	METHYLACRYLATE		0.03	7	6	0.348				-0.51			Rat, TerraTox	skin
0000079-22-1	METHYLCHLOROFORMATE				17									
0005124-30-1	METHYLENE BIS(4-			0.054										
0000101-14-4	METHYLENEBISCHLORO ←	2A	0	0.11		313.85				-0.38			Mouse,	skin
0000101-68-8	METHYLENEBISPHENYL			0.051						-0.94			Mouse,	
0000078-93-3	METHYLETHYLKETONE		0.6	590	-3	0.3005				-1.67	-1.65	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000108-10-1	METHYLISOBUTYLKETO		0.08	205	13	2.5473				-1.32	-0.71	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000080-62-6	METHYLMETHACRYLATE		0.08	410	10	2.9498				-1.56	-0.41	96hr, FHM, Static, TerraTox	Mouse,	
0001634-04-4	METHYLTBUTYLET			144	-10	1.5136				-1.66	-0.88	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000090-94-8	MICHLERSKETONE					538.75								
0000075-04-7	MONOETHYLAMINE			9.2	-16	0.1247		10.81		-0.95			Rat, TerraTox	skin
0000924-42-5	N-METHYLOLACRYLAMIDE													
0000091-20-3	NAPHTHALENE		0.04	52	79	426.58				-0.62	1.32	96hr, FHM, Static, TerraTox	Mouse,	
0007440-02-0	NICKEL	2B	0.02	0.5										
0000373-02-4	NICKEL ACETATE			0.05										soluble Ni cmpds
0006018-89-9	NICKEL ACETATE TETRAHYDRATE			0.05										soluble Ni cmpds
0037211-05-5	NICKEL AND COMPOUNDS			0.05										soluble Ni cmpds
0007761-88-8	NITRATE COMPOUNDS			0.01						0.53	4.28	96hr, FHM, Static, TerraTox	Mouse,	soluble Ag cmpds
0007697-37-2	NITRICACID			5.2			>0							
0010102-43-9	NITRICOXIDE			31										
0000098-95-3	NITROBENZENE		0	5	88	15.136				-0.6	0.01	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0010102-44-0	NITROGEN DIOXIDE			5.6										
0000088-75-5	NITROPHENOLA					6.9641	7.23			-0.38	0	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000099-55-8	NITROTOLUIDINE					1.784				-0.58	0.35	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0020325-40-0	O-DIANISIDINE DIHYDROCHLORIDE													
0030525-89-4	PARAFORMALDEHYDE				71									
0000594-42-3	PERCHLOROMETHYLMERCAPTAN			0.76	none									
0000108-95-2	PHENOL		0.6	19	79	17.378	9.99			-0.46	0.51	96hr, FHM, Static, TerraTox	Mouse,	skin
0000106-50-3	PHENYLENEDIAMINE		0.19	0.1		0.0411				0.13			Rat, TerraTox	
0000075-44-5	PHOSGENE			0.4		0.037								
0007664-38-2	PHOSPHORICACID			1			2.12		CRC					
0010025-87-3	PHOSPHORUS OXYCHLORIDE			0.63						-0.39			Rat, TerraTox	
X 0000117-81-7	PHTHALATE ESTERS	2B	0.02	5	207	851.14				-1.89	1.8	96hr, goldf, static, TerraTox	Rat, TerraTox	
0000085-44-9	PHTHALICANHYDRIDE		2	6.1	151	0.0446				-1.43			Rat, TerraTox	
0000109-06-8	PICOLINE				26	1.6753				-0.86	-0.98	96hr, FHM, Static, TerraTox	Mouse,	
0001336-36-3	POLYCHLORINATEDBIPH ←	2A	0	0.5										skin; TLV for chlorodiphenyl (0011097-69-1)
0009016-87-9	POLYMERIC DIPHENYLMETHANE													
0001310-58-3	POTASSIUMHYDROXIDE			no TWA				>0						
0007722-64-7	POTASSIUMPERMANGANATE			0.2										TLV for Manganese and inorganic compounds
0000079-09-4	PROPIONICACID			30	51	0.3268	4.87			-1.55			Rat, TerraTox	
0000107-12-0	PROPIONITRILE				6	0.2289				0.19	-1.44	96hr, FHM, Static, TerraTox	Mouse,	
0000075-55-8	PROPYLENEIMINE	2B		4.7	-15					0.48			Rat, TerraTox	skin

CAS Number	Chemical Name	IARC	RFD	TLV(TWA in mg/m^3)	FP (C)	BCF	pKa	pKa (ca)	pK notes	LD50, pT	c LC50 , pT	Aquatic LC50 notes	LD50 notes	TLV Notes
0000075-56-9	PROPYLENEOXIDE	2B		48	-37	0.1936				-0.82	-0.39	96hr, bgill, static, TerraTox	Rat, TerraTox	
0000110-86-1	PYRIDINE		0	16	20	0.639		5.23		-1.05	-0.1	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000108-46-3	RESORCINOL			45		0.875	9.4			-0.26	0.04	96hr, FHM, Static, TerraTox	Mouse,	
0000057-12-5	SELENIUM		0.02	0.2										and compounds
0007782-49-2	SELENIUM		0.01	0.2										and compounds
0007446-08-4	SELENIUM AND COMPOUNDS			0.2										and compounds
0007783-00-8	SELENIUM CMPD?		0.01	0.2										and compounds
0007488-56-4	SELENIUM DIOXIDE			0.2						0.02			Rat, TerraTox	and compounds
0007783-79-1	SELENIUM HEXAFLUORIDE			0.16										as Selenium
0012033-59-9	SELENIUM NITRIDE			0.2										and compounds
0014832-90-7	SELENIUM OXIDE			0.2										and compounds
0007440-22-4	SILVER		0.01	0.1										
0007783-90-6	SILVER AND COMPOUNDS			0.01										sol cmpds, as Silver
0007783-91-7	SILVER CHLORITE			0.01										sol cmpds, as Silver
0007784-01-2	SILVER CHROMATE			0.01										sol cmpds, as Silver
0000506-64-9	SILVER CYANIDE		0.1	0.01										sol cmpds, as Silver
0007761-88-8	SILVER NITRATE			0.01						0.53	4.28	96hr, FHM, Static, TerraTox	Mouse,	sol cmpds, as Silver
0007761-88-8	SILVERNITRATE			0.01						0.53	4.28	96hr, FHM, Static, TerraTox	Mouse,	sol cmpds, as Silver
0007440-23-5	SODIUM													
0010588-01-9	SODIUM BICHROMATE ←	1		0.01										insol Cr (VI) cmpds
0007631-90-5	SODIUM BISULFITE			5						-1.28	0.64	96hr, mosqf, static, TerraTox	Rat, TerraTox	
0000143-33-9	SODIUM CYANIDE (Na(CN))		0.04	no TWA		0.0047				0.88	2.46	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000128-04-1	SODIUM DIMETHYLDITHIOCARBAMATE									-0.84	1.74	96hr, guppy, static, TerraTox	Rat, TerraTox	
0025155-30-0	SODIUM													
0007681-49-4	SODIUM FLUORIDE													
0016721-80-5	SODIUM HYDROSULFIDE													
0001310-73-2	SODIUM HYDROXIDE			no TWA				>0						
0007681-52-9	SODIUM HYPOCHLORITE													
0010022-70-5	SODIUM HYPOCHLORITE													
0000124-41-4	SODIUM METHYLATE													
0007632-00-0	SODIUM NITRITE					0.0011					1.48	96hr, FHM, Static, TerraTox		
0007558-79-4	SODIUM PHOSPHATE, DIBASIC							12.67	CRC					
0007601-54-9	SODIUM PHOSPHATE, TRIBASIC										0.76	96hr, mosqf, static, TerraTox		
0007758-29-4	SODIUM PHOSPHATE, TRIBASIC													
0010101-89-0	SODIUM PHOSPHATE, TRIBASIC													
0000100-42-5	STYRENEMONOMER	2B	0.2	85	31	97.464				-0.48	1.41	96hr, FHM, Static, TerraTox	Mouse,	skin
0007664-93-9	SULFURICACID	1		1			>0						H2SO4 in strong inorg acid mists	
0008014-95-7	SULFURICACID (FUMING)						>0							
0000127-18-4	TETRACHLOROETHYLENE	2B	0.01	170	none	38.905				-1.26	1.09	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000108-98-5	THIOPHENOL		0		51	32.137	6.52			0.38			Rat, TerraTox	
0000062-56-6	THIOUREA	2B				0.0206				-0.22			Rat, TerraTox	
0000108-88-3	TOLUENE		0.2	188	4	45.879				-1.74	0.43	96hr, FHM, Static, TerraTox	Rat, TerraTox	skin
0000091-08-7	TOLUENEDIISOCYANATEA	2B				411.34								
0000584-84-9	TOLUENEDIISOCYANATEB	2B		0.036	121	411.34				-1.52	0.02	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0026471-62-5	TOLUENEDIISOCYANATEC	2B								-1.05			Mouse,	
0000071-55-6	TRICHLOROETHANEA			1910	none	8.9125				-1.92	0.45	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000079-01-6	TRICHLOROETHYLENE	2A		269	none	19.851				-1.26	0.47	96hr, FHM, Static, TerraTox	Mouse,	
0000075-69-4	TRICHLOROMONOFLUOROMETHANE		0.3	no TWA	none	32.817				-1.77			Rat, TerraTox	
0000121-44-8	TRIETHYLAMINE			4.1	-6	3.3449		10.72		-0.66			Rat, TerraTox	skin
0000075-63-8	TRIFLUOROBROMOMETHANE			6090		8.0641								

CAS Number	Chemical Name	IARC	RFD	TLV(TWA in mg/m^3)	FP (C)	BCF	pKa	pKa (ca)	pK notes	LD50, pT	c LC50 , pT	Aquatic LC50 notes	LD50 notes	TLV Notes
0000075-50-3	TRIMETHYLAMINE			12	-6	0.2289		9.79						
0000095-63-6	TRIMETHYLBENZ				48	327.2					1.21	96hr, FHM, Static, TerraTox		
0000108-05-4	VINYLACETATE	2B	1	35	-6	0.5754				-1.27	0.57	96hr, FHM, Static, TerraTox	Mouse,	
0000095-47-6	XYLENEB		2	434	32	112.83				-1.67	0.81	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0000106-42-3	XYLENEC		2	434	27	120.14				-1.67	1.21	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0001330-20-7	XYLENEMIXEDISOMER		2	434	29	120.14				-1.61	0.87	96hr, FHM, Static, TerraTox	Rat, TerraTox	
0007440-66-6	ZINC		0.3											
0001314-13-2	ZINC AND COMPOUNDS			5						-1.99			Mouse,	TLV for Zinc dust=10
0001314-13-2	ZINC OXIDE FUME			5						-1.99			Mouse,	
0007733-02-0	ZINC SULFATE													
0014639-98-6	ZINCAMMONIUM CHLORIDE													
0001332-07-6	ZINCBORATE													
0007733-02-0	ZINCSULFATE													
		47	35	190	114	136	21	14		137	102	102	137	94

Appendix H: Category 3 Chemicals with CAS Numbers

CAS Number	Chemical Name
1717-00-6	1,1-DICHLORO - 1 FLUOROETHANE
507-55-1	1,3-DICHLORO-1,1,2,2,3-PENTAFLUOROPROPANE
872-50-4	1-METHYL-2-PYRROLIDONE
540-84-1	2,2,4-TRIMETHYLPENTANE
612-83-9	3,3'DICHLOROBENZIDINE DIHYDROCHLORIDE
55406-53-6	3-IODO-2-PROPYNYL BUTYLCARBAMATE
75-07-0	ACETALDEHYDE
108-24-7	ACETIC ANHYDRIDE
75-05-8	ACETONITRILE
98-86-2	ACETOPHENONE
79-10-7	ACRYLICACID
124-04-9	ADIPIC ACID
107-05-1	ALLYLCHLORIDE
7429-90-5	ALUMINUM
1344-28-1	ALUMINUMOXIDE
10043-01-3	ALUMINUMSULFATE
7664-41-7	AMMONIA
1341-49-7	AMMONIUMBIFLUORIDE
12125-02-9	AMMONIUMCHLORIDE
12125-01-8	AMMONIUMFLUORIDE
1336-21-6	AMMONIUMHYDROXIDE
7773-06-0	AMMONIUMSULFAMATE
62-53-3	ANILINE
7440-36-0	ANTIMONY
01-00-0	ANTIMONY COMPOUNDS
1309-64-4	ANTIMONYTRIOXIDE
7440-39-3	BARIUM
01-00-2	BARIUM COMPOUNDS
94-36-0	BENZOYLPEROXIDE
92-52-4	BIPHENYL
103-23-1	BISETHYLHEXYL
7726-95-6	BROMINE
353-59-3	BROMOCHLORODIFLUOROMETHANE (HALON 1211)
74-83-9	BROMOMETHANE
110-19-0	BUTYL ACETATE-I
540-88-5	BUTYL ACETATE-T
123-86-4	BUTYLACETATE
141-32-2	BUTYLACRYLATE
75-65-0	BUTYLALCOHOLC
85-68-7	BUTYLBENZYLPHTHALA
84-74-2	BUTYLPHTHALATE
123-72-8	BUTYRALDEHYDE
107-92-6	BUTYRIC ACID
75-20-7	CALCIUM CARBIDE
7778-54-3	CALCIUM HYPOCHLORITE
105-60-2	CAPROLACTAM DUST AND VAPOR
106-47-8	CHLOROANILINE
108-90-7	CHLOROBENZENE
75-45-6	CHLORODIFLUOROMETHANE
74-87-3	CHLOROMETHANE
95-57-8	CHLOROPHENOL

Appendix H: Category 3 Chemicals with CAS Numbers

CAS Number	Chemical Name
7790-94-5	CHLOROSULFONIC ACID
1897-45-6	CHLOROTHALONIL
10101-53-8	CHROMIC SULFATE
28407-37-6	CI DIRECT BLUE 218
2832-40-8	CIDISPERSEYELLOW
81-88-9	CIFOODRED15
97-56-3	CISOLVENTYELLOWA
7440-48-4	COBALT
01-01-3	COBALT COMPOUNDS
7440-50-8	COPPER
01-01-5	COPPER COMPOUNDS
8001-58-9	CREOSOTE
108-39-4	CRESOLA
95-48-7	CRESOLB
1319-77-3	CRESOLMIXEDISOMER
98-82-8	CUMENE
3251-23-8	CUPRIC NITRATE
7758-98-7	CUPRIC SULFATE
110-82-7	CYCLOHEXANE
108-94-1	CYCLOHEXANONE
1163-19-5	DECABROMODIPHENYLOX
95-50-1	DICHLOROBENZENEA
106-46-7	DICHLOROBENZENEC
25321-22-6	DICHLOROBENZENEMIX
75-27-4	DICHLOROBROMOMETHANE
75-71-8	DICHLORODIFLUOROMETHANE
156-60-5	DICHLOROETHYLENE
75-09-2	DICHLOROMETHANE
76-14-2	DICHLOROTETRAFLUOROETHANE
111-42-2	DIETHANOLAMINE
109-89-7	DIETHYLAMINE
117-81-7	DIETHYLHEXYLPHT
84-66-2	DIETHYLPHTHALATE
822-06-0	DIISOCYANATES
124-40-3	DIMETHYLAMINE
121-69-7	DIMETHYLANILINE
131-11-3	DIMETHYLPHTALATE
117-84-0	DIOCTYLPHTHALATE
27176-87-0	DODECYLBENZENESULFONIC ACID
5952-26-1	ETHANOL, 2,2-OXYDI, DICARBAMATE
110-80-5	ETHOXYETHANOL
140-88-5	ETHYLACRYLATE
100-41-4	ETHYLBENZENE
74-85-1	ETHYLENE
142-59-6	ETHYLENE BIS DITHIOCARBAMATE
107-15-3	ETHYLENEDIAMINE
60-00-4	ETHYLENEDIAMINE-TETRAACETIC ACID (EDTA)
96-45-7	ETHYLENETHIOUREA
60-29-7	ETHYLETHER
133-07-3	FOLPET
64-18-6	FORMIC ACID

Appendix H: Category 3 Chemicals with CAS Numbers

CAS Number	Chemical Name
1336-36-3	POLYCHLORINATEDBIPH
9016-87-9	POLYMERIC DIPHENYLMETHANE DIISOCYANATE
1310-58-3	POTASSIUMHYDROXIDE
7722-64-7	POTASSIUMPERMANGANATE
79-09-4	PROPIONICACID
107-12-0	PROPIONITRILE
110-86-1	PYRIDINE
108-46-3	RESORCINOL
7440-22-4	SILVER
01-03-7	SILVER AND COMPOUNDS
7761-88-8	SILVERNITRATE
7440-23-5	SODIUM
10588-01-9	SODIUM BICHROMATE
7631-90-5	SODIUM BISULFITE
128-04-1	SODIUM DIMETHYLDITHIOCARBAMATE
25155-30-0	SODIUM DODECYLBENZENESULFONATE
7681-49-4	SODIUM FLUORIDE
16721-80-5	SODIUM HYDROSULFIDE
1310-73-2	SODIUM HYDROXIDE
7681-52-9	SODIUM HYPOCHLORITE
10022-70-5	SODIUM HYPOCHLORITE
124-41-4	SODIUM METHYLATE
7632-00-0	SODIUM NITRITE
100-42-5	STYRENEMONOMER
108-98-5	THIOPHENOL
62-56-6	THIOUREA
108-88-3	TOLUENE
71-55-6	TRICHLOROETHANEA
75-69-4	TRICHLOROMONOFLUOROMETHANE
121-44-8	TRIETHYLAMINE
75-63-8	TRIFLUOROBROMOMETHANE
75-50-3	TRIMETHYLAMINE
95-63-6	TRIMETHYLBENZ
108-05-4	VINYLACETATE
95-47-6	XYLENEB
106-42-3	XYLENEC
1330-20-7	XYLENEMIXEDISOMER
7440-66-6	ZINC
01-03-9	ZINC AND COMPOUNDS
1314-13-2	ZINC OXIDE FUME
14639-98-6	ZINCAMMONIUM CHLORIDE

Note: This list of Category 3 chemicals does not contain the names of chemicals that have never been reported under TURA.

Appendix H: Category 3 Chemicals with CAS Numbers

CAS Number	Chemical Name
76-13-1	FREON113
110-17-8	FUMARIC ACID
109-99-9	FURAN, TETRAHYDRO-
98-01-1	FURFURAL
01-02-2	GLYCOL ETHERS
422-56-0	HCFC-225CA
110-54-3	HEXANE (N-HEXANE)
7647-01-0	HYDROCHLORICACID
74-90-8	HYDROGEN CYANIDE
7664-39-3	HYDROGENFLUORIDE
78-59-1	ISOPHORONE
4098-71-9	ISOPHORONE DIISOCYANATE
67-63-0	ISOPROPYLALCOHOL
80-05-7	ISOPROPYLIDENED
554-13-2	LITHIUM CARBONATE
14307-35-8	LITHIUM CHROMATE
110-16-7	MALEICACID
108-31-6	MALEICANHYDRIDE
7439-96-5	MANGANESE
01-02-7	MANGANESE COMPOUNDS
126-98-7	METHACRYLONITRILE
109-86-4	METHOXYETHANOL
96-33-3	METHYLACRYLATE
79-22-1	METHYLCHLOROFORMATE
5124-30-1	METHYLENE BIS(4-CYCLOHEXYLISOCYANATE)
101-14-4	METHYLENEBISCHLORO
108-10-1	METHYLISOBUTYLKETO
80-62-6	METHYLMETHACRYLATE
1634-04-4	METHYLTBUTYLET
75-79-6	METHYLTIRCHLOROSILANE
90-94-8	MICHLERSKETONE
75-04-7	MONOETHYLAMINE
91-20-3	NAPHTHALENE
7440-02-0	NICKEL
01-09-0	NITRATE COMPOUNDS
7697-37-2	NITRICACID
10102-43-9	NITRICOXIDE
10102-44-0	NITROGEN DIOXIDE
88-75-5	NITROPHENOLA
99-55-8	NITROTOLUIDINE
924-42-5	N-METHYLOLACRYLAMIDE
20325-40-0	O-DIANISIDINE DIHYDROCHLORIDE
30525-89-4	PARAFORMALDEHYDE
594-42-3	PERCHLOROMETHYLMERCAPTAN
108-95-2	PHENOL
106-50-3	PHENYLENEDIAMINE
7664-38-2	PHOSPHORICACID
10025-87-3	PHOSPHORUS OXYCHLORIDE
01-03-3	PHTHALATE ESTERS
85-44-9	PHTHALICANHYDRIDE
109-06-8	PICOLINE