

# **Technical Appendix B**

## **Physicochemical Properties for TRI Chemicals and Chemical Categories**

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# 1 Introduction

To predict the environmental fate and transport of the reportable TRI chemicals and chemical categories, the RSEI model relies on a chemical table<sup>1</sup>, which contains physicochemical properties and estimates of chemical removal efficiencies at incinerators and at publicly owned treatment works (POTWs). The physicochemical properties in the database include rates of chemical decay in air and water; organic carbon-water, octanol-water, and soil-water partition coefficients ( $K_{oc}$ ,  $K_{ow}$ , and  $K_d$ , respectively); water solubilities; bioconcentration factors; Henry's Law constants ( $K_H$ ); and molecular weights. To evaluate the effects of treatment and disposal, the model also requires incinerator destruction and removal efficiencies (DREs) as well as removal efficiencies for POTWs, including estimates of the percent of chemical removed due to volatilization, biodegradation, and sorption to sludge within a POTW. However, not all of the properties included in the model are currently used for modeling. Maximum Contaminant Levels (MCLs) for chemicals in drinking water also are included in the database as a resource.

The sources of values in this database were originally documented in November, 1992. Since that time, the data have been significantly updated, with several new sources being used. The most significant new data sources were the experimental and estimation databases from Syracuse Research Corporation (SRC, Inc.) (Environmental Fate Data Base, PHYSPROP, CHEMFATE, and the Estimation Programs Interface (EPI) suite of estimation programs) and EPA's Risk Reduction Engineering Laboratory (RREL)'s Treatability Database Version 5.0 (U.S. EPA, 1994). Table B-1 lists each parameter, its field name in the chemical database and the main data source(s) or estimation methods used to obtain chemical-specific values.

**Table B-1. Physicochemical Properties and Data Sources**

Parameter	Field Name	Main Data Source(s)
Rate of Chemical Decay in Air	AirDecay	AOPWIN (SRC) PHYSPROP (SRC)
Organic Carbon-Water Partition Coefficient ( $K_{oc}$ )	Koc	CHEMFATE (SRC) Lyman et al. (1990) PCKOC (SRC)
Rate of Chemical Decay in Water	H2ODecay	HYDROWIN (SRC)
Log of Octanol-Water Partition Coefficient ( $\log K_{ow}$ )	LogKow	PHYSPROP (SRC)
Soil-Water Partition Coefficient ( $K_d$ )	Kd	Gerritse et al. (1982)
Water Solubility	WaterSolubility	PHYSPROP (SRC)
Total Removal Efficiency for POTWs	POTWPartition(Removal)	RREL (U.S. EPA, 1994) STPWIN (SRC)
Within-POTW Sorption to Sludge	POTWPartition(Sludge)	EFDB (SRC) STPWIN (SRC)

<sup>1</sup> The current version of the chemical table is posted on the [Chemical Data](#) page of the RSEI Data Dictionary

<b>Parameter</b>	<b>Field Name</b>	<b>Main Data Source(s)</b>
Within-POTW Volatilization to Air	POTWPartition(Volatil)	EFDB (SRC) STPWIN (SRC)
Within-POTW Biodegradation	POTWPartition(Biod)	EFDB (SRC) STPWIN (SRC)
Incinerator Destruction and Removal Efficiency	IncineratorDRE	Assumed
Bioconcentration Factor	BCF	CHEMFATE (SRC) Lyman et al. (1990)
Henry's Law Constant	Henrys	PHYSPROP (SRC)
Maximum Contaminant Level	MCL	U.S. EPA, Safe Drinking Water Act (SDWA). <sup>2</sup>
Molecular Weight	Molecular Weight	PHYSPROP (SRC)

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<sup>2</sup> EPA maintain a [current list of Maximum Contaminant Levels](#).

## 2 Physicochemical Properties of Chemicals Included in the RSEI Model

This technical appendix describes the methods used to update the chemical database and provides the sources for all of the data. Values for the physicochemical parameters for the TRI chemicals and chemical categories are provided in a separate spreadsheet that can be found on the [RSEI website](#). Explanations for the reference codes and full citations for the data sources can be found on the “Notes” page of the spreadsheet. The following sections discuss the data sources and special issues for each physicochemical parameter presented. The methods for treating chemical categories are also presented, followed by a summary of the resolution of certain TRI reporting issues which affect the exposure modeling.

### 2.1 Rate of Chemical Decay in Air ( $\text{hr}^{-1}$ )

This parameter describes how fast a chemical degrades in air, primarily due to photooxidation by hydroxyl radicals. The daughter products of photodegradation are not modeled in RSEI further; that is, it is assumed that all chemicals are photodegraded into non-toxic compounds. The main source for decay rates is SRC, Inc.’s Atmospheric Oxidation Program for Windows (AOPWIN), which estimates the second-order rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. For the RSEI model, a concentration of hydroxyl radicals of  $1.5 \times 10^6$  molecules / cubic centimeter ( $\text{cm}^3$ ) is used to convert the second-order rate constant provided in AOPWIN to a first-order rate constant. Furthermore, the rate is divided by a factor of two to reflect an assumed average day length of 12 hours:

$$\text{AirDecay}(\text{hr}^{-1}) = \text{AOPWINestimate} \left( \frac{\text{cm}^3}{\text{molecule}} * \text{sec} \right) * 1.5 * 10^6 \left( \frac{\text{molecules}}{\text{cm}^3} \right) * 3600 \frac{\text{sec}}{\text{hr}} * 1/2$$

For details on the methodology used in AOPWIN, see Meylan and Howard (1993).

### 2.2 Organic Carbon-Water Partition Coefficient ( $K_{oc}$ , in units of L/kg)

$K_{oc}$  is “the ratio of the amount of chemical adsorbed per unit weight of organic carbon (oc) in the soil or sediment to the concentration of the chemical in solution at equilibrium” (Lyman et al., 1990; p. 4-1).  $K_{oc}$  provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic systems. The  $K_{oc}$  values have units of liter (L) per kilogram (kg) (L/kg).

Several sources were used for  $K_{oc}$  values. CHEMFATE, part of SRC Inc.’s Environmental Fate Data Base (EFDB), is an online database that presents experimental and estimated values for various parameters. CHEMFATE was the preferred data source. If an appropriate value from CHEMFATE was not available, regression equations from Lyman et al. (1990) were used to estimate  $K_{oc}$ . If a solubility value was available, the following equation (Eq. 4-5 in Lyman et al., 1990) was used to estimate  $K_{oc}$ :

$$\log(K_{oc}) = -0.55 \log(S) + 3.64$$

Note that in this equation, solubility ( $S$ ) must be entered in units of milligrams per liter (mg/L). In total, 261 chemicals were used to obtain this regression equation, which has an  $r^2$  of 0.71. Solubility values ranged between approximately  $5 \times 10^{-4}$  mg/L to 1,000,000 mg/L.

If a solubility value was not available, or it did not fall within the range of solubility values used to develop the regression equation, then another equation, based on  $\log(K_{ow})$ , was used. If a  $\log(K_{ow})$  value was available, Eq. 4-8 in Lyman et al. (1990) was used to estimate  $K_{oc}$ :

$$\log(K_{oc}) = 0.544 \log(K_{ow}) + 1.377$$

Fifty chemicals were used to obtain this regression equation, which has an  $r^2$  of 0.74. Values of  $\log(K_{ow})$  ranged between approximately -3 and 6.6.

If a  $\log(K_{ow})$  value was not available, or it did not fall within the range of  $\log(K_{ow})$  values used to develop the regression equation, then CHEMFATE or SRC Inc.'s estimation program PCKOC was used. PCKOC uses an estimation method based on a first-order molecular conductivity index and a series of statistically derived fragment contribution factors for polar compounds to predict  $K_{oc}$  values. For details on the methodology used in this program, see Meylan et al. (1992).

### 2.3 Rate of Chemical Decay in Water ( $\text{hr}^{-1}$ )

The primary source of water decay rates was SRC Inc.'s estimation program HYDROWIN, which was developed for EPA. The program estimates abiotic hydrolysis rate constants and half-lives for esters, carbamates, epoxides, halomethanes, and selected alkyl halides. For the RSEI model, the half-life estimated for a pH of 7 was converted to a rate using the following equation:

$$k = -\ln(0.5)/t_{1/2}$$

For some chemicals, HYDROWIN stated that "Even at low pH, the hydrolysis rate is very fast:  $t_{1/2} < 10$  minutes." For these chemicals, a first-order decay rate of 4.2/hr was used.

For details on the methodology used in HYDROWIN, see Mill et al. (1987). A few decay rates were obtained from the Office of Pesticide Program's OneLiner database, as included in PIRANHA (U.S. EPA, 1991).

For a few chemicals which do not undergo hydrolysis, a water decay rate was estimated based on information in CHEMFATE on photodegradation. Twelve hours of sunlight per day were assumed, and thus the rates provided in CHEMFATE for photodegradation in water were halved to estimate an average rate over a 24 hour period.

## 2.4 Log of Octanol-Water Partition Coefficient ( $\log(K_{ow})$ , unitless)

$\log(K_{ow})$  describes a chemical's lipophilic or hydrophobic properties. It is the ratio of a chemical's concentration in the octanol phase to its concentration in the aqueous phase of a two-phase system at equilibrium. It has been strongly correlated with environmental fate and transport parameters such as  $K_{oc}$  and bioconcentration factor (BCF) and therefore is often used to estimate values for those two parameters.

The primary source for values of  $\log(K_{ow})$  was SRC Inc.'s PHYSPROP database, which contains experimental and estimated values. A few values were estimated using SRC Inc.'s program KOWWIN. KOWWIN uses a fragment constant methodology, in which a compound's structure is divided into functional fragments, and the coefficients for all groups are summed to obtain the compound's coefficient. Coefficients for individual fragments are derived from multiple regressions of more than 2,400 reliably measured values. For details on the methodology used, see Meylan and Howard (1995). Note that the parameter  $\log(K_{ow})$  has no units because it is the ratio of two concentrations.

## 2.5 Soil-Water Partition Coefficient ( $K_d$ , in units of L/kg)

In the RSEI chemical database, explicit values for this soil-water partition coefficient parameter ( $K_d$ ) are provided only for inorganic compounds. Organic compounds are modeled by combining chemical-specific  $K_{oc}$  values, as listed in the chemical database, with an estimate of the fraction of organic carbon,  $f_{oc}$ , to obtain a soil-water partition coefficient. For all the metals except aluminum,  $K_d$  values were estimated from column studies by Gerritse et al. (1982) using sand with an  $f_{oc}$  value of 0.0355 g/g, a cation exchange capacity of 0.22 meq/g, zero clay content, and a solution pH of 5.<sup>3</sup> The median of the range of  $K_d$  values for each metal was taken, assuming a log-normal distribution. For classes of inorganic compounds, the same values were used as for the elemental inorganic compound. For aluminum, the  $K_d$  value is based on Langmuir isotherm data presented in Bodek et al. (1988). The  $K_d$  values presented have units of L/kg.

## 2.6 Water Solubility (mg/L)

Water solubility values were primarily obtained from SRC Inc.'s PHYSPROP database. The water solubility values have units of mg/L.

## 2.7 POTW Removal Efficiencies and Within-POTW Partitioning Percentages

The publicly owned treatment works (POTW) removal efficiency and the three within-POTW partitioning percentages describe the fate of chemicals during treatment at POTWs. The 'POTW

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<sup>3</sup>The assumption that the waste in landfills is similar to the above conditions results in a conservative estimate of the leachate concentration of metals, because low clay content and relatively low pH tend to increase the mobility of metals.

Partition Removal' is the total POTW removal efficiency, or the total percentage of the chemical removed by the POTW (influent concentration minus effluent concentration divided by influent concentration). The three within-POTW partitioning percentages describe the fate of the total amount of chemical removed by the POTW; the chemical may be removed by sorbing to sludge (POTW Partition Sludge), by volatilizing into the air (POTW Partition Volatil) or by being biodegraded by microorganisms (POTW Partition Biodeg). Note that the within-POTW partitioning percentages sum to 100 percent.

POTW removal efficiencies were obtained primarily from the Treatability Database maintained by EPA's Office of Research and Development (ORD), National Risk Management Research Laboratory (NRMRL), Risk Reduction Engineering Laboratory (RREL) (U.S. EPA, 1994). For any given chemical, the RREL Treatability Database provided a list of POTW removal efficiencies published in the scientific literature. Each value is characterized by the technology used, the type of influent, and the scale of the experiment. For all values associated with activated sediment and full-scale experiments, a geometric mean was derived and used as the POTW removal efficiency. Within-POTW partitioning values were obtained for most organic chemicals from EPA's Exposure Assessment Branch (EAB), now presently grouped in the Existing Chemicals Risk Assessment Division (ECRAD) within the Office of Pollution Prevention and Toxics (OPPT). Inorganic chemicals, except for ammonia, were assumed to partition 100% to sludge. For chemicals without data from these sources, SRC, Inc.'s Sewage Treatment Plant Fugacity Model (STPWIN) was used to estimate total POTW removal efficiencies and within-POTW partitioning values. Details on the methodology used in STPWIN can be found in Clark et al. (1995). One value was obtained from Howard et al. (1991).

## 2.8 Bioconcentration Factor (L/kg)

Bioconcentration factors (BCFs) are used to describe the equilibrium concentrations of chemicals in aquatic organisms living in contaminated water. The BCF is defined as the ratio of the chemical concentration in the organism (mg/kg) to that in the surrounding water (mg/L). Many experimental and estimated BCF values were obtained from SRC Inc.'s CHEMFATE database. If an appropriate BCF value from CHEMFATE was not available, regression equations from Lyman et al. (1990) were used to estimate BCF values, as described below.

If a  $\log(K_{ow})$  value was available for a chemical and was within the range used to develop the regression equation (0.90 to 6.9), Eq. 5-2 in Lyman et al. (1990) was used to estimate a BCF:

$$\log BCF = 0.76 \log(K_{ow}) - 0.23$$

Two hundred and fifty-five chemicals used this regression equation, which has an  $r^2$  of 0.823.

If a  $\log(K_{ow})$  value was not available, or it did not fall within the range of values used to develop the regression equation, then another equation, based on water solubility, was used. If a water solubility value was available and within the range of 0.001 to 50,000 mg/L, Eq. 5-3 in Lyman et al. (1990) was used to estimate a BCF:



$$\log BCF = 2.791 - 0.564 \log (S)$$

Thirty-nine chemicals were used to obtain this regression equation, which has an  $r^2$  of 0.49.

If the above two equations could not be applied to estimate BCF values, then CHEMFATE or SRC Inc.'s BCFWIN program was used.

## 2.9 Incinerator Destruction and Removal Efficiencies

This parameter describes the percentage of a chemical removed or destroyed during combustion in an incinerator. The RSEI model assumes that the typical municipal waste combustor destruction and removal efficiency (DRE) for organics is 99 percent. This assumption ignores the fact that chemicals of concern, such as dioxins, may be formed during the incineration process. The exceptions to the 99 percent DRE assumption are for polychlorinated biphenyls (PCBs) and dioxin and dioxin-like compounds, both of which are assumed to have a DRE of 99.9999 percent, as required by Toxic Substances Control Act (TSCA) regulations.

For incinerator destruction and removal efficiencies for inorganic chemicals, values were taken from multiple hearth sludge incinerator studies, as reported in U.S. EPA, 1992.

## 2.10 Henry's Law Constant ( $K_H$ , in units of atm·m<sup>3</sup>/mol)

The Henry's Law constant ( $K_H$ ) is defined as the ratio of a chemical concentration in air (often expressed as a partial pressure with units of atmospheres (atm)) to the chemical concentration in water (often expressed as moles (mol) per cubic meter (m<sup>3</sup>) under equilibrium conditions. This constant is used to model volatilization from off-site landfills. The primary source for this parameter is SRC Inc.'s PHYSPROP database. The units of the Henry's Law constants are atm·m<sup>3</sup>/mol.

## 2.11 Maximum Contaminant Level (mg/L)

Maximum Contaminant Levels (MCLs)<sup>4</sup> are enforceable standards for chemicals in drinking water and are to be set as close to the Maximum Contaminant Level Goals (MCLGs), which are based on health effects, as is feasible. MCLs are based upon the availability of analytical methods, treatment technologies, and costs for achieving various levels of removal. MCLs have not been set for most TRI chemicals. For those chemicals that do have MCLs, the RSEI model limits the concentrations in drinking water so that they cannot exceed the appropriate MCLs.

## 2.12 Molecular Weight (g/mol)

The molecular weight is not specifically used in the RSEI model, but values are provided as part of the RSEI chemical database. The primary source for molecular weights is SRC Inc.'s PHYSPROP database.

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<sup>4</sup> EPA maintain a [current list of Maximum Contaminant Levels](#).

### 3 Chemical Categories

EPA's annual Toxic Chemical Release Inventory Reporting Forms and Instructions<sup>5</sup> describes the reporting requirements for individually-listed toxic chemicals and for listed chemical categories. For most listed chemical categories, subject reporting facilities are not required to disclose the specific category member's identity in their Toxics Release Inventory (TRI) reporting forms. Because the identities and specific proportions of individual chemical waste management activity quantities within each reported chemical category are not known, professional judgment is used to assign surrogate values for various physicochemical properties of each chemical category. For the majority of cases, the most toxic chemical of each chemical category, based on its calculated toxicity weight, is selected, and the toxicity and physicochemical data for that chemical are assigned to the entire chemical category.

The rest of this section describes the decisions made for certain TRI chemical categories. Note that a TRI chemical category does not have a Chemical Abstracts Service Registry Number (CASRN) in the chemical database; instead, it has a three digit category code number preceded by an 'N.'

#### 3.1 Metal Compounds

Generally, metal compounds (e.g., nickel compounds such as nickel chloride) are reportable to the TRI Program in addition to their parent (elemental form) metal (e.g., nickel). The RSEI model combines TRI-listed metal compound categories (e.g., nickel compounds) together with the TRI-listed parent metal (e.g., nickel) into one consolidated RSEI chemical category (e.g., nickel and nickel compounds).<sup>6</sup> The physicochemical properties for the parent metal are used as a surrogate to represent the combined RSEI chemical category, unless otherwise noted. Table B-2 shows the metal compound categories included in TRI. Most categories include any unique chemical substance that contains the metal as part of that chemical's infrastructure. Any additional restrictions are noted in the table.

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<sup>5</sup> [https://ordspub.epa.gov/ords/guideme\\_ext/f?p=guideme:rfi-home](https://ordspub.epa.gov/ords/guideme_ext/f?p=guideme:rfi-home)

<sup>6</sup> Both nickel and nickel compounds are reported to TRI to reflect the quantities of the nickel parent metal that is ultimately released to the environment or otherwise managed as waste. This applies to most metal compounds categories.

**Table B-2. Metal Compound Categories**

Category Code	Name	Exclusions
N010	Antimony compounds	None.
N020	Arsenic compounds	None.
N040	Barium compounds	Does not include barium sulfate (CASRN 7727-43-7).
N050	Beryllium compounds	None.
N078	Cadmium compounds	None.
N090	Chromium compounds	Does not include chromite ore mined in the Transvaal Region of South Africa and the unreacted ore component of the chromite ore processing residue (COPR). COPR is the solid waste remaining after aqueous extraction of oxidized chromite ore that has been combined with soda ash and kiln roasted at approximately 2,000 °F.
N096	Cobalt compounds	None.
N100	Copper compounds	Does not include copper phthalocyanine compounds that are substituted with only hydrogen, and/or chlorine, and/or bromine.
N420	Lead compounds	None.
N450	Manganese compounds	None.
N458	Mercury compounds	None.
N495	Nickel compounds	None.
N725	Selenium compounds	None.
N740	Silver compounds	None.
N760	Thallium compounds	None.
N770	Vanadium compounds	None.
N982	Zinc compounds	None.

### 3.2 Chlorophenols

Of the 19 chlorophenols which have the formula  $C_6OHCl_xH_{(5-x)}$ , where  $x = 1$  to  $5$ , toxicity data were available for six. For the chlorophenols chemical category (N084), pentachlorophenol (CASRN 87-86-5) has the highest toxicity value, so that chemical is used as a surrogate for the category for both toxicity and physicochemical data.

### 3.3 Cyanide Compounds

The cyanide compounds chemical category (N106) includes only chemicals that can be represented by the formula  $X^{y+}(CN^-)_y$ , where  $X^{y+}$  = any group or ion (except for  $H^+$ ) where a formal dissociation can be made, for example, KCN or  $Ca(CN)_2$ . Because cyanide compounds in a gaseous state exhibit markedly different properties than compounds in solution, two surrogate compounds are used for toxicity and physicochemical data for the chemical category. For the inhalation toxicity scoring, the air decay rate and the Henry's Law constant were used based on the properties of hydrogen cyanide (HCN, CASRN 74-90-8). For the oral exposure pathway, toxicity data were collected for metal cyanide compounds, the most toxic group of nongaseous cyanide compounds. Copper cyanide ( $Cu(CN)_2$ , CASRN 4367-08-2) was found to be the most toxic metal cyanide compound. Thus, for the oral toxicity score and for all physicochemical properties other than the air decay rate and the Henry's Law constant, the properties of ( $Cu(CN)_2$ ) are used for this chemical category.

### 3.4 Diisocyanates

This chemical category (N120) only includes the 20 chemicals listed in Table B-3. At this time, physicochemical data have not been obtained or estimated for this chemical category.

**Table B-3. Members of Diisocyanates Chemical Category**

CASRN	Name
822-06-0	Hexamethylene-1,6-diisocyanate
101-68-8	4,4'-Methylenedi(phenyl isocyanate)
38661-72-2	1,3-Bis(methylisocyanate)cyclohexane
10347-54-3	1,4-Bis(methylisocyanate)cyclohexane (1,4-Bis(isocyanatomethyl)cyclohexane)
2556-36-7	1,4-Cyclohexane diisocyanate
134190-37-7	Diethyldiisocyanatobenzene
4128-73-8	4,4'-Diisocyanatodiphenyl ether
75790-87-3	2,4'-Diisocyanatodiphenyl sulfide
91-93-0	3,3'-Dimethoxybenzidine-4,4'-diisocyanate
91-97-4	3,3'-Dimethyl-4,4'-diphenylene diisocyanate
139-25-3	3,3'-Dimethyldiphenylmethane-4,4'-diisocyanate
4098-71-9	Isophorone diisocyanate
75790-84-0	4-Methyldiphenylmethane-3,4-diisocyanate
5124-30-1	1,1-Methylenebis(4-isocyanatocyclohexane)
3173-72-6	1,5-Naphthalene diisocyanate
123-61-5	1,3-Phenylene diisocyanate
104-49-4	1,4-Phenylene diisocyanate
9016-87-9	Polymeric diphenylmethane diisocyanate
16938-22-0	2,2,4-Trimethylhexamethylene diisocyanate
15646-96-5	2,4,4-Trimethylhexamethylene diisocyanate

### 3.5 Dioxin and Dioxin-like Compounds

This chemical category (N150) includes manufacturing and the processing or otherwise use of dioxin and dioxin-like compounds if the dioxin and dioxin-like compounds are present as contaminants in a chemical and if they were created during the manufacture of that chemical. Of the 17 congeners reportable under this category and shown below in Table B-4, physicochemical data were available only for 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD), which was used as a surrogate for the entire category. However, POTW removal rates were not available, so dioxin and dioxin-like compound transfers to POTWs are not currently modeled in RSEI. Fugitive and

stack air releases, direct releases to water and transfers off site to incineration are modeled. The incineration destruction and removal efficiency is assumed to be 99.9999, as required by TSCA regulations.

**Table B-4. Members of the Dioxin and Dioxin-like Compounds Chemical Category**

CASRN	Dioxin and Dioxin-like Compounds Name
1746-01-6	2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin
40321-76-4	1,2,3,7,8-Pentachlorodibenzo- <i>p</i> -dioxin
39227-28-6	1,2,3,4,7,8-Hexachlorodibenzo- <i>p</i> -dioxin
57653-85-7	1,2,3,6,7,8-Hexachlorodibenzo- <i>p</i> -dioxin
19408-74-3	1,2,3,7,8,9-Hexachlorodibenzo- <i>p</i> -dioxin
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo- <i>p</i> -dioxin
3268-87-9	1,2,3,4,6,7,8,9-Octachlorodibenzo- <i>p</i> -dioxin
51207-31-9	2,3,7,8-Tetrachlorodibenzofuran
57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran
57117-31-4	2,3,4,7,8-Pentachlorodibenzofuran
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran
72918-21-9	1,2,3,7,8,9-Hexachlorodibenzofuran
60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran
67562-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran
55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran
39001-02-0	1,2,3,4,6,7,8,9-Octachlorodibenzofuran

### 3.6 Ethylenebisdithiocarbamic Acid, Salts and Esters

This chemical category (N171) includes any unique chemical substance that contains an ethylenebisdithiocarbamic acid or an ethylenebisdithiocarbamic acid salt or ester as a part of that chemical's infrastructure. According to EPA's 1998 Status of Pesticides in Registration, Reregistration, and Special Review (The Rainbow Report), chemicals typically associated with this chemical category include maneb, mancozeb, metiram, nabam, zineb, and amobam. Maneb, metiram, nabam, and zineb are individually listed for TRI reporting purposes. Toxicity data were

available for four compounds (mancozeb, maneb, metiram, and zineb); of these, metiram had the highest toxicity weight. Therefore, metiram is used as the surrogate for physicochemical data.

### 3.7 Certain Glycol Ethers

This chemical category (N230) includes chemicals that can be represented by the formula  $R-(OCH_2CH_2)_n-OR'$  where  $n = 1, 2, \text{ or } 3$ ;  $R = \text{alkyl C7 or less, or, } R = \text{phenyl or alkyl substituted phenyl}$ ;  $R' = H, \text{ or alkyl C7 or less}$ ; or,  $OR'$  consists of carboxylic acid ester, sulfate, phosphate, nitrate, or sulfonate. Eight common glycol ethers were identified: ethylene glycol monobutyl ether (CASRN 111-76-2), dipropylene glycol monomethyl ether (CASRN 34590-94-8), ethylene glycol diethyl ether (CASRN 629-14-1), ethylene glycol monoethyl ether acetate (CASRN 11-15-9), ethylene glycol monoethyl ether (CASRN 110-80-5), monomethyl ether acetate (CASRN 110-49-6), ethylene glycol monomethyl ether (CASRN 109-86-4), and propylene glycol monomethyl ether (CASRN 107-98-2). Of these, four chemicals had available toxicity data. Ethylene glycol monomethyl ether (2-methoxyethanol) had the highest toxicity weight of the four and therefore is used as a surrogate for the category for both the toxicity data and the physicochemical data.

### 3.8 Nicotine and Salts

This chemical category (N503) includes any unique chemical substance that contains nicotine or a nicotine salt as part of that chemical's infrastructure. Nicotine was selected as a surrogate for both toxicity and physicochemical values.

### 3.9 Nitrate Compounds

This chemical category (N511) only includes compounds that are water dissociable and are reportable only when in an aqueous solution. Toxicity data for nitrate were available from IRIS; however, at this time, physicochemical data have not been fully determined for this category.

### 3.10 Polybrominated Biphenyls (PBBs)

This chemical category (N575) includes chemicals that can be represented by the formula  $C_{12}Br_xH_{(10-x)}$ , where  $x = 1 \text{ to } 10$ . Toxicity data for a PBB mixture were available from HEAST. However, no physicochemical data were available for PBB mixtures. According to the International Agency for Research on Cancer (IARC), hexabromobiphenyl (CASRN 36355-01-8) was the most commercially significant PBB in the United States (WHO, 1986). Therefore, this chemical is used as a surrogate for the entire category for physicochemical data.

### 3.11 Polychlorinated Alkanes

This chemical category (N583) includes chemicals that can be represented by the formula  $C_xH_{2x-y}Cl_y$ , where  $x = 10 \text{ to } 13$  and  $y = 3 \text{ to } 12$ , and the average chlorine content ranges from 40 to 70 percent, with the limiting molecular formulas  $C_{10}H_{19}Cl_3$  and  $C_{13}H_{16}Cl_{12}$ . At this time, toxicity and physicochemical data have not been determined for this category.

### 3.12 Polycyclic Aromatic Compounds (PACs)

There are 25 members of this chemical category (N590) that are reportable to TRI and shown below in Table B-5. Of these 25 chemicals, only benzo[a]pyrene (CASRN 50-32-8) and benzo[j,k]fluorine (fluoranthene) (CASRN 206-44-0) had available toxicity data. The toxicity weight for benzo[j,k]fluorine (fluoranthene) (tox weight = 13) is approximately 1,000-fold lower than that for benzo[a]pyrene (tox weight = 15,000). However, absent information on the composition of the total PAC emissions, the model uses a conservative approach and uses the benzo[a]pyrene value to represent the chemical category. This chemical was selected as a surrogate for the entire chemical category for physicochemical data. For toxicity data, the toxicity of this group is assumed to be 18% of the toxicity for benzo[a]pyrene. This approach follows that used in EPA's National-Scale Air Toxics Assessment (NATA) evaluation for polycyclic organic matter (POM).

**Table B-5. Members of Polycyclic Aromatic Compounds Chemical Category**

CASRN	Name
56-55-3	Benz[a]anthracene
205-99-2	Benzo[b]fluoranthene
205-82-3	Benzo[j]fluoranthene
207-08-9	Benzo[k]fluoranthene
206-44-0	Benzo[j,k]fluorine (Fluoranthene)
189-55-9	Benzo[r,s,t]pentaphene (Dibenzo[a,i]pyrene)
218-01-9	Benzo[a]phenanthrene (Chrysene)
50-32-8	Benzo[a]pyrene
226-36-8	Dibenz[a,h]acridine
224-42-0	Dibenz[a,j]acridine
53-70-3	Dibenzo[a,h]anthracene (Dibenz[a,h]anthracene)
194-59-2	7H-Dibenzo[c,g]carbazole
5385-75-1	Dibenzo[a,e]fluoranthene
192-65-4	Dibenzo[a,e]pyrene
189-64-0	Dibenzo[a,h]pyrene
191-30-0	Dibenzo[a,l]pyrene
57-97-6	7,12-Dimethylbenz[a]anthracene
42397-64-8	1,6-Dinitropyrene



CASRN	Name
42397-65-9	1,8-Dinitropyrene
193-39-5	Indeno[1,2,3-cd]pyrene
56-49-5	3-Methylcholanthrene
3697-24-3	5-Methylchrysene
7496-02-8	6-Nitrochrysene
5522-43-0	1-Nitropyrene
57835-92-4	4-Nitropyrene

### 3.13 Strychnine and Salts

This chemical category (N746) includes any unique chemical substance that contains strychnine or a strychnine salt as part of that chemical's infrastructure. Strychnine (CASRN 57-24-9) is used as a surrogate for both toxicity and physicochemical data for this category.

### 3.14 Warfarin and Salts

This chemical category (N874) includes any unique chemical substance that contains warfarin or a warfarin salt as part of that chemical's infrastructure. Warfarin (CASRN 81-81-2) is used as a surrogate for both toxicity and physicochemical data for this category.

## **4 Summary of Resolution of Certain TRI Reporting Issues**

In March 1996, several reporting issues pertaining to the TRI chemicals ammonia, ammonium sulfate, and mineral acids were resolved. These issues and the corresponding modifications or recommendations which were agreed upon are summarized below.

### **4.1 Ammonia and Ammonium Sulfate**

Effective for the 1994 reporting year, only the ammonia (CASRN 7664-41-7) or a fraction of the water-dissociable portion of ammonia in a compound are reportable to TRI. This includes anhydrous ammonia, aqueous ammonia, and ammonia from water-dissociable ammonium salts and other sources (the latter includes ammonium sulfate). The total quantity of ammonia is calculated, but only 10% of this quantity counts towards threshold levels for reporting and it is this 10% which is actually reported. To re-calculate the original quantity of ammonia, one must multiply the reported quantity of releases and transfers (e.g., to POTWs) to water and land by 10 (air emissions are reported at 100%).

Because of these reporting changes, comparisons should not be made between ammonia reporting before 1995 and after 1995.

### **4.2 Mineral Acids**

Mineral acids include sulfuric acid (CASRN 7664-93-9) and hydrochloric acid (CASRN 7647-01-0). The Agency has made the decision to modify reporting to include only the more highly toxic exposures to aerosol releases of these acids. The acid aerosols include mists, vapors, gas, fog and other airborne forms of any particle size. For sulfuric acid, this change in reporting took place in 1994, while for hydrochloric acid the change took place for reporting year 1995. The very high decay rate in water of these acids will greatly reduce any risk-based impacts associated with releases or transfers to water.

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