

AIChE/DIPPR[®] Project 911

Environmental, Safety and Health Data Compilation

Policy and Procedures Guidelines

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Policy and Procedures Guideline

1.0 Introduction

Design Institute for Physical Property Data (DIPPR)[®] Project 911 entitled Environmental, Safety and Health Data Compilation is responding to a need for a critically evaluated, internally consistent, documented and computerized database covering the title properties for a select list of pure chemicals with known hazards. The project is anticipated to satisfy industrial needs for more accurate and complete property data in order to respond effectively to regulatory requirements. The project scope was developed around the 275 chemicals in the Clean Air Act Amendments of 1990 (CAAA) and the Occupational Safety and Health (OSHA) Act of 1970, Federal Register No. 1910.119 with six blocks of properties covering specific areas of interest. In 1994, the 84 chemicals of the Environmental Protection Agency's Risk Management Program (EPA-RMP) were added to the project chemical list. The updates to the chemical list from 1994 to the present have included sponsor-selected chemicals. Thirty-two sponsor-selected chemicals were added in 1994, 87 in 1995, 110 in 1996, 102 in 1997, and 105 in 1998.

Michigan Technological University was chosen as the prime contractor to develop the Project 911 database with assistance from software and database consultants. This document describes the policy and guidelines which Project 911 staff have used to develop the Environmental, Safety and Health Data Compilation. Each section describes in detail the methods, assumptions, and procedures used by Project 911 staff to complete the tasks set forth.

1.1 Project Approach

The team assembled by Michigan Technological University consists of chemical and environmental engineers, chemists, biologists, and software and database consultants. This team has set the following objectives:

1. Develop a data compilation for each property and chemical identified by the AIChE/DIPPR[®] Technical Steering Committee. This compilation would include the values and units for each of the properties and for each of the chemicals as well as the quality rating, literature citation, appropriate comments, and experimental conditions where available.
2. Provide a comprehensive search of all available, reliable data resources both domestic and foreign. These sources include standard library literature as well as industrial reports, commercially available computerized databases, government reports, and Project 801 data.
3. Evaluate each piece of data on the basis of consistency with other properties of that chemical, fundamental thermodynamics, statistical correlations, and the documentable quality assurance/quality control (QA/QC) behind each study.
4. Develop a DOS software product incorporating features such as CAS number indexing, literature citations, quality codes, temperature dependent graphing capabilities, and built-in conversion of units. The final DOS software product (sponsor version 6.0) was released to the Project 911 Steering Committee in July 1998. Future public dissemination of Project 911 data in electronic form will be done through a third party vendor, EPCON International (www.epcon.com). In 1998, the steering committee granted EPCON the rights to license the 911 database to third party users. Sponsor companies continue to receive the Project 911 data files from MTU prior to public release.
5. In a companion project, Project 912, MTU evaluated existing and developed new estimation methods for many of the properties in Project 911. These Project 912 methods are used to estimate data not available in the literature and to test available data for consistency.

In order to efficiently manage and track the number of individual pieces of data as well as the amount of data source material, the Project 911 team chose to develop, with the assistance of software and database consultants, a computerized data management and tracking system. A detailed discussion of each of the components including

properties and chemicals of interest, literature searches, quality screening methods, data tracking system, and demonstration software in the Project 911 effort is provided in separate sections below.

2.0 Project 911 Parameters

2.1 List of Parameters

The Technical Steering Committee has identified six blocks of parameters or properties to be included in the Project 911 effort. These are:

Block Number	Block Title
1	Oxygen Demand
2	Partitioning Parameters
3	General Physical Properties
4	Vapor-Liquid Equilibrium
5	Fire and Explosion Parameters
6	Sensory, Health and Toxicity Impacts

Each block contains three or more parameters. The properties requested by the Technical Steering Committee have been incorporated into the data management and tracking system. The list of property names and property codes as used by Project 911 and as established by the Technical Steering Committee can be found in Table 1. In order to incorporate this list in the data management and tracking system, the list was revised slightly from the original layout. In some cases additional properties have been added to provide unique descriptors of each property such as for Flammability Limits. It was also necessary to shorten some names to provide more room on the final software product screens.

2.2 Definitions of Parameters

The following is a listing of the definitions of each of the properties as used in Project 911. A discussion of the units used for each definition is contained in Section 2.2.7.

2.2.1 Block 1 Oxygen Demand

1a. Biochemical oxygen demand (BOD) is a measure of the oxygen consumed by microbial life while assimilating and oxidizing the organic matter present in a wastewater. The standard BOD tests are typically run for 5 days at 20°C in the dark.

1b. Chemical oxygen demand (COD) is another method of obtaining the equivalent of oxygen demand of the organic matter by oxidizing the sample using a strong chemical oxidant such as potassium dichromate or permanganate. Since COD tests are very severe and interference from chloride ions can be a problem if not accounted for during testing, it should be noted that COD is not a true measure of biodegradable organic carbon. Two property codes have been created for COD to reflect the two most commonly used test procedures. The property code for COD using potassium dichromate as the oxidant is *1b*, and the property code for COD using potassium permanganate as the oxidant is *1bp*.

1c. Theoretical Oxygen Demand (ThOD) is estimated for specific organic compounds based on the stoichiometry of a balanced chemical reaction which describes the reaction of the organic chemical with oxygen to produce theoretical inorganic end products. The following guidelines were used to determine the reaction's

inorganic end products. Organic chemicals which contain only carbon and hydrogen were assumed to be converted to CO₂ and H₂O; organic chemicals which contain carbon, hydrogen, and sulfur were assumed to be converted to CO₂, H₂O, and SO₄²⁻; organic chemicals which contain carbon, hydrogen, and phosphorus were assumed to be converted to CO₂, H₂O and orthophosphate forms (i.e., H₂PO₄⁻ or HPO₄²⁻); organic chemicals which contain carbon, hydrogen, and halogens (e.g., chlorine, bromine) were assumed to be converted to CO₂, H₂O and the respective halogen ion (e.g., Cl⁻, Br⁻); and, organic chemicals which contain carbon, hydrogen, and nitrogen were assumed to be converted to CO₂, H₂O, and ammonia. In the later case the oxygen demand associated with nitrogenous theoretical oxygen demand was found by showing the stoichiometric amount of oxygen required to oxidize the ammonia to nitrate.

An exception to these rules is chemicals with nitro (NO₂) or nitroso (NO) groups. The nitrogen in a nitro or nitroso group will be converted to ammonia under anaerobic, reducing conditions. Under aerobic conditions the nitro or nitroso group will go directly to nitrite and subsequently to nitrate. In order to calculate the carbonaceous ThOD for chemicals with nitro or nitroso groups, the stoichiometry was drawn out by hand assuming nitro or nitroso groups go to nitrate and all other nitrogen goes to ammonia. For combined carbonaceous and nitrogenous oxygen demand all the nitrogen was assumed to go to nitrate.

Both ThOD based on oxidation of C and H (carbonaceous) and ThOD based on oxidation of all elements (including N) to their highest oxidation state in the environment (combined) are provided for the Project 911 chemicals. The property code for carbonaceous ThOD is *Icc*, and the property code for combined carbonaceous and nitrogenous ThOD is *Icn*.

2.2.2 Block 2 Partitioning Parameters

2a. 1-Octanol/water partition coefficient (K_{ow}) is defined as the ratio of the equilibrium concentrations of a dissolved chemical in a 1-octanol-rich phase and a water-rich phase. The 1-octanol and water phases are nearly immiscible. It is dimensionless and is expressed as the coefficient (K_{ow}) or its base 10 logarithm (log K_{ow}). All partitioning parameters are measured at 298.15 K unless stated otherwise.

2b. Soil/water partition coefficients relate the concentration of an organic solute associated with the aqueous and solid phases at equilibrium. It is defined by the relationship $S = K_p C^{1/n}$ where S is the sorbed chemical concentration, K_p is the soil/water partition coefficient, C is the aqueous concentration and n is the Freundlich exponent. If the aqueous concentration of the pollutant is less than 10⁻⁵ M or one half its aqueous solubility (whichever is lower), the Freundlich isotherm has been found to be linear (i.e. n=1). Because K_p's can vary dramatically for different soil types and are typically developed from knowledge of a chemical's K_{oc} (K_{oc} = K_p/OC, where K_{oc} is the soil/water partition normalized for organic carbon on a unit basis and OC is the fraction of organic carbon in the soil) and the fraction of organic carbon in a soil, Project 911 has not incorporated K_p data into the data management system. In the software, the equation $K_p = K_{oc} \times (\% \text{ OC}/100)$ will be displayed if no comment is available. The user can then use the percentage of organic carbon in their soil sample to calculate the soil/water partition coefficient.

2c. Organic carbon/water partition coefficients are used in many environmental situations where the amount of organic carbon present in the sorbent dominates sorption (organic carbon >0.1%). Thus, partition coefficients are normalized with respect to organic carbon or organic matter content. Although the value given in the Project 911 is the log of the coefficient, units of cm³/g OC are assigned to the value to indicate the antilog units applied to the value.

2d. Bioconcentration factor (BCF) is defined as concentration of the chemical in the organism at equilibrium divided by the concentration of the chemical in water. This parameter is dimensionless and can be determined experimentally by dosing water containing the organism and dividing the concentration in the organism by the concentration in water once equilibrium is reached. If equilibration is slow, the rate of uptake and loss can be used to calculate the bioconcentration factor at equilibrium. The BCFs are collected for freshwater fish species. BCF values in the Project 911 database may not necessarily be at 25°C, as BCF tests are conducted at temperatures that are dependent on the species. For example, experiments using a cold-water species such as trout are usually conducted at 16°C, as most trout would die during a BCF test at a higher temperature. Temperatures for specific BCF data values are found as part of the reference information in the Project 911 database.

2.2.3 Block 3 General Physical Properties

Unless otherwise noted, properties of liquids below the normal boiling point are at 1 atm, and those above the normal boiling point are at saturation conditions; solid and vapor properties are at 1 atm or low pressure. For property values, quality codes, indicating source and accuracy, and references are included. For temperature dependent properties, discrete data at or near 25°C ($\pm 5^\circ\text{C}$) is collected. The temperature associated with the discrete data is also included. In addition to the discrete data, temperature dependent correlations have also been developed, concentrating on the temperature range of environmental interest, 250 to 500 K. For these properties, equation-fit statistics and the upper and lower temperature limits of applicability and values computed at these limits are included. Temperature dependent data are calculated from a temperature dependent correlation and displayed at the default temperature of 25°C (298.15 K) or can be viewed in a graphical form in the Project 911 software. See Table 2 for units and unit conversions.

3a. Molecular Weight is defined as the sum of the atomic weights of all the atoms in the molecule based on the IUPAC list of 1993 (*J. Phys. Chem Ref. Data* **24**, 1561 (1995)). This is expressed in units of kg/kmol. The molecular weight data is used as a means to cross check the accuracy of articles using SQC. The highest rated molecular weight values in the Project 911 datafiles will be the IUPAC calculation.

3b and 3bt. Liquid Density (ρ) is the ratio of the mass of a substance to its volume. Density can also be determined by dividing the molecular weight by the molar volume or by correcting for the density of water where molar volume or specific gravity are given in the source material.

Specific gravity is frequently given in data collections and is written in the form displayed in Equations (1) and (2).

$$\frac{\text{Density of liquid at } t_1}{\text{Density of water at } t_2} = \frac{\rho_l}{\rho_w} \quad 1$$

$$\text{Example: } 0.668 \frac{20}{4} \quad 2$$

In equation 2, the superscript number is the temperature of the liquid, and the subscript denotes the temperature of the water. The density of water is 1.00000 g/mL at 277.15 K. In Project 911 specific gravities are converted to densities by multiplying the density of water and the specific gravity. Data are presented at or near 25°C (3b) or calculated from a temperature dependent correlation (3bt) and expressed in units of kg/m³. If the substance is a solid at 298.15 K, the density may be given with a note that it is for the solid.

3c. Solubility in Water (s_a) is defined as the relative mass of the chemical dissolved in aqueous solution which is in equilibrium with an excess of the substance. The dissolved chemical may be a solid, liquid, or gas. For any binary solute-solvent system which has limited miscibility, there is a corresponding solubility limit of the solvent in the solute. These two endpoints of the equilibrium "tie-line" are related through equal-fugacity expressions at a given temperature and pressure and are not independent. Under Project 911, we are attempting to tabulate (or estimate) both chemical-in-water and water-in-chemical solubilities. The water-in-chemical solubilities, if given, are recorded in the comments (literature section) of the chemical-in-water solubility. Values listed are at 298.15 K unless noted otherwise and in units of ppm(wt). When the literature reports a chemical as "infinitely soluble", a value of 1,000,000 ppm (wt) has been placed in the Project 911 database in the "value" and "unit" fields.

For environmental purposes (temperature range of 20° to 30°C), solubilities of gases in water in the Project 911 database are assumed to be at 1 atm total pressure, unless otherwise noted in the reference information or comments. For applications outside an environmental range, the partial pressure of the chemical must be considered.

3d. Melting Point (T_{MP}) is defined as the temperature at which both liquid and solid exist in equilibrium at a pressure of 1 atmosphere. These are presented in units of K.

3e. Normal Boiling Point (T_{BP}) is defined as the temperature at which the liquid exerts an equilibrium vapor pressure of 1 atm. These are presented in units of K.

3f and 3g. The Vapor Pressure (P_{vp}) of a pure chemical is the pressure which the chemical will exert at a given temperature; i.e., it is the pressure of the vapor above the chemical at equilibrium. In a closed vessel, a chemical is in a dynamic state of equilibrium in which the molecules of the chemical are constantly shifting between chemical and vapor states. The presence of this vapor creates a pressure termed the vapor pressure. Vapor pressure is temperature dependent and is presented in Project 911 at or near 25°C (temperature stated if not 298.15 K) (3f) or calculated from a temperature dependent correlation (3g). Both 3f and 3g are presented in units of Pa.

3h and 3i. Molecular Diffusivity (D_{AB}) is a measure of the mass transfer through a homogeneous gas,

liquid, or solid phase as defined by Fick's Law: $N = D_{AB} \frac{dCA}{dx}$, where N is the molar flux and $\frac{dCA}{dx}$ is the concentration

or potential gradient for species A in a phase B. This mass transfer results from gradients in chemical potential and the diffusion coefficient relates the potential difference (usually represented by concentration or partial pressure) to the rate of diffusion. Diffusivity values are presented in Project 911 in air (3h) and in water (3i) at or near 25°C unless otherwise noted and in cm²/s.

3j. Vapor Viscosity (η_v) is analogous to the viscosity of a liquid. If atoms in a fast moving layer travel into a slower moving layer, they transfer their excess momentum to the atoms in the slow moving layer. If the opposite occurs, the atoms from the slow layer retard the motion of the faster layer. The rate at which these atom transfers occur is proportional to the vapor density and to the average velocity gradient. Data are calculated from a temperature dependent empirical correlation in Pa-s or can be viewed in a graphical form in the Project 911 software product. The viscosity used here is the dynamic viscosity.

3k. Liquid Viscosity (η_L) is a measure of the resistance of a fluid to dynamic change. When a force is applied to a fluid, it begins to flow at a velocity which is proportional to the force. This flow is not uniform because of the fluid's resistance to motion. Data are calculated from a temperature dependent empirical correlation in Pa-s. The viscosity used here is the dynamic viscosity.

3l and 3lt. Surface Tension (σ) is a contracting force parallel to a liquid surface which forms a boundary between the liquid and gas phases or liquid/liquid interface. In mathematical terms it is the force per unit length required to create a new unit area of the gas-liquid interface. The surface tension cited is the interfacial tension between the pure component and air at or near 298.15 K. Data in Project 911 are presented at or near 25°C (temperature stated if not 298.15 K; 3l) and calculated from a temperature dependent correlation (3lt) in N/m.

3m. Thermal Conductivity (λ_l and λ_v) is defined as the time rate of heat transfer by conduction through unit thickness, across unit area for a unit difference in temperature. It is typically measured as Watts per meter times K (W/m-K). Thermal conductivity is calculated in Project 911 for the liquid (λ_l) (3ml) and vapor (λ_v) (3mv) from a temperature dependent property. Information for solids is also included when available.

3n. Standard Enthalpy of Formation ($\Delta H_{f,298.15}^\circ$), also known as the Ideal Gas Heat of Formation, is defined as the change in enthalpy associated with the reaction of forming one mole of the given compound in the ideal gas state from the elements in their standard state at 298.15 K. The standard state of the element is the form which is the most stable at 298.15 K. Enthalpy of formation is given in joules per kilomole (J/kmol). When ideal gas values are not available for inorganic compounds solid at 298.15 K, the values for the solid are given in the comments. If both the ideal gas and the solid values are available, the solid value is placed in the comments.

If values are not located in the literature, they are calculated by the method of Rhodes (1984). This method uses Benson (1976) groups, by the ASTM's CHETAH (1974) program which uses known heat of formation values for designated compounds as well as Benson groups, or from Benson groups available in Danner and Daubert (1987).

3o. Liquid Heat Capacity (C_p) is the energy required to change the temperature of a liquid by a specified thermal quantity. It can be defined in at least three ways: heat capacity at constant pressure, heat capacity at constant

volume, and saturated liquid heat capacity. Unless otherwise stated in the comments, the Project 911 values cited are for heat capacity at constant pressure. Data are calculated from a temperature dependent correlation and presented in J/kmol·K. Information for solids may be included when it is available.

3p. Vapor Heat Capacity (C_p), also known as the Ideal Gas Heat Capacity, is the energy required to change the temperature of a vapor by specified thermal quantity. It can be defined in at least four ways: heat capacity at constant pressure, heat capacity at constant volume, saturated vapor heat capacity, and ideal gas heat capacity. Unless otherwise stated in the comments, the Project 911 values cited are for ideal gas heat capacity. Data are calculated from a temperature dependent correlation and presented in J/kmol·K.

3q. Critical Temperature (T_c) is the highest temperature at which a pure substance can exist in vapor-liquid equilibrium. This critical point has the coordinates critical pressure (P_c) and critical temperature (T_c). The critical temperature is where density of the liquid equals the density of the saturated vapor and the heat of vaporization becomes zero. The pressure at this temperature is the critical pressure. Critical temperature is presented in units of K.

3r. Critical Pressure (P_c) is the pressure at the highest temperature at which a pure substance can exist in vapor-liquid equilibrium. This critical point has the coordinates critical pressure (P_c) and critical temperature (T_c). Critical pressure is presented in Pa.

3s. Critical Volume (V_c) is the molar volume at the critical point and is presented in $m^3/kmol$.

3t, 3tt, and 3tz. The Latent enthalpy of Vaporization (ΔH_{vb}) is defined as the enthalpy required in the phase change from a liquid to a gas. This value is usually obtained for the normal boiling point. The nomenclature for latent enthalpy of vaporization at the normal boiling point is ΔH_{vb} . Data are collected and presented for three forms: ΔH_{vb} at or near 298.15 K (3t), calculated from a temperature dependent correlation (3tt), and at the normal boiling point for that chemical (3tz) all in J/kmol.

2.2.4 Block 4 Vapor-Liquid Equilibrium

4a and 4b. Activity Coefficients (γ) are a measure of the nonideal behavior of a chemical mixture relative to ideal behavior (Lewis-Randall or Henry's law) equilibrium calculations. The Lewis-Randall standard state for a chemical is commonly chosen to be the pure liquid at the system temperature and pressure and the activity coefficient has a value of one. If $\gamma > 1.0$, there are said to be positive deviations from ideal behavior in which the molecules of the different components in solution are dissimilar and have no preferential interaction between the species. If $\gamma < 1$, there are negative deviations from ideal behavior in which the molecules of the different components exhibit preferential attractive forces (such as hydrogen bonding, etc.) that do not occur for either species alone. In aqueous systems activity coefficients for hydrophobic chemicals are often expressed as infinite dilution activity coefficients γ_1^∞ based on the Lewis-Randall standard state. The Project 911 group is compiling activity coefficients at infinite dilution of the chemical in water (4a) and of water in the chemical (4b). Values are for 298.15 K unless stated otherwise and are dimensionless.

4c. Aqueous Henry's Law Constant (H) is defined as the ratio of a chemical's concentration in the gas phase to its concentration in the water phase at equilibrium, and is often called an air/water partitioning coefficient. This form of Henry's Law constant is dimensionless [mole of chemical (gas phase)/mole of chemical (liquid phase)]. Two other forms of Henry's constant with units also exist: one relates gas-phase partial pressure to liquid-phase molar concentration (units of Pa·m³/mol), and the other relates gas-phase partial pressure to liquid-phase mole fraction (units of Pa). This last form of Henry's constant, by definition, is the product of the Lewis-Randall infinite dilution activity coefficient and the pure component vapor pressure. The temperature is 298.15 K unless stated otherwise. Henry's constants are presented in units of kPa·mol/mol.

2.2.5 Block 5 Fire and Explosion Parameters

5a. Flammability Limits in Air are defined as the boundary line mixtures of gas with air, which if ignited will just propagate flame. They are presented in terms of percentage by volume of gas in the air. Both the upper (5au) and lower (5al) flammability limits are presented in Project 911 in units of vol% in air.

5b. The Flash Point is the lowest temperature (presented here in Kelvin) at which a liquid gives off sufficient vapor to form an ignitable mixture with air near the surface of the liquid or within the vessel used. The preferred experimental method is closed cup. In Project 911, the experimental method is noted with the value where it has been explicitly given. The value for closed cup is in the “values” field. Any value for open cup will be in the “comments” field. Sataflash is a closed cup method and Cleveland is an open cup method.

5c. Autoignition Temperature is the minimum temperature for a substance to initiate self-combustion in air in the absence of a spark or flame.

5d. Standard net enthalpy (heat) of combustion - The standard net enthalpy of combustion is the increase in enthalpy when a substance in its standard state at 298.15 K and 101325 Pa undergoes oxidation to products obtained in complete combustion. Unless otherwise stated the value is for the combustion of the gaseous substance to produce H₂O(g), CO₂(g), F₂(g), Cl₂(g), Br₂(g), I₂(g), SO₂(g), N₂(g), H₃PO₄(s), and SiO₂(cristobalite). It is given in joules per kilomole (J/kmol) at 298.15 K. Heat of combustion values in the Project 911 database are defined as negative values for purposes of sign convention. The standard net enthalpy heat of combustion is also known as the Net Heating Value or the Lower Heating Value (LHV). For Project 911 chemicals that are the gaseous combustion products given above, the value field in the database has been left blank, and “property inappropriate for this compound” has been placed in the comment field.

For compounds containing C, H, and O if a gross heat of combustion (also known as the Higher Heating Value (HHV)), (H₂O(liquid)) value is available, the net value is calculated by adding the enthalpy of vaporization for the appropriate amount of water. Again, the negative sign convention for heats of combustion is used here. The user is cautioned that the absolute value of the net heat of combustion should always be less than the absolute value of the gross heat of combustion, by an amount equal to the enthalpy of vaporization of the appropriate amount of water, as stated earlier. In addition, the enthalpy of combustion is calculated from the accepted enthalpies of formation (in the ideal gas state) to check for consistency with the enthalpy of combustion obtained from the gross enthalpy of combustion. This calculation involves subtracting the enthalpy of vaporization of the compound at 298.15 K, so that the enthalpy of formation is for the standard state. The enthalpy of vaporization value used is that calculated from the regression equation. The agreement is usually excellent; if it is not, the enthalpy of combustion calculated from the enthalpies of formation is accepted. For some compounds, no experimental values are available but a value for enthalpy of combustion can be predicted by Benson's method and the CHETAH program. These values are entered based on the ideal gas state and are so noted.

To convert net enthalpy of combustion values for any compound to gross enthalpy of combustion values where the end products are HCl(g), HF(g), P₄O₁₀(g), and H₂O(liquid), rather than Cl₂(g), F₂(g), H₃PO₄(s), and H₂O(g), respectively, use the following for H(a), Cl(b), F(c), P(d):

$$\Delta H_c(\text{gross}) = \Delta H_c(\text{net}) + (b)\Delta H_f^\circ(\text{HCl})(\text{g}) - \left(\frac{b}{2}\right)\Delta H_f^\circ(\text{Cl}_2)(\text{g}) + (c)\Delta H_f^\circ(\text{HF})(\text{g}) - \left(\frac{c}{2}\right)\Delta H_f^\circ(\text{F}_2)(\text{g}) + \left(\frac{d}{4}\right)\Delta H_f^\circ(\text{P}_4\text{O}_{10})(\text{g}) - (d)\Delta H_f^\circ(\text{H}_3\text{PO}_4)(\text{s}) + (a-b-c)/2\Delta H_f^\circ(\text{H}_2\text{O})(\text{liquid}) - (a-3d)/2\Delta H_f^\circ(\text{H}_2\text{O})(\text{g})$$

2.2.6 Block 6 Sensory, Health and Toxicity Impacts

6a-6i. Acute Aquatic Toxicity is defined as the potential a chemical has to cause adverse effects in an aquatic organism over four or fewer days. The end-points used in Block 6a-i, Acute Aquatic Toxicity, are:

LC50: the median lethal concentration of material which results in mortality of 50% of test organisms;

EC50: the median effective concentration of material which results in a sublethal response, such as a behavioral change, in 50% of test organisms.

Pimephales promelas (fathead minnow), *Daphnia magna* (water flea), Salmonidae (trout and salmon family) Mysidacea (opossum shrimp order), two toxicity endpoints (EC50, LC50), and three exposure times (24, 48, 96 hours) are incorporated under this block. Initially, the literature was searched for each combination of organism, endpoint, and time. However, it became apparent that few data were available for some of these combinations, and a number of property codes were deleted as indicated by an asterisk (*) below:

<u>Property Code</u>	<u>Name</u>	<u>Endpoint</u>	<u>Test Duration</u>
6ab	fathead minnow	EC50	48 hours
6ac	fathead minnow	EC50	96 hours
6ba	fathead minnow	LC50	24 hours
6bb	fathead minnow	LC50	48 hours
6bc	fathead minnow	LC50	96 hours
6ca	<i>Daphnia magna</i>	EC50	24 hours
6cb	<i>Daphnia magna</i>	EC50	48 hours
*6cc	<i>Daphnia magna</i>	EC50	96 hours
6da	<i>Daphnia magna</i>	LC50	24 hours
6db	<i>Daphnia magna</i>	LC50	48 hours
*6dc	<i>Daphnia magna</i>	LC50	96 hours
*6ea	Salmonidae	EC50	24 hours
*6eb	Salmonidae	EC50	48 hours
*6ec	Salmonidae	EC50	96 hours
6fa	Salmonidae	LC50	24 hours
6fb	Salmonidae	LC50	48 hours
6fc	Salmonidae	LC50	96 hours
*6ga	Mysidacea	EC50	24 hours
*6gb	Mysidacea	EC50	48 hours
*6gc	Mysidacea	EC50	96 hours
*6ha	Mysidacea	LC50	24 hours
*6hb	Mysidacea	LC50	48 hours
6hc	Mysidacea	LC50	96 hours
6i	Other	Those property numbers designated with and asterisk (*) are grouped into this general property code	

Bioconcentration factors are collected for the following species: fathead minnow, *Pimephales promelas*; common water flea, *Daphnia magna*; Atlantic salmon, *Salmo salar*; brown trout, *Salmo trutta*; lake trout, *Salmo trutta lacustris*; arctic char, *Salvelinus alpinus*; brook trout, *Salvelinus fontinalis*; white spotted char, *Salvelinus leucomaenis*; Dolly Varden, *Salvelinus malma*; lake trout, siscowet, *Salvelinus namaycush*; golden trout, *Oncorhynchus aguabonita*; cutthroat trout, *Oncorhynchus clarki*; gila trout, *Oncorhynchus gilae*; pink salmon, *Oncorhynchus gorbuscha*; chum salmon, *Oncorhynchus keta*; coho salmon, silver salmon, *Oncorhynchus kisutch*; cherry salmon, yamame trout, *Oncorhynchus masou*; rainbow trout, Donaldson trout, *Oncorhynchus mykiss*; sockeye salmon, *Oncorhynchus nerka*; chinook salmon, *Oncorhynchus tshawytscha*; and the opossum shrimp order Mysidacea, *Bowmaniella dissimilis*, *Leptomysis mediterranea*, *Mysidopsis bahia*, *Mysidopsis bigelowi*, *Mysidopsis almyra*, *Mysis relicta*, *Neomysis americana*, *Neomysis awatschensis*, *Neomysis integer*, *Taphromysis louisianae*.

2.2.7 Units

Data are entered into the Project 911 database in the original units from the data source material. In some cases the data are converted to simplify the conversion routine. For example, solubility units given in log mmol/L are converted with inverse log to get mmol/L. A unit conversion routine has been developed in which the data extracted for the Project 911 software product are converted into a default unit. The routine then gives options of SI or CGS units. Table 2 provides a list of the default units for each property, selection of unit options and the mathematical

expression to convert to them. The default unit is the unit to which all the values for that property have been converted and will be displayed on the software screen unless the user chooses a different unit from the list of unit options. In all cases where it is necessary to incorporate the density of water, it was assumed to be 1 g/mL.

The conversion routines are based on a temperature of 298.15 K. If there are values in the database at temperatures other than 298.15 K, the conversion is calculated by hand and entered into the database in the default units. The original value and units as stated in the literature source is entered into the comments section. This is used especially for Henry's constants (4c) and solubility.

This "hard-coding" is also employed for solubility (3c) values which exceed 10,000 ppm(wt). The automatic conversion routines and relationships for solubility are only applicable for values < 10,000 ppm(wt). Again, the original value and units are entered in the comments section of the database.

3.0 Description of Chemical List

The stated purpose of Project 911 data compilation effort is to focus on chemicals of environmental, safety, and health concerns. Initially the chemicals listed in the CAAA were chosen by the Project 911 Technical Steering Committee as the focus. This list consists of 172 chemicals identified by the Chemical Abstract Service (CAS) number as well as an additional 17 chemicals, such as cadmium compounds, which can be listed with multiple CAS numbers. The 1992 effort focused on those with single CAS numbers although information has been collected on the other chemicals as well. In 1993, 109 chemicals from the OSHA list were added to the database. The 1994 additions included the EPA-RMP list and a list of sponsor-selected chemicals. The current additions to the list are 90 sponsor-selected chemicals. These numbers include chemical numbers 382.0 to 1021.0 for a total of 1011 chemicals.

Several problems were discovered in regard to the CAAA list and have been discussed with EPA staff. First, several chemicals identified by specific CAS number are for salts, esters or mixtures of species such as 2,4-D, Aroclors, 4,6-dinitro-o-cresol, and dibenzofurans. The DIPPR[®] projects are interested in pure chemicals. Unique CAS numbers exist for the salts and esters or for the different dibenzofurans. Second, the CAS number given in the CAAA list for DDE is incorrect. The correct CAS number is used in Project 911. Third, CAS number 121697 for N,N-Diethylaniline in the CAAA list is actually for the N,N-Dimethylaniline. Project 911 has incorporated the CAS numbers for both chemicals until a decision from EPA is made regarding which chemical should be listed. The Project 911 list has also distinguished between the isomers of 1,3-Dichloropropene. There are three forms of phosphorus: white, yellow and red. Priority for entry into the database has been given in the following order: white, yellow, red. Data for yellow or red phosphorus are placed in the comments where appropriate.

In the OSHA list, incorrect CAS numbers were identified for Propyl Nitrate, Ammonium Permanganate, Oleum and Trichloro(dichlorophenyl)silane and the correct CAS numbers were incorporated into the database. Another change made to the OSHA list was that Project 911 distinguishes between the isomers of Ethyl Methyl Ketone Peroxide in the database. Additional chemical suggested by sponsors are also included in the database.

In order to conform to software constraints, each chemical was assigned an arbitrary number based on alphabetical order for the CAAA list and, starting with number 173, in numerical order based on CAS number for the OSHA list (Table 3). The number continues for the EPA-RMP list and the sponsor-selected chemicals.

4.0 Literature Search

4.1 General Approach

There are a number of sources of data which are incorporated into the Project 911 database. They include the following: 1) values from AIChE/DIPPR[®] Project 801 where Project 801 and Project 911 have common chemicals and parameters; 2) principal literature sources where data are readily available; 3) available literature compilations, commercially available electronic databases, and other electronic sources; and 4) international literature to obtain source materials to fill the additional parameters and data gaps. The method followed for each of these steps is discussed below.

4.2 Project 801 Release

Communication among Pennsylvania State University and Brigham Young University, DIPPR Project 801, and MTU, DIPPR Project 911, is ongoing in the exchange of new methods of prediction and new ideas. This allows each team to keep abreast of general progress of each of the projects. An example of this exchange has been in the prediction of Block 5 Fire and Explosion parameters. Project 801 has been utilizing the new prediction methods developed and utilized by Project 911.

AICHe/DIPPR[®] Project 801 is a data compilation project for physical, thermodynamic, and transport property data. Some properties and chemicals are common to both Project 801 and Project 911. In order to avoid duplicating efforts, Project 911 receives and extracts the Project 801 data release on a set of diskettes each year. In the past, the data were provided on a set of magnetic tapes which were then extracted on the MTU mainframe. The Project 801 data, references, supplementary coefficients, policies and procedures, and footnotes are contained in separate files on the diskettes. A Fortran program is employed to extract the desired data with the associated references and footnotes.

To conduct the data extraction for the Project 911 chemical list, a software routine is used to pull the appropriate values with the associated references, units, quality codes, equation numbers, correlation coefficients, and footnotes, rearrange the field locations as necessary, and insert them into the Project 911 database. This effort was coordinated between Principal Investigator, Tony Rogers, Software Consultant, Kenneth Clark, and Database Liaison, JCM Environmental. Only those values which were labeled as acceptable by Project 801 are extracted.

An update of release of Project 801 of 1996 was done in September in compliance with the contract agreement. At this time, nearly 400 data values were downloaded to the Project 911 database. The update was performed by tagging the code system which Project 801 uses. For example, Project 801 labeled values entered during 8/1/91 to 1/31/92 with a L and so on alphabetically until the 2/1/96-7/31/96 which was marked with an X. Changes made to Project 801 data which have already been downloaded by Project 911 is designated with a C or & or @ which permits the extraction of all the updates of the Project 801 database. These updates and extractions have been occurring annually since August of 1991.

Some differences in format and field length between the Project 801 files and the Project 911 database cannot be resolved in the software routine. In particular, the comments from Project 801 are longer than the 120 characters set aside in Project 911. In these cases the Project 801 comments are manually edited by Project 911 staff.

4.3 Principal Literature Search

Literature reviews, thorough searches of available journals, chemical supply catalogs, and published compilations are conducted at Michigan Technological University's Van Pelt Library. Source materials not available from the Van Pelt Library are requested by interlibrary loan. Certain source materials were found to be particularly productive sources of high quality data. These principal literature sources are given in Table 4 by block number and the journals are reviewed regularly for additional data. If data are not available from the principal sources a more detailed search is conducted.

4.3.1 Blocks 1 and 2 Oxygen Demand and Soil/Water Partitioning

A literature search was conducted in 1992, 1993, and 1995 primarily with a Wilsondisc CD-ROM information retrieval system developed by the H. W. Wilson Co. of Bronx, New York. This is an electronic data base system that contains approximately 800 journals from four major indexes: Readers Guide, Biological and Agricultural, Applied Science and Technology, and Business Periodicals. The majority of this search was spent in the Applied Science and Technology, and Biological and Agricultural indexes. The system at the MTU J. Robert Van Pelt Library only covers back to approximately 1983 for most references, though information was obtained from sources dating back as far as 1967. Any relevant titles and keywords were searched on this system by entering the words; partitioning, sorption, K_{oc} and distribution coefficient to name just a few. In addition, *Environ. Sci. Technol.*, *Water Res.*, *Soil Sci. Soc. Am. J.* and *J. Agric. Food Chem.* were individually searched back to 1965 because several articles on the subject were referenced to these journals. The 1995 search generated many more first-hand data sources for BOD dating back to 1932. These

sources included Purdue waste conferences from 1946 to present, Sewage Works Journal, Sewage and Industrial Wastes Engineering, and several German sources. One difficulty with BOD values is the lack of measured values in the past two decades.

Another search that turned out to be more productive came from searching through glossaries of two books that had previously compiled data on partitioning. These books were K. Verschueren, *Handbook of Environmental Data on Organic Chemicals* (1983) and the Mackay, et al., *Illustrated Handbook of Physical Chemical Properties and Environmental Fate for Organic Chemicals* (1992). An excellent source of experimental COD data was a German publication *Chemische Oxidierbarkeit organischer Wasserinhaltsstoffe* which contains nearly 600 values for COD by both dichromate and permanganate methods. A complete list of references is found in Table 4 (Blocks 1 & 2).

Oxygen demand data were compiled using two basic criteria: 1) only chemicals listed in the Technical Steering Committee list were considered; and 2) the study must have followed standard procedures in the obtaining of these data. For example, COD values were obtained for methods using either a dichromate oxidant in the presence of a silver sulfate catalyst for *Ib* or permanganate oxidant for *Ibp*. Experimental data were not found for all the chemicals. Estimates were then used to fill in gaps in the data base. This is described in more detail under Estimation Methods below.

Due to the nature of the Biochemical Oxygen Demand (BOD) test, the rating criteria used differed from the system used for other DIPPR properties. A rating system specifically for BOD was created based on the conditions that critically affect the results of the BOD test. For convenience a copy of the rating form is provided in Table 6.

The experimental technique used is of utmost importance in the BOD test as the results tend to be highly variable. Those experiments not following the 1992, 18th Edition of Standard Methods for Examination of Wastewater and Water (APHA, AWWA, WEF) (Standard Methods) produce data that are not comparable to other BOD values. For this reason, those papers following Standard Methods were given a higher ranking than those not following Standard Methods.

Just as the experimental technique is important, so too is the temperature at which the experiment is conducted. Most biological processes are a function of temperature. To insure that data from different sources are comparable with respect to temperature, Standard Methods recommends performing the BOD test 20°C. In some instances temperature is intentionally manipulated for the purpose of the experiment. For example, an experiment may be designed to show the effect on BOD of seasonal changes in a waste water. In such cases the rating system does not penalize a paper for running the experiment at a temperature other than 20°C. A paper is only penalized if the temperature is not reported. The comment field will indicate the temperature of all experiments run at a temperature other than 20°C.

The state of seed acclimation also plays an important role in the BOD test. An organism that is not acclimated to a specific chemical may experience a lag phase during which the organism adapts itself to the compound of interest. The length of this lag phase is highly variable. If the lag phase is greater than the five days allowed for the test, the chemical may appear to be nonbiodegradable or perhaps less biodegradable than if an acclimated seed was used. An acclimated seed receives a higher rating than a nonacclimated seed in the rating criteria, which in turn receives a higher rating than those paper in which acclimation is not reported. Both the seed used and the state of acclimation will be reported in the comment field.

The initial chemical concentration can also affect the results of the BOD test. It is important that the concentration is not toxic to the seed organisms and that an adequate amount of dissolved oxygen is present in the test container to degrade the compound of interest. Standard Methods states that a dilution which results in a residual dissolved oxygen concentration of at least 1 mg/L and a dissolved oxygen uptake of at least 2 mg/L after five days incubation produces the most reliable results. Papers were evaluated on whether or not the initial chemical concentration was reported to indicate the author's thorough understanding of the BOD test.

Finally, the BOD of a chemical must be less than or equal to the chemical's theoretical oxygen demand. The comparison of the results of the BOD test to the chemical's theoretical oxygen demand was used to show internal consistency.

Based on the literature review conducted in 1992, 1993, and 1995 for soil/water partitioning, it appears that it will be very difficult to develop an extensive, good quality data base for most chemicals for a number of reasons. Three important reasons for this are: 1) many DIPPR chemicals are not strongly sorbed to soils/sediments; therefore, their sorptive properties have not been investigated intensively; 2) there is no standard method for determining soil/water partition coefficients or units of reporting; thus, much of the data reviewed for this project were judged unacceptable; and, 3) a major problem not accounted for by many researchers when measuring soil water partition coefficients is that the target chemical can be lost by biological degradation, volatilization, or sorption onto surfaces other than the soil (e.g., onto glassware).

Many values were judged unacceptable because the reported units could not be normalized to one common standardized unit. Soil/water partition coefficients are typically normalized to some measurement of organic carbon. This allows application of a partition coefficient to most circumstances, as long as the amount of organic carbon is known. Unfortunately, researchers normalize the partition coefficient on either a basis of organic carbon (OC) or organic matter (OM). OM is the organic fraction of the soil and includes organic carbon, nitrogen, phosphorus, and sulfur. However, OC only accounts for the organic carbon fraction of soil. While, OM is typically related to OC by multiplying OC by 1.724, a number of studies suggest that the conversion factor may actually range from 1.9 to 2.5 (Nelson, D.W. and L.E. Sommers, *Total Carbon, Organic Carbon, and Organic Matter*, American Society of Agronomy, Madison, WI, 1982). Thus, values of a soil/water partition coefficient which are reported as K_{om} , instead of K_{oc} , were not used unless the researcher reported a specific conversion ratio (OC/OM) for their test system.

Where possible, soil/water partition data were obtained according to the following conditions: 1) the isotherms were performed with several soils of varying organic carbon content and the data were fit to a straight line, or a Freundlich isotherm with $1/n=1$. When the data were fit to a Freundlich isotherm with $1/n$ between 0.9 and 1.1, these data were refit to a straight line to obtain K_{oc} . Experiments have shown that if $1/n$ is between 0.9 and 1.1 it is statistically more valid to assume that the isotherm is linear (J.C. Crittenden, Dept. of Civil and Environmental Eng., Michigan Tech, personal communication with James Baker, September, 1993); 2) either the soils were sterilized to inhibit biological degradation of the chemical or other tests were performed to account for no biotic loss of the chemical; 3) sorption equilibrium was confirmed by previous results or sequential sampling; 4) the water was free of dissolved organics; and 5) the pH of the solution was near neutral. These criteria were developed to follow a proposed American Society of Testing and Materials method for activated carbon adsorption studies (J.C. Crittenden, Department of Civil and Environmental engineering, Michigan Technological University, personal communication with Dr. James Mihelcic, August 1992). The system for rating papers in the area of Soil/Water Partitioning is provided in Table 5. When multiple sources of K_{oc} that did not meet all the above criteria were available, the source that fit the most criteria was chosen. Articles that provided data that did not fit any of the criteria were discarded. For example the extensive data base of G.G. Briggs, *J. Agric. Food Chem.* **29**, 1050 (1981) was discarded because the samples in this study were only equilibrated for 2 hours.

Table 7 provides the reliable sources obtained for K_{oc} and the criteria used for evaluation. The first row of Table 7 has the proposed ASTM method. This table was used to decide which references were most reliable in the case where different values for the same chemical were in different papers. Important criteria from above are listed here such as equilibration time, method of sterilization, source of water used, number of soils used and the range of organic carbon in the soil, the pH at which the isotherms were performed, and the specific method used.

4.3.2 Block 3 General Physical Properties

As stated earlier, the Project 801 data have served as a very important starting point for the compilation of general physical properties. Approximately 60 percent of the chemicals of interest to Project 911 are found in the Project 801 data compilation. These chemicals and properties coincidental to both Projects 911 and 801 are electronically extracted as described earlier. The properties not found in Project 801 have been the subject of an open literature search as described previously. Examples of the sources scrutinized are listed in Table 4 (Block 3). The search to date has included both properties at 298.15 K and those as a function of temperature. Some of the temperature dependent data have not yet been correlated with parameterized equations, and may not yet appear in the DIPPR® 911 electronic database. The results of the extractions are summarized in master database table (VALUES.DB). The coefficients of the temperature dependents are also contained in the VALUES table.

4.3.3 Block 4 Vapor-Liquid Equilibrium

In addition to data sources typically used by chemists, chemical engineers, and environmental scientists, the Project 911 team has broadened the search for partitioning/equilibrium data to medicinal and pharmacological journals. The latter are particularly good sources for Quantitative Structure Activity Relationships (QSAR) predictive methods. The team is also investigating collections of data compiled by U.S. EPA contractors, as well as the software data files associated with process simulator packages and wastewater fate and transport models. Table 4 summarizes the primary literature citations used to date.

4.3.4 Block 5 Fire and Explosions

A large amount of high quality data are available from international reference material. Project 911 has obtained data from: A.N. Baratov, A.Ya. Korol'chenko, G.I. Kravchukh, et al., *The Handbook for Flammability and Explosability of Chemicals and Substances, and Means of Extinguishing*, Khimia, Moscow, 1990; and K. Nabert and G. Schön, *Sicherheitstechnische Kennzahlen brennbarer Gas and Dampfe*, Deutscher Eichuerlag Gmbtl., Berlin, 1963. The Russian translation was conducted by a native speaker, who translated the introductory material, a summary of methods used in the compilations, and the data. Project 911 found this compilation to be a very rich source of Fire and Explosion data. Fire and explosion data were also translated from the German handbook as well as data for General Physical Properties. A list of principal sources is provided in Table 4 (Block 5).

4.3.5 Block 6 Sensory, Health & Toxicity Impacts and 2d Bioconcentration Factors

In addition to the Wilsondisc library search described in Section 4.3.1, the reference sections of collected papers were also searched for relevant titles in the area of Aquatic Toxicity and bioconcentration factor. Consequently, papers were collected from over 40 journals and other research compilations. Journals checked regularly are listed in Table 4 (Block 6). An on-line Current Contents search of the tables of contents of journals not received at MTU is performed periodically.

In addition, the U.S. Environmental Protection Agency's (EPA) Aquatic Toxicity Information Retrieval Data Base (AQUIRE) was purchased from the National Technical Information Service (NTIS). This source contains ecotoxicology data, literature references, and EPA data quality codes.

The AQUIRE ecotoxicology data are distributed over nine files: master record file with pointers to data in the other eight files; test chemical purity; concentration of the chemical in water and/or bioconcentration factor and confidence interval; test temperature, hardness, dissolved oxygen, alkalinity, and pH; species name code; CAS number for each record; CAS numbers and corresponding chemical names; comments; references. An additional nine files define the structure of the nine corresponding data files.

These 18 files were uploaded from magnetic tape to MTU's Sun network and converted to text files from VMS-VAX format. A search program was developed to extract all the AQUIRE ecotoxicology information, EPA quality codes, and literature references for a specified species/chemical combination. Each record has 64 fields. The output may be viewed on screen on a Sun terminal, or it can be imported into a spreadsheet or database program as a text file.

A final program is used to aid in condensing the 64 AQUIRE fields into 20 Project 911 fields, reformatting the AQUIRE citations, and translating the EPA review codes into Project 911 rating codes. Removal of key violations (where a paper has more than one data point per species/chemical/citation combination) and consolidation of the 7, 60-character AQUIRE comment fields into 1, 120-character 911 field must be performed manually. Finally, when AQUIRE reports a range for the temperature, pH, or hardness field, the median value is reported and the range is manually entered as a \pm value in the Project 911 Comments field.

5.0 Evaluation Criteria

5.1 Quality Assurance

Every effort is made to ensure that the thousands of pieces of data in the Project 911 database are recorded accurately. The quality assurance procedures for the data entry process are threefold; 1) a screening by the reviewer, 2) a screening of the data entry, and item by item check where necessary, and 3) a review for consistency with data from other source materials.

The first review is conducted by the technical reviewer. This initial evaluation consists of an examination of the data generation and collection procedures which are outlined in the literature. The paper is then rated based on the experimental procedures followed.

The second review is conducted by the data entry personnel. The data are transcribed from the literature source onto a data entry form and it is determined if all necessary information is present. The data entry form is then entered directly into an Excel© spreadsheet. A printout of the spreadsheet is compared to the original publication prior to incorporation into the Project 911 database.

The third review is a quantitative assessment for consistency with other data, thermodynamic relationships, or other theoretical principles. A Delphi based error flagging program utilizing Statistical Quality Control (SQC) techniques has been developed which can perform an error analysis on data files for which the units have been converted to a common units system. The program uses the highest rated value as the basis for the test, which is referred to as a "Level 1" test by Project 911 personnel. Presently, any value exceeding the percent error defined for that particular property is labeled as an outlier and is reviewed in detail. The percent error is set differently within each different physical property depending on the general quality of the data available. Table 16 summarizes the percent errors used for the various properties. The values that are flagged are double-checked with the literature for entry errors. If the value is correctly entered but greatly disagrees with the other reported values at the same temperature, an "AF" code (Anomaly flagged) note is placed in the Anomaly column of the project 911 database. If the current highest rated data value does not agree with other available data, the highest rated data point is labeled as "AD" (Anomaly Dropped) in the Anomaly column, the rating is lowered, and a new highest rated data point is determined. The SQC software is then used to compare all available data to the new highest rated data point. During the SQC review process, MTU investigators are asked for any adjustments to the evaluations or ratings based upon agreement with other work, past experience with a particular data source, or other factors. All values which have undergone Level 1 scrutiny are then coded with a "Q1" in the Keywords column. Additional information on the results of the SQC analysis has been made available to Project 911 sponsors at the semi-annual steering committee meetings. The use of the SQC software to do thermodynamic based comparisons (Level 2 check) across several physical properties (e.g., Henry's Constant should be greater than or equal to the ratio of Vapor Pressure to Aqueous Solubility) is ongoing. Those data points that have completed a Level 2 analysis are labeled with a "Q2" in the Keywords column.

5.2 Qualitative Review

A required component of Project 911 is to provide a critical evaluation and quality assessment of each of the data points in the data compilation. The Project 911 investigator evaluates the data source material based on 5 basic criteria (Table 8) where each is ranked on a scale from 0 to 2. This system provides that well documented primary sources receive a higher score than incompletely documented or secondary sources. Separate evaluation criteria for BOD and Soil/Water Partition Coefficient as stated in Section 4.3.1 are shown in Table 6 and Table 7. As mentioned previously, the data and data analysis for the Acute Aquatic Toxicity Block are managed differently from the engineering parameters and therefore also have separate evaluation criteria as illustrated in Table 9.

The data from Project 801 automatically receive a rating higher than the data gathered by the Project 911 team because of the rigorous data entry, testing and quality checking procedures. The quality codes used by Project 801 have been incorporated into the Project 911 data management and tracking system. However, they are not completely compatible. To make them compatible, the Project 801 ratings were translated into the same scale as Project 911 ratings. Project 911 ratings range from 0 to 10. The Project 801 ratings were given ratings which ranged from 11 to 14 with 14 being the highest rating. This was performed by allocating points to Project 801 coding as shown in Table 10. This provided the ability for the software product to preferentially choose Project 801 values over Project 911 values. In the cases where Project 801's type of data is predicted, defined, smoothed, unknown, or extrapolated, the rating is left blank as stated in Table 10. In these cases, Project 911 data are chosen. Project 911 data are also chosen preferentially

in some Fire and Explosion data values because of past complications in Project 801 data. Any changes to the Project 801 ratings are communicated to the Project 801 staff.

Data in AQUIRE are rated by the EPA on a 5-number scale. The AQUIRE Technical Support Document defines these review codes as follows:

- 1 = Thorough methods and documentation;
- 2 = Documentation generally satisfactory, but one or more of the pieces of information are missing from either the methods or results section, such as control information or chemical concentrations are unmeasured;
- 3 = Insufficient methods and results documentation;
- 4 = Indicates data is available only in a limited format, such as conference proceeding abstracts or English language abstracts for untranslated international papers;
- 5 = This file contains laboratory data for acute toxicity of organic chemicals, using a single test species (30-day fathead minnows). The information was transferred via computer files and was not subjected to the standard AQUIRE procedures. All test results, including data not available on-line, are available in five volumes titled: Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), (Center for Lake Superior Environmental Studies; University of Wisconsin-Superior; 1984, 1985, 1986, 1988, and 1990).

Review codes are converted to Project 911's ten-point scale rating codes as follows: 1 = 9; 2 = 5; 3 = 1; 4 = 0; 5 = 10.

Ratings for AQUIRE in general are not based on an author's reputation. Rather, they are based on subjective impressions of Project 911 investigators about the data set based on the completeness of detail in the experimental methods. A data digest is attached to each paper reviewed. If key experiment details are not available (such as: test temperature; whether values reported are nominal or measured, especially for volatile organics; whether system was static or flow through; whether dosing was constant or intermittent; whether controls were missing; whether pH was reported, especially for metals; etc.) the rating will be low because the reliability to the end user is reduced. Lower rated values should always be used only with caution.

5.3 Quantitative Reviews

The Qualitative Review rating system provides an initial screen of data but is not intended to replace more quantitative analysis by each investigator. Once enough data have been received and reviewed, a more quantitative evaluation for physical and thermodynamic consistency is conducted. The first evaluation is a visual inspection for "smoothness" and consistency. Consistent values from differing data sources are considered more trustworthy than values which are scattered. Tests for accuracy include investigator examination of the methods by which the data were obtained to see if acceptable experimental and quality assurance procedures were followed. The investigators look particularly for analytical methods which can be traced back to quantitative primary standards.

The data sets are also examined for their consistency with theoretical relationships and empirical predictive methods of Project 912. Since the Project 911 effort concentrates on collecting data on many interrelated properties, data from more than one property code can be checked to confirm their consistency with simple theoretical relationships or more complex interactions. After such quantitative analysis, the investigators assign a final quality code to the data which then can be drawn into the software product.

5.3.1 Statistical Quality Control (SQC)

Prior to December of 1996, the date at which time SQC was applied to the Project 911 database, a manually intensive program using QBASIC language performed similar tasks. The QBASIC Program was a quantitative assessment for consistency with other data, thermodynamic relationships, or other theoretical principals. It consisted of two steps: conversion of units and percent error analysis, both of which utilize computer programs generated for the Project 911 project. The original data collected from the literature are reported in many different units and entered into

the database in the original units. An automated unit conversion routine was employed to put the data into consistent units (SI, or user-defined).

A more automated system is now employed using a Windows software utility to review the Project 911 database. This software applies SQC techniques to compare data values in some of the same ways as the older QBASIC routines. The SQC program uses the highest rated value as the basis for the test. The internal comparison to the highest rated data value for a particular chemical and property code combination is referred to as a "Level 1" SQC review. Presently, any value exceeding a defined percent error tolerance value is identified as an outlier in the output file. The percent error tolerance value is set differently for each property within the different property blocks depending on the general quality of the data available, e.g. 10% error for most of Block 3 and 50% error for Block 6. The outlying values are double checked with the literature to identify entry errors. If the value has been correctly entered, but greatly disagrees with the other reported values at the same temperature, a note is placed in the comments indicating such. The project investigators are asked for any adjustments to the evaluations or ratings of that particular entry based upon "agreement with other work."

All values which have undergone a quantitative review are coded with a Q character in the Keywords column of the VALUES table. The data analyzed using the older QBASIC routines received a code of "Q" when they passed the review criteria. The newer SQC system uses codes of "Q1" for data values passing the Level 1 check, and "Q2" for passing a Level 2 review, as defined below.

The Level 2 data evaluation is a comparison of physical properties using additional SQC criteria. It involves the comparison of data values for a given property code to another property, an algebraic calculation involving one or more properties, or comparison to a specified range. Examples of Level 2 data evaluations are confirming that all melting points are less than their corresponding normal boiling points, or that the Henry's Law Constant is greater than or equal to the ratio of the vapor pressure to solubility. Data values successfully completing a Level 2 review are designated in the Project 911 software with a "Q2" quality code.

5.3.2 Classification of Errors Using SQC

When performing an analysis using the SQC system, the "actual error" rate and "flag" rate must be carefully separated. Each data value flagged by the SQC software is examined and analyzed to determine the classification or type of error. All data that successfully pass the SQC check will have a "Q1" or "Q2" entered into the database column which will be seen in the Project 911 software product.

For those data values that do not pass the SQC criteria, the original article is reviewed so that an error code can be attached to the data value. Those values receiving an error code of "AF" (Anomaly Flagged) or "AD" (Anomaly, Rating Dropped) are reviewed by an MTU investigator to determine their accuracy, and a recommendation made as to their disposition. Data values that are determined to be data entry mistakes will be flagged as "DE" (Data Entry Error) and corrected in the Project 911 data files.

Values that have been flagged with an "AF" code are values that are outside the tolerance range when compared to the highest qualitatively rated data value for a particular chemical and physical property, but the value has been correctly transcribed from the original literature reference. An anomaly flag of "AD" is used when a number of literature sources report data values that are in agreement with each other, but are outside the tolerance range when compared to the highest qualitatively rated data value. The original literature references are reviewed, and a determination is made as to whether a transcription error has occurred with the highest rated value, or whether different experimental conditions or techniques were used for the various literature sources. A reliability assessment is also made about the authors of the literature source, based on the experience of MTU investigators. If an error in transcription has occurred, the highest rated value is corrected and labeled "DE." If it is found that the highest rated value uses a less reliable experimental technique, or there are questions about the quality of work based on the authors, the highest rated value is labeled "AD", the qualitative numeric rating is lowered, and the SQC system is run again to check the data against the new highest rated value. The "DE", "AF", and "AD" codes are not displayed within the Project 911 DOS software product, but they are documented by the SQC tracking system and are available in the Paradox format sponsor release datafile.

Data values that are flagged with an error code of "DE" are rechecked by the SQC system during the next SQC review of the Project 911 database. At that time, it is anticipated that the error will not be repeated, and the values will receive a rating of "Q1" or "Q2". An Anomaly Tracking Form is kept with the database reference article so that MTU staff have a complete record of any changes made to data values from a particular reference. The output files from the SQC system, which are a compilation of all errors identified for the criteria checks run, are logged and dated in a notebook and maintained in a file according to the physical property on which the SQC analysis was completed. The SQC output files can be cross referenced to the individual data errors on the Anomaly Tracking Forms attached to each Project 911 database reference paper. Table 19 contains the current results from the SQC Review System.

6.0 Data Tracking and Management

6.1 General Overview

An integral part of the compilation effort is to organize into an efficient software system the thousands of reference materials and tens of thousands of pieces of data. Ideally the organizational system would allow the Project 911 team quick and easy access to the data as well as data source materials and provide a mechanism to download the data for quantitative review and for the final software product. To accomplish this task the Project 911 team, with the assistance of a software and database consultant, developed the data management and tracking system based on a relational database approach. This tracking database is designed around a Paradox[®] driver and customized according to the needs of Project 911.

The purpose of the tracking database is to provide a method to identify, track, and store information about the Project 911 chemical and property lists, data source materials, data values, units, and qualitative rating. In order to efficiently design the database, these types of information were separated into tables and key relationships among them were established. For an efficient database design, relationships are made between categories by assigning a key field to the categories one wishes to relate and by assigning an arbitrary numbering or coding system to that key field. In the tracking database, the chemical, property, and source materials lists are separate tables, each with an assigned number and/or code. The values for each chemical and property combination are kept in a separate table and related to the chemical, property, and citation lists by the appropriate numbers and codes. In this manner, the data source material can be sorted, tagged and downloaded independently of the data associated with it. Conversely, each piece of data is identified by its source.

6.2 Datafiles Description

The data source tables are distributed to project sponsors on an annual basis in the Paradox[®] format. A brief description of each table and its purpose and structure is given below.

The VALUES table is the primary data table which contains the chemical number, property code, quality code, citation number, data value, unit, comment, and rating. The structure of the table is provided in Table 11 with a brief description of what each field contains. The data contained in VALUES is quantitatively assessed for errors and is in the original units given in the source material. Since this table is the primary data table a multitude of forms, scripts, and reports are generated from it. These are described in greater detail below.

The CITATION Table contains the data about the source material, i.e. the author, title, journal or book, and publication date. The Project 911 data entry personnel have developed a standard format for entering data into this table from different data sources. This format is not completely compatible with the references which are obtained from Project 801 data files. The Project 801 reference numbers have been given paper numbers starting from 80000 to distinguish them from Project 911 data sources. In addition to these Project 801 datafiles, a number of calculations have been performed over the course of Projects 911 and 912 by different researchers which must be documented. Therefore it has become necessary to develop a system of identifying these with distinct citation numbers. These citation numbers are identified by project number, year, and sequence. For example, the first set of calculations performed by Project 911 in the year 1995 are given the number 911951. The second set would be designated 911952, and so on. The year 1995 follows the project year: June 1, 1995 - May 31, 1996. The structure of the CITATION table is given in Table 12. This table is also used in the Project 911 DOS Version 6.0 software described below.

The PROPERTY Table contains information about the Project 911 properties. This includes the property code name, reviewer name, and default units for that property. A "Y" indicates that the property is temperature dependent. This table is used in the Project 911 commercial software and the structure is given in Table 13.

The CHEMICAL Table contains information about the chemical list in Project 911. The structure and information in the CHEMICAL Table are provided in Table 14. The CHEMLIST Table has almost the same structure and provides the same information as the CHEMICAL Table except the CAS numbers have the hyphens in the appropriate locations. These provide a valuable link between the software and the VALUES table because they contain the CAS number and VALUES table does not.

The CONVUNIT Table contains the unit conversion information. It contains fields listing the default units and original literature units, and the multipliers and addends required to convert between the two. The structure is provided in Table 15. This table is used in three locations; 1) in the batch program which draws down the best data for the Project 911 software and builds the VALUESF table (discussed below); 2) in the batch program which converts the units of a temporary table to the default units; and 3) in the units conversion routine in the Project 911 software product. The unit conversion data are defined by the Project 911 staff and conversions may be added or changed as necessary to satisfy user needs.

To aid in the data entry process, a temporary table is used. This table, called GENRPT, is identical in structure to the VALUES table. In Paradox 5.0, any number of reports of varying styles may be generated based on one table. Three such reports are used to print out data which have been entered and formatted in the Project 911 database. They are: GENRPT for Blocks 1-5 non-temperature dependent data, TOXIC for Block 6 and TEMPDEP for all temperature dependent data.

Another temporary table is the CMPREPRT table. Based on the data which are entered in the VALUES table, this completion report is an output of the chemicals and property codes for which there are data entered. It is a good method of determining where there are holes in the database which need to be filled. The completeness report identifies where at least one value has been entered for each chemical for each property with an "X". A "-" illustrates where there is an attached comment in the literature screen but no value in the Value field. A summary of the number of data points per property is generated at the end of the report. The purpose of this report is to identify gaps in data, and set priorities for data entry and data searches. This table is furnished upon request.

6.3 Data Entry System

In the initial organization of Project 911, a data entry system was requested from the software consultants. The purpose of this system was to provide a user friendly and "foolproof" method for data entry. Data entry template software and forms were custom designed in Paradox[®] for Project 911. Paradox[®] tables were set up to easily update the VALUES, CHEMICAL, CITATION, PROPERTY, and CONVUNIT tables. These tables allow the data entry personnel to enter, delete or modify records which have been entered.

A system has been developed to track and handle data source material and to provide a uniform method for data entry. Once a data source has been located, it is immediately attached to a DIPPR[®] Tracking Form (Figure 1). A Citation Entry Format (Figure 2) is used to provide uniform entry for varied material such as journal articles, books, chapters from books, government or industrial reports, or staff-generated materials. The original tracking form is forwarded to the appropriate reviewer. The reviewer rates the paper, offers comments concerning the quality of the data, and notes the chemicals and properties contained in the paper.

The data entry personnel then check the assigned chemical #'s against the chemical list and copy the appropriate (highlighted) data from the publication to data entry forms (Figure 3). The data are then entered directly into an Excel[™] spreadsheet. A printout of this spreadsheet is then double checked against the original publication for any transcription errors. The data are then imported into Paradox[®] and entered directly into the VALUES Table. Once the data have been entered into the data base, the source material along with the data entry form and Excel[™] printout of the exact data which have been entered into VALUES is filed by citation number in a central file "library."

The data for property Block 6, Acute Aquatic Toxicity, is very different from the engineering related data so the values template is used in a slightly different manner from the other property blocks. This data entry format is shown in Figure 4.

7.0 Temperature Dependent Properties

Several of the properties to be evaluated in Project 911 show temperature dependency as noted in Table 1. The tracking database handles these properties by accepting equation numbers and correlation coefficients as identified under the VALUES table structure (Table 11). All temperature dependent coefficients are developed using temperature units of Kelvin. The temperature range for which the correlation is developed is placed in the value and temperature fields for lower and upper limits (T_{\min} and T_{\max}), respectively. Equations used in the Project 911 database are assigned the same numbers as used by Project 801. All sets of coefficients are assigned a citation number which identifies the investigator(s) who developed the coefficients.

Although the source material for temperature dependent data is tracked in the tracking database, the database is not designed to accept multiple values for the same chemical, property, and citation. Thus the tracking database cannot be used as the data repository for the data to determine new correlations. This is done via an Excel® spreadsheet application for which a standard format has been developed.

Where it is appropriate, more than one correlation may be developed to accommodate different behavior in different temperature regimes. In those cases, more than one record is added to the tracking database.

An ongoing effort is finding data for the temperature dependent properties to enlarge our data sets for developing temperature dependent correlations. As a rule of thumb, the DIPPR® 911 project will employ the DIPPR® 801 format for all common properties. For data sets of properties not in common with DIPPR® 801, or those covering a different range, we have developed two additional equation forms and have included them in the Project 911 database as equations 200 and 201. Correlation coefficients for a specific chemical and property are being continually added to the Project 911 database. A minimum of ten data points is needed before we use curve fitting software to generate correlation coefficients. We are continuing our effort to use Project 912 predictive methods to generate predicted data values to supplement experimental data sets that do not meet the minimum requirement of 10 data points.

As decided at the June 1994 DIPPR® 911/912 meeting at MTU, and reconfirmed at the June 1999 meeting at MTU, we are concerned principally with a temperature range of 250 to 500 K. Literature data that fall outside this temperature range are still used in developing the coefficient correlations, if the data fit the appropriate equation form. MTU personnel review all temperature dependent data plots for expected curve shapes. Values for T_{\min} and T_{\max} are selected based on curve shape, temperature range of available data, and to eliminate any inflection points on the plots of temperature dependent data. It is not recommended that a user of the Project 911 database extrapolate a set of coefficients to a temperature outside the range of T_{\min} to T_{\max} .

8.0 Estimation Methods

Even after a thorough literature search, gaps still remain for many properties and chemicals. These gaps are identified by running a completion report as described above. Various estimation methods are utilized to fill these gaps. Values developed from estimation methods are identified in color in the Project 911 software product and details on the method used are provided in the comments. The estimation technique methods that have already been used in the Project 911 software product are summarized in Table 17 and some are described in more detail briefly below. Some data gaps remain to be filled using appropriate, validated estimation techniques. Full documentation of the methods used and their selection criteria are to be reported in the 1994 DIPPR® Project 912 Progress Report.

8.1 Biochemical Oxygen Demand

BOD is estimated by substituting it for the ThOD in the equation below. This provides a potentially overly optimistic value for BOD. This is especially true because even if a chemical is readily biodegradable, its ThOD and

ultimate BOD may be similar, but its 5-day BOD may not. Therefore a comment is inserted which states "This BOD₅ value is estimated from the chemical's ThOD and may be overly optimistic of its biodegradability."

8.2 Chemical Oxygen Demand

COD is a measure of the oxygen consumed by oxidizing a sample under harsh oxidizing conditions of the COD test. Under these conditions COD was estimated for the following classes of compounds by equating it to the ThOD

$$\text{COD} = \text{ThOD}$$

ThOD is the theoretical oxygen demand, or the amount of oxygen stoichiometrically required to oxidize an organic chemical to end products such as CO₂ and H₂O. Calculation of ThOD is explained in Section 8.3.

Aromatic compounds: phenols, chloroquinones, nitroquinones, aromatic acids, aromatic amines, aromatic thiols, polycyclic aromatic hydrocarbons. The user can have 90% statistical confidence that the COD for these compounds will be within the range of 0.91 * ThOD and 1.0 * ThOD.

Nonaromatic compounds: esters, ethers, nitriles, aldehydes, ketones, acids, glycerine esters. The user can have 90% statistical confidence that the COD for these compounds will be within the range of 0.92 * ThOD and 1.0 * ThOD.

If the COD for a chemical, not included in the above mentioned classes, is required, measure the value if the accuracy is crucial. The COD test is relatively quick (several hours) and inexpensive. Many companies have the facilities to perform this test in the labs associated with their wastewater treatment plants. If the correct oxidation end products are assumed, the experimental COD should never be greater than the ThOD. Therefore COD = ThOD will always be a conservative estimate of oxygen demand.

8.3 Theoretical Oxygen Demand

Theoretical Oxygen Demand (ThOD) is estimated for specific organic compounds based on the stoichiometry of a balanced chemical reaction which describes the reaction of the organic chemical with oxygen to produce theoretical inorganic end products. The following guidelines were utilized to determine the reaction's inorganic end products. Organic chemicals which contain only carbon and hydrogen were assumed to be converted to CO₂ and H₂O; organic chemicals which contain carbon, hydrogen, and sulfur were assumed to be converted to CO₂, H₂O, and SO₄²⁻; organic chemicals which contain carbon, hydrogen, and phosphorus were assumed to be converted to CO₂, H₂O and orthophosphate forms (i.e., H₂PO₄⁻ or HPO₄²⁻); organic chemicals which contain carbon, hydrogen, and halogens (e.g., chlorine, bromine) were assumed to be converted to CO₂, H₂O and the respective halogen ion (e.g., Cl⁻, Br⁻); and, organic chemicals which contain carbon, hydrogen, and nitrogen were assumed to be converted to CO₂, H₂O, and ammonia. In the later case the oxygen demand associated with nitrogenous theoretical oxygen demand was found by showing the stoichiometric amount of oxygen required to oxidize the ammonia to nitrate.

An exception to these rules is chemicals with nitro or nitroso groups. The nitrogen in nitro or nitroso groups will be converted to ammonia under anaerobic, reducing conditions. Under aerobic conditions the nitro or nitroso groups will go directly to nitrite and subsequently to nitrate. In order to calculate the carbonaceous ThOD for chemicals with nitro or nitroso groups, the stoichiometry was drawn out by hand assuming nitro or nitroso groups go to nitrate and all other nitrogen goes to ammonia. For combined carbonaceous and nitrogenous oxygen demand all the nitrogen was assumed to go to nitrate.

8.4 Partitioning/Equilibrium Parameters

To fill data gaps in Blocks 2 and 4, the UNIFAC activity coefficient model is being used to provide estimates for those properties involving nonideal liquids. From fundamental principles, all the partitioning and equilibrium properties are functions of liquid-phase activity coefficients. Under DIPPR[®] Project 912, a software algorithm has been developed to implement phase equilibrium and partitioning calculations based on UNIFAC activity coefficients. Three UNIFAC parameter sets are available in the software: (1) a published UNIFAC-VLE set, derived primarily from vapor-

liquid equilibrium data; (2) a published UNIFAC-LLE set recommended for liquid-liquid equilibrium calculations; and (3) the UNIFAC-ENV, a new parameter set developed at MTU and optimized for environmental systems, e.g. dilute aqueous mixtures. Testing UNIFAC against data compiled under Project 911 has led to a preferred choice of parameter sets for each property. This ranking is described below.

8.4.1 Solubility of a Chemical in Water

Mutual miscibility can be calculated rigorously for any partially miscible binary mixture by assuming solute-rich and solvent-rich phases in contact at equilibrium. In such a case, the solute is defined as the dissolved organic and the solvent as water. For a binary system, equal solute and solvent chemical potentials in the two phases at equilibrium give rise to two coupled nonlinear algebraic equations. The two unknowns are the organic solubility in the water-rich phase and the water solubility in the organic-rich phase. These quantities are found numerically by a computer program based on the UNIFAC liquid-phase activity coefficient model.

8.4.2 Solubility of Water in a Chemical

Most models of aqueous solubility focus on the dissolved solute and ignore the mutual miscibility of the solvent in a solute-rich phase at equilibrium. However, the phase equilibrium (activity coefficient) approach outlined earlier has the advantage of predicting both ends of the binary miscibility tie-line. The endpoints of the tie-line are referred to as the solubility of the chemical in water and of water in the chemical, respectively.

Recommended UNIFAC Parameters for Solubility: The UNIFAC-LLE parameter set is recommended as the first choice and UNIFAC-ENV as the second choice. Test calculations have shown comparable accuracy for the two sets. The UNIFAC-VLE set is used when both LLE and ENV parameters are missing.

8.4.3 1-Octanol/Water Partition Coefficient (K_{ow})

A UNIFAC-based model of 1-octanol/water partitioning is an extension of the general procedure for liquid-liquid equilibrium calculations. UNIFAC activity coefficients permit phase equilibrium calculations for the binary 1-octanol/water system. Because the two components are almost immiscible in each other, two phases will form: an 1-octanol-rich phase containing dissolved water, and a water-rich phase containing dissolved 1-octanol. Once the phase compositions are known, infinite dilution activity coefficients for a third component in each phase can be calculated. The 1-octanol/water partition coefficient is directly proportional to the ratio of the infinite dilution activity coefficients for a third component distributed between the water-rich and 1-octanol-rich phases.

Summarizing, the 1-octanol/water partition coefficient is calculated from an activity coefficient model (e.g., UNIFAC) by a series of steps:

- (1) Perform a binary 1-octanol/water equilibrium calculation at the temperature of interest. Component 1 is 1-octanol, component 2 is water, and component 3 is the distributing chemical. The 1-octanol-rich phase is designated Phase I, and the water-rich phase is designated Phase II.
- (2) Define K_{ow} as the ratio of the concentrations of a third component distributed between the 1-octanol-rich and water-rich phases. As the mole fraction of the distributed chemical in the two phases approaches zero (i.e., approaches infinite dilution of component 3), the K_{ow} concentration ratio approaches a constant value.
- (3) Determine the total molar densities of Phases I and II from the calculated phase compositions. The concentration of component 3 in each phase is the product of its mole fraction and the total molar density of that phase.
- (4) Use the calculated compositions of Phases I and II to estimate the activity coefficients of component 3 at infinite dilution in each phase. At equilibrium, component 3 must have equal fugacities in the two phases, so the mole fraction ratio of component 3 in Phases I and II is equal to the activity coefficient ratio in Phases II and I.

(5) Calculate K_{ow} as the ratio of total molar densities of Phases I and II multiplied by the ratio of infinite dilution activity coefficients of component 3 in Phases II and I. The CLOGP software was also used as a source of estimated values.

8.4.4 Soil/Water Partitioning

Soil water partition coefficients normalized to organic carbon, K_{oc} , were estimated from the following relationship which relates K_{oc} to K_{ow} . This method is valid for chemicals which follow: $1.7 \leq \log K_{ow} < 7.0$.

$$\log K_{oc} = 0.903 \log K_{ow} + 0.094; r^2=0.91$$

8.4.5 Bioconcentration Factor

Estimates are taken from an empirical correlation to $\log_{10}K_{ow}$ presented by G. Briggs, *Journal of Agricultural and Food Chemistry* 29:1050-1059 (1981), or if molecular connectivity indices are available, then R. Kock, pp.207-222 in K.L.E. Kaiser (ed.) *QSAR in Environmental Toxicology*, D. Reidel Publishing Co., Dordrecht, Netherlands (1984), or if solubility is available, then E.E. Kenaga and C.A.I. Goring, pp. 78-115 in J.G. Eaton, P.R. Parrish, and A.C. Hendricks (eds.) *Aquatic Toxicology: Proceedings of the Third Annual Symposium on Aquatic Toxicology*. ASTM STP 707, ASTM, Philadelphia, PA (1980).

8.4.6 Activity Coefficients

To fill data gaps, the UNIFAC algorithm is being used to calculate activity coefficient estimates from chemical structure. The DIPPR[®] Project 911 compilation contains infinite dilution activity coefficients for the chemical in water and for water in the chemical. Because the Henry's constant data upon which UNIFAC-ENV was derived is considered to be of high quality, the infinite dilution activity coefficients for the chemical in water come from the UNIFAC-ENV parameter set. The UNIFAC-VLE and UNIFAC-LLE parameters are used as second and third selections, respectively. Generally, we lack validated data for water solubility in chemicals, so the activity coefficient of water in a chemical is computed from the standard UNIFAC-LLE model. The UNIFAC-VLE parameters are used as a second estimation source, while the UNIFAC-ENV model is used as a last choice.

8.4.7 Henry's Law Constant

This is the product of the infinite dilution activity coefficient and the pure component vapor pressure. The latter is obtained from the temperature-dependent equation in DIPPR[®] Project 801 or from data compiled under DIPPR[®] Project 911. The UNIFAC-ENV parameter set is the first choice for calculating the infinite dilution activity coefficient, followed by UNIFAC-VLE and UNIFAC-LLE.

9.0 Database Software (Sponsor Version and ENVIRON 2001)

9.1 Description

A completed objective of Project 911 was to provide a DOS software product incorporating features such as CAS number indexing, literature citations, quality codes, and temperature dependent graphing capabilities. The first version of this software was developed during the 1992 effort. The software was written in C language, based on Paradox[®] engine, with Hiscreen Pro by Softway screen package, and Quinn-Curtis Science and Engineering graphic package. The product was designed to run on any 286 or higher IBM compatible computer with 640 RAM and a VGA or EGA monitor. The software was mouse compatible. The final DOS software product (Sponsor Version 6.0) was released to the Project 911 Steering Committee in July 1998.

Future public dissemination of Project 911 data in electronic form will be done through a third party vendor, EPICON International (www.epcon.com) within a product entitled ENVIRON2001[®]. ENVIRON2001[®] utilizes a MS Visual Basic[™] Version 5.0 user interface. The Paradox[®] format database structure that has been in use since 1992 by Project 911 has been retained for purposes of data entry, data manipulation, and overall database structure. The VALUESF,

CITATION, and CHEMICAL Paradox© format files are translated into MS Access™ format for easier use with the Visual Basic™ interface. The user help file for ENVIRON 2001 gives details of use which should be examined before using this product.

9.2 Software Tables

Project 911 sponsors continue to receive the Project 911 database prior to public release. At present, the sponsors receive all data in Paradox© format as described in the tables contained within. The primary data table, VALUES, contains all data collected within the Project 911 effort. The highest rated data is extracted through a batch utility program that selects the highest rated value for each chemical and property and converts the values into the default unit system. The resulting table is called VALUESF. Like the VALUES table in the data management software, VALUESF contains the value, unit, property code, chemical number, citation, comment, rating and other information associated with the data points. VALUESF contains an additional field which is used for determining the highest quality code from the VALUES table. This data table is used in the ENVIRON 2001 commercial product.

Table 1: Property List

Property Code	Project 911 Description	Technical Steering Committee Description
Block 1	Oxygen Demand	Oxygen Demand
1a	Biochemical O ₂ Demand (BOD)	Biochemical Oxygen Demand (BOD)
1b	Dichromate Chemical O ₂ Demand (COD)	Chemical Oxygen Demand (COD)
1bp	Permanganate Chemical O ₂ Demand (COD)	Chemical Oxygen Demand (COD)
1cc	Theoretical O ₂ Demand, Carbonaceous	Theoretical Oxygen Demand
1cn	Theoretical O ₂ Demand, Combined (C+N)	
Block 2	Partitioning Parameters	Partitioning Parameters
2a	1-Octanol/Water Partitioning	1-Octanol/Water Partition Coefficient
2b	Soil/Water Partitioning (K _p)	Soil/Water Partition Coefficient
2c	Organic Carbon/Water Partitioning (K _{oc})	Organic Carbon/Water Partition Coefficient
2d	Bioconcentration Factor	Bioconcentration Factor
Block 3	General Physical Properties	General Physical Properties
3a	Molecular Weight	Molecular Weight
b	Liquid Density at 298.15 K	Liquid Density at 298.15 K
3bt	Liquid Density	Liquid Density vs. Temperature
3c	Solubility in Water	Solubility in Water
3d	Melting Point	Melting Point
3e	Normal Boiling Point	Normal Boiling Point (Normal BP)
3f	Vapor Pressure at 298.15 K	Vapor Pressure at 298.15 K
3g	Vapor Pressure	Vapor Pressure vs. Temperature
3h	Molecular Diffusivity in Air	Molecular Diffusivity in Air
3i	Molecular Diffusivity in Water	Molecular Diffusivity in Water
3j	Vapor Viscosity	Vapor Viscosity vs. Temperature
3k	Liquid Viscosity	Liquid Viscosity vs. Temperature
3l	Surface Tension at 298.15 K	Surface Tension at 298.15 K
3lt	Surface Tension	Surface Tension vs. Temperature
3ml	Thermal conductivity, liquid	Thermal Conductivity, liquid vs. Temperature

Table 1: Property List (cont.)

Property Code	Project 911 Description	Technical Steering Committee Description
3mv	Thermal conductivity, vapor	Thermal Conductivity, vapor vs. Temperature
3n	Enthalpy of Formation at 298.15 K	Enthalpy of Formation at 298.15 K
3o	Liquid Heat Capacity	Liquid Heat Capacity vs. Temperature
3p	Vapor Heat Capacity	Vapor Heat Capacity vs. Temperature
3q	Critical Temperature	Critical Temperature
3r	Critical Pressure	Critical Pressure
3s	Critical Volume	Critical Volume
3t	Enthalpy of Vaporization at 298.15 K	Enthalpy of Vaporization at 298.15 K
3tt	Enthalpy of Vaporization	Enthalpy of Vaporization vs. Temperature
3tz	Enthalpy of Vaporization at Normal BP	Enthalpy of Vaporization at Normal BP
Block 4	Vapor-Liquid Equilibrium	Vapor-Liquid Equilibrium
4a	Activity Coefficient of Chemical	Activity Coefficient in Water
4b	Activity Coefficient of Water	Activity Coefficient of Water in Chemical
4c	Aqueous Henry's Law Constant	Henry's Law Constant for Water Mixtures
Block 5	Fire and Explosion Parameters	Fire and Explosion Parameters
5al	Lower Flammability Limit in Air	Flammability Limits in Air vs. Temperature
5au	Upper Flammability Limit in Air	
5b	Flash Point	Flash Point
5c	Autoignition Temperature	Autoignition Temperature
5d	Enthalpy of Combustion at 298.15 K	Enthalpy of Combustion at 298.15 K

Table 1: Property List (cont.)

Property Code	Project 911 Description	Technical Steering Committee Description
Block 6	Sensory, Health and Toxicity Impacts	Sensory, Health, and Toxicity Impacts
6a-6i	Acute Aquatic Toxicity	Aquatic Toxicity
6ab	Fathead minnow, 48h, EC50	
6ac	Fathead minnow, 96h, EC50	
6ba	Fathead minnow, 24h, LC50	
6bb	Fathead minnow, 48h, LC50	
6bc	Fathead minnow, 96h, LC50	
6ca	Daphnia magna, 24h, EC50	
6cb	Daphnia magna, 48h, EC50	
6da	Daphnia magna, 24h, LC50	
6db	Daphnia magna, 48h, LC50	
6fa	Salmonidae, 24h, LC50	
6fb	Salmonidae, 48h, LC50	
6fc	Salmonidae, 96h, LC50	
6hc	Mysid, 96h, LC50	
6i	Other	

Table 2: Default Units and Mathematical Expressions to Convert to Unit Options

Property Code	Project 911 Description	Default Units	Unit Options
Block 1	Oxygen Demand		
1a	Biochemical O ₂ Demand (BOD)	g O ₂ /g chem	x 1000 = mg O ₂ /g chem
1b	Dichromate Chemical O ₂ Demand (COD)	g O ₂ /g chem	x 1000 = mg O ₂ /g chem
1bp	Permanganate Chemical O ₂ Demand (COD)	g O ₂ /g chem	x 1000 = mg O ₂ /g chem
1cc	Theoretical O ₂ Demand, Carbonaceous	g O ₂ /g chem	x 1000 = mg O ₂ /g chem
1cn	Theoretical O ₂ Demand, Combined	g O ₂ /g chem	x 1000 = mg O ₂ /g chem
Block 2	Partitioning Parameters		
2a	1-Octanol/Water Partitioning	Log K _{ow} , K _{ow} is unit-less	
2b	Soil/Water Partitioning	cm ³ /g soil	
2c	Organic Carbon/Water Partitioning	cm ³ /g OC cm ³ /g OM	
2d	Bioconcentration Factor	unit-less	
Block 3	General Physical Properties		
3a	Molecular Weight	kg/kmol	= g/mol = lb/lbmol
3b	Liquid Density at 298.15 K	kg/m ³	x 0.001 = g/cm ³ x 0.001 = g/mL ÷ 3a = kmol/m ³ x 0.062435 = lb/ft ³
3bt	Liquid Density	kmol/m ³	x 3a x 0.001 = g/cm ³ x 3a x 0.001 = g/mL x 3a = kg/m ³ x 3a x 0.062435 = lb/ft ³
3c	Solubility in Water	ppm(wt)	= mg/L ÷ 3a x 1.802 x 10 ⁻⁵ = mol frac. x 10 ⁻⁶ = mass frac.
3d	Melting Point	K	-273.15 = °C x 1.8 - 459.67 = °F
3e	Normal Boiling Point	K	-273.15 = °C x 1.8 - 459.67 = °F

Table 2: Default Units and Mathematical Expressions to Convert to Unit Options (cont.)

Property Code	Project 911 Description	Default Units	Unit Options
3f	Vapor Pressure at 298.15 K	Pa	$\div 101325 = \text{atm}$ $\times 10^{-5} = \text{bar}$ $\div 1000 = \text{kPa}$ $\times 0.02089 = \text{lb/ft}^2$ $\times 7.5 \times 10^{-3} = \text{mm Hg}$ $\times 1.45 \times 10^{-4} = \text{psia}$ $\times 7.5 \times 10^{-3} = \text{torr}$
3g	Vapor Pressure	Pa	$\div 101325 = \text{atm}$ $\times 10^{-5} = \text{bar}$ $\div 1000 = \text{kPa}$ $\times 0.02089 = \text{lb/ft}^2$ $\times 7.5 \times 10^{-3} = \text{mm Hg}$ $\times 1.45 \times 10^{-4} = \text{psia}$ $\times 7.5 \times 10^{-3} = \text{torr}$
3h	Molecular Diffusivity in Air	cm^2/s	$\times 0.155 = \text{in}^2/\text{s}$ $\times 1.076 \times 10^{-3} = \text{ft}^2/\text{s}$ $\times 10^{-4} = \text{m}^2/\text{s}$
3i	Molecular Diffusivity in Water	cm^2/s	$\times 0.155 = \text{in}^2/\text{s}$ $\times 1.076 \times 10^{-3} = \text{ft}^2/\text{s}$ $\times 10^{-4} = \text{m}^2/\text{s}$
3j	Vapor Viscosity	Pa·s	$\times 1000 = \text{cp}$ $\times 3600 = \text{kg/m}\cdot\text{hr}$ $\times 2419 = \text{lb/ft}\cdot\text{hr}$ $\times 0.6719 = \text{lb/ft}\cdot\text{s}$ $\times 0.02089 = \text{slug/ft}\cdot\text{s}$
3k	Liquid Viscosity	Pa·s	$\times 1000 = \text{cp}$ $\times 3600 = \text{kg/m}\cdot\text{hr}$ $\times 2419 = \text{lb/ft}\cdot\text{hr}$ $\times 0.6719 = \text{lb/ft}\cdot\text{s}$ $\times 0.02089 = \text{slug/ft}\cdot\text{s}$
3l	Surface Tension at 298.15 K	N/m	$\times 1000 = \text{dynes/cm}$ $\times 0.06852 = \text{lb/ft}$ $\times 5.7 \times 10^{-3} = \text{lb/in}$
3lt	Surface Tension	N/m	$\times 1000 = \text{dynes/cm}$ $\times 0.06852 = \text{lb/ft}$ $\times 5.7 \times 10^{-3} = \text{lb/in}$
3ml	Thermal Conductivity, liquid	W/m·K	$\times 0.5781 = \text{BTU/ft}\cdot\text{hr}\cdot\text{F}$ $\times 2.39 \times 10^{-3} = \text{cal/cm}\cdot\text{s}\cdot^\circ\text{C}$ $\times 0.8604 = \text{kcal/m}\cdot\text{hr}\cdot\text{C}$
3mv	Thermal Conductivity, vapor	W/m·K	$\times 0.5781 = \text{BTU/ft}\cdot\text{hr}\cdot\text{F}$ $\times 2.39 \times 10^{-3} = \text{cal/cm}\cdot\text{s}\cdot^\circ\text{C}$ $\times 0.8604 = \text{kcal/m}\cdot\text{hr}\cdot\text{C}$

Table 2: Default Units and Mathematical Expressions to Convert to Unit Options (cont.)

Property Code	Project 911 Description	DefaultUnits	UnitOptions
3n	Enthalpy of Formation at 298.15 K	J/kmol	$\times 4.299 \times 10^{-4} = \text{BTU/lb}$ $\times 0.001 = \text{J/mol}$ $\div 3a \times 2.39 \times 10^{-4} = \text{cal/g}$ $\times 0.1084 = \text{cal/lbmol}$ $\div 3a \times 0.001 = \text{kJ/kg}$ $\times 0.001 = \text{kJ/kmol}$
3o	Liquid Heat Capacity	J/kmol·K	$\div 3a \times 2.389 \times 10^{-4} = \text{BTU/lb}\cdot^{\circ}\text{F}$ $\div 3a \times 2.39 \times 10^{-7} = \text{cal/g}\cdot^{\circ}\text{C}$ $\div 3a \times 0.001 = \text{kJ/kg}\cdot\text{K}$ $\times 0.001 = \text{kJ/kmol}\cdot\text{K}$
3p	Vapor Heat Capacity	J/kmol·K	$\div 3a \times 2.389 \times 10^{-4} = \text{BTU/lb}\cdot^{\circ}\text{F}$ $\div 3a \times 2.39 \times 10^{-7} = \text{cal/g}\cdot^{\circ}\text{C}$ $\div 3a \times 0.001 = \text{kJ/kg}\cdot\text{K}$ $\times 0.001 = \text{kJ/kmol}\cdot\text{K}$
3q	Critical Temperature	K	$-273.15 = ^{\circ}\text{C}$ $\times 1.8 - 460 = ^{\circ}\text{F}$
3r	Critical Pressure	Pa	$\div 101325 = \text{atm}$ $\times 10^{-5} = \text{bar}$ $\div 1000 = \text{kPa}$ $\times 0.02089 = \text{lbf/ft}^2$ $\times 7.5 \times 10^{-3} = \text{mm Hg}$ $\times 1.45 \times 10^{-4} = \text{psia}$ $\times 7.5 \times 10^{-3} = \text{torr}$
3s	Critical Volume	m ³ /kmol	$\times 1000 = \text{L/kmol}$ $\times 16.02 = \text{ft}^3/\text{lbmol}$
3t	Enthalpy of Vaporization at 298.15 K	J/kmol	$\times 4.299 \times 10^{-4} = \text{BTU/lb}$ $\times 0.001 = \text{J/mol}$ $\div 3a \times 2.39 \times 10^{-4} = \text{cal/g}$ $\times 0.1084 = \text{cal/lbmol}$ $\div 3a \times 0.001 = \text{kJ/kg}$ $\times 0.001 = \text{kJ/kmol}$
3tt	Enthalpy of Vaporization vs Temperature	J/kmol	$\times 4.299 \times 10^{-4} = \text{BTU/lb}$ $\times 0.001 = \text{J/mol}$ $\div 3a \times 2.39 \times 10^{-4} = \text{cal/g}$ $\times 0.1084 = \text{cal/lbmol}$ $\div 3a \times 0.001 = \text{kJ/kg}$ $\times 0.001 = \text{kJ/kmol}$
3tz	Enthalpy of Vaporization at Normal Boiling Point	J/kmol	$\times 4.299 \times 10^{-4} = \text{BTU/lb}$ $\times 0.001 = \text{J/mol}$ $\div 3a \times 2.39 \times 10^{-4} = \text{cal/g}$ $\times 0.1084 = \text{cal/lbmol}$ $\div 3a \times 0.001 = \text{kJ/kg}$ $\times 0.001 = \text{kJ/kmol}$

Table 2: Default Units and Mathematical Expressions to Convert to Unit Options (cont.)

Property Code	Project 911 Description	Default Units	Unit Options
Block 4	Vapor-Liquid Equilibrium		
4a	Activity Coefficient of Chemical	unit-less	
4b	Activity Coefficient of Water	unit-less	
4c	Aqueous Henry's Law Constant 25°C assumed (Air-water Partition Coeff.)	kPa·mol/mol	$\times 1.78 \times 10^{-4} = \text{atm}\cdot\text{L}/\text{mol}$ $\times 1.78 \times 10^{-7} = \text{atm}\cdot\text{m}^3/\text{mol}$ $\times 9.87 \times 10^{-3} = \text{atm}\cdot\text{mol}/\text{mol}$ $\times 0.01802 = \text{kPa}\cdot\text{m}^3/\text{kmol}$ $\times 0.001 = \text{MPa}\cdot\text{mol}/\text{mol}$ $\times 1000 = \text{Pa}\cdot\text{mol}/\text{mol}$ $\times 7.5 = \text{Torr}\cdot\text{mol}/\text{mol}$ $\times 1.38 \times 10^5 = \text{unit-less}$
Block 5	Fire and Explosion Parameters		
5al	Lower Flammability Limit in Air	vol% in air	
5au	Upper Flammability Limit in Air	vol% in air	
5b	Flash Point	K	$-273.15 = ^\circ\text{C}$ $\times 1.8 - 460 = ^\circ\text{F}$
5c	Autoignition Temperature	K	$-273.15 = ^\circ\text{C}$ $\times 1.8 - 460 = ^\circ\text{F}$
5d	Enthalpy of Combustion at 298.15 K	J/kmol	$\times 4.299 \times 10^{-4} = \text{BTU}/\text{lb}$ $\times 0.001 = \text{J}/\text{mol}$ $\div 3a \times 2.39 \times 10^{-4} = \text{cal}/\text{g}$ $\times 0.1084 = \text{cal}/\text{lbmol}$ $\div 3a \times 0.001 = \text{kJ}/\text{kg}$ $\times 0.001 = \text{kJ}/\text{kmol}$
Block 6	Sensory, Health and Toxicity Impacts		
6a-i	Acute Aquatic Toxicity	mg/L	

Table 3 :Chemical List

C#	CAS #	Description	Molecular Formula (Hill ordering system)
1.0	75-07-0	Acetaldehyde	C ₂ H ₄ O
2.0	60-35-5	Acetamide	C ₂ H ₅ NO
3.0	75-05-8	Acetonitrile	C ₂ H ₃ N
4.0	98-86-2	Acetophenone	C ₈ H ₈ O
5.0	53-96-3	2-Acetylaminofluorene	C ₁₅ H ₁₃ NO
6.0	107-02-8	Acrolein	C ₃ H ₄ O
7.0	79-06-1	Acrylamide	C ₃ H ₅ NO
8.0	79-10-7	Acrylic Acid	C ₃ H ₄ O ₂
9.0	107-13-1	Acrylonitrile	C ₃ H ₃ N
10.0	107-05-1	Allyl Chloride	C ₃ H ₅ Cl
11.0	92-67-1	4-Aminobiphenyl	C ₁₂ H ₁₁ N
12.0	62-53-3	Aniline	C ₆ H ₇ N
13.0	90-04-0	o-Anisidine	C ₇ H ₉ NO
14.0	1332-21-4	Asbestos	
15.0	71-43-2	Benzene	C ₆ H ₆
16.0	92-87-5	Benzidine	C ₁₂ H ₁₂ N ₂
17.0	98-07-7	Benzotrichloride	C ₇ H ₅ Cl ₃
18.0	100-44-7	Benzyl Chloride	C ₇ H ₇ Cl
19.0	92-52-4	Biphenyl	C ₁₂ H ₁₀
20.0	117-81-7	Bis(2-ethylhexyl) Phthalate (DEHP)	C ₂₄ H ₃₈ O ₄
21.0	542-88-1	Bis(chloromethyl) Ether	C ₂ H ₄ Cl ₂ O
22.0	75-25-2	Bromoform	CHBr ₃
23.0	106-99-0	1,3-Butadiene	C ₄ H ₆
24.0	156-62-7	Calcium Cyanamide	CCaN ₂
25.0	105-60-2	Caprolactam, ε	C ₆ H ₁₁ NO
26.0	133-06-2	Captan	C ₉ H ₈ Cl ₃ NO ₂ S
27.0	63-25-2	Carbaryl	C ₁₂ H ₁₁ NO ₂
28.0	75-15-0	Carbon Disulfide	CS ₂
29.0	56-23-5	Carbon Tetrachloride	CCl ₄
30.0	463-58-1	Carbonyl Sulfide	COS
31.0	120-80-9	Catechol	C ₆ H ₆ O ₂
32.0	133-90-4	Chloramben	C ₇ H ₅ Cl ₂ NO ₂
33.0	57-74-9	Chlordane	C ₁₀ H ₆ Cl ₈
34.0	7782-50-5	Chlorine	Cl ₂
35.0	79-11-8	Chloroacetic Acid	C ₂ H ₃ ClO ₂
36.0	532-27-4	2-Chloroacetophenone	C ₈ H ₇ ClO
37.0	108-90-7	Chlorobenzene	C ₆ H ₅ Cl
38.0	510-15-6	Chlorobenzilate	C ₁₆ H ₁₄ Cl ₂ O ₃
39.0	67-66-3	Chloroform	CHCl ₃
40.0	107-30-2	Chloromethyl Methyl Ether	C ₂ H ₅ ClO
41.0	126-99-8	Chloroprene	C ₄ H ₅ Cl
42.0	1319-77-3	Cresols/Cresylic Acid (isomers & mixture)	C ₇ H ₈ O
43.0	95-48-7	o-Cresol	C ₇ H ₈ O
44.0	108-39-4	m-Cresol	C ₇ H ₈ O
45.0	106-44-5	p-Cresol	C ₇ H ₈ O

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
46.0	98-82-8	Cumene	C ₉ H ₁₂
47.0	94-75-7	2,4-D, salts and esters	C ₈ H ₆ Cl ₂ O ₃
48.0	72-55-9	DDE	C ₁₄ H ₈ Cl ₄
49.0	334-88-3	Diazomethane	CH ₂ N ₂
50.0	132-64-9	Dibenzofuran	C ₁₂ H ₈ O
51.0	96-12-8	1,2-Dibromo-3-chloropropane	C ₃ H ₅ Br ₂ Cl
52.0	84-74-2	Dibutyl Phthalate	C ₁₆ H ₂₂ O ₄
53.0	106-46-7	1,4-Dichlorobenzene	C ₆ H ₄ Cl ₂
54.0	91-94-1	3,3-Dichlorobenzidine	C ₁₂ H ₁₀ Cl ₂ N ₂
55.0	111-44-4	Dichloroethyl Ether (Bis(2-chloroethyl) Ether)	C ₄ H ₈ Cl ₂ O
56.0	542-75-6	1,3-Dichloropropene, mixture	C ₃ H ₄ Cl ₂
56.1	10061-01-5	1,3-Dichloropropene, Z (cis)	C ₃ H ₄ Cl ₂
56.2	10061-02-6	1,3-Dichloropropene, E (trans)	C ₃ H ₄ Cl ₂
57.0	62-73-7	Dichlorvos	C ₄ H ₇ Cl ₂ O ₄ P
58.0	111-42-2	Diethanolamine	C ₄ H ₁₁ NO ₂
59.0	121-69-7	N,N-Dimethylaniline	C ₈ H ₁₁ N
59.1	91-66-7	N,N-Diethylaniline	C ₁₀ H ₁₅ N
60.0	64-67-5	Diethyl Sulfate	C ₄ H ₁₀ O ₄ S
61.0	119-90-4	3,3'-Dimethoxybenzidine	C ₁₄ H ₁₆ N ₂ O ₂
62.0	60-11-7	4-(Dimethylamino)azobenzene	C ₁₄ H ₁₅ N ₃
63.0	119-93-7	3,3'-Dimethylbenzidine	C ₁₄ H ₁₆ N ₂
64.0	79-44-7	Dimethylcarbamyl Chloride	C ₃ H ₆ ClNO
65.0	68-12-2	Dimethyl Formamide	C ₃ H ₇ NO
66.0	57-14-7	1,1-Dimethylhydrazine	C ₂ H ₈ N ₂
67.0	131-11-3	Dimethyl Phthalate	C ₁₀ H ₁₀ O ₄
68.0	77-78-1	Dimethyl Sulfate	C ₂ H ₆ O ₄ S
69.0	534-52-1	4,6-Dinitro-o-cresol, and salts	C ₇ H ₆ N ₂ O ₅
70.0	51-28-5	2,4-Dinitrophenol	C ₆ H ₄ N ₂ O ₅
71.0	121-14-2	2,4-Dinitrotoluene	C ₇ H ₆ N ₂ O ₄
72.0	123-91-1	1,4-Dioxane (1,4-Diethyleneoxide)	C ₄ H ₈ O ₂
73.0	122-66-7	1,2-Diphenylhydrazine	C ₁₂ H ₁₂ N ₂
74.0	106-89-8	Epichlorohydrin	C ₃ H ₅ ClO
75.0	106-88-7	1,2-Epoxybutane	C ₄ H ₈ O
76.0	140-88-5	Ethyl Acrylate	C ₅ H ₈ O ₂
77.0	100-41-4	Ethylbenzene	C ₈ H ₁₀
78.0	51-79-6	Ethyl Carbamate (Urethane)	C ₃ H ₇ NO ₂
79.0	75-00-3	Ethyl Chloride (Chloroethane)	C ₂ H ₅ Cl
80.0	106-93-4	Ethylene Dibromide (Dibromoethane)	C ₂ H ₄ Br ₂
81.0	107-06-2	Ethylene Dichloride (1,2-Dichloroethane)	C ₂ H ₄ Cl ₂
82.0	107-21-1	Ethylene Glycol	C ₂ H ₆ O ₂
83.0	151-56-4	Ethylene Imine (Aziridine)	C ₂ H ₅ N
84.0	75-21-8	Ethylene Oxide	C ₂ H ₄ O
85.0	96-45-7	Ethylene Thiourea	C ₃ H ₆ N ₂ S
86.0	75-34-3	Ethylidene Dichloride (1,1-Dichloroethane)	C ₂ H ₄ Cl ₂
87.0	50-00-0	Formaldehyde	CH ₂ O
88.0	76-44-8	Heptachlor	C ₁₀ H ₅ Cl ₇
89.0	118-74-1	Hexachlorobenzene	C ₆ Cl ₆

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
90.0	87-68-3	Hexachlorobutadiene	C ₄ Cl ₆
91.0	77-47-4	Hexachlorocyclopentadiene	C ₅ Cl ₆
92.0	67-72-1	Hexachloroethane	C ₂ Cl ₆
93.0	822-06-0	Hexamethylene-1,6-diisocyanate	C ₈ H ₁₂ N ₂ O ₂
94.0	680-31-9	Hexamethylphosphoramide	C ₆ H ₁₈ N ₃ OP
95.0	110-54-3	Hexane	C ₆ H ₁₄
96.0	302-01-2	Hydrazine	H ₄ N ₂
97.0	7647-01-0	Hydrochloric Acid	ClH
98.0	7664-39-3	Hydrogen Fluoride (Hydrofluoric acid)	FH
99.0	123-31-9	Hydroquinone	C ₆ H ₆ O ₂
100.0	78-59-1	Isophorone	C ₉ H ₁₄ O
101.0	58-89-9	Lindane (all isomers)	C ₆ H ₆ Cl ₆
102.0	108-31-6	Maleic Anhydride	C ₄ H ₂ O ₃
103.0	67-56-1	Methanol	CH ₄ O
104.0	72-43-5	Methoxychlor	C ₁₆ H ₁₅ Cl ₃ O ₂
105.0	74-83-9	Methyl Bromide (Bromomethane)	CH ₃ Br
106.0	74-87-3	Methyl Chloride (Chloromethane)	CH ₃ Cl
107.0	71-55-6	Methyl Chloroform (1,1,1-trichloroethane)	C ₂ H ₃ Cl ₃
108.0	78-93-3	Methyl Ethyl Ketone (2-Butanone)	C ₄ H ₈ O
109.0	60-34-4	Methylhydrazine	CH ₆ N ₂
110.0	74-88-4	Methyl Iodide (Iodomethane)	CH ₃ I
111.0	108-10-1	Methyl Isobutyl Ketone (Hexone)	C ₆ H ₁₂ O
112.0	624-83-9	Methyl Isocyanate	C ₂ H ₃ NO
113.0	80-62-6	Methyl Methacrylate	C ₅ H ₈ O ₂
114.0	1634-04-4	<i>tert</i> -butyl Methyl Ether	C ₅ H ₁₂ O
115.0	101-14-4	4,4'-Methylenebis(2-chloroaniline)	C ₁₃ H ₁₂ Cl ₂ N ₂
116.0	75-09-2	Methylene Chloride (Dichloromethane)	CH ₂ Cl ₂
117.0	101-68-8	4,4'-Methylenebis(phenyl isocyanate) (MDI)	C ₁₅ H ₁₀ N ₂ O ₂
118.0	101-77-9	4,4'-Methylenedianiline	C ₁₃ H ₁₄ N ₂
119.0	91-20-3	Naphthalene	C ₁₀ H ₈
120.0	98-95-3	Nitrobenzene	C ₆ H ₅ NO ₂
121.0	92-93-3	4-Nitrobiphenyl	C ₁₂ H ₉ NO ₂
122.0	100-02-7	4-Nitrophenol	C ₆ H ₅ NO ₃
123.0	79-46-9	2-Nitropropane	C ₃ H ₇ NO ₂
124.0	684-93-5	N-Nitroso-N-methylurea	C ₂ H ₅ N ₃ O ₂
125.0	62-75-9	N-Nitrosodimethylamine	C ₂ H ₆ N ₂ O
126.0	59-89-2	N-Nitrosomorpholine	C ₄ H ₈ N ₂ O ₂
127.0	56-38-2	Parathion	C ₁₀ H ₁₄ NO ₅ PS
128.0	82-68-8	Pentachloronitrobenzene (Quintobenzene)	C ₆ Cl ₅ NO ₂
129.0	87-86-5	Pentachlorophenol	C ₆ HCl ₅ O
130.0	108-95-2	Phenol	C ₆ H ₆ O
131.0	106-50-3	p-Phenylenediamine	C ₆ H ₈ N ₂
132.0	75-44-5	Phosgene	CCl ₂ O
133.0	7803-51-2	Phosphine	H ₃ P
134.0	7723-14-0	Phosphorus, white	P ₄
135.0	085-44-9	Phthalic Anhydride	C ₈ H ₄ O ₃
136.0	1336-36-3	Polychlorinated Biphenyls (Aroclors)	

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
137.0	1120-71-4	1,3-Propane Sultone	C ₃ H ₆ O ₃ S
138.0	57-57-8	beta-Propiolactone	C ₃ H ₄ O ₂
139.0	123-38-6	Propionaldehyde	C ₃ H ₆ O
140.0	114-26-1	Propoxur (Baygon)	C ₁₁ H ₁₅ NO ₃
141.0	78-87-5	Propylene Dichloride (1,2-Dichloropropane)	C ₃ H ₆ Cl ₂
142.0	75-56-9	Propylene Oxide	C ₃ H ₆ O
143.0	75-55-8	1,2-Propylene Imine	C ₃ H ₇ N
144.0	91-22-5	Quinoline	C ₉ H ₇ N
145.0	106-51-4	Quinone	C ₆ H ₄ O ₂
146.0	100-42-5	Styrene	C ₈ H ₈
147.0	96-09-3	Styrene Oxide	C ₈ H ₈ O
148.0	1746-01-6	2,3,7,8-Tetrachlorodibenzo-p-dioxin	C ₁₂ H ₄ Cl ₄ O ₂
149.0	79-34-5	1,1,2,2-Tetrachloroethane	C ₂ H ₂ Cl ₄
150.0	127-18-4	Tetrachloroethylene (Perchloroethylene)	C ₂ Cl ₄
151.0	7550-45-0	Titanium Tetrachloride	Cl ₄ Ti
152.0	108-88-3	Toluene	C ₇ H ₈
153.0	95-80-7	2,4-Toluenediamine	C ₇ H ₁₀ N ₂
154.0	584-84-9	Tolylene 2,4-Diisocyanate	C ₉ H ₆ N ₂ O ₂
155.0	95-53-4	o-Toluidine	C ₇ H ₉ N
156.0	8001-35-2	Toxaphene (chlorinated camphene)	
157.0	120-82-1	1,2,4-Trichlorobenzene	C ₆ H ₃ Cl ₃
158.0	79-00-5	1,1,2-Trichloroethane	C ₂ H ₃ Cl ₃
159.0	79-01-6	Trichloroethylene	C ₂ HCl ₃
160.0	95-95-4	2,4,5-Trichlorophenol	C ₆ H ₃ Cl ₃ O
161.0	88-06-2	2,4,6-Trichlorophenol	C ₆ H ₃ Cl ₃ O
162.0	121-44-8	Triethylamine	C ₆ H ₁₅ N
163.0	1582-09-8	Trifluralin	C ₁₃ H ₁₆ F ₃ N ₃ O ₄
164.0	540-84-1	2,2,4-Trimethylpentane	C ₈ H ₁₈
165.0	108-05-4	Vinyl Acetate	C ₄ H ₆ O ₂
166.0	593-60-2	Vinyl Bromide	C ₂ H ₃ Br
167.0	75-01-4	Vinyl Chloride	C ₂ H ₃ Cl
168.0	75-35-4	Vinylidene Chloride (1,1-dichloroethylene)	C ₂ H ₂ Cl ₂
169.0	1330-20-7	Xylenes (isomers & mixture)	C ₈ H ₁₀
170.0	95-47-6	o-Xylene	C ₈ H ₁₀
171.0	108-38-3	m-Xylene	C ₈ H ₁₀
172.0	106-42-3	p-Xylene	C ₈ H ₁₀
173.0	627-13-4	Propyl Nitrate	C ₃ H ₇ NO ₃
174.0	74-89-5	Methylamine	CH ₅ N
175.0	74-90-8	Hydrogen Cyanide	CHN
176.0	74-93-1	Methyl Mercaptan	CH ₄ S
177.0	75-04-7	Ethylamine	C ₂ H ₇ N
178.0	75-31-0	Isopropylamine	C ₃ H ₉ N
179.0	75-52-5	Nitromethane	CH ₃ NO ₂
180.0	75-74-1	Tetramethyl Lead	C ₄ H ₁₂ Pb
181.0	75-78-5	Dimethyldichlorosilane	C ₂ H ₆ Cl ₂ Si
182.0	75-79-6	Methyltrichlorosilane	CH ₃ Cl ₃ Si
183.0	75-91-2	tert-Butyl Hydroperoxide	C ₄ H ₁₀ O ₂

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
184.0	76-06-2	Chloropicrin	CCl ₃ NO ₂
185.0	78-85-3	Methacrolein	C ₄ H ₆ O
186.0	79-21-0	Peracetic Acid	C ₂ H ₄ O ₃
187.0	79-22-1	Methyl Chloroformate	C ₂ H ₃ ClO ₂
188.0	79-38-9	Trifluorochloroethylene	C ₂ ClF ₃
189.0	79-84-4	Methyl Vinyl Ketone	C ₄ H ₆ O
190.0	80-15-9	Cumene Hydroperoxide	C ₉ H ₁₂ O ₂
191.0	94-36-0	Dibenzoyl Peroxide	C ₁₄ H ₁₀ O ₄
192.0	96-10-6	Chlorodiethylaluminum	C ₄ H ₁₀ AlCl
193.0	97-00-7	1-Chloro-2,4-dinitrobenzene	C ₆ H ₃ ClN ₂ O ₄
194.0	97-02-9	2,4-Dinitroaniline	C ₆ H ₅ N ₃ O ₄
195.0	100-01-6	4-Nitroaniline	C ₆ H ₆ N ₂ O ₂
196.0	105-64-6	Diisopropyl Peroxydicarbonate	C ₈ H ₁₄ O ₆
197.0	105-74-8	Dilauroyl Peroxide	C ₂₄ H ₄₆ O ₄
198.0	106-96-7	3-Bromopropyne	C ₃ H ₃ Br
199.0	107-11-9	Allylamine	C ₃ H ₇ N
200.0	107-44-8	Sarin	C ₄ H ₁₀ FO ₂ P
201.0	109-95-5	Ethyl Nitrite	C ₂ H ₅ NO ₂
202.0	110-00-9	Furan	C ₄ H ₄ O
203.0	110-05-4	Di- <i>tert</i> -butyl Peroxide	C ₈ H ₁₈ O ₂
204.0	110-22-5	Diacetyl Peroxide (Conc>70%)	C ₄ H ₆ O ₄
205.0	116-14-3	Tetrafluoroethylene	C ₂ F ₄
206.0	124-40-3	Dimethylamine	C ₂ H ₇ N
207.0	126-98-7	Methacrylonitrile	C ₄ H ₅ N
208.0	353-50-4	Carbonyl Fluoride	CF ₂ O
209.0	371-62-0	Ethylene Fluorhydrin	C ₂ H ₅ FO
210.0	421-20-5	Methyl Fluorosulfate	CH ₃ FO ₃ S
211.0	453-18-9	Methyl Fluoroacetate	C ₃ H ₅ FO ₂
212.0	460-19-5	Cyanogen	C ₂ N ₂
213.0	463-51-4	Ketene	C ₂ H ₂ O
214.0	506-77-4	Cyanogen Chloride	CClN
215.0	557-20-0	Diethylzinc	C ₄ H ₁₀ Zn
216.0	594-42-3	Perchloromethyl Mercaptan	CCl ₄ S
217.0	614-45-9	<i>tert</i> -Butyl Perbenzoate	C ₁₁ H ₁₄ O ₃
218.0	675-14-9	Cyanuric Fluoride	C ₃ F ₃ N ₃
219.0	684-16-2	Hexafluoroacetone	C ₃ F ₆ O
220.0	7787-71-5	Bromine Trifluoride	BrF ₃
221.0	814-68-6	Acryloyl Chloride	C ₃ H ₃ ClO
222.0	920-46-7	Methacryloyl Chloride	C ₄ H ₅ ClO
223.0	33817-91-3	Ethyl Methyl Ketone Peroxide Z (cis)	C ₈ H ₁₆ O ₄
223.1	1338-23-4	Ethyl Methyl Ketone Peroxide (Conc>60%)	C ₈ H ₁₆ O ₄
223.2	33817-92-4	Ethyl Methyl Ketone Peroxide E (trans)	C ₈ H ₁₆ O ₄
224.0	1558-25-4	Trichloro(chloromethyl)silane	CH ₂ Cl ₄ Si
225.0	2487-90-3	Trimethoxysilane	C ₃ H ₁₀ O ₃ Si
226.0	5714-22-7	Disulfur Decafluoride	F ₁₀ S ₂
227.0	4109-96-0	Dichlorosilane	Cl ₂ H ₂ Si

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
228.0	7446-09-5	Sulfur Dioxide	O ₂ S
229.0	7446-11-9	Sulfur Trioxide, alpha	O ₃ S
229.1	13771-24-9	Sulfur Trioxide, gamma	O ₃ S
229.2	27118-91-8	Sulfur Trioxide, beta	O ₃ S
230.0	7572-29-4	Dichloroacetylene	C ₂ Cl ₂
231.0	7601-90-3	Perchloric Acid (Conc.>60%)	ClHO ₄
232.0	7616-94-6	Perchloryl Fluoride	ClFO ₃
233.0	7637-07-2	Boron Trifluoride	BF ₃
234.0	7664-41-7	Ammonia solutions (>44 wt% Ammonia)	
234.1	7664-41-7	Ammonia	H ₃ N
235.0	7697-37-2	Nitric Acid	HNO ₃
236.0	7719-09-7	Thionyl Chloride	Cl ₂ OS
237.0	7719-12-2	Phosphorus Trichloride	Cl ₃ P
238.0	7722-84-1	Hydrogen Peroxide (≥52 wt%)	H ₂ O ₂
239.0	7726-95-6	Bromine	Br ₂
240.0	7782-41-4	Fluorine	F ₂
241.0	7783-07-5	Hydrogen Selenide	H ₂ Se
242.0	7783-41-7	Oxygen Difluoride	F ₂ O
243.0	7783-54-2	Nitrogen Trifluoride	F ₃ N
244.0	7783-60-0	Sulfur Tetrafluoride	F ₄ S
245.0	7783-79-1	Selenium Hexafluoride	F ₆ Se
246.0	7783-80-4	Tellurium Hexafluoride	F ₆ Te
247.0	7784-42-1	Arsine	AsH ₃
248.0	13446-10-1	Ammonium Permanganate	H ₄ MnNO ₄
249.0	7789-30-2	Bromine Pentafluoride	BrF ₅
250.0	7790-91-2	Chlorine Trifluoride	ClF ₃
251.0	7790-98-9	Ammonium Perchlorate	ClH ₄ NO ₄
252.0	7803-49-8	Hydroxylamine	H ₃ NO
253.0	7803-52-3	Stibine	H ₃ Sb
254.0	8014-95-7	Oleum (65-85 wt%)	H ₂ O ₇ S ₂
255.0	9004-70-0	Cellulose Nitrate (@>12.5% nitrogen)	
256.0	10025-78-2	Trichlorosilane	Cl ₃ HSi
257.0	10025-87-3	Phosphorus Oxychloride	Cl ₃ OP
258.0	10028-15-6	Ozone	O ₃
259.0	10035-10-6	Hydrogen Bromide	BrH
260.0	10036-47-2	Tetrafluorohydrazine	F ₄ N ₂
261.0	10049-04-4	Chlorine Dioxide	ClO ₂
262.0	10102-43-9	Nitric Oxide	NO
263.0	10102-44-0	Nitrogen Dioxide	NO ₂
264.0	10294-34-5	Boron Trichloride	BCl ₃
265.0	10544-72-6	Dinitrogen Tetroxide	N ₂ O ₄
266.0	10544-73-7	Dinitrogen Trioxide	N ₂ O ₃
267.0	13463-39-3	Nickel Carbonyl	C ₄ NiO ₄
268.0	13463-40-6	Iron Pentacarbonyl	C ₅ FeO ₅
269.0	13637-63-3	Chlorine Pentafluoride	ClF ₅
270.0	13863-41-7	Bromine Chloride	BrCl

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
271.0	19287-45-7	Diborane	B ₂ H ₆
272.0	19624-22-7	Pentaborane	B ₅ H ₉
273.0	20816-12-0	Osmium Tetroxide	O ₄ Os
274.0	27137-85-5	Trichloro(dichlorophenyl)silane	C ₆ H ₃ Cl ₅ Si
275.0	30674-80-7	Methacroyloxyethyl Isocyanate	C ₇ H ₉ N ₃ O
276.0	64-19-7	Acetic Acid	C ₂ H ₄ O ₂
277.0	75-86-5	Acetone Cyanohydrin	C ₄ H ₇ NO
278.0	74-86-2	Acetylene	C ₂ H ₂
279.0	107-18-6	Allyl Alcohol	C ₃ H ₆ O
280.0	5332-73-0	3-Methoxypropylamine	C ₄ H ₁₁ NO
281.0	7783-70-2	Antimony Pentafluoride	F ₅ Sb
282.0	7784-34-1	Arsenic Trichloride	AsCl ₃
283.0	98-87-3	Benzal Chloride	C ₇ H ₆ Cl ₂
284.0	98-16-8	Benzenamine, 3-(Trifluoromethyl)	C ₇ H ₆ F ₃ N
285.0	140-29-4	Benzyl Cyanide	C ₈ H ₇ N
286.0	353-42-4	Boron Trifluoride with Methyl Ether (1:1)	C ₂ H ₆ BF ₃ O
287.0	598-73-2	Bromotrifluorethylene	C ₂ BrF ₃
288.0	106-97-8	Butane	C ₄ H ₁₀
289.0	25167-67-3	Butene	C ₄ H ₈
290.0	106-98-9	1-Butene	C ₄ H ₈
291.0	107-01-7	2-Butene	C ₄ H ₈
291.1	624-64-6	2-Butene, E (<i>trans</i>)	C ₄ H ₈
291.2	590-18-1	2-Butene, Z (<i>cis</i>)	C ₄ H ₈
292.0	85-68-7	Butyl Benzyl Phthalate	C ₁₉ H ₂₀ O ₄
293.0	7791-21-1	Dichlorine Monoxide	Cl ₂ O
294.0	79-04-9	Chloroacetyl Chloride	C ₂ H ₂ Cl ₂ O
295.0	107-07-3	Chloroethanol	C ₂ H ₅ ClO
296.0	590-21-6	1-Chloropropylene	C ₃ H ₅ Cl
296.1	16136-85-9	1-Chloropropylene, E (<i>trans</i>)	C ₃ H ₅ Cl
296.2	16136-84-8	1-Chloropropylene, Z (<i>cis</i>)	C ₃ H ₅ Cl
297.0	557-98-2	2-Chloropropylene	C ₃ H ₅ Cl
298.0	4170-30-3	Crotonaldehyde	C ₄ H ₆ O
298.1	123-73-9	Crotonaldehyde, E (<i>trans</i>)	C ₄ H ₆ O
298.2	15798-64-8	Crotonaldehyde, Z (<i>cis</i>)	C ₄ H ₆ O
299.0	108-91-8	Cyclohexylamine	C ₆ H ₁₃ N
300.0	75-19-4	Cyclopropane	C ₃ H ₆
301.0	75-37-6	1,1-Difluoroethane	C ₂ H ₄ F ₂
302.0	2524-03-0	Dimethyl Chlorothiophosphate	C ₂ H ₆ ClO ₂ PS
303.0	463-82-1	2,2-Dimethylpropane	C ₅ H ₁₂
304.0	101-84-8	Diphenyl Oxide	C ₁₂ H ₁₀ O
305.0	74-84-0	Ethane	C ₂ H ₆
306.0	141-78-6	Ethyl Acetate	C ₄ H ₈ O ₂
307.0	107-00-6	Ethyl Acetylene	C ₄ H ₆
308.0	60-29-7	Ethyl Ether	C ₄ H ₁₀ O
309.0	75-08-1	Ethyl Mercaptan	C ₂ H ₆ S
310.0	74-85-1	Ethylene	C ₂ H ₄
311.0	107-15-3	Ethylenediamine	C ₂ H ₈ N ₂

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
312.0	107-16-4	Formaldehyde Cyanohydrin	C ₂ H ₃ NO
313.0	764-42-1	Fumaronitrile	C ₄ H ₂ N ₂
314.0	142-82-5	Heptane	C ₇ H ₁₆
315.0	1333-74-0	Hydrogen (equilibrium)	H ₂
316.0	7783-06-4	Hydrogen Sulfide	H ₂ S
317.0	103-90-2	4-Hydroxyacetanilide	C ₈ H ₉ NO ₂
318.0	99-93-4	4-Hydroxyacetophenone	C ₈ H ₈ O ₂
319.0	75-28-5	Isobutane	C ₄ H ₁₀
320.0	78-82-0	Isobutyronitrile	C ₄ H ₇ N
321.0	78-78-4	Isopentane	C ₅ H ₁₂
322.0	78-79-5	Isoprene	C ₅ H ₈
323.0	75-29-6	Isopropyl Chloride	C ₃ H ₇ Cl
324.0	108-23-6	Isopropyl Chloroformate	C ₄ H ₇ ClO ₂
325.0	78-97-7	Lactonitrile	C ₃ H ₅ NO
326.0	928-53-0	Maleonitrile	C ₄ H ₂ N ₂
327.0	79-41-4	Methacrylic Acid	C ₄ H ₆ O ₂
328.0	74-82-8	Methane	CH ₄
329.0	115-10-6	Methyl Ether	C ₂ H ₆ O
330.0	107-31-3	Methyl Formate	C ₂ H ₄ O ₂
331.0	556-64-9	Methyl Thiocyanate	C ₂ H ₃ NS
332.0	563-46-2	2-Methyl-1-butene	C ₅ H ₁₀
333.0	563-45-1	3-Methyl-1-butene	C ₅ H ₁₀
334.0	109-87-5	Methylal	C ₃ H ₈ O ₂
335.0	115-11-7	2-Methylpropene	C ₄ H ₈
336.0	100-54-9	Nicotinonitrile	C ₆ H ₄ N ₂
337.0	100-00-5	p-Nitrochlorobenzene	C ₆ H ₄ ClNO ₂
338.0	836-30-9	p-Nitrodiphenylamine	C ₁₂ H ₁₀ NO ₂
339.0	504-60-9	1,3-Pentadiene	C ₅ H ₈
339.1	2004-70-8	1,3-Pentadiene, E (<i>trans</i>)	C ₅ H ₈
339.2	1574-41-0	1,3-Pentadiene, Z (<i>cis</i>)	C ₅ H ₈
340.0	109-66-0	Pentane	C ₅ H ₁₂
341.0	109-67-1	1-Pentene	C ₅ H ₁₀
341.1	646-04-8	2-Pentene, E (<i>trans</i>)	C ₅ H ₁₀
341.2	627-20-3	2-Pentene, Z (<i>cis</i>)	C ₅ H ₁₀
342.0	122-79-2	Phenyl acetate	C ₈ H ₈ O ₂
343.0	1314-80-3	Phosphorus Pentasulfide	P ₄ S ₁₀
344.0	1314-56-3	Phosphorus Pentoxide	O ₁₀ P ₄
345.0	110-89-4	Piperidine	C ₅ H ₁₁ N
346.0	463-49-0	Propadiene	C ₃ H ₄
347.0	74-98-6	Propane	C ₃ H ₈
348.0	107-12-0	Propionitrile	C ₃ H ₅ N
349.0	109-61-5	Propyl Chloroformate	C ₄ H ₇ ClO ₂
350.0	115-07-1	Propylene	C ₃ H ₆
351.0	74-99-7	Propyne	C ₃ H ₄
352.0	140-76-1	2-Methyl-5-vinylpyridine	C ₈ H ₉ N
353.0	289-95-2	Pyrimidine	C ₄ H ₄ N ₂
354.0	69-72-7	Salicylic Acid	C ₇ H ₆ O ₃

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
355.0	7803-62-5	Silane	H ₄ Si
356.0	497-19-8	Sodium Carbonate	CNa ₂ O ₃
357.0	110-61-2	Succinonitrile	C ₄ H ₄ N ₂
358.0	10545-99-0	Sulfur Dichloride	Cl ₂ S
359.0	10025-67-9	Sulfur Monochloride	Cl ₂ S ₂
360.0	7664-93-9	Sulfuric Acid	H ₂ O ₄ S
361.0	75-64-9	<i>Tert</i> -Butylamine	C ₄ H ₁₁ N
362.0	75-76-3	Tetramethylsilane	C ₄ H ₁₂ Si
363.0	509-14-8	Tetranitromethane	CN ₄ O ₈
364.0	108-98-5	Thiophenol	C ₆ H ₆ S
365.0	91-08-7	Toluene 2,6-Diisocyanate	C ₉ H ₆ N ₂ O ₂
366.0	26471-62-5	Toluene Diisocyanate (unspecified isomer)	C ₉ H ₆ N ₂ O ₂
367.0	110-57-6	<i>trans</i> -1,4-Dichloro-2-butene	C ₄ H ₆ Cl ₂
368.0	115-21-9	Trichloroethylsilane	C ₂ H ₃ Cl ₃ Si
369.0	75-50-3	Trimethylamine	C ₃ H ₉ N
370.0	75-77-4	Trimethylchlorosilane	C ₃ H ₉ ClSi
371.0	77-99-6	Trimethylolpropane	C ₆ H ₁₄ O ₃
372.0	689-97-4	Vinyl Acetylene	C ₄ H ₄
373.0	109-92-2	Vinyl Ethyl Ether	C ₄ H ₈ O
374.0	75-02-5	Vinyl Fluoride	C ₂ H ₃ F
375.0	107-25-5	Vinyl Methyl Ether	C ₃ H ₆ O
376.0	75-38-7	Vinylidene Fluoride	C ₂ H ₂ F ₂
377.0	18600-41-4	3-Methoxypropylamine Hydrochloride	C ₄ H ₁₁ NO·HCl
378.0	141-43-5	Monoethanolamine	C ₂ H ₇ NO
379.0	2002-24-6	Monoethanolamine Hydrochloride	C ₂ H ₇ NO·HCl
380.0	108-01-0	N,N-Dimethylethanolamine	C ₄ H ₁₁ NO
381.0	2498-25-1	N,N-Dimethylethanolamine Hydrochloride	C ₄ H ₁₁ NO·HCl
382.0	7440-36-0	Antimony	Sb
383.0	1309-64-4	Antimony(III) Oxide	O ₃ Sb ₂
384.0	28300-74-5	Antimony Potassium Tartarate (Hydrate)	C ₈ H ₄ K ₂ O ₁₂ Sb ₂ ·3H ₂ O
385.0	7440-38-2	Arsenic	As
386.0	1327-53-3	Arsenic Trioxide	As ₂ O ₃
387.0	7784-46-5	Sodium Arsenite	AsNaO ₂
388.0	7440-41-7	Beryllium	Be
389.0	1304-56-9	Beryllium Oxide	BeO
390.0	7787-56-6	Beryllium Sulfate Tetrahydrate	BeO ₄ S·4H ₂ O
391.0	7440-43-9	Cadmium	Cd
392.0	10108-64-2	Cadmium Chloride	CdCl ₂
393.0	1306-19-0	Cadmium Oxide	CdO
394.0	7440-47-3	Chromium	Cr
395.0	1333-82-0	Chromium Trioxide	CrO ₃
396.0	7778-50-9	Potassium Dichromate	Cr ₂ K ₂ O ₇
397.0	7440-48-4	Cobalt	Co
398.0	10026-24-1	Cobalt(II) Sulfate Heptahydrate	CoO ₄ S·7H ₂ O
399.0	109-16-8	2-Picoline	C ₆ H ₇ N
400.0	108-99-6	3-Picoline	C ₆ H ₇ N

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
401.0	108-89-4	4-Picoline	C ₆ H ₇ N
402.0	110-86-1	Pyridine	C ₅ H ₅ N
403.0	151-50-8	Potassium Cyanide	KCN
404.0	506-64-9	Silver Cyanide	AgCN
405.0	506-61-6	Silver Potassium Cyanide	C ₂ AgKN ₂
406.0	143-33-9	Sodium Cyanide	CNNa
407.0	629-14-1	Ethylene Glycol Diethyl Ether	C ₆ H ₁₀ O ₂
408.0	110-71-4	Ethylene Glycol Dimethyl Ether	C ₄ H ₁₀ O ₂
409.0	111-76-2	Ethylene Glycol Monobutyl Ether	C ₆ H ₁₄ O ₂
410.0	122-99-6	Ethylene Glycol Monophenyl Ether	C ₈ H ₁₀ O ₂
411.0	7439-92-1	Lead	Pb
412.0	6080-56-4	Lead(II) Acetate, Trihydrate	C ₄ H ₆ O ₄ Pb·3H ₂ O
413.0	1309-60-0	Lead Dioxide	O ₂ Pb
414.0	1335-32-6	Lead(II) Subacetate	C ₄ H ₁₀ O ₈ Pb ₃
415.0	1314-41-6	Red Lead	O ₄ Pb ₃
416.0	7439-96-5	Manganese	Mn
417.0	10034-96-5	Manganese(II) Sulfate, Monohydrate	MnO ₄ S·H ₂ O
418.0	7439-97-6	Mercury	Hg
419.0	7487-94-7	Mercuric Chloride	HgCl ₂
420.0	7440-02-1	Nickel	Ni
421.0	7791-20-0	Nickel Chloride Hexahydrate	Cl ₂ Ni·6H ₂ O
422.0	1313-99-1	Nickel(II) Oxide	NiO
423.0	7786-81-4	Nickel Sulfate	NiSO ₄
424.0	10101-97-0	Nickel Sulfate Hexahydrate	NiO ₄ S·6H ₂ O
425.0	12674-11-2	Aroclor 1016	
426.0	11104-28-2	Aroclor 1221	
427.0	11141-16-5	Aroclor 1232	
428.0	53469-21-9	Aroclor 1242	
429.0	12672-29-6	Aroclor 1248	
430.0	11096-82-5	Aroclor 1260	
431.0	37324-23-5	Aroclor 1262	
432.0	11100-14-4	Aroclor 1268	
433.0	120-12-7	Anthracene	C ₁₄ H ₁₀
434.0	50-32-8	Benzo[a]pyrene	C ₂₀ H ₁₂
435.0	218-01-9	Chrysene	C ₁₈ H ₁₂
436.0	85-01-8	Phenanthrene	C ₁₄ H ₁₀
437.0	129-00-0	Pyrene	C ₁₆ H ₁₀
438.0	7440-14-4	Radium	Ra
439.0	14859-67-7	Radon	Rn
440.0	7782-49-2	Selenium	Se
441.0	7783-00-8	Selenious Acid	H ₂ O ₃ Se
442.0	112-07-2	Ethylene Glycol Monobutyl Ether Acetate	C ₈ H ₁₆ O ₃
443.0	111-15-9	Ethylene Glycol Monoethyl Ether Acetate	C ₆ H ₁₂ O ₃
444.0	112-36-7	Diethylene Glycol Diethyl Ether	C ₈ H ₁₈ O ₃
445.0	111-96-6	Diethylene Glycol Dimethyl Ether	C ₆ H ₁₄ O ₃
446.0	2807-30-9	Ethylene Glycol Monopropyl Ether	C ₅ H ₁₂ O ₂

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
447.0	110-80-5	Ethylene Glycol Monoethyl Ether	C ₄ H ₁₀ O ₂
448.0	109-86-4	Ethylene Glycol Monomethyl Ether	C ₃ H ₈ O ₂
449.0	112-15-2	Diethylene Glycol Monoethyl Ether Acetate	C ₈ H ₁₆ O ₄
450.0	112-34-5	Diethylene Glycol Monobutyl Ether	C ₈ H ₁₈ O ₃
451.0	112-49-2	Triethylene Glycol Dimethyl Ether	C ₈ H ₁₈ O ₄
452.0	111-77-3	Diethylene Glycol Monomethyl Ether	C ₅ H ₁₂ O ₃
453.0	111-90-0	Diethylene Glycol Monoethyl Ether	C ₆ H ₁₄ O ₃
454.0	84-15-1	o-Terphenyl	C ₁₈ H ₁₄
455.0	92-94-4	p-Terphenyl	C ₁₈ H ₁₄
456.0	92-06-8	m-Terphenyl	C ₁₈ H ₁₄
457.0	135-70-6	p-Quaterphenyl	C ₂₄ H ₁₈
458.0	128-37-0	BHT, 2,6-Di- <i>tert</i> -butyl-p-cresol	C ₁₅ H ₂₄ O
459.0	6484-52-2	Ammonium Nitrate	H ₄ N ₂ O ₃
460.0	96-24-2	alpha-Chlorohydrin	C ₃ H ₇ ClO ₂
461.0	96-23-1	alpha-Dichlorohydrin	C ₃ H ₆ Cl ₂ O
462.0	616-23-9	beta-Dichlorohydrin	C ₃ H ₆ Cl ₂ O
463.0	637-92-3	Ethyl <i>tert</i> -butyl Ether	C ₆ H ₁₄ O
464.0	556-52-5	Glycidol	C ₃ H ₆ O ₂
465.0	56-55-3	Benz[a]anthracene	C ₁₈ H ₁₂
466.0	110-49-6	Ethylene Glycol Monomethyl Ether Acetate	C ₅ H ₁₀ O ₃
467.0	542-92-7	Cyclopentadiene	C ₅ H ₆
468.0	77-73-6	Dicyclopentadiene	C ₁₀ H ₁₂
469.0	617-94-7	Dimethylbenzyl Alcohol	C ₉ H ₁₂ O
470.0	141-79-7	Mesityl Oxide	C ₆ H ₁₀ O
471.0	116-09-6	Hydroxyacetone	C ₃ H ₆ O ₂
472.0	7732-18-5	Water	H ₂ O
473.0	3037-72-7	(4-Aminobutyl)diethoxymethylsilane	C ₉ H ₂₃ NO ₂ Si
474.0	956-36-1	2,4-Trimethylbenzene	C ₉ H ₁₂
475.0	95-50-1	1,2-Dichlorobenzene	C ₆ H ₄ Cl ₂
476.0	540-59-0	1,2-Dichloroethylene (unspecified cis- or trans-)	C ₂ H ₂ Cl ₂
477.0	88-05-1	2,4,6-Trimethylaniline	C ₉ H ₁₃ N
478.0	120-83-2	2,4-Dichlorophenol	C ₆ H ₄ Cl ₂ O
479.0	606-20-2	2,6-Dinitrotoluene	C ₇ H ₆ N ₂ O ₄
480.0	95-57-8	2-Chlorophenol	C ₆ H ₅ ClO
481.0	90-43-7	2-Phenylphenol	C ₁₂ H ₁₀ O
482.0	504-24-5	4-Aminopyridine	C ₅ H ₆ N ₂
483.0	95-83-0	4-Chloro- <i>o</i> -phenylenediamine	C ₆ H ₇ ClN ₂
484.0	3697-24-3	5-Methylchrysene	C ₁₉ H ₁₄
485.0	134-32-7	alpha-Naphthylamine	C ₁₀ H ₉ N
486.0	83-32-9	Acenaphthene	C ₁₂ H ₁₀
487.0	208-96-8	Acenaphthylene	C ₁₂ H ₈
488.0	67-64-1	Acetone	C ₃ H ₆ O
489.0	111-69-3	Adiponitrile	C ₆ H ₈ N ₂
490.0	116-06-3	Aldicarb	C ₇ H ₁₄ N ₂ O ₂ S
491.0	309-00-2	Aldrin	C ₁₂ H ₈ Cl ₆
492.0	1344-28-1	Aluminum Oxide	Al ₂ O ₃
493.0	7787-36-2	Barium Permanganate	BaMn ₂ O ₈

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
494.0	7783-20-2	Ammonium Sulfate	H ₈ N ₂ O ₄ S
495.0	71-41-0	Amyl Alcohol	C ₅ H ₁₂ O
496.0	1303-28-2	Arsenic Pentoxide	As ₂ O ₅
497.0	1912-24-9	Atrazine	C ₈ H ₁₄ ClN ₅
498.0	91-59-8	beta-Naphthylamine	C ₁₀ H ₉ N
499.0	7440-39-3	Barium	Ba
500.0	55-21-0	Benzamide	C ₇ H ₇ NO
501.0	598-31-2	Bromoacetone	C ₃ H ₅ BrO
502.0	141-32-2	Butyl Acrylate	C ₇ H ₁₂ O ₂
503.0	78-92-2	Butyl Alcohol, sec-	C ₄ H ₁₀ O
504.0	123-72-8	Butyraldehyde	C ₄ H ₈ O
505.0	7778-44-1	Calcium Arsenate	As ₂ Ca ₃ O ₈
506.0	16887-00-6	Chloride ion	Cl ⁻
507.0	18540-29-9	Chromium ion (hexavalent)	Cr ⁶⁺
508.0	10025-73-7	Chromium(III) Chloride	Cl ₃ Cr
509.0	7440-50-8	Copper	Cu
510.0	57-12-5	Cyanide ion	CN ⁻
511.0	110-82-7	Cyclohexane	C ₆ H ₁₂
512.0	111-92-2	Dibutylamine	C ₈ H ₁₉ N
513.0	2050-92-2	Dipentylamine	C ₁₀ H ₂₃ N
514.0	541-73-1	1,3-Dichlorobenzene	C ₆ H ₄ Cl ₂
515.0	75-27-4	Bromodichloromethane	CHBrCl ₂
516.0	149-74-6	Dichloromethylphenylsilane	C ₇ H ₈ Cl ₂ Si
517.0	75-71-8	Dichlorodifluoromethane	CCl ₂ F ₂
518.0	156-59-2	<i>cis</i> -1,2-Dichloroethylene	C ₂ H ₂ Cl ₂
518.1	156-60-5	<i>trans</i> -1,2-Dichloroethylene	C ₂ H ₂ Cl ₂
519.0	60-57-1	Dieldrin	C ₁₂ H ₈ Cl ₆ O
520.0	84-66-2	Diethyl Phthalate	C ₁₂ H ₁₄ O ₄
521.0	109-89-7	Diethylamine	C ₄ H ₁₁ N
522.0	1615-80-1	1,2-Diethylhydrazine	C ₄ H ₁₂ N ₂
523.0	674-82-8	Diketene	C ₄ H ₄ O ₂
524.0	75-18-3	Dimethyl Sulfide	C ₂ H ₆ S
525.0	67-68-5	Dimethyl Sulfoxide	C ₂ H ₆ OS
526.0	64-17-5	Ethanol	C ₂ H ₆ O
527.0	86-73-7	Fluorene	C ₁₃ H ₁₀
528.0	144-49-0	Fluoroacetic Acid	C ₂ H ₃ FO ₂
529.0	75-12-7	Formamide	CH ₃ NO
530.0	98-01-1	Furfural	C ₅ H ₄ O ₂
531.0	124-09-4	Hexamethylenediamine	C ₆ H ₁₆ N ₂
532.0	7439-89-6	Iron	Fe
533.0	78-84-2	Isobutyraldehyde	C ₄ H ₈ O
534.0	67-63-0	Isopropyl Alcohol	C ₃ H ₈ O
535.0	301-04-2	Lead(II) Acetate	C ₄ H ₆ O ₄ Pb
536.0	7446-27-7	Lead Phosphate	O ₈ P ₂ Pb ₃
537.0	121-75-5	Malathion	C ₁₀ H ₁₉ O ₆ PS ₂
538.0	21908-53-2	Mercuric Oxide	HgO
539.0	01600-27-7	Mercuric Acetate	C ₄ H ₆ HgO ₄

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
540.0	16752-77-5	Methomyl	C ₅ H ₁₀ N ₂ O ₂ S
541.0	96-33-3	Methyl Acrylate	C ₄ H ₆ O ₂
542.0	624-92-0	Methyl Disulfide	C ₂ H ₆ S ₂
543.0	75-54-7	Dichloromethylsilane	CH ₄ Cl ₂ Si
544.0	74-95-3	Methylene Bromide	CH ₂ Br ₂
545.0	1313-27-5	Molybdenum Trioxide	MoO ₃
546.0	123-86-4	Butyl Acetate	C ₆ H ₁₂ O ₂
547.0	71-36-3	Butyl Alcohol	C ₄ H ₁₀ O
548.0	1116-54-7	N-Nitrosodiethanolamine	C ₄ H ₁₀ N ₂ O ₃
549.0	86-30-6	N-Nitrosodiphenylamine	C ₁₂ H ₁₀ N ₂ O
550.0	54-11-5	Nicotine	C ₁₀ H ₁₄ N ₂
551.0	55-63-0	Nitroglycerin	C ₃ H ₅ N ₃ O ₉
552.0	88-75-5	2-Nitrophenol	C ₆ H ₅ NO ₃
553.0	108-03-2	1-Nitropropane	C ₃ H ₇ NO ₂
554.0	111-36-4	Butyl Isocyanate	C ₅ H ₉ NO
555.0	4685-14-7	Paraquat ion	C ₁₂ H ₁₄ N ₂
556.0	2074-50-2	Paraquat Methylsulfate	C ₁₄ H ₂₀ N ₂ O ₈ S ₂
557.0	8030-30-6	Petroleum Naphtha	
558.0	103-71-9	Phenyl Isocyanate	C ₇ H ₅ NO
559.0	103-85-5	Phenylthiourea	C ₇ H ₈ N ₂ S
560.0	7664-38-2	Phosphoric Acid	H ₃ O ₄ P
561.0	10026-13-8	Phosphorus Pentachloride	Cl ₅ P
562.0	88-89-1	Picric Acid	C ₆ H ₃ N ₃ O ₇
563.0	7758-01-2	Potassium Bromate	BrKO ₃
564.0	625-55-8	Isopropyl Formate	C ₄ H ₈ O ₂
565.0	109-90-0	Ethyl Isocyanate	C ₃ H ₅ NO
566.0	108-20-3	Isopropyl Ether	C ₆ H ₁₄ O
567.0	81-07-2	Saccharin	C ₇ H ₅ NO ₃ S
568.0	7631-89-2	Sodium Arsenate (mixture mono,di,tri basic salts)	
569.0	1310-73-2	Sodium Hydroxide	HNaO
570.0	57-24-9	Strychnine	C ₂₁ H ₂₂ N ₂ O ₂
571.0	100-21-0	Terephthalic Acid	C ₈ H ₆ O ₄
572.0	75-65-0	<i>tert</i> -Butyl Alcohol	C ₄ H ₁₀ O
573.0	78-00-2	Tetraethyllead	C ₈ H ₂₀ Pb
574.0	109-99-9	Tetrahydrofuran	C ₄ H ₈ O
575.0	62-56-6	Thiourea	CH ₄ N ₂ S
576.0	13463-67-7	Titanium Dioxide	O ₂ Ti
577.0	98-13-5	Trichlorophenylsilane	C ₆ H ₅ Cl ₃ Si
578.0	998-30-1	Triethoxysilane	C ₆ H ₁₆ O ₃ Si
579.0	7440-62-2	Vanadium (fume or dust)	V
580.0	1314-62-1	Vanadium Pentoxide	O ₅ V ₂
581.0	628-63-7	Pentyl Acetate	C ₇ H ₁₄ O ₂
582.0	71-23-8	1-Propanol	C ₃ H ₈ O
583.0	70-69-9	Aminopropiophenone, 4'-	C ₉ H ₁₁ NO
584.0	1341-49-7	Ammonium Bifluoride	F ₂ H ₅ N ₂
585.0	12125-02-9	Ammonium Chloride	ClH ₄ N
586.0	12125-01-8	Ammonium Fluoride	FH ₄ N
587.0	10022-31-8	Barium Nitrate	BaN ₂ O ₆
588.0	13813-79-1	Boric Acid	BH ₃ O ₃
589.0	109-72-8	Butyllithium	C ₄ H ₉ Li

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
590.0	7778-54-3	Calcium Hypochlorite	CaCl ₂ O ₂
591.0	124-38-9	Carbon Dioxide	CO ₂
592.0	630-08-0	Carbon Monoxide	CO
593.0	9004-36-8	Cellulose Acetate Butyrate	
594.0	7738-94-5	Chromic(VI) Acid	CrH ₂ O ₄
595.0	13530-68-2	Dichromic Acid	Cr ₂ H ₂ O ₇
596.0	544-92-3	Copper(I) Cyanide	CCuN
597.0	108-93-0	Cyclohexanol	C ₆ H ₁₂ O
598.0	124-18-5	Decane	C ₁₀ H ₂₂
599.0	621-64-7	Dipropylnitrosamine	C ₆ H ₁₄ N ₂ O
600.0	39156-41-7	Diaminoanisole Sulfate, 2,4-	C ₇ H ₁₂ N ₂ O ₅ S
601.0	101-80-4	Diaminodiphenyl Ether, 4,4'-	C ₁₂ H ₁₂ N ₂ O
602.0	111-46-6	Diethylene Glycol	C ₄ H ₁₀ O ₃
603.0	105-10-2	N,N'-Dimethyl-p-phenylenediamine	C ₈ H ₁₂ N ₂
604.0	33204-76-1	Diphenylhexamethylcyclotetrasiloxane, 2,6- <i>cis</i>	C ₁₈ H ₂₈ O ₄ Si ₄
605.0	72-20-8	Endrin	C ₁₂ H ₈ Cl ₆ O
606.0	379-79-3	Ergotamine Tartrate	C ₃₅ H ₃₈ N ₅ O ₈
607.0	9004-57-3	Ethyl Cellulose	
608.0	538-07-8	Ethylbis(2-chloroethyl)amine	C ₆ H ₁₃ Cl ₂ N
609.0	64-18-6	Formic Acid	CH ₂ O ₂
610.0	7782-42-5	Graphite	C
611.0	18406-41-2	Hexakis(methoxy)disilylethane	C ₈ H ₂₂ O ₆ Si ₂
612.0	109-49-9	Hexen-2-one, 5-	C ₆ H ₁₀ O
613.0	118-93-4	Hydroxyacetophenone, 2-	C ₈ H ₈ O ₂
614.0	15687-27-1	Ibuprofen	C ₁₃ H ₁₈ O ₂
615.0	7553-56-2	Iodine	I ₂
616.0	110-19-0	Isobutyl Acetate	C ₆ H ₁₂ O ₂
617.0	78-83-1	Isobutyl Alcohol	C ₄ H ₁₀ O
618.0	8008-20-6	Kerosene	
619.0	50-21-5	Lactic Acid	C ₃ H ₆ O ₃
619.1	598-82-3	dl-Lactic Acid	C ₃ H ₆ O ₃
619.2	79-33-4	L, S, & d-Lactic Acid	C ₃ H ₆ O ₃
619.3	326-41-7	D & l-Lactic Acid	C ₃ H ₆ O ₃
620.0	12141-20-7	Lead Oxide Phosphate	HO ₅ PPb ₃
621.0	68476-85-7	Liquefied Petroleum Gas	
622.0	10377-66-9	Manganous Nitrate	MnN ₂ O ₆
623.0	872-50-4	Methyl-2-pyrrolidinone, 1-	C ₅ H ₉ NO
624.0	108-87-2	Methylcyclohexane	C ₇ H ₁₄
625.0	101-61-1	Methylenebis(N,N-dimethyl) benzeneamine, 4,4'-	C ₁₇ H ₂₂ N ₂
626.0	64091-91-4	Methylnitrosoamino-1-(3-pyridyl)-1-butanone	C ₁₀ H ₁₃ N ₃ O ₂
627.0	1317-33-5	Molybdenum Disulfide	MoS ₂
628.0	4835-11-4	N,N'-Dibutylhexamethylenediamine	C ₁₄ H ₃₂ N ₂
629.0	3710-84-7	N,N-Diethylhydroxylamine	C ₄ H ₁₁ NO
630.0	04062-60-6	N,N'-Di- <i>tert</i> -butylethylenediamine	C ₁₀ H ₂₄ N ₂
631.0	18328-90-0	N-Ethyl-2-methylallylamine	C ₆ H ₁₃ N
632.0	2424-01-3	N-Methyldiallylamine	C ₇ H ₁₃ N
633.0	924-16-3	N-Nitrosodibutylamine	C ₈ H ₁₈ N ₂ O
634.0	55-18-5	N-Nitrosodiethylamine	C ₄ H ₁₀ N ₂ O
635.0	10595-95-6	N-Nitrosomethylethylamine	C ₃ H ₈ N ₂ O
636.0	4549-40-0	N-Nitrosomethylvinylamine	C ₃ H ₆ N ₂ O
637.0	373-02-4	Nickel(II) Acetate	C ₄ H ₆ NiO ₄

638.0	7718-54-9	Nickel(II) Chloride	Cl ₂ Ni
639.0	13770-89-3	Nickel(II) Sulfamate	H ₄ N ₂ NiO ₆ S ₂

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
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640.0	111-84-2	Nonane	C ₉ H ₂₀
641.0	111-65-9	Octane	C ₈ H ₁₈
642.0	30525-89-4	Paraformaldehyde	(CH ₂ O) _x
643.0	2570-26-5	Pentadecylamine	C ₁₅ H ₃₃ N
644.0	9002-84-0	Polytetrafluoroethylene	(C ₂ F ₄) _x
645.0	877-24-7	Potassium Acid Phthalate	C ₈ H ₅ KO ₄
646.0	584-08-7	Potassium Carbonate	CK ₂ O ₃
647.0	13746-66-2	Potassium Ferricyanide	C ₆ FeK ₃ N ₆
648.0	16923-95-8	Potassium Fluorozirconate	F ₆ K ₂ Zr
649.0	13967-50-5	Potassium Gold(I) Cyanide	C ₂ AuKN ₂
650.0	1310-58-3	Potassium Hydroxide	HKO
651.0	12142-33-5	Potassium Stannate	K ₂ O ₃ Sn
652.0	107-19-7	Propargyl Alcohol	C ₃ H ₄ O
653.0	123-75-1	Pyrrolidine	C ₄ H ₉ N
654.0	35574-23-3	Pyrrolidinium Acetate	C ₆ H ₁₃ NO ₂
655.0	112945-52-5	Silica (fumed)	O ₂ Sn
656.0	127-09-3	Sodium Acetate	C ₂ H ₃ O ₂ Na
657.0	144-55-8	Sodium Bicarbonate	CHNaO ₃
658.0	7647-14-5	Sodium Chloride	ClNa
659.0	6132-04-3	Sodium Citrate (dihydrate)	C ₆ H ₅ Na ₃ O ₇ ·2H ₂ O
660.0	10588-01-9	Sodium Dichromate	Cr ₂ Na ₂ O ₇
661.0	13755-29-8	Sodium Fluoroborate	BF ₄ Na
662.0	16721-80-5	Sodium Hydrosulfide	HNaS
663.0	7681-52-9	Sodium Hypochlorite	ClNaO
664.0	7681-53-0	Sodium Hypophosphite	H ₂ NaO ₂ P
665.0	7632-00-0	Sodium Nitrite	NNaO ₂
666.0	1344-08-7	Sodium Polysulfide	Na ₂ S _x
667.0	16893-85-9	Sodium Silicofluoride	F ₆ Na ₂ Si
668.0	12201-54-6	Sodium Stannate	Na ₄ O ₄ Sn
669.0	7757-82-6	Sodium Sulfate	Na ₂ O ₄ S
670.0	1313-82-2	Sodium Sulfide	Na ₂ S
671.0	126-33-0	Sulfolane	C ₄ H ₈ O ₂ S
672.0	7704-24-9	Sulfur	S
673.0	14807-96-6	Talc	H ₂ Mg ₃ O ₁₂ Si ₄
674.0	112-60-7	Tetraethylene Glycol	C ₈ H ₁₈ O ₅
675.0	112-27-6	Triethylene Glycol	C ₆ H ₁₄ HO ₄
676.0	555-77-1	Tris(2-Chloroethyl)amine	C ₆ H ₁₂ Cl ₃ N
677.0	7646-85-7	Zinc Chloride	Cl ₂ Zn
678.0	13530-65-9	Zinc Chromate	CrO ₄ Zn
679.0	557-21-1	Zinc Cyanide	C ₂ N ₂ Zn
680.0	1314-13-2	Zinc Oxide	OZn
681.0	10026-11-6	Zirconium (IV) Chloride	Cl ₄ Zr
682.0	111-87-5	1-Octanol	C ₈ H ₁₈ O
683.0	75-98-9	Propanoic Acid, 2, 2-Dimethyl-	C ₅ H ₁₀ O ₂
684.0	156-10-5	p-Nitrosodiphenylamine	C ₁₂ H ₁₀ N ₂ O
704.0	108-24-7	Acetic Anhydride	C ₄ H ₆ O ₃
705.0	124-04-9	Adipic Acid	C ₆ H ₁₀ O ₄
706.0	11097-69-1	Aroclor 1254	

707.0	65-85-0	Benzoic Acid	C ₇ H ₆ O ₂
708.0	2467-02-9	Bis(2-Hydroxyphenyl)methane	C ₁₃ H ₁₂ O ₂

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
709.0	107-88-0	1,3-Butanediol	C ₄ H ₁₀ O ₂
710.0	110-63-4	1,4-Butanediol	C ₄ H ₁₀ O ₂
711.0	4435-50-1	1,2,3-Butanetriol	C ₄ H ₁₀ O ₃
712.0	592-84-7	Butyl Formate	C ₅ H ₁₀ O ₂
713.0	590-01-2	Butyl Propionate	C ₇ H ₁₄ O ₂
714.0	107-92-6	Butyric Acid	C ₄ H ₈ O ₂
715.0	77-92-9	Citric Acid	C ₆ H ₈ O ₇
716.0	592-57-4	1,3-Cyclohexadiene	C ₆ H ₈
717.0	110-83-8	Cyclohexane	C ₆ H ₁₀
718.0	292-64-8	Cyclooctane	C ₈ H ₁₆
719.0	287-92-3	Cyclopentane	C ₅ H ₁₀
720.0	50-29-3	DDT	C ₁₄ H ₉ Cl ₅
721.0	872-05-9	1-Decene	C ₁₀ H ₂₀
722.0	5989-27-5	<i>d</i> -Limonene	C ₁₀ H ₁₆
723.0	13029-08-8	2,2'-Dichlorobiphenyl	C ₁₂ H ₈ Cl ₂
724.0	2050-68-2	4,4'-Dichlorobiphenyl	C ₁₂ H ₈ Cl ₂
725.0	100-37-8	N,N-Diethylethanolamine	C ₆ H ₁₅ NO
726.0	624-72-6	1,2-Difluoroethane	C ₂ H ₄ F ₂
727.0	75-83-2	2,2-Dimethylbutane	C ₆ H ₁₄
728.0	2207-01-4	<i>cis</i> -1,2- Dimethylcyclohexane	C ₈ H ₁₆
729.0	638-04-0	<i>cis</i> -1,3- Dimethylcyclohexane	C ₈ H ₁₆
730.0	624-29-3	<i>cis</i> -1,4- Dimethylcyclohexane	C ₈ H ₁₆
731.0	581-42-0	2,6-Dimethylnaphthalene	C ₁₂ H ₁₂
732.0	582-16-1	2,7-Dimethylnaphthalene	C ₁₂ H ₁₂
733.0	14426-20-1	2-Diethylaminoethanol hydrochloride	C ₆ H ₁₅ NO·ClH
734.0	1678-91-7	Ethylcyclohexane	C ₈ H ₁₆
735.0	3553-80-8	Ethyl Diethylcarbamate	C ₇ H ₁₅ NO ₂
736.0	109-94-4	Ethyl Formate	C ₃ H ₆ O ₂
737.0	110-17-8	Fumaric Acid	C ₄ H ₄ O ₄
738.0	96-48-0	Gamma-Butyrolactone	C ₄ H ₆ O ₂
739.0	591-50-4	Iodobenzene	C ₆ H ₅ I
740.0	107-08-4	1-Iodopropane	C ₃ H ₇ I
741.0	110-16-7	Maleic Acid	C ₄ H ₄ O ₄
742.0	141-82-2	Malonic Acid	C ₃ H ₄ O ₄
743.0	79-20-9	Methyl Acetate	C ₃ H ₆ O ₂
744.0	547-63-7	Methyl Isobutyrate	C ₅ H ₁₀ O ₂
745.0	623-42-7	Methyl Butyrate	C ₅ H ₁₀ O ₂
746.0	590-67-0	1-Methylcyclohexanol	C ₇ H ₁₄ O
747.0	90-12-0	1-Methylnaphthalene	C ₁₁ H ₁₀
748.0	91-57-6	2-Methylnaphthalene	C ₁₁ H ₁₀
749.0	691-38-3	4-Methyl-2-pentene	C ₆ H ₁₂
750.0	100-80-1	m-Methylstyrene	C ₉ H ₁₀
751.0	622-97-9	p-Methylstyrene	C ₉ H ₁₀
752.0	616-44-4	3-Methylthiophene	C ₅ H ₆ S
753.0	88-74-4	o-Nitroaniline	C ₆ H ₆ N ₂ O ₂
754.0	79-24-3	Nitroethane	C ₂ H ₅ NO ₂
755.0	111-66-0	1-Octene	C ₈ H ₁₆
756.0	144-62-7	Oxalic Acid	C ₂ H ₂ O ₄

757.0	110-85-0	Piperazine	C ₄ H ₁₀ N ₂
758.0	10430-90-7	1-Piperazinecarboxylic Acid	C ₅ H ₁₀ N ₂ O ₂

Table 3: Chemical List (cont.)

C#	CAS #	Description	Molecular Formula
759.0	2762-32-5	2-Piperazinecarboxylic Acid	C ₅ H ₁₀ N ₂ O ₂
760.0	7709-80-0	1,4-Piperazinedicarboxylic Acid	C ₈ H ₁₅ NO
761.0	142-64-3	Piperazine Dihydrochloride	C ₄ H ₁₀ N ₂ ·2ClH
762.0	6091-62-9	Piperazine Dihydrochloride Monohydrate	C ₄ H ₁₀ N ₂ ·2ClH·H ₂ O
763.0	57-55-6	1,2-Propanediol	C ₃ H ₈ O ₂
764.0	504-63-2	1,3-Propanediol	C ₃ H ₈ O ₂
765.0	79-09-4	Propionic Acid	C ₃ H ₆ O ₂
766.0	106-36-5	Propyl Propionate	C ₆ H ₁₂ O ₂
767.0	108-30-5	Succinic Anhydride	C ₄ H ₄ O ₃
768.0	586-62-9	Terpinolene	C ₁₀ H ₁₆
769.0	12408-10-5	Tetrachlorobenzene (general)	C ₆ H ₂ Cl ₄
769.1	634-66-2	1,2,3,4- Tetrachlorobenzene	C ₆ H ₂ Cl ₄
769.2	95-94-3	1,2,4,5- Tetrachlorobenzene	C ₆ H ₂ Cl ₄
769.3	634-90-2	1,2,3,5- Tetrachlorobenzene	C ₆ H ₂ Cl ₄
770.0	26914-33-0	Tetrachlorobiphenyl (general)	C ₁₂ H ₆ Cl ₄
771.0	811-97-2	1,1,1,2- Tetrafluoroethane	C ₂ H ₂ F ₄
772.0	359-35-3	1,1,2,2- Tetrafluoroethane	C ₂ H ₂ F ₄
773.0	119-64-2	Tetralin	C ₁₀ H ₁₂
774.0	108-70-3	1,3,5- Trichlorobenzene	C ₆ H ₃ Cl ₃
775.0	25323-68-6	Trichlorobiphenyl (general)	C ₁₂ H ₇ Cl ₃
776.0	16747-26-5	2,2,4- Trimethylhexane	C ₉ H ₂₀
777.0	16747-28-7	2,3,3- Trimethylhexane	C ₉ H ₂₀
778.0	16747-31-2	3,3,4- Trimethylhexane	C ₉ H ₂₀
779.0	106-43-4	Benzene, 1-chloro-4-methyl	C ₇ H ₇ Cl
780.0	620-14-4	Benzene, 1-ethyl-3-methyl	C ₉ H ₁₂
781.0	25619-60-7	Benzene, tetramethyl- (general)	C ₁₀ H ₁₄
781.1	527-53-7	1,2,3,5- Tetramethylbenzene	C ₁₀ H ₁₄
781.2	488-23-3	1,2,3,4- Tetramethylbenzene	C ₁₀ H ₁₄
782.0	98-83-9	Benzene, (1-methylethenyl)-	C ₉ H ₁₀
783.0	108-67-8	Benzene, 1,3,5-trimethyl-	C ₉ H ₁₂
784.0	99-87-6	Benzene, 1-methyl-4-(1-methylethyl)-	C ₁₀ H ₁₄
785.0	95-93-2	Benzene, 1,2,4,5-tetramethyl-	C ₁₀ H ₁₄
786.0	526-73-8	Benzene, 1,2,3,-trimethyl-	C ₉ H ₁₂
787.0	55880-77-8	Pentachlor-1,3-butadiene (general)	C ₄ HCl ₅
788.0	464-06-2	Butane, 2,2,3-trimethyl-	C ₇ H ₁₆
789.0	1502-38-1	Cyclooctane, methyl-	C ₉ H ₁₈
790.0	96-37-7	Cyclopentane, methyl-	C ₆ H ₁₂
791.0	630-20-6	Ethane, 1,1,1,2- tetrachloro-	C ₂ H ₂ Cl ₄
792.0	589-34-4	Hexane, 3-methyl-	C ₇ H ₁₆
792.1	6131-24-4	Hexane, 3-Methyl-, (S)-	C ₇ H ₁₆
792.2	78918-91-9	Hexane, 3-Methyl-, (R)-	C ₇ H ₁₆
793.0	28699-88-9	Naphthalene, dichloro- (general)	C ₁₀ H ₆ Cl ₂
794.0	593-45-3	Octadecane	C ₁₈ H ₃₈
795.0	2216-33-3	Octane, 3-methyl-	C ₉ H ₂₀
796.0	107-83-5	Pentane, 2-methyl-	C ₆ H ₁₄
797.0	576-26-1	Phenol, 2,6-dimethyl-	C ₈ H ₁₀ O
798.0	34652-54-5	Propane, bromochloro- (general)	C ₃ H ₆ BrCl
799.0	67708-83-2	Propane, dibromochloro- (general)	C ₃ H ₅ Br ₂ Cl

800.0	554-14-3	Thiophene, 2-methyl-	C ₅ H ₆ S
801.0	110-15-6	Succinic Acid	C ₄ H ₆ O ₄

Table 3: Chemical List (cont.)

C#	CAS#	Description	Molecular Formula
802.0	629-73-2	1-Hexadecene	C ₁₆ H ₃₂
803.0	2532-58-3	<i>cis</i> -1,3-Dimethylcyclopentane	C ₇ H ₁₄
804.0	822-50-4	<i>trans</i> -1,2-Dimethylcyclopentane	C ₇ H ₁₄
805.0	1759-58-6	<i>trans</i> -1,3-Dimethylcyclopentane	C ₇ H ₁₄
806.0	1638-26-2	1,1-Dimethylcyclopentane	C ₇ H ₁₄
807.0	112-47-0	1,10-Decanediol	C ₁₀ H ₂₂ O ₂
808.0	7440-21-3	Silicon	Si
809.0	590-19-2	1,2-Butadiene	C ₄ H ₆
811.0	591-95-7	1,2-Pentadiene	C ₅ H ₈
812.0	646-06-0	1,3-Dioxolane	C ₃ H ₆ O ₂
813.0	26519-91-5	Methyl-1,3-cyclopentadiene	C ₆ H ₈
814.0	628-41-1	1,4-Cyclohexadiene	C ₆ H ₈
815.0	591-93-5	1,4-Pentadiene	C ₅ H ₈
816.0	13048-33-4	1,6-Hexanediol Diacrylate	C ₁₂ H ₁₈ O ₄
817.0	109-79-5	1-Butanethiol	C ₄ H ₁₀ S
818.0	10026-04-7	Silicon Tetrachloride	Cl ₄ Si
821.0	592-76-7	1-Heptene	C ₇ H ₁₄
823.0	36653-82-4	1-Hexadecanol	C ₁₆ H ₃₄ O
825.0	592-41-6	1-Hexene	C ₆ H ₁₂
826.0	947-19-3	1-Hydroxycyclohexyl Phenyl Ketone	C ₁₃ H ₁₆ O ₂
829.0	2885-00-9	1-Octadecanethiol	C ₁₈ H ₃₈ S
832.0	622-96-8	1-Ethyl-4-methylbenzene	C ₉ H ₁₂
838.0	24650-42-8	2,2-Dimethoxy-2-phenylacetophenone	C ₁₆ H ₁₆ O ₃
839.0	4032-93-3	2,3,6-Trimethylheptane	C ₁₀ H ₂₂
840.0	513-85-9	2,3-Butanediol	C ₄ H ₁₀ O ₂
841.0	5341-95-7	<i>meso</i> -2,3-Butanediol	C ₄ H ₁₀ O ₂
842.0	79-29-8	2,3-Dimethylbutane	C ₆ H ₁₄
843.0	565-59-3	2,3-Dimethylpentane	C ₇ H ₁₆
844.0	591-96-8	2,3-Pentadiene	C ₅ H ₈
845.0	108-08-7	2,4-Dimethylpentane	C ₇ H ₁₆
846.0	79-74-3	2,5-Di- <i>tert</i> -pentylhydroquinone	C ₁₆ H ₂₆ O ₂
847.0	75-26-3	2-Bromopropane	C ₃ H ₇ Br
849.0	3404-71-5	2-Ethyl-1-pentene	C ₇ H ₁₄
850.0	543-49-7	2-Heptanol	C ₇ H ₁₆ O
851.0	110-43-0	2-Heptanone	C ₇ H ₁₄ O
852.0	611-14-3	1-Ethyl-2-methylbenzene	C ₉ H ₁₂
853.0	26741-29-7	2-Hexadecene	C ₁₆ H ₃₂
854.0	626-93-7	2-Hexanol	C ₆ H ₁₄ O
855.0	75-30-9	2-Iodopropane	C ₃ H ₇ I
856.0	763-29-1	2-Methyl-1-pentene	C ₆ H ₁₂
857.0	591-76-4	2-Methylhexane	C ₇ H ₁₆
858.0	611-15-4	2-Methylstyrene	C ₉ H ₁₀
860.0	123-96-6	2-Octanol	C ₈ H ₁₈ O
861.0	6032-29-7	2-Pentanol	C ₅ H ₁₂ O
863.0	4032-92-2	2,4,4-Trimethylheptane	C ₁₀ H ₂₂
864.0	4032-86-4	3,3-Dimethylheptane	C ₉ H ₂₀
865.0	562-49-2	3,3-Dimethylpentane	C ₇ H ₁₆
866.0	4038-04-4	3-Ethyl-1-pentene	C ₇ H ₁₄

867.0	15869-80-4	3-Ethylheptane	C ₉ H ₂₀
868.0	619-99-8	3-Ethylhexane	C ₈ H ₁₈

Table 3: Chemical List (cont.)

C#	CAS#	Description	Molecular Formula
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869.0	617-78-7	3-Ethylpentane	C ₇ H ₁₆
870.0	589-38-8	3-Hexanone	C ₆ H ₁₂ O
871.0	96-14-0	3-Methylpentane	C ₆ H ₁₄
872.0	3404-61-3	3-Methyl-1-hexene	C ₇ H ₁₄
873.0	760-20-3	3-Methyl-1-pentene	C ₆ H ₁₂
874.0	7784-13-6	Aluminum Chloride (6-Hydrate)	AlCl ₃ ·6H ₂ O
875.0	584-02-1	3-Pentanol	C ₅ H ₁₂ O
876.0	123-19-3	4-Heptanone	C ₇ H ₁₄ O
877.0	691-38-3	<i>cis</i> -4-Methyl-2-pentene	C ₆ H ₁₂
878.0	691-37-2	4-Methyl-1-pentene	C ₆ H ₁₂
879.0	3178-29-8	4-Propylheptane	C ₁₀ H ₂₂
880.0	98-29-3	4- <i>tert</i> -Butylcatechol	C ₁₀ H ₁₄ O ₂
881.0	103-84-4	Acetanilide	C ₈ H ₉ NO
882.0	123-54-6	Acetylacetone	C ₅ H ₈ O ₂
883.0	260-94-6	Acridine	C ₁₃ H ₉ N
884.0	7446-70-0	Aluminum Chloride (Anhydrous)	AlCl ₃
885.0	21645-51-2	Aluminum Hydroxide	AlH ₃ O ₃
886.0	145-08-8	1-Nonanol	C ₉ H ₂₀ O
887.0	100-66-3	Anisole	C ₇ H ₈ O
888.0	84-65-1	Anthraquinone	C ₁₄ H ₈ O ₂
889.0	225-11-6	Benz(a)acridine	C ₁₄ H ₁₁ N
890.0	100-52-7	Benzaldehyde	C ₇ H ₆ O
891.0	207-08-9	Benzo(k)fluoranthene	C ₂₀ H ₁₂
892.0	100-47-0	Benzonitrile	C ₇ H ₅ N
893.0	140-11-4	Benzyl Acetate	C ₉ H ₁₀ O ₂
894.0	100-51-6	Benzyl Alcohol	C ₇ H ₈ O
895.0	539-30-0	Benzyl Ethyl Ether	C ₉ H ₁₂ O
896.0	104-57-4	Benzyl Formate	C ₈ H ₈ O ₂
897.0	100-46-9	Benzylamine	C ₇ H ₉ N
899.0	75-62-7	Bromotrichloromethane	CBrCl ₃
900.0	75-63-8	Bromotrifluoromethane	CBrF ₃
901.0	111-34-2	Butyl Vinyl Ether	C ₆ H ₁₂ O
902.0	109-73-9	Butylamine	C ₄ H ₁₁ N
903.0	104-51-8	Butylbenzene	C ₁₀ H ₁₄
904.0	471-34-1	Calcium Carbonate	CCaO ₃
905.0	1305-62-0	Calcium Hydroxide	CaH ₂ O ₂
906.0	7789-82-4	Calcium Molybdate	CaMoO ₄
907.0	75-73-0	Carbon Tetrafluoride	CF ₄
908.0	610-31-1	1,2,4-Trinitrobenzene	C ₆ H ₃ N ₃ O ₆
909.0	7688-21-3	<i>cis</i> -2-Hexene	C ₆ H ₁₂
910.0	12192-29-9	Cobalt Carbide	Co ₂ C
911.0	7447-39-4	Cupric Chloride (Anhydrous)	Cl ₂ Cu
912.0	287-23-0	Cyclobutane	C ₄ H ₈
913.0	291-64-5	Cycloheptane	C ₇ H ₁₄
914.0	108-94-1	Cyclohexanone	C ₆ H ₁₀ O
915.0	931-87-3	(<i>z</i>)-Cyclooctene	C ₈ H ₁₄
916.0	120-92-3	Cyclopentanone	C ₅ H ₈ O
917.0	142-29-0	Cyclopentene	C ₅ H ₈

918.0	112-30-1	1-Decanol	C ₁₀ H ₂₂ O
919.0	96-22-0	Diethyl Ketone	C ₅ H ₁₀ O

Table 3: Chemical List (cont.)

C#	CAS#	Description	Molecular Formula
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920.0	142-96-1	Butyl Ether	C ₈ H ₁₈ O
921.0	142-84-7	Dipropylamine	C ₆ H ₁₅ N
922.0	7783-28-0	Ammonium Hydrogenphosphate	H ₉ N ₂ O ₄ P
923.0	53-70-3	Dibenz(a,h)anthracene	C ₂₂ H ₁₄
924.0	189-64-0	Dibenzo(a,h)pyrene	C ₂₄ H ₁₄
925.0	103-50-4	Benzyl Ether	C ₁₄ H ₁₄ O
926.0	1067-33-0	Dibutyltin Diacetate	C ₁₂ H ₂₄ O ₄ Sn
927.0	352-9-32	Ethyl Sulfide	C ₄ H ₁₀ S
928.0	623-81-4	Diethyl Sulfite	C ₄ H ₁₀ O ₃ S
929.0	75-10-5	Difluoromethane	CH ₂ F ₂
930.0	75-11-6	Diiodomethane	CH ₂ I ₂
931.0	628-55-7	Isobutyl Ether	C ₈ H ₁₈ O
932.0	51363-64-5	Diisodecyl Phenyl Phosphate	C ₂₆ H ₄₇ O ₄ P
933.0	26761-40-0	Diisodecyl Phthalate	C ₂₈ H ₄₆ O ₄
934.0	123-28-4	Didodecyl 3,3'-Thiodipropionate	C ₃₀ H ₅₈ O ₄ S
935.0	624-48-6	Dimethyl Maleate	C ₆ H ₈ O
936.0	971-15-3	Dipentamethylenethiuram Hexasulfide	C ₁₂ H ₂₀ N ₂ S ₈
937.0	120-54-7	Dipentamethylenethiuram Tetrasulfide	C ₁₂ H ₂₀ N ₂ S ₆
938.0	25265-71-8	Dipropylene Glycol	C ₆ H ₁₄ O ₃
939.0	112-40-3	Dodecane	C ₁₂ H ₂₆
940.0	565-69-5	Ethyl Isopropyl Ketone	C ₆ H ₁₂ O
941.0	540-67-0	Ethyl Methyl Ether	C ₃ H ₈ O
942.0	105-37-3	Ethyl Propionate	C ₅ H ₁₀ O ₂
943.0	628-32-0	Ethyl Propyl Ether	C ₅ H ₁₂ O
944.0	103-69-5	N-Ethylaniline	C ₈ H ₁₁ N
945.0	542-10-9	Ethylidene Diacetate	C ₆ H ₁₀ O ₄
947.0	206-44-0	Fluoranthene	C ₁₆ H ₁₀
948.0	462-06-6	Fluorobenzene	C ₆ H ₅ F
949.0	353-36-6	Fluoroethane	C ₂ H ₅ F
950.0	593-53-3	Fluoromethane	CH ₃ F
951.0	103-70-8	Formanilide	C ₇ H ₇ NO
952.0	56-81-5	Glycerine	C ₃ H ₈ O ₃
953.0	111-70-6	Heptyl Alcohol	C ₇ H ₁₆ O
954.0	87-82-1	Hexabromobenzene	C ₆ Br ₆
955.0	544-76-3	Hexadecane	C ₁₆ H ₃₄
956.0	392-56-3	Hexafluorobenzene	C ₆ F ₆
957.0	142-62-1	Hexanoic Acid	C ₆ H ₁₂ O ₂
958.0	111-27-3	Hexyl Alcohol	C ₆ H ₁₄ O
959.0	288-32-4	Imidazole	C ₃ H ₄ N ₂
960.0	5888-33-5	Isobornyl Acrylate	C ₁₃ H ₂₀ O ₂
961.0	78-81-9	Isobutylamine	C ₄ H ₁₁ N
962.0	538-93-2	Isobutylbenzene	C ₁₀ H ₁₄
963.0	79-31-2	Isobutyric Acid	C ₄ H ₈ O ₂
964.0	29590-42-9	Isooctyl Acrylate	C ₁₁ H ₂₀ O ₂
965.0	108-21-4	Isopropyl Acetate	C ₅ H ₁₀ O ₂
966.0	78448-33-6	Isopropyl Isobutyl Ether	C ₇ H ₁₆ O ₂
967.0	112-53-8	1-Dodecanol	C ₁₂ H ₂₆ O
968.0	7758-97-6	Lead Chromate	CrO ₄ Pb

969.0	7447-41-8	Lithium Chloride	CLi
970.0	546-93-0	Magnesium Carbonate	CMgO ₃

Table 3: Chemical List (cont.)

C#	CAS#	Description	Molecular Formula
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971.0	298-00-0	Methyl Parathion	C ₈ H ₁₀ NO ₅ PS
972.0	628-28-4	Butyl Methyl Ether	C ₅ H ₁₂ O
973.0	142-47-2	Monosodium Glutamate	C ₅ H ₈ NNaO ₄
974.0	924-42-5	N-(Hydroxymethyl)acrylamide	C ₄ H ₇ NO
975.0	109-74-0	Butyronitrile	C ₄ H ₇ N
976.0	142-92-7	Hexyl Acetate	C ₈ H ₁₆ O ₂
977.0	105-59-9	N-Methyldiethanolamine	C ₅ H ₁₃ NO ₂
978.0	109-60-4	Propyl Acetate	C ₅ H ₁₀ O ₂
979.0	88-12-0	N-Vinyl-2-pyrrolidone	C ₆ H ₉ NO
980.0	554-84-7	3-Nitrophenol	C ₆ H ₅ NO ₃
981.0	124-19-6	Nonanal	C ₉ H ₁₈ O
982.0	108-82-7	2,6-Dimethyl-4-heptanol	C ₉ H ₂₀ O
983.0	279-23-2	Norbornane	C ₇ H ₁₂
984.0	498-66-8	Norbornene	C ₇ H ₁₀
985.0	528-29-0	o-Dinitrobenzene	C ₆ H ₄ N ₂ O ₄
986.0	112-96-9	Octadecycl Isocyanate	C ₁₉ H ₃₇ NO
987.0	124-13-0	Octanal	C ₈ H ₁₆ O
988.0	124-07-2	Octanoic Acid	C ₈ H ₁₆ O ₂
989.0	538-68-1	Pentylbenzene	C ₁₁ H ₁₆
990.0	122-60-1	Phenyl Glycidyl Ether	C ₉ H ₁₀ O ₂
991.0	536-74-3	Phenylacetylene	C ₈ H ₆
992.0	88-99-3	Phthalic Acid	C ₈ H ₆ O ₄
993.0	7447-40-7	Potassium Chloride	ClK
994.0	111-43-3	Propyl Ether	C ₆ H ₁₄ O
995.0	103-65-1	Propylbenzene	C ₉ H ₁₂
996.0	151-21-3	Sodium Docecyl Sulfate	C ₁₂ H ₂₅ NaO ₄ S
997.0	7631-99-4	Sodium Nitrate	NNaO ₃
998.0	1313-60-6	Sodium Peroxide	Na ₂ O ₂
999.0	7772-99-8	Stannous Chloride	Cl ₂ Sn
1000.0	57-11-4	Stearic Acid	C ₁₈ H ₃₆ O ₂
1001.0	121-57-3	Sulfanilic Acid	C ₆ H ₇ NO ₃ S
1002.0	540-88-5	<i>tert</i> -Butyl Acetate	C ₆ H ₁₂ O ₂
1003.0	762-75-4	<i>tert</i> -Butyl Formate	C ₅ H ₁₀ O ₂
1004.0	631-36-7	Tetraethylsilane	C ₈ H ₂₀ Si
1005.0	3333-52-6	Tetramethylsuccinonitrile	C ₈ H ₁₂ N ₂
1006.0	7705-07-9	Titanium Trichloride	Cl ₃ Ti
1007.0	76-03-9	Trichloroacetic Acid	C ₂ HCl ₃ O ₂
1008.0	102-71-6	Triethanolamine	C ₆ H ₁₅ NO ₃
1009.0	143-22-6	Triethylene Glycol Monobutyl Ether	C ₁₀ H ₂₂ O ₄
1011.0	76-05-1	Trifluoroacetic Acid	C ₂ HF ₃ O ₂
1012.0	122-20-3	Triisopropanolamine	C ₉ H ₂₁ NO ₃
1013.0	99-35-4	1,3,5-Trinitrobenzene	C ₆ H ₃ N ₃ O ₆
1014.0	115-86-6	Triphenyl Phosphate	C ₁₈ H ₁₅ O ₄ P
1015.0	102-69-2	Tripropylamine	C ₉ H ₂₁ N
1016.0	42978-66-5	Tripropylene Glycol Diacrylate	C ₁₅ H ₂₄ O ₆
1017.0	57-13-6	Urea	CH ₄ N ₂ O
1018.0	692-45-5	Vinyl Formate	C ₃ H ₄ O ₂
1019.0	105-38-4	Vinyl Propionate	C ₅ H ₈ O ₂

1020.0	78-78-4	Methylbutane, 2-	C ₅ H ₁₂
1021.0	19132-06-0	2,3-Butanediol, (2S,3S)-(+)-	C ₄ H ₁₀ O ₂

Table 4: Principal Literature Sources

BLOCK 1 - Oxygen Demand

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JOURNAL

ABBREVIATION

Acta Hydrochimica Hydrobiologica	Acta Hydrochim. Hydrobiol.
American Dyestuff Reporter	Amer. Dyestuff Reporter
American Public Health Association (APHA)	Am. Public Health Assoc. Yearb.
Applied Microbiology	Appl. Microbiol.
Annual Book of ASTM Standards	Ann. Book ASTM Stand.
Chemosphere	(same)
Industrial and Engineering Chemistry	Ind. Eng. Chem.
Industrial Pollution Control Handbook	(same)
Journal of Industrial Microbiology	J. Ind. Microbiol.
Journal of the Water Pollution Control Federation	J. Water Poll. Cont. Fed.
Plant Engineering Handbook	
Proceedings of the Purdue Industrial Waste Conference	
Proceedings of the American Association of Textile Chemists and Colorists	Proc. Amer. Assoc. Text. Chem & Colorists
Sewage and Industrial Wastes	Sew. Ind. Wastes
Vodosnabzhenie i Sanitarnaya Tekhnika	Vodosnabzh. Sanit. Tekh.
Vom Wasser	
Water Research	Water Res.

Table 4: Principal Literature Sources (cont.)

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Table 4: Principal Literature Sources (cont.)

BLOCK 2 - Soil/Water Partitioning (cont.)

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JOURNAL

ABBREVIATION

American Society of Agronomy	Am. Soc. Agron., Sp. Publ.
Bulletin of the Chemical Society of Japan	Bull. Chem. Soc. Jpn.
Ecotoxicology and Environmental Safety	Ecotoxicol. Environ. Saf.
Environmental Health Perspectives	Environ. Health Perspect.
Environmental Science and Technology	Environ. Sci. Technol.
Hazardous Waste and Hazardous Materials	Hazard. Waste Hazard. Mater.
Illinois Institute of Natural Resources, St. Geological Survey	Bull.-Ill. State Water Surv.
Journal of Agricultural and Food Chemistry	J. Agric. Food Chem.
Journal of Chemical and Engineering Data	J. Chem. Eng. Data
Journal of Environmental Quality	J. Environ. Qual.
Journal of Hazardous Materials	J. Hazard. Mater.
Reviews of Environmental Contamination and Toxicology	Rev. Environ. Contam. Toxicol.
Soil Science	Soil Sci.
Water Research	Water Res.

Table 4: Principal Literature Sources (cont.)

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Table 4: Principal Literature Sources (cont.)**BLOCK 3 - General Physical Properties (cont.)**Yaws, C.L., *Handbook of Thermal Conductivity, Vol. 1-3*, Gulf Publishing, Houston, 1995Yaws, C.L., *Thermodynamic & Physical Property Data*, Gulf Publishing, Houston, 1992

JOURNALS

AIChE Journal
 Analytica Chimica Acta
 Analytical Chemistry
 Angewante Chemie
 Canadian Journal of Chemistry
 Chemical Abstracts
 Chemical Engineering
 Chemical Reviews
 Chemosphere
 Environmental and Toxicological Chemistry
 Environmental Science and Technology
 Fluid Phase Equilibria
 Environmental Contamination and Toxicology
 Industrial and Engineering Chemistry Research
 J. Chemical Society of Japan (Nippon Kagaku Kaishi)
 J. of Applied Polymer Science
 J. of Applied Toxicology
 J. of Chemical and Engineering Data
 J. of Chemical Engineering of Japan
 J. of Chemical Information and Computer Science
 J. of Chemical Physics
 J. of Chemical Thermodynamics
 J. of Environmental Engineering
 J. of Hazardous Materials
 J. of Pharmaceutical Science
 J. of Physical Chemistry
 J. of Research of the National Bureau of Standards
 J. of Solution Chemistry
 J. of the American Chemical Society
 J. of the Chemical Society (London)
 J. Physical and Chemical Reference Data
 Makromolekular Chemie
 Materials Chemistry and Physics
 Mobay Technical Data Sheet for 2,4-Toluene Diisocyanate
 SAR and QSAR in Environmental Research
 Science
 Thermochemica Acta
 Water Research

ABBREVIATION

AIChE J.
 Anal. Chim. Acta
 Anal. Chem.
 Angew. Chem.
 Can. J. Chem.
 Chem. Abstr.
 Chem. Eng.
 Chem. Rev.
 (same)
 Environ. Toxicol. Chem.
 Environ. Sci. Technol.
 Fluid Phase Equilib.
 Environ. Contam. Toxicol.
 Ind. Eng. Chem. Res.
 J. Chem. Soc. Jpn.
 J. Appl. Polym. Sci.
 J. Appl. Toxicol.
 J. Chem. Eng. Data
 J. Chem. Eng. Jpn.
 J. Chem. Inf. Comput. Sci.
 J. Chem. Phys.
 J. Chem. Thermodyn.
 J. Environ. Eng.
 J. Hazard. Mater.
 J. Pharm. Sci.
 J. Phys. Chem.
 J. Res. Nat. Bur. Stand.
 J. Solution Chem.
 J. Am. Chem. Soc.
 J. Chem. Soc.
 J. Phys. Chem. Ref. Data
 Makromol. Chem.
 Mater. Chem. Phys.

 SAR QSAR Environ. Res.
 Sci.
 Thermochem. Acta
 Water Res.

Table 4: Principal Literature Sources (cont.)

BLOCK 4 - Partitioning/Equilibrium

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JOURNAL

AICHe Journal
Analytical Chemistry
Bulletin of the Chemical Society of Japan
Chemical Engineering
Chemical Engineering Progress
Chemosphere
Environmental Science and Technology
Environmental Toxicology and Chemistry
European Journal of Medicinal Chemistry
J. American Water Works Association
J. Chemical Engineering Data
J. Chemical Engineering of Japan
J. Chemical Society Japan (Nippon Kagaku Kaishi)
J. Physical Chemical Reference Data
J. Medicinal Chemistry
J. of Hazardous Materials
J. Solution Chemistry

ABBREVIATION

AICHe J.
Anal. Chem.
Bull. Chem. Soc. Jpn.
Chem. Eng.
Chem. Eng. Prog.
(same)
Environ. Sci. Technol.
Environ. Toxicol. Chem.
Eur. J. Med. Chem.
J. Am. Water Works Assoc.
J. Chem. Eng. Data
J. Chem. Eng. Jpn.
J. Chem. Soc. Jpn.
J. Phys. Chem. Ref. Data
J. Med. Chem.
J. Hazard. Mater.
J. Solution Chem.

Table 4: Principal Literature Sources (cont.)

BLOCK 5-Fire & Explosion

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JOURNAL

Chemical Engineering
Chemical Reviews
Chemicals and Products
Fire and Materials
Industrial and Engineering Chemistry (Research)
J. Chemical Engineering Data
J. of Hazardous Materials
J. of Research of the National Bureau of Standards
Soviet Chemical Industry

ABBREVIATION

Chem. Eng.
Chem. Rev.
Chem. Prod.
Fire Mater.
Ind. Eng. Chem. Res.
J. Chem. Eng. Data
J. Hazard. Mater.
J. Res. Nat. Bur. Stand.
Sov. Chem. Ind.

Table 4: Principal Literature Sources (cont.)**BLOCK 6 - Aquatic Toxicity**

JOURNAL	ABBREVIATION
Ambio	(same)
Aquatic Toxicology	Aquat. Toxicol.
Archives of Environmental Contamination and Toxicology.	Arch. Environ. Contam. Toxicol.
Archives of Environmental Health	Arch. Environ. Health
Bulletin of Environmental Contamination and Toxicology	Bull. Environ. Contam. Toxicol.
Canadian Journal of Fisheries and Aquatic Science	Can. J. Fish. Aquat. Sci.
Comparative Biochemistry and Physiology, C	Comp. Biochem. Physiol. C
Current Contents (A)	(same)
Ecotoxicology and Environmental Safety	Ecotoxicol. Environ. Saf.
Environment and Technology	Environ. Technol.
Environment and Ecology	Environ. Ecol.
Environmental Health Perspectives	Environ. Health Perspect.
Environmental Pollution, Series A	Environ. Pollut., Ser. A
Environmental Science and Technology	Environ. Sci. Technol.
Environmental Toxicology and Chemistry	Environ. Toxicol. Chem.
Freshwater Biology	Freshwater Biol.
Health	(same)
Hydrobiologia	(same)
Journal of Agricultural and Food Chemistry	J. Agric. Food Chem.
Journal of Environmental Quality	J. Environ. Qual.
Journal of Experimental Biology	J. Exp. Biol.
Journal of Experimental Marine Biology and Ecology	J. Exp. Mar. Biol. Ecol.
Journal of Fish Biology	J. Fish Biol.
Journal of Marine Research	J. Mar. Res.
Journal of the Fisheries Research Board of Canada (changed to Can. J. Fish. Aquat. Sci.)	J. Fish. Res. Board Can.
Journal of the Water Pollution Control Federation	J. Water Pollut. Control Fed.
Journal of Toxicology and Environmental Health	J. Toxicol. Environ. Health
Marine Biology	Mar. Biol.
Marine Ecology Progress Series	Mar. Ecol. Progr. Ser.
Marine Fisheries Review	Mar. Fish. Rev.
NAPCA Abstract Bulletin	(same)
Oikologia	(same)
Oikos	(same)
Progressive Fish Culturist	Prog. Fish Cult.
Reviews in Fish Biology and Fisheries Science	Rev. Fish Biol. and Fish. Science
Science and the Total Environment	Sci. Total Environ.
Sewage Works Journal (changed to J. Water Pollut. Control Fed.)	Sewage Works J.
Sewage and Industrial Wastes (changed to J. Water Pollut. Control Fed.)	Sewage Ind. Wastes
Transactions of the American Fisheries Society	Trans. Am. Fish. Soc.
Water Environment Research	Water Env. Res.
Water Research	Water Res.
Water and Sewage Works	Water Sewage Works
Water, Air, and Soil Pollution	Water Air Soil Poll.

Table 5: Evaluation Criteria for Soil/Water Partition Coefficient

Criteria	Score		
	0	1	2
Experimental Conditions	Data not from primary source	Paper does not report that the sample was sterilized/measured for byproducts.	Paper reports that the samples was sterilized/measured for byproducts.
Purity of Chemicals	Data not from primary source	All others	Supplier reported
Experimental Techniques	1 soil tested	2 - 4 soils tested	³ 4 soils tested
Reported Accuracy/Internal Precision*	No consideration given to relevant conditions	Some relevant conditions monitored and reported	All relevant conditions monitored and reported
Agreement with other work	Low scores for previous evaluation criteria and no discussion of comparison to other work and/or poor comparability	High scores for previous evaluation criteria and no discussion of comparison to other work and good comparability of data	High scores for previous evaluation criteria and discusses work done by others with good comparability of data

* Important considerations include: equilibration, removal of solids from dilution water, soil pH, temperature and general quality of work and journal.

NOTE: The relevance of these conditions varies for different chemicals and different types of tests. Designations are determined by the reviewer and explained in the comment section specific to the value.

Table 6: BOD Rating Criteria

PAPER INFORMATION

Title _____

Author(s) _____

Comments _____

=====

Rating Criteria

Followed Standard Methods (temperature not included)

Yes (2)

No or cannot tell from information provided (0)

Temperature Reported?

Yes (2)

No (0)

Acclimation

Acclimated seed was used (3)

Non-Acclimated seed was used (1)

Acclimation not reported (0)

Concentration Reported?

Yes (1)

No (0)

Internal Consistency

Compared results to ThoD (2)

No comparison to ThoD (1)

TOTAL

Table 7: Some Reliable References and Criteria for Soil/Water Partitioning

Reference	Equil time	Sterilization	Water source	# of soils	pH	OC%	Method
ASTM, 1991	³ 48 hours ¹	Mass balance ²	Source or Reagent Grade ³	³ 4	6	-	BP1
Barber, 1992	48 hours	None	NS	4	NS	0.8-5.7	BP2
Lee, 1991	NA CS	MW radiation	NS	1	NS	0.39	MD
Ball, 1991	9-100 days	Autoclaved	NS	8	NS	0.015-0.099	BP2
Boyd, 1982	24 hours ⁴	Anaerobic	NS	1	NS	5.10(OM)	BP3
Schellenberg, 1984	15-20 hours ⁴	None	NS	3	NS	0.84-9.4	BP2
Brown, 1981	24-72 hours ⁴	None	NS	1	NS	3.27	BP1
Chin, 1988	120 hours ⁴	None	NS ⁵	2	NS	0.13-1.42	BP4
Russell, 1986	25 hours	sodium azide	NS	2	NS	0.26-1.59	BP2
Walters, 1989	2 days	sodium azide	NS ⁵	1	7	0.66	BP3
Hassett, 1980	20-24 hours	None ⁶	NS	14	NS	0.11-2.38	BP2
Karickhoff, 1979	24-48 hours ⁴	None	NS ⁵	3	NS	0.086-3.29	BP2
Abdul, 1987	24 hours ⁴	None	Milli-Q	3	NS	0.04-2.2	BP2
Rippen, 1982	24 hours ⁴	None	NS	3	NS	0.69-2.24	BP2
Garbini, 1985	~24 hours	None	NS	2	NS	0.23-0.41	BP5

Abbreviations: NS=Not stated in article, BP1=Bottle point with varying sorbent amount, BP2=Bottle point with more than one sorbent of varying organic carbon concentration, BP3=Bottle point with varying chemical concentration in solution, BP4=Bottle point with one soil and one point, BP5=Bottle point with different sorbents of varying sorbent organic carbon concentration where the gas phase was sampled, NA=Not applicable, CS=Column study, GP=Gas purge, MD=Miscible displacement, MW=Microwave

Footnotes: 1=Preliminary tests should be done to determine appropriate equilibrium time, 2=Used to determine if degradation has occurred, 3=Source water should be treated to remove particulate matter, 4=Equilibrium was confirmed with kinetic studies or by sequential sampling, 5=Particulate matter removed by washing, 6=Byproducts of degradation were looked for in the form of unidentified peaks in the gas chromatograph recording.

References:

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 Walters, R.W., S.A. Ostazewski, and A. Guiseppi, *Environ. Sci. Technol.* **23** 480 (1989)

Table 8: Evaluation Criteria for Block 3

Criteria	Score		
	0	1	2
Experimental Conditions	Not stated	Stated without range	Stated with range
Purity of Chemicals	Not stated	Stated with no range or as received with range	Stated with range, purified, or calculated
Experimental Technique	Not stated or Not acceptable	Stated briefly	Described in detail
Reported Accuracy and/or Internal Precision- QA/QC Procedures	Not stated or >20%	Stated with 5-20%	Stated with 1-5%
Qualitative Agreement with Other Work	Does not agree	Agrees	Agrees well with other work

Table 9: Evaluation Criteria for Block 6

* Essential Information

	Score		
	0	1	2
Experimental Conditions Temperature and DT* Animal Loading* Volume Additions* Water Chemistry* Water Source* Photo-period Food before experiment	Essentials not all reported or secondary source.	Reported as given elsewhere (other source); standard techniques named but few essentials reported; non-standard technique with all conditions reported.	Standard technique with all essentials listed.
Purity of Chemicals Source of chemical* Verification of experimental conc.* Purity of chemical from source reported	Not stated or secondary source.	Source listed or concentration verified.	Sources reported and concentrations verified.
Experimental Technique (Standard) technique reported or described* Number of replicates reported* Random assignment* Age, size, and supplier of organism rptd* Concentration of chemical verified throughout experiment (24 intervals)* Control used when chemical is dissolved in solvent.	Not reported or standard method without details or secondary source.	Standard method listed with incomplete report of essentials; non-standard technique with full report of essentials.	Standard method with full report.
Accuracy/Precision Statistical tests named & appropriate* No pseudo-replication* Confidence limits reported*	1 significant figure with 20% confidence or secondary source.	2 significant figures and 5-20% confidence with essentials.	2 significant figures and 1-5% confidence with essentials.
Agreement with others		Agrees with own work.	Agrees with other's work or reports comparisons.

Table 10: Translation of DIPPR® 801 Evaluation Codes to DIPPR® 911 Evaluation Codes

Type of Data	Definition	Points Allocated
X	Experimental	1
P	Predicted	Rating will be blank
D	Defined	Rating will be blank
S	Smoothed	Rating will be blank
?	Unknown	Rating will be blank
T	Extrapolated	Rating will be blank
Nature of Data Source		
E	Evaluated Source	1
U	Unevaluated Source	0
"blank"	Predicted, Interpolated, or derived from the definition by the project staff	0
Reliability of Data		
"blank"	Predicted or derived at PSU	0
0	Unknown Accuracy	0
1	< 0.2% Error	2
2	< 1% Error	2
3	< 3% Error	2
4	< 5% Error	1
5	< 10% Error	1
6	< 25% Error	0
7	< 50% Error	0
8	< 100% Error	0
9	> 100% Error	0

Table 11: Structure for Values Table

Field Name	Purpose	Field Type and Size
C#	Chemical Number	N*
Property Code	Property Code	A3*
Article #	Citation Number	N*
Rating	Quality Rating	N
Desc/Method	Experimental Method or 801 Quality Code	A30
Keywords	Keywords	A30
Value	Value or Lower Temperature Limit	N
Units	Units	A11
Temperature	Experimental Conditions or Upper Temperature Limit	A13
Equation	Correlation Equation Number	A3
Coef1	Coefficient for Equation or Lower Confidence Limit (Block 6)	N
Coef2	Coefficient for Equation or Upper Confidence Limit (Block 6)	N
Coef3	Coefficient for Equation or Hardness (Block 6)	N
Coef4	Coefficient for Equation or pH (Block 6)	N
Coef5	Coefficient for Equation	N
Ref2	Project 801 Second Reference	N
Ref3	Project 801 Third Reference	N
FootN	Project 801 Footnote Code	A2
Pressure	Experimental Conditions or Life stage of Organism (Block 6)***	A13
Comment	Comment	A120

* Key Field

Table 12: Structure of Citation Table

Field Name	Purpose	Field Type and Size
Paper #	Data Source Number	N*
Title	Title	A120
Author	Author	A120
Journal	Journal	A120
Date	Date of Publication	A15
Volume	Volume	A15
Number	Journal Number	A15
Pages	Page Number	A15
Pcode1	Property code for tracking	A3
Pcode2	Property code for tracking	A3
Pcode3	Property code for tracking	A3
Pcode4	Property code for tracking	A3
Pcode5	Property code for tracking	A3
Pcode6	Property code for tracking	A3
Date Assigned	Date for tracking	D

* Key Field

Table 13: Structure of Property Table

Field Name	Purpose	Field Type and Size
Property Code	Property Code	A3
Description	Property Name	A45
Reviewer	Technical Reviewer	A30
Default Units	Default Units for the Property	A11
T. Dep.	Temperature Dependent?	A1

Table 14: Structure of Chemical Table

Field Name	Purpose	Field Type and Size
C#	Project 911 Chemical Number	N*
CAS#	Chemical Abstract Number	N
Description	Clean Air Act Name	A50
Molecular Formula	Molecular Formula	A25
Structural Formula	Structural Formula	A25
Common Name	Common Name	A50
Chem. Abstracts Name	CAS Name	A50
Family Group (see Table 20)	Chemical Family Group	A2

* Key Field

Table 15: Structure of Convunit Table

Field Name	Purpose	Field Type and Size
From Units	Units from the database (VALUES Table)	A11*
To Units	Default Units or Unit Options	A11*
Multiplier Property	Multiplier Property	A3
Multiplier	Multiplier	N
Addend	Addend	N
Mult Property Flag	Multiplier Property Flag	A1
Comment	States for which properties units are used	A20

* Key Field

Table 16: Criteria for Flagging Data Entry Errors and Significant Outliers

Property Code	Project 911 Description	Error Analysis
Block 1	Oxygen Demand	
1a	Biochemical O ₂ Demand (BOD)	1a <= 1cn
1b & 1bp	Dichromate Chemical O ₂ Demand (COD) Permanganate Chemical O ₂ Demand (COD)	1b <= 1cc 1bp <= 1b
1cc & 1cn	Theoretical O ₂ Demand, Carbonaceous Theoretical O ₂ Demand, Combined	1cc <= 1cn
Block 2	Partitioning Parameters	
2a	1-Octanol/Water Partitioning	Log K _{ow} vs. Log K _{oc} Scatter Plot
2c	Organic Carbon/Water Partitioning	Log K _{oc} vs. Log K _{ow} Scatter Plot
2d	Bioconcentration Factor	> ±1 logarithmic unit
Block 3	General Physical Properties	
3a	Molecular Weight	> 5%
3b	Liquid Density at 298.15 K (±5 K)	> 10%
3d	Melting Point	> 10%
3e	Normal Boiling Point	> 10%
3f	Vapor Pressure at 298.15 K (±5 K)	> 50%
3h	Molecular Diffusivity in Air	> 30%
3i	Molecular Diffusivity in Water	> 30%
3l	Surface Tension at 298.15 K (±5 K)	> 10%
3n	Enthalpy of Formation at 298.15 K (±5 K)	> 20%
3q	Critical Temperature	> 10%
3r	Critical Pressure	> 10%
3s	Critical Volume	> 10%
3t	Enthalpy of Vaporization at 298.15 K	> 20%
Block 5	Fire and Explosion Parameters	
5al	Lower Flammability Limit in Air	> 25%
5au	Upper Flammability Limit in Air	> 50%
5b	Flash Point	> 10%
5c	Autoignition Temperature	> 15%
5d	Enthalpy of Combustion at 298.15 K	> 10%
Block 6	Sensory, Health and Toxicity Impacts	
6..	Acute Aquatic Toxicity	> 50%

Table 17: Project 912 Estimation Methods Included in Project 911 Software Product

PROPERTY (CODE)	ESTIMATION TECHNIQUE
Biochemical Oxygen Demand (BOD) (1a)	None
Chemical Oxygen Demand (COD) (1b)	COD = ThOD for 14 chemical classes.
Theoretical Oxygen Demand, Carbonaceous (ThOD) (1cc)	Baker (1994; corrected, 1999) Baker (1994)
Theoretical Oxygen Demand, Combined (ThOD) (1cn)	Baker (1994)
Octanol Water Partitioning (Log K _{ow}) (2a)	UNIFAC (Fredenslund, 1975) with choice of interaction parameter set ENV- Environmental Parameter Set (Rogers, 1994) GBL- Global (Rogers, 1994) VLE- Vapor Liquid Parameter Set (Hansen, 1991) LLE- Liquid Liquid Parameter Set (Gemhling, 1982) Kenga-Goring (1980) Hansch (1968)
Organic Carbon Water Partitioning Log(K _{oc}) (2c)	Baker et al. (1997)
Bioconcentration Factor (2d)	Kobayashi (1981) Kenaga and Goring (1980)
Molecular Weight (3a)	Estimate from addition of UNIFAC chemical fragment groups, if necessary
Liquid Density (3b)	Bhirud (Bhirud, 1978) Modified Racket equation (Spencer, 1972), using critical properties.
Solubility in Water (3c)	Yalkowsky and Mishra (1990) UNIFAC (See above)
Solubility of Water in Chemical	UNIFAC (See above)
Melting Point (3d)	Taft and Starek (1930: Horvath, 1992) Lorenz and Hertz (1922: Horvath 1992)
Molecular Diffusivity in Air (3h)	Wilke-Lee (1955)
Molecular Diffusivity in Water (3i)	Hayduk and Minhas (1982). Hayduk and Laudie (1974). Polson (1950) Wilkie and Chang (1955).
Surface Tension (3l)	Brock and Bird (Danner, 1983)
Heat of Vaporization at 25° (3t)	Watson (1931; Reid, <u>et al.</u> , 1986)
Heat of Vaporization at NBP	Klein (1949: Lyman, 1982) Chen (1965) Watson (1931; Reid, <u>et al.</u> , 1986)
Activity Coeff. Of Water in Chemical (4b)	UNIFAC (See above)
Henry's Law Constant (4c)	UNIFAC (SEE ABOVE)
Upper and Lower Flammability Limit in Air (5a and 5b)	MTU Group Contribution Method (Pintar, 1999) MTU Combustion Reaction Method (Pintar, 1999) Penn State Group Contribution Method (Danner, 1986)

Table 18: Family Grouping Codes

AA Normal Alkanes	OT Other ethers/diethers
MA Methylalkanes	CT Epoxides
DA Dimethylalkanes	
OA Other alkanes	TT Peroxides
CA Cycloalkanes	AH C1/C2 Aliphatic chlorides
	HH C3 and higher aliphatic chloride
GA Alkylcyclopentanes	RH Aromatic chlorides
HA Alkylcyclohexanes	VH C,H,Br Compounds
RA Multiring cycloalkanes	
AE 1-Alkenes	WH C,H,I Compounds
BE 2,3, or 4-Alkenes	FH C,H,F Compounds
	PH C,H, Multihalogen compounds
ME Methylalkenes	AM Normal aliphatic primary amines
EE Ethyl and higher alkenes	BM Other aliphatic amines
CE Cycloalkenes	
DE Dialkenes	RM Aromatic amines
YY Alkynes	OM Other amines, imines
	NX Nitriles
AR Normal alkylbenzenes	TN C,H, NO ₂ Compounds
BR Other alkylbenzenes	YN Isocyanates/diisocyanates
MR Other monoaromatics	
DR Naphthalenes	DZ Diazoalkanes
OR Other condensed rings	SD Mercaptans
	SF Sulfides/thiophenes
PR Diphenyl/polyaromatics	SU Sultones
TR Terpenes	PC Polyfunctional acids
HR Other hydrocarbon rings	
IG Inorganic gases	PS Polyfunctional esters
LD Aldehydes	PO Other polyfunctional C,H,O
	NP Polyfunctional nitriles
KK Ketones	TM Nitroamines
AL Normal alcohols	PM Polyfunctional amides/amines
OL Other aliphatic alcohols	
CL Cycloaliphatic alcohols	PN Polyfunctional C,H,O,N
RL Aromatic alcohols	SP Polyfunctional C,H,O,S
	HP Polyfunctional C,H,O,halide
PL Polyols	BP Polyfunctional C,H,N,halide,(O)
AC Normal aliphatic acids	OP Other polyfunctional organics
OC Other aliphatic acids	
DC Dicarboxylic acids	LX Elements
RC Aromatic carboxylic acids	SX Silanes/siloxanes
	GI Organic/inorganic compounds
HD Anhydrides	IC Inorganic acids
FS Formates	IB Inorganic bases
ES Acetates	
BS Propionates and butyrates	GS Organic salts
SS Other saturated aliphatic esters	XS Sodium salts
US Unsaturated aliphatic esters	OS Other inorganic salts
RS Aromatic esters	IH Inorganic halides
AT Aliphatic ethers	OI Other inorganics

Table 19: Results of SPC Review

Physical Property	Number of Values Evaluated	Number and Type of Error AF / DE / AD	Level 1 Tolerance Value	Quality Code
Molecular Weight	5669	5 / 16 / 1	± 5%	Q1
Melting Point	3891	88 / 20 / 5	± 10%	Q1
Normal Boiling Point	5628	20 / 34 / 10	± 10%	Q1
Diffusivity in Air	1282	8 / 1 / 0	± 30%	Q1
Diffusivity in Water	1141	63 / 4 / 1	± 30%	Q1
Heat of Formation	1510	173 / 50 / 21	± 20%	Q1
Critical Temperature	3469	22 / 5 / 0	± 10%	Q1
Flash Point	3256	73 / 121 / 25	± 10%	Q1
Heat of Combustion	1285	76 / 10 / 9	± 10%	Q1
TOTAL	27,131	508 / 261 / 72		
		AF2 / DE / AD		
Melting Point less than Normal Boiling Point	3635	56 / 7 / 1		Q2

AF: Anomaly Flagged, Level 1; value is correct as transcribed from literature source

AF2: Anomaly Flagged, Level 2; value is correct as transcribed from literature source

DE: Data Entry Error

AD: Anomaly, Rating Dropped; highest rated value is transcribed correctly from literature source, but does not agree with multiple other literature values.

Figure 1: DIPPR® 911 Tracking Form

Figure 2: Citation Formats

Books

(complete - not a compilation)

Author : Author or Editor(s)
Title : Book Title
Journal : Publisher and City, State
Volume : If given
Number : Chapter or Subheading
Pages : Starting Page #
Date : Year

Books

(compilation)

Author : Chapter Author(s)
Title : Title of Chapter
Journal : Book Title, Editor(s), Publisher, Place of Publication
Volume : If given
Number : Chapter
Pages : Starting Page #
Date : Year

Industrial Reports

Author : Company and Division
Title : Title (or subject); if sales literature note such in parentheses
Journal : Company Address
Volume :
Number : Report Number (if given)
Pages :
Date : Date

Figure 4: Acute Aquatic Toxicity Entry Format

Values Table Fields

C #	DIPPR chemical number
Property Code	DIPPR property code
Article #	DIPPR article number
Rating	quality code assigned by reviewer (0-10; 0 if predicted, 1 if secondary)
Desc/Method	experiment method*
Keywords	species tested For toxicity, note species here if it is a Salmonidae or Mysidacea)
Value	toxicity or BCF value from article
Units	mg/L for toxicity; unit-less for BCF; If author reports as log of a value but does not report the original units, then record the log value, leave units blank, and provide a note in comment.
Temperature	test temp. or temp. range, °C If a temp. range is given, put median in "Temperature;" include range as a ±... in "Comment."
Equation	unused field
Coef1	lower 95% confidence limit
Coef2	upper 95% confidence limit
Coef3	pH (If pH is a range, put median in "Coef3;" include range as a ±... in "Comment.")
Coef4	hardness (mg/L as CaCO ₃) (If hardness is a range, put median in "Coef4;" include range as a ±... in "Comment.")
Coef5	unused field
Ref2	unused field
Ref3	unused field
FootN	unused field
Pressure	life stage of organism**
Comment	additional pertinent details (For: < or > EC50, LC50, or BCF values; data which do not fit in other fields; ±values or ranges of temperature, pH, hardness. For BCFs, include exposure duration in "Comment." Note when data at other test conditions are available. Note whether QSARs are available. For secondary sources, list the reference for the data). Example--describe coefficients 1 and 2 if they are not the lower and upper confidence limits; report hardness as hard or soft if author reports this but no values are given.

* Standard methods are abbreviated:

APHA = American Public Health Association USEPA = United States Environmental Protection Agency
 ASTM = American Society for Testing and Materials AWWA = American Water Works Association
 OECD = Organization for Economic Cooperation and Development WPCF = Water Pollution Control Federation

If a standard method was used, follow method abbreviation with a hyphen and an abbreviation of the exposure system:

f = flow-through fc = flow-through, covered system to limit volatilization
 s = static sc = static, covered vessel to limit volatilization
 sr = static with renewal src = static with renewal, covered vessel to limit volatilization
 r = recirculation rc = recirculation, covered system to limit volatilization

Example: EPA-s means the author used the U.S. Environmental Protection Agency method in a static water system.

** Pressure field is used for the organism's life stage information (weight, length, age). Use the following abbreviations:

g = gram	mm = millimeter	y = years
mg = milligram	cm = centimeter	mo = months
ug = microgram		w = weeks
		d = days

If the author uses a term rather than an age, note the term in comments (ex: juvenile; larval; smolt).

Conversions to mg/L

from g/m³, no change

from g/L, multiply by 1000

from ppm (parts per million), no change

from ppb (parts per billion), divide by 1000

from mol/L, multiply by molecular weight and by 1000

from mmol/L, multiply by molecular weight

from German dH° hardness to mg/L CaCO₃, divide by .056

Salmonidacea (salmon and trout family)

scientific name

Salmo salar

Salmo trutta

Salmo trutta lacustris

Salvelinus alpinus

Salvelinus fontinalis

Salvelinus leucomaenis

Salvelinus malma

Salvelinus namaycush

Salvelinus sp.***

Oncorhynchus aguabonita

Oncorhynchus clarki

Oncorhynchus gilae

Oncorhynchus gorbuscha

Oncorhynchus keta

Oncorhynchus kisutch

Oncorhynchus masou

Oncorhynchus mykiss

or Salmo Gairdneri

Oncorhynchus nerka

Oncorhynchus tshawytscha

common name

Atlantic salmon

Brown trout

Lake trout

Arctic char (or charr)

Brook trout

White spotted char (or charr)

Dolly varden

Lake trout

Siscowet

Trout, charr

Golden trout

Cutthroat trout

Gila trout

Pink salmon

Chum salmon

Coho salmon

Silver salmon

Cherry salmon

Yamame trout

Rainbow trout

Donaldson trout

Sockeye salmon

Chinook salmon

Mysidacea (Opossum shrimp order)

scientific name

Mysidopsis almyra

Mysidopsis bahia

Mysidopsis bigelowi

Mysis relicta

Neomysis americana

Neomysis awatschensis

Neomysis integer

Neomysis sp.***

Leptomysis lingvura

Leptomysis mediterranea

*** sp. = species, any species of the given genus.