Background Document on:

The Selection of Initial HWIR Chemicals

for the Proposed

Hazardous Waste Identification Rule

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1.0 Introduction and Selection Process

As part of the Hazardous Waste Identification Rule (HWIR), EPA developed a multi-pathway risk model that will be used to determine concentrations (i.e., levels) of chemicals below which wastes containing these chemicals could become exempt from RCRA Subtitle C Regulations. The preamble to the proposed rule discusses how EPA developed a Master List of Chemicals that are currently "of concern" to the RCRA program. From this Master List, EPA then determined which of these chemicals had toxicity benchmarks with sufficient quality to run this multi-pathway risk model.

The complexity of the risk model, however, in conjunction with both data and time limitations precluded EPA from developing exemption levels for all of these chemicals consistent with the schedule for the proposed rule. EPA then determined that the risk model needed to be tested using a smaller set of chemicals. This document discusses how the EPA selected this set of "representative" chemicals. The preamble to the proposed rule provides more detail on the circumstances surrounding the need for this smaller set of chemicals.

1.1 What was the first step?

As a starting point, EPA took all of the chemicals with at least one toxicological benchmark and sorted them into 16 groups of somewhat similar chemical, physical and structural properties. The criteria used to establish these groups included: 1) the degree of aromaticity (e.g., aromatic hydrocarbons vs polynuclear aromatic hydrocarbons); 2) the range of volatility (e.g., all of the chlorinated hydrocarbons tend to be relatively volatile); 3) the presence or absence of different kinds of halogens in the chemical structure (e.g., bromine vs chlorine); 4) the presence or absence of other key elements (e.g., oxygen, nitrogen, sulfur and/or phosphorus); 5) the use of the chemical (e.g., pesticides); 6) the presence or absence of certain organic functional groups (e.g., phenols and carbamates); and/or 7) the ionic state in aqueous systems (e.g., cationic vs anionic metals).

1.2 What are the 16 Groups of Chemicals?

The following table presents a summary of the 16 groups of chemicals that EPA developed. The first column provides a reference to the section of this document that explains how each chemical within that group was selected. This table also provides a summary of the number of chemicals in each group and the number of chemicals selected as representatives of that group. At the beginning of the selection process, EPA had identified a total of 188 chemicals with at least one toxicity benchmark. Since the risk assessors and model developers needed to begin obtaining and verifying physical and chemical parameters for this reduced set of chemicals, it was necessary to temporarily "freeze" the number of chemicals from which the selection process would proceed. In the mean time, EPA continued to investigate the availability of toxicity benchmarks for the chemicals remaining on the Master List. This document does not include information on any other chemicals for which additional toxicity data has since been obtained.

Summary of the 16 Groups			
Discussed in Section	**Chemical Group Used to Select Representatives**	**# chemicals in group**	**# chemicals selected**
2.1	Aromatic Hydrocarbons	6	2
2.2	Polynuclear Aromatics	13	2
2.3	Brominated Hydrocarbons	7	1
2.4	Chlorinated Hydrocarbons	26	6
2.5	Chlorinated Aromatics	8	1
2.6	Chlorinated Pesticides	23	2
2.7	Chlorinated Phenolics	6	1
2.8	Halogenated Dioxins and Furans*	1	1
2.9	Miscellaneous Chlorinated Organics	10	1
2.10	Oxygen, Hydrogen and Carbon Chemicals	32	4
2.11	Organonitrogen Chemicals	31	5
2.12	Carbamates and Related Structures**	0	1
2.13	Sulfur and/or Phosphorus Containing Chemicals	11	1
2.14	Cationic Metals***	8	8
2.15	Anionic Metals	6	6
2.16	Cyanides and Inorganics****	0	0
	Totals:	188	42

* - This group was included based on the perception that EPA may want to add all of the 16 Halogenated Dioxins and Furans isomers that can be measured in wastes. When this group was developed, no determination had been made as to whether these 16 extra isomers had to be modeled individually or whether exemption levels could be extrapolated using toxicity equivalency factors based on 2,3,7,8-TCDD.

** - This group was included based on an anticipated need for modeling these chemicals in order to cover the relatively "new" listings associated with them. When this group was developed, benchmarks had not been fully investigated. Thiram was selected with the hopes of testing the model for at least representative of this group.

*** - Lead and Silver were included in this group, even though their benchmarks were not completely evaluated when this document was first developed. They were added in order to complete the characterization of wastes containing metals. "Total Mercury" is also considered to be a representative of Phenyl mercury acetate, which has a separate benchmark.

**** - Decisions on appropriate benchmarks for Cyanide, Fluoride and Sulfide had not been made when this document was being developed so there were no "representatives" selected for this group.

1.3 What criteria were used to select chemicals within the 16 groups?

A team of EPA scientists with collective experience in toxicology, fate and transport modeling, waste chemistry and programmatic policy reviewed the chemicals with benchmarks and selected a total of 42 representative chemicals. The selection process further involved considerations such as: 1) the total number of chemicals within a group; 2) the range of expected toxicity of the chemicals within the group; 3) availability of verified chemical and physical property; 4) the differences in chemical structures within the group; 5) the differences in degree or type of halogenation (chlorinated vs. brominated); 6) the representativeness of the toxicity data for chemical isomers (mixed vs individual); 7) the need for modeling degradation products for that chemical; 8) the significance of the chemicals to other programs in EPA; and/or 9) the number of waste streams and types of industrial processes that generate wastes containing these chemicals. Further details on which of these factors were used to select each representative chemical are presented in Section 2 of this document.

1.4 What databases were used to support the selection of chemicals?

EPA used two databases to assist in determining which chemicals were expected to be the most frequently encountered in RCRA hazardous waste streams, the ***1996 National Hazardous Waste Constituent Survey (NHWCS) Database*** and the ***Toxic Release Inventory (TRI) Data for 1994.*** These data were very important in helping select the representatives from *within* each group.

1.5 What data were used and what were their limitations?

The NHWCS database provided information on the relative number of RCRA waste streams that were *known* to contain these chemicals. Since it was a survey and since it only contains data from RCRA-regulated facilities that treat, store or dispose of hazardous wastes (i.e., referred to as TSDFs), it does not necessarily provide an accurate picture of the number of *generators* of wastes containing these chemicals. At the same time, the NHWCS database does represent the vast majority of wastes being handled nationally *on a volume basis*. (NOTE: This is because most generators send their wastes to TSDFs for treatment, storage or disposal. The problem arises from the fact that TSDFs aggregate these wastes and many facilities reported the constituent concentrations for their aggregated wastes. As such, these data do not reflect the true number of wastes containing these chemicals that were received by these facilities.)

In order to supplement the NHWCS data with regards to the number of *potential* waste generators, EPA decided to include the number of TRI report forms submitted in 1994 for these chemicals. While the number of forms submitted for a given chemical can be greater than the number of facilities submitting the forms, EPA felt that this was still a good *surrogate* measure for the frequency of *potential occurrence* in wastes. (NOTE: Even though there are more recent data than 1994 currently available, the 1994 TRI data were readily available to the EPA analysts. Since the data from both of these sources were only used to compare the relative frequency of occurrence of these chemicals, the dates of these data was deemed less important.)

EPA did not use volumes of wastes containing these chemicals from the NHWCS nor did it use pounds of chemicals released in the TRI to compare relative frequency of occurrence. EPA felt that the *number* of NHWCS wastes containing these chemicals and the *number* of TRI forms submitted by industry was a more accurate reflection of the *frequency* of potential occurrence of these chemicals.

For some specific chemicals (e.g., PCBs) and groups of chemicals (e.g., PAHs and Chlorinated Dioxins/Furans) EPA felt, however, that both of these data sources probably under represented the potential frequency of occurrence in RCRA wastes. These cases of probable under representation are explained later in this document under the discussion of the appropriate group of chemicals.

2.0 Selection of the Representative Chemicals

This section of this document discuss EPA's reasoning behind selecting each of the 42 representative chemicals from the 16 Groups of Chemicals. In general, each subsection discusses the following five issues, as appropriate.

What chemicals are represented by this group? This section provides a list of chemicals which fall under the group. This section also provides data on the frequency of appearance of these chemicals in RCRA hazardous wastes as presented by the number of wastes reported to contain them according to EPA's 1996 National Hazardous Waste Constituent Survey (NHWCS). The table also includes the number of forms submitted for each chemical under the requirements of EPA's Toxics Release Inventory (TRI) that were submitted for the 1994 reporting period.
What was the basis for creating the group? This section provides a discussion of the similarities in structures, use, or industries generating or using these chemicals.
What chemicals were selected for the first round of constituents? This section clearly lists which chemicals were selected from that group.
Why were they chosen? This section provides a discussion for each chemical that was selected
Why weren't others chosen? This section provides a brief discussion of other chemicals that could have been selected and why certain others were not.

2.1 Aromatic Hydrocarbons

2.1.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	Hydrocarbon on the Benzene Ring	# of Waste Streams in NHWCS	# of TRI Forms in 1994
71-43-2	Benzene	yes	none	300	491
108-88-3	Toluene	yes	methyl	357	3,566
1330-20-7	Xylene(s) o-Xylene m-Xylene p-Xylene	no	two methyls	305	3,346
98-82-8	Ethyl benzene	no	ethyl	212	969
100-41-4	Cumene	no	isopropyl	6	237
100-42-5	Styrene	no	vinyl	25	1,489

2.1.2 What was the basis for creating the group?

All of the chemicals in this group have one benzene ring as the core structure and except for benzene, they also have a relatively simple hydrocarbon structure (e.g., methyl, ethyl, etc) attached to the ring. All of these chemicals have a reasonably high volatility.

2.1.3 What chemicals were selected for the first round of constituents?

Benzene and Toluene.

2.1.4 Why were they chosen?

Benzene was chosen because it is the backbone structure of the group, but more importantly it is also a known carcinogen and is one of the most toxic chemicals in the group. Toluene was chosen over the others in this group because it was reported to be present in the largest number of waste streams in the NHWCS and had the greatest number of 1994 TRI reports submitted on it. Toluene was also selected as a representative of one with relatively low toxicity.

2.1.5 Why weren't others chosen?

Xylenes was a strong candidate for selection because it was reported present in a large number of wastes and there were a lot of TRI forms for it. However, this chemical represents a mixture of three isomers and EPA decided in general that it was not going to test the model *in this phase* with chemicals that involve more than one isomer. EPA has not determined whether the model should use physical/chemical data and toxicity data for each isomer or for the mix of isomers. Ethyl benzene was also a strong candidate for the first round because it was also reported to be contained in a relatively high number of wastes in the NHWCS. Ethyl benzene and Xylenes are often found with Benzene and Toluene in wastes from the petroleum refining industry or from the use of petroleum products. Since these wastes tend to be high volume wastes, EPA would most likely include Ethyl benzene and Xylenes in an expanded list of chemicals.

Styrene is used in making plastics and, as such, there were a significant number of 1994 TRI reports submitted on it. However, there were a relatively small number of wastes reported in the NHWCS to have contained Styrene. On exposure to light and air, Styrene slowly undergoes self-polymerization which can pose difficulties during testing of environmental samples. Styrene is not on the Universal Treatment Standards List (UTS). As a result of all of these factors, Styrene was not chosen for the first round.

Cumene is used in the production of some high volume organic chemicals such as phenol and acetone. This may be why the number of TRI reports for Cumene were relatively high; however, Cumene was not reported to be contained in very many wastes in the NHWCS. Cumene is not on the Universal Treatment Standards List (UTS) because it is not easily measured with standard Gas Chromatography - Mass Spectrometry (GCMS) equipment. As a result of all of these factors, Cumene was also not chosen for the first round.

2.2 Polynuclear Aromatics

2.2.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	Number of Aromatic Rings	# of Waste Streams in NHWCS	# of TRI Forms in 1994
91-20-3	Naphthalene	no	2	93	527
83-32-9	Acenaphthene	no	3	28	none
86-73-7	Fluorene	no	3	31	none
206-44-0	Fluoranthene	no	4	6	none
56-55-3	Benz[a]anthracene	no	4	34	none
218-01-9	Chrysene	no	4	40	none
129-00-0	Pyrene	no	4	44	none
57-97-6	7,12-Dimethylbenz[a]anthracene	no	4	1	none
205-99-2	Benzo[b]fluoranthene	no	5	4	none
56-49-5	3-Methylcholanthrene	no	5	none	none
50-32-8	Benzo[a]pyrene	yes	5	38	none
53-70-3	Dibenz[a,h]anthracene	yes	5	4	none
193-39-5	Indeno[1,2,3-cd]pyrene	no	6	4	none

2.2.2 What was the basis for creating the group?

All of the chemicals in this group consist of two or more “aromatic” rings. All of the chemicals except for Naphthalene (which consists of only two “fused” benzene rings) share double bonds with another benzene ring, a cyclopentane ring , a cyclopentadiene ring, or a pyridine ring. This series of interconnected “aromatic” rings is referred to as “polynuclear aromatic”. All of these chemicals are semivolatiles; however, Naphthalene has a high enough vapor pressure that it sublimes (i.e., goes directly to a gaseous state from a solid state) and is often considered to be a volatile rather than semivolatile chemical. All of these chemicals are typically found together in different proportions primarily in wastes from the petroleum and coking industries.

2.2.3 What chemicals were selected for the first round of constituents?

Benzo[a]pyrene and Dibenz[a,h]anthracene.

2.2.4 Why were they chosen?

Benzo[a]pyrene and Dibenz[a,h]anthracene were chosen because both of them are recognized carcinogens and have toxicity benchmarks. They were also chosen because they have a higher number of rings (five) than most of the others and are supposed to be more difficult to break down and relatively immobile. These chemicals were specifically chosen to test the performance of the model for these difficult criteria.

2.2.5 Why weren't others chosen?

Naphthalene was a very strong candidate for selection in the first round of performance testing because it was reported present in a great number of wastes and there were a lot of TRI reports submitted on it. However, this chemical has only two benzene rings and would not be a good representative of chemicals with four, five or six rings and because it is much more volatile than the others.

Some of the toxicity benchmarks for the chemicals that were not selected are often "extrapolated" or "interpolated" using structure activity relationship factors from toxicity data from others within the group. For many of them, a Toxicity Equivalency Factor (TEF) is often calculated. It was decided not to include any of these chemicals in the first round because of the additional calculations that this would require. Except for Naphthalene, these chemicals are not manufactured in the United States in significant quantities. Most are manufactured only in very small amounts and only for toxicity research or for standard analytical test solutions. The majority of these chemicals are found as natural components of petroleum, coal and wood products or in their associated wastes. They are also found in low concentrations in almost all combustion residues, as a result of incomplete combustion. The NHWCS data is, thus, believed to under-represent their presence in wastes because facilities do not always test for all of the individual chemicals.

2.3 Brominated Hydrocarbons

2.3.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	# of Br/Cl	# of Waste Streams in NHWCS	# of TRI Forms in 1994
74-83-9	Methyl bromide [Bromomethane]	no	1 Br	6	48
74-95-3	Methylene bromide [Dibromomethane]	no	2 Br	1	6
75-25-2	Bromoform [Tribromomethane]	no	3 Br	3	0
75-27-4	Bromodichloromethane	no	1 Br; 2 Cl	3	1
124-48-1	Dibromochloromethane	no	2 Br; 1 Cl	2	none
106-93-4	Ethylene dibromide [1,2-Dibromoethane]	yes	2 Br	2	16

CASRN	Chemical Name	Chosen	# of Br/Cl	# of Waste Streams in NHWCS	# of TRI Forms in 1994
96-12-8	1,2-Dibromo-3-chloropropane	no	2 Br; 1 Cl	none	0

2.3.2 What was the basis for creating the group?

All of the chemicals in this group consist of a low molecular weight hydrocarbon structure (e.g., methane, ethane or propane) that has at least one bromine substituted on the carbon. A good number of them are used for their pesticidal properties as fumigants.

2.3.3 What chemical was selected for the first round of constituents?

Ethylene dibromide.

2.3.4 Why was it chosen?

Ethylene dibromide was chosen because it is one of only two chemicals in this group that have specific listed RCRA hazardous waste codes associated with its' production. Ethylene dibromide was also chosen because it is a heavy liquid like most of the other chemicals in this group. It had the highest number of TRI reports submitted in 1994 compared to the rest of the liquid brominated aliphatics.

2.3.5 Why weren't others chosen?

Although Methyl bromide was reported in only six wastes in the NHWCS, it was a strong candidate for selection in the first round because it had the largest number of TRI reports submitted on it. Along with Ethylene dibromide, it is the second of only two chemicals in this group that have specific listed RCRA hazardous waste codes associated with its' production. The biggest problem in selecting Methyl bromide as a representative of this group is that, it is a gas at room temperature while all the others are liquids.

Most of these brominated hydrocarbons are not very likely to be found in listed RCRA waste streams except those specifically from the manufacturing of Methyl bromide and Ethylene dibromide. All of these chemicals have somewhat limited and very specific uses as fumigants and pesticides. Some of these uses are now restricted or have been canceled. In addition, Methyl bromide, being a gas, would not be expected to be present in wastes for very long so developing an exemption level .

2.4 Chlorinated Hydrocarbons

2.4.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	Hydrocarbon Structure (# Cl atoms)	# of Waste Streams in NHWCS	# of TRI Forms in 1994
74-87-3	Methyl Chloride [Chloromethane]	no	methane (1)	13	109
75-09-2	Methylene chloride [Dichloromethane]	yes	methane (2)	232	1,030
67-66-3	Chloroform [Trichloromethane]	yes	methane (3)	85	167
56-23-5	Carbon tetrachloride [Tetrachloromethane]	no	methane (4)	105	69
75-71-8	Dichlorodifluoromethane	no	methane (2)	1	169
75-69-4	Trichlorofluoromethane	no	methane (3)	70	82
76-13-1	1,1,2-Trichloro-1,2,2-trifluoroethane	no	methane (3)	80	237
75-34-3	1,1-Dichloroethane	no	ethane (2)	11	3
107-06-2	1,2-Dichloroethane	no	ethane (2)	69	79
71-55-6	1,1,1-Trichloroethane	yes	ethane (3)	189	1,207
79-00-5	1,1,2-Trichloroethane	no	ethane (3)	81	23
630-20-6	1,1,1,2-Tetrachloroethane	no	ethane (4)	8	7
79-34-5	1,1,2,2-Tetrachloroethane	no	ethane (4)	13	16
67-72-1	Hexachloroethane	no	ethane (6)	32	19
75-01-4	Vinyl chloride [Chloroethylene]	yes	ethylene (1)	38	43
75-35-4	1,1-Dichloroethylene	no	ethylene (2)	44	22
156-59-2	cis-1,2-Dichloroethylene	no	ethylene (2)	2	22
156-60-5	trans-1,2-Dichloroethylene	no	ethylene (2)	6	22
79-01-6	Trichloroethylene	yes	ethylene (3)	159	783
127-18-4	Tetrachloroethylene	yes	ethylene (4)	190	459
78-87-5	1,2-Dichloropropane	no	propane (2)	11	13
96-18-4	1,2,3-Trichloropropane	no	propane (3)	2	none
107-05-1	Allyl chloride	no	propene (1)	2	20
542-75-6	1,3-Dichloropropene, mixed isomers	no	propene (2)	5	11
10061-01-5	cis-1,3-Dichloropropene	no	propene (2)	5	11
10061-02-6	trans-1,3-Dichloropropene	no	propene (2)	5	11

2.4.2 What was the basis for creating the group?

All of the chemicals in this group are primarily hydrocarbons substituted with mostly chlorine. This group also includes a few chlorofluorocarbons. The chlorinated hydrocarbons are key hazardous constituents in a significant number of listed RCRA wastes generated from the production of organic chemicals. The majority of these chemicals, however, were used as solvents in a vast assortment of industries and end up in listed solvent wastes. When not mixed with other nonhalogenated solvents, the listed solvent wastes are identified as F001 or F002, but they are quite often found mixed with other nonhalogenated solvents and therefore are also identified as F003 and F005. The NHWCS data show that many of the chemicals in this group have significant numbers of wastes associated with them. As such, more chemicals were selected

from this group than from other organic groups.

2.4.3 What chemicals were selected for the first round of constituents?

Methylene chloride, Chloroform, 1,1,1-Trichloroethane, Vinyl chloride, Trichloroethylene and Tetrachloroethylene

2.4.4 Why were they chosen?

Methylene chloride, Chloroform, 1,1,1-Trichloroethane, Trichloroethylene and Tetrachloroethylene were chosen because they are the most common halogenated solvents that are used by so many industries. Even though Vinyl chloride is a gas at room temperature, it was selected because it is believed to a breakdown product of some of the other chlorinated solvents when present in the environment. Vinyl chloride should be an interesting test of the model for a chemical with such interesting chemical and physical properties.

2.4.5 Why weren't others chosen?

Carbon tetrachloride, Chloromethane, Chloroethane, 1,2-Dichloroethane, Dichlorodifluoromethane, Trichlorofluoromethane, and 1,1,2-Trichloro-1,2,2-trifluoroethane were also strong candidates for the first round because they were also reported present in a great number of wastes and there were also a reasonable number of TRI reports on them. However, Chloromethane, Chloroethane and Dichlorodifluoromethane are gases and are not good representatives of the other halogenated hydrocarbons. The three chlorinated fluorocarbons also typically used as refrigerants rather than solvents, which is probably why the number of TRI forms is significantly higher than the number of NHWCS wastes containing these chemicals. Both the NHWCS and TRI data also show that chlorinated propanes, propenes and butenes are not found as often as the chlorinated methanes, ethanes, and ethylenes.

2.5 Chlorinated Aromatics

2.5.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	# of Cl	# of Waste Streams in NHWCS	# of TRI Forms in 1994
108-90-7	Chlorobenzene	yes	1 Cl	121	65
95-50-1	1,2-Dichlorobenzene	no	2 Cl	79	33
106-46-7	1,4-Dichlorobenzene	no	2 Cl	34	23
120-82-1	1,2,4-Trichlorobenzene	no	3 Cl	7	33
95-94-3	1,2,4,5-Tetrachlorobenzene	no	4 Cl	16	none
608-93-5	Pentachlorobenzene	no	5 Cl	2	none
118-74-1	Hexachlorobenzene	no	6 Cl	32	9
1336-36-3	Polychlorinated biphenyls (PCBs)	no	variable	none	13

2.5.2 What was the basis for creating the group?

All of the chemicals in this group are benzene or biphenyl (i.e., two benzene rings joined by a single bond) with various numbers of chlorine atoms bonded directly to the benzene ring. These chlorinated benzenes are found in a relatively limited number of listed RCRA wastes from the production of organic chemicals and the tri- and tetra- substituted ones can be often found associated with PCBs at contaminated sites.

2.5.3 What chemical was selected for the first round of constituents?
Chlorobenzene.

2.5.4 Why was it chosen?
Chlorobenzene was chosen because it was the chlorinated aromatic with the highest number of TRI forms and the greatest number of NHWCS wastes containing it. It was also chosen for comparison to other chemicals that represent a benzene ring with a single functional group attached such as phenol, nitrobenzene and aniline.

2.5.5 Why weren't others chosen?
The data on the other chemicals in this group indicate that there are relatively lower number of wastes containing them. 1,2-Dichlorobenzene had the second highest number of wastes containing it and was a reasonable second candidate for study from this group. However, when compared to other chemicals that were not selected as representatives of other groups (e.g., Xylenes), the frequency of occurrence of 1,2-Dichlorobenzene was significantly lower. As such, only Chlorobenzene was selected from this group.

The NHWCS database is believed to significantly under count the number of wastes containing PCBs, because PCBs are regulated as hazardous materials under TSCA rather than RCRA. PCBs were not, however, chosen for study in this round because of complications associated with performing toxicity calculations for complex mixtures like PCBs. PCBs can have over 100 different individual chlorinated biphenyls in them.

2.6 Chlorinated Pesticides

2.6.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	Basic Structure	# of Waste Streams in NHWCS	# of TRI Forms in 1994
50-29-3	p,p'-DDT	no	diphenyl	4	none
72-54-8	p,p'-DDD	no	diphenyl	3	none
72-55-9	p,p'-DDE	no	diphenyl	3	none
72-43-5	Methoxychlor	yes	diphenyl	11	3
510-15-6	Chlorobenzilate	no	diphenyl	none	none
309-00-2	Aldrin	no	bicyclic	4	none
60-57-1	Dieldrin	no	bicyclic	5	none
72-20-8	Endrin	no	bicyclic	24	none
115-29-7	Endosulfan, mixed isomers	no	bicyclic	3	none
76-44-8	Heptachlor	no	bicyclic	9	1
1024-57-3	Heptachlor epoxide	no	bicyclic	7	none
143-50-0	Kepone	no	bicyclic	none	none
319-84-6	alpha-Hexachlorocyclohexane	no	cyclohexane	9	none

CASRN	Chemical Name	Chosen	Basic Structure	# of Waste Streams in NHWCS	# of TRI Forms in 1994
319-85-7	beta-Hexachlorocyclohexane	no	cyclohexane	8	none
58-89-9	gamma-Hexachlorocyclohexane [Lindane]	no	cyclohexane	18	8
57-74-9	Chlordane	no	mixture	14	1
8001-35-2	Toxaphene	no	mixture	14	0
94-75-7	2,4-D	yes	phenoxyacid	14	29
93-76-5	2,4,5-Trichlorophenoxyacetic acid	no	phenoxyacid	none	none
93-72-1	Silvex	no	phenoxyacid	9	none
2303-16-4	Diallate	no	chloro-nitrogen	none	none
82-68-8	Pentachloronitrobenzene	no	chloro-nitrogen	none	12
23950-58-5	Pronamide	no	chloro-nitrogen	none	1

2.6.2 What was the basis for creating the group?

All of the chemicals in this group are chlorinated organics that have been used primarily as pesticides. Most of these chemicals are not expected to be found in any listed RCRA wastes except those from production of Chlordane, Heptachlor, 2,4-D and Toxaphene. At the same time, almost all of the chlorinated pesticides in this group are no longer being manufactured in the United States, so there is less of a need to develop exemption levels for most of these pesticides. Wastes containing these pesticides tend to be contaminated soils and media being generated solely from RCRA corrective actions and Superfund clean-up.

2.6.3 What chemicals were selected for the first round of constituents?

Methoxychlor and 2,4-D.

2.6.4 Why were they

Methoxychlor has a DDT-like, chlorinated diphenyl structure and is still being produced in this country. 2,4-D was chosen as a representative of the chlorophenoxyacid derivatives. Both of these pesticides do not have the isomer problem, as explained below, that is associated with so many of the other pesticides in this group that were not selected. While there are not many wastes in the NHWCS that contain any of these pesticides, Methoxychlor and 2,4-D were reasonably represented by the data.

2.6.5 Why weren't others chosen?

The majority of these chlorinated pesticides were not chosen for the first round, because so many of them are isomers or degradation products of each other. For example, commercial DDT almost always has a little DDD and DDE in it. All three of these have benchmarks for the p,p'-isomers, but not the o,p'- isomers and they are hardly ever found without both isomers in them.

Commercial Endosulfan contains two isomers, Endosulfan I and Endosulfan II. Heptachlor is always found with some Heptachlor epoxide in it and Aldrin, Dieldrin and Endrin are also often found together. Early toxicity data for many of these pesticides was often based on the testing of commercial products and, as such, actually represents the combined effects of all isomers that were present in the commercial mixture. For example, Lindane is the commercial name for a mixture of Hexachlorocyclohexane isomers in which the gamma-isomer is the predominant active chemical. Lindane mixtures contained significant amounts of the alpha-, beta- and delta- isomers. In another example, commercial products with Endrin in them, contain degradation products such as Endrin aldehyde and Endrin ketone.

EPA decided overall that it was not going to test the model *in this phase* with chemicals that involve more than one isomer or are otherwise interrelated. EPA has not determined whether the model should use physical/chemical data and toxicity data for each isomer/related chemical or for the mix of isomers/related chemicals. While these issues present interesting aspects of the model, it was deemed to be better suited for later study, when there would be more time to study how the model handles these chemical relationships. Wastes expected to contain any one of these more "complicated" chlorinated pesticides would not likely to become exempt from RCRA until the related chlorinated pesticides were also modeled.

Toxaphene and Chlordane were not chosen for the initial testing of the risk model because they are not single chemicals, but rather are multiple component commercial pesticides with a *significant number* of isomers and congeners. These pesticides were considered to be too complex to be used for the initial tests.

2.7 Chlorinated Phenolics

2.7.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	# of Cl	# of Waste Streams in NHWCS	# of TRI Forms in 1994
95-57-8	2-Chlorophenol	no	1	3	none
120-83-2	2,4-Dichlorophenol	no	2	2	5
95-95-4	2,4,5-Trichlorophenol	no	3	4	0
88-06-2	2,4,6-Trichlorophenol	no	3	5	1
58-90-2	2,3,4,6-Tetrachlorophenol	no	4	1	none
87-86-5	Pentachlorophenol	yes	5	19	35

2.7.2 What was the basis for creating the group?

All of the chemicals in this group contain phenol with a varying amount of chlorine atoms attached in different positions around the benzene ring. The hydrogen atom of the phenolic hydroxy group is acidic and varies in strength based on where the chlorine atoms are positioned

around the benzene ring. The water solubility of all of these chemicals thus varies greatly and depends a lot on the pH of the leaching media. All of these chlorinated phenolics have pesticidal activity on their own, but are often used as building blocks for other chlorinated pesticides. There are several listed RCRA wastes associated with these chlorinated phenols (and their derivatives), but the most predominant wastes are from wood preserving. F027 is the RCRA waste code for off-spec discontinued pesticides containing these Chlorinated phenolics. Most of these wastes tend to come from RCRA corrective actions and Superfund clean-up.

2.7.3 What chemical was selected for the first round of constituents?

Pentachlorophenol.

2.7.4 Why was it chosen?

Pentachlorophenol was reported to be present in the greatest number of NHWCS wastes and had the greatest number of TRI forms submitted when compared to the other Chlorinated phenolics. Pentachlorophenol has a somewhat significant, albeit limited, commercial use as a wood preservative, while the others do not.

2.7.5 Why weren't others chosen?

Most of these chlorophenols are no longer being used in the United States as pesticides or being used to manufacture other chlorinated pesticides. There were very few wastes and TRI reports submitted for them.

2.8 Halogenated Dioxins and Furans

2.8.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	# of Cl	# of Waste Streams in NHWCS	# of TRI Forms in 1994
1746-01-6	2,3,7,8-Tetrachlorodibenzo-p-dioxin	yes	4	none	not covered
51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	NA	4	none	not covered
40321-76-4	1,2,3,7,8-Pentachlorodibenzo-p-dioxin	NA	5	none	not covered
57117-41-6	1,2,3,7,8-Pentachlorodibenzofuran	NA	5	none	not covered
57117-31-4	2,3,4,7,8-Pentachlorodibenzofuran	NA	5	none	not covered
39227-28-6	1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	NA	6	none	not covered
57653-85-7	1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	NA	6	none	not covered
19408-74-3	1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	NA	6	none	not covered
70648-26-9	1,2,3,4,7,8-Hexachlorodibenzofuran	NA	6	none	not covered
57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	NA	6	none	not covered
72918-21-9	1,2,3,7,8,9-Hexachlorodibenzofuran	NA	6	none	not covered
60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	NA	6	none	not covered
35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	NA	7	none	not covered

CASRN	Chemical Name	Chosen	# of Cl	# of Waste Streams in NHWCS	# of TRI Forms in 1994
67562-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	NA	7	none	not covered
55673-89-7	1,2,3,4,7,8,9-Heptachlorodibenzofuran	NA	7	none	not covered
3268-87-9	Octachlorodibenzo-p-dioxin	NA	8	none	not covered
39001-02-0	Octachlorodibenzofuran	NA	8	none	not covered

NA - Not Applicable. Benchmarks were not investigated for this document.

2.8.2 What was the basis for creating the group?

All of the chemicals in this group are isomers and congeners of chlorinated dioxins and furans. *If found*, they are expected to be found *together* and probably in the same types of wastes (e.g., combustion residues from burning wastes containing chlorinated organics). While there was only one isomer, 2,3,7,8-TCDD, that was reported with specific toxicity benchmarks, this group was developed based on the *potential need* to expand the number of Halogenated Dioxins and Furans isomers. This may be deemed necessary if it is decided that all of these isomers and congeners need to be measured in wastes. At the time of developing these groups, no policy decision had been made as to how to handle these isomers.

2.8.3 What chemical was selected for the first round of constituents?

2,3,7,8-Tetrachlorodibenzo-p-dioxin.

2.8.4 Why was it chosen?

2,3,7,8-Tetrachlorodibenzo-p-dioxin forms the basis for estimating the toxicity of all other isomers and congeners in this group.

2.8.5 Why weren't others chosen?

Since all the chemicals in this group are based on the toxicity of 2,3,7,8-Tetrachlorodibenzo-p-dioxin, there may be no need to test (or possibly even run) the model for the other congeners or isomers. EPA is continuing to study the potential use of Toxicity Equivalency Factors for all these chemicals.

2.9 Miscellaneous Chlorinated Organics

2.9.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	Fundamental Structure (# Cl)	# of Waste Streams in NHWCS	# of TRI Forms in 1994
126-99-8	Chloroprene [2-Chloro-1,3-butadiene]	no	diene (1)	7	14
87-68-3	Hexachloro-1,3-butadiene	yes	diene (6)	37	7
77-47-4	Hexachlorocyclopentadiene	no	diene (6)	7	4

CASRN	Chemical Name	Chosen	Fundamental Structure (# Cl)	# of Waste Streams in NHWCS	# of TRI Forms in 1994
111-44-4	Bis-(2-Chloroethyl)ether	no	ether (2)	4	11
39638-32-9	Bis-(2-Chloroisopropyl)ether [2,2'-Oxybis(2-chloropropane)]	no	ether (2)	1	none
106-89-8	Epichlorohydrin [1-Chloro-2,3-epoxypropane]	no	epoxide (1)	none	68
100-44-7	Benzyl chloride	no	aromatic (1)	3	48
70-30-4	Hexachlorophene	no	aromatic (6)	none	2
106-47-8	4-Chloroaniline	no	aromatic amine (1)	3	none
91-94-1	3,3'-Dichlorobenzidine	no	aromatic amine (2)	1	5

2.9.2 What was the basis for creating the group?

All of the chemicals in this group have at least one chlorine atom attached to a relatively simple organic structure. Most of these do not necessarily "fit" very well into the other chlorinated organic groups. Hardly any of these chemicals are found in most listed RCRA wastes; however, there are a few very specific "K" wastes from the production of specific chlorinated organics that may contain them.

2.9.3 What chemical was selected for the first round of constituents?

Hexachloro-1,3-butadiene.

2.9.4 Why was it chosen?

Hexachloro-1,3-butadiene was chosen because it was the only miscellaneous chlorinated organic that was found in a significant number of wastes reported in the NHWCS.

2.9.5 Why weren't others chosen?

While there were 68 TRI forms submitted indicating releases of Epichlorohydrin, there were no wastes reported in the NHWCS that were reported to contain it. There were 48 TRI forms submitted indicating releases of Benzyl chloride, but there were only 3 wastes reported in the NHWCS that were reported to contain it. Most of the chemicals in this group are not expected to be present in RCRA listed wastes.

2.10 Oxygen, Hydrogen and Carbon Chemicals

2.10.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	primary functional group	# of Waste Streams in NHWCS	# of TRI Forms in 1994
67-56-1	Methanol	no	alcohol	212	2,439
71-36-3	n-Butyl alcohol	no	alcohol	164	1,145

CASRN	Chemical Name	Chosen	primary functional group	# of Waste Streams in NHWCS	# of TRI Forms in 1994
78-83-1	Isobutyl alcohol	no	alcohol	84	none
100-51-6	Benzyl alcohol	no	alcohol	3	none
67-64-1	Acetone	no	ketone	290	none
78-93-3	Methyl ethyl ketone	yes	ketone	261	2,389
108-10-1	Methyl isobutyl ketone	no	ketone	198	1,031
98-86-2	Acetophenone	no	ketone	31	35
78-59-1	Isophorone	no	cyclic ketone	15	none
60-29-7	Ethyl ether	no	ether	69	none
110-80-5	2-Ethoxyethanol	no	ether	65	40
123-91-1	1,4-Dioxane	no	epoxide	7	55
110-00-9	Furan	no	epoxide	1	none
50-00-0	Formaldehyde	no	aldehyde	15	781
107-02-8	Acrolein	no	aldehyde	8	17
64-18-6	Formic Acid	no	acid	11	213
141-78-6	Ethyl acetate	no	ester	193	none
80-62-6	Methyl methacrylate	yes	ester	15	262
97-63-2	Ethyl methacrylate	no	ester	2	none
131-11-3	Dimethyl phthalate	no	di-ester	25	75
84-66-2	Diethyl phthalate	no	di-ester	22	63
84-74-2	Di-n-butyl phthalate	no	di-ester	39	126
117-84-0	Di-n-octyl phthalate	no	di-ester	30	none
117-81-7	Bis-(2-Ethylhexyl) phthalate	yes	di-ester	50	307
85-68-7	Butyl benzyl phthalate	no	di-ester	21	none
108-95-2	Phenol	yes	phenol	101	719
95-48-7	o-Cresol	no	phenol	81	25
108-39-4	m-Cresol	no	phenol	74	24
106-44-5	p-Cresol	no	phenol	82	27
105-67-9	2,4-Dimethylphenol	no	phenol	24	21
94-59-7	Safrole	no	complex ohc	none	0
56-53-1	Diethylstilbestrol, trans-	no	complex ohc	none	none

2.10.2 What was the basis for creating the group?

Except for Safrole and Diethylstilbestrol, all of the chemicals in this group have at least one oxygen atom attached to a relatively simple hydrocarbon structure. The majority of these chemicals represent the more traditional organic "functional groups" comprised of just oxygen, carbon and hydrogen known as alcohols, aldehydes, ketones, acids, ethers, esters and epoxides. Safrole and Diethylstilbestrol have a more complex hydrocarbon structure, but also contain only carbon, hydrogen and oxygen in their structure. Both the TRI and the NHWCS data support that the majority of these chemicals are found in a significant number of wastes streams.

2.10.3 What chemicals were selected for the first round of constituents?

Phenol, Methyl ethyl ketone, Methyl methacrylate and Bis-(2-ethylhexyl) phthalate.

2.10.4 Why were they chosen?

Methyl ethyl ketone was chosen because it is a very common solvent and is present in a very large group of wastes. It is expected to be in the middle of the range of toxicity values for the oxygenated hydrocarbons. Phenol was chosen because it is the basis of substituted phenolic chemicals found in this and other chemical groups and because it can be related and compared to other single substituted benzenes such as aniline, nitrobenzene and chlorobenzene. Methyl methacrylate was chosen as an example of one of the more reactive esters that are often used in the manufacturing of plastics. Bis-(2-Ethylhexyl) phthalate was chosen to represent the phthalate esters (i.e., di-esters) that are relatively ubiquitous in wastes owing to their use as plasticizers.

2.10.5 Why weren't others chosen?

Methanol, n-Butyl alcohol, Isobutyl alcohol, Acetone, Methyl isobutyl ketone, Ethyl acetate, Formaldehyde, Ethyl ether, 2-Ethoxyethanol, o-Cresol, m-Cresol, and p-Cresol are also high volume oxygenated hydrocarbons. Any of these could easily have been chosen as additional representatives of this group, however, many of these tend to be of relatively low toxicity.

2.11 Organonitrogen Chemicals

2.11.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	primary functional group	# of Waste Streams in NHWCS	# of TRI Forms in 1994
122-39-4	Diphenylamine	no	amine	7	none
62-53-3	Aniline	yes	aromatic amine	12	67
95-53-4	o-Toluidine	no	aromatic amine	4	23
106-49-0	p-Toluidine	no	aromatic amine	2	none
95-80-7	2,4-Toluenediamine	no	aromatic amine	3	4
108-45-2	1,3-Phenylenediamine	no	aromatic amine	none	none
92-87-5	Benzidine	no	aromatic amine	none	1
119-93-7	3,3'-Dimethylbenzidine	no	aromatic amine	none	none
119-90-4	3,3'-Dimethoxybenzidine	no	aromatic amine	none	3
62-75-9	N-Nitrosodimethylamine	no	nitrosamine	none	0
55-18-5	N-Nitrosodiethylamine	no	nitrosamine	none	none
10595-95-6	N-Nitroso-N-methylethylamine	no	nitrosamine	none	none
621-64-7	N-Nitrosodi-n-propylamine	no	nitrosamine	2	none
924-16-3	N-Nitrosodi-n-butylamine	no	nitrosamine	none	none
86-30-6	N-Nitrosodiphenylamine	no	nitrosamine	2	1
930-55-2	N-Nitrosopyrrolidine	no	nitrosamine	none	none
100-75-4	N-Nitrosopiperidine	no	nitrosamine	none	none
75-05-8	Acetonitrile	yes	nitrile	44	86
107-13-1	Acrylonitrile	yes	nitrile	27	114
126-98-7	Methacrylonitrile	no	nitrile	7	3
79-46-9	2-Nitropropane	no	nitro aliphatic	44	7
98-95-3	Nitrobenzene	yes	nitro aromatic	87	14
99-65-0	1,3-Dinitrobenzene	no	nitro aromatic	none	2
99-35-4	1,3,5-Trinitrobenzene	no	nitro aromatic	none	none
121-14-2	2,4-Dinitrotoluene	no	nitro aromatic	31	2

CASRN	Chemical Name	Chosen	primary functional group	# of Waste Streams in NHWCS	# of TRI Forms in 1994
606-20-2	2,6-Dinitrotoluene	no	nitro aromatic	3	1
51-28-5	2,4-Dinitrophenol	no	nitro aromatic	7	6
88-85-7	Dinoseb [2-sec-Butyl-4,6-dinitrophenol]	no	nitro aromatic	2	none
79-06-1	Acrylamide	no	amide	17	76
110-86-1	Pyridine	yes	heterocycle	97	35
57-24-9	Strychnine and salts	no	heterocycle	none	none

2.11.2 What was the basis for creating the group?

All of the chemicals in this group have at least one nitrogen atom attached to a relatively simple hydrocarbon or oxygenated hydrocarbon structure. These chemicals represent the basic organonitrogen structures known as amines (i.e., primary, secondary, tertiary, nitroso and aromatic amines), amides, nitriles, isocyanates, heterocycles, and nitro aromatics. While these represent a wide variety of different types of chemicals, both the TRI and the NHWCS data indicate that a relatively few number of these chemicals are found in wastes.

2.11.3 What chemicals were selected for the first round of constituents?

Aniline, Acetonitrile, Acrylonitrile, Nitrobenzene, and Pyridine.

2.11.4 Why were they chosen?

Aniline, Acetonitrile, Acrylonitrile, Nitrobenzene, and Pyridine were chosen because the data indicated they represented the largest number of wastes containing any of these organonitrogen chemicals. These five organonitrogen chemicals also appear to contain the basic structures that comprise this group of chemicals. Nitrobenzene and Aniline also provide an opportunity to further investigate the effect that various functional groups have when substituted on benzene.

2.11.5 Why weren't others chosen?

2-Nitropropane and Acrylamide could also have been chosen because of the number of TRI forms, but the NHWCS data indicated a relatively small universe of wastes containing them. No Nitrosoamines were selected because they were reported as being present in so few wastes.

2.12 Carbamates and Related Structures

2.12.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	"Carbamate" Type	# of Waste Streams in NHWCS	# of TRI Forms in 1994
116-06-3	Aldicarb	NA	Oxime	not covered	not covered
1646-88-4	Aldicarb sulfone	NA	Oxime	not covered	not covered
16752-77-5	Methomyl	NA	Oxime	not covered	not covered

CASRN	Chemical Name	Chosen	"Carbamate" Type	# of Waste Streams in NHWCS	# of TRI Forms in 1994
23135-22-0	Oxamyl	NA	Oxime	not covered	not covered
39196-18-4	Thiofanox	NA	Oxime	not covered	not covered
17804-35-2	Benomyl	NA	Carbamate	not covered	not covered
63-25-2	Carbaryl	NA	Carbamate	not covered	24
1563-66-2	Carbofuran	NA	Carbamate	not covered	not covered
55285-14-8	Carbosulfan	NA	Carbamate	not covered	not covered
122-42-9	Propham	NA	Carbamate	not covered	not covered
114-26-1	Propoxur	NA	Carbamate	not covered	3
23564-05-8	Thiophanate-methyl	NA	Carbamate	not covered	not covered
2008-41-5	Butylate	NA	Thiocarbamate	not covered	not covered
759-94-4	S-Ethyl dipropylthiocarbamate	NA	Thiocarbamate	not covered	not covered
2212-67-1	Molinate	NA	Thiocarbamate	not covered	not covered
1114-71-2	Pebulate	NA	Thiocarbamate	not covered	not covered
2303-17-5	Triallate	NA	Thiocarbamate	not covered	not covered
1929-77-7	Vernolate	NA	Thiocarbamate	not covered	not covered
148-18-5	Sodium diethyldithiocarbamate	NA	Dithiocarbamate	not covered	not covered
137-26-8	Thiram	yes	Dithiocarbamate	1	54

NA - Not Applicable. Benchmarks were not investigated for this document.

2.12.2 What was the basis for creating the group?

All of the chemicals in this group are in the general category of Carbamates and could have been considered subcategories of organonitrogen chemicals. These are split into four "carbamate" types; carbamates, thiocarbamates, dithiocarbamates, and oximes (which are not carbamates but have similar functional groups). Most of these chemicals are expected to be primarily found only in the relatively "new" listed RCRA waste streams from the manufacturing of these chemicals. In commerce, all of these chemicals have somewhat limited and very specific uses. Most are used primarily as pesticides; however, Thiram and a few others are also used in manufacturing rubber and rubber products (as rubber accelerators in the vulcanization process).

2.12.3 What chemical was selected for the first round of constituents?

Thiram.

2.12.4 Why was it chosen?

Thiram, a dithiocarbamate, was chosen primarily because it had the highest number of TRI reports submitted in 1994 compared to the other two chemicals in this group. This group was developed based on an *anticipated need* for representation of these chemicals in the model. At the time of developing these groups, benchmarks had not been fully investigated for any of these chemicals. Thiram was selected so that benchmark data could be obtained and then the model could be tested for a representative of this group of chemicals.

2.12.5 Why weren't others chosen?

Since these wastes were not officially "listed" as hazardous wastes for the time period measured by the NHWCS, the waste stream data does not adequately reflect the frequency of occurrence of these chemicals in RCRA wastes. At the same time, only Carbaryl, Propoxur and Thiram were required to be reported under the TRI in 1994. Very few wastes are represented by any of these chemicals and toxicity benchmarks have not been completely investigated.

2.13 Sulfur and/or Phosphorus Containing Chemicals

2.13.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	primary functional group	# of Waste Streams in NHWCS	# of TRI Forms in 1994
75-15-0	Carbon disulfide	yes	org-sulfur	73	82
62-50-0	Ethyl methanesulfonate	no	org-sulfur	none	none
96-45-7	Ethylene thiourea	no	org-sulfur	none	10
60-51-5	Dimethoate	no	phosphorothioate	none	none
298-02-2	Phorate	no	phosphorothioate	3	none
298-04-4	Disulfoton	no	phosphorothioate	3	none
56-38-2	Parathion	no	phosphorothioate	none	2
298-00-0	Methyl parathion	no	phosphorothioate	4	none
3689-24-5	Sulfotepp [Tetraethyldithiopyrophosphate]	no	phosphorothioate	none	none
126-72-7	Tris-(2,3-Dibromopropyl) phosphate	no	org-phosphorus	none	none
152-16-9	Octamethylpyrophosphoramide	no	org-phosphorus	none	none

2.13.2 What was the basis for creating the group?

All of the chemicals in this group contain either a sulfur and/or phosphorus moiety as a functional group. Many of them contain both elements, so it was difficult to separate them into two different groups. It was also logical to group many of these because they tend to be pesticides or are derived from the production of pesticides.

2.13.3 What chemical was selected for the first round of constituents?

Carbon disulfide.

2.13.4 Why was it chosen?

Carbon disulfide was chosen because it was the only chemical in this group that had significant number of wastes that contain it. Although it is the simplest chemical in the group, it is also a relatively toxic degradation product of some of the thiocarbamates and dithiocarbamates. Carbon

disulfide also has several commercial non-pesticide uses, especially as a specialty solvent. Owing to its' unique and somewhat offensive odor, most solvent wastes containing carbon disulfide are readily identified and are typically managed by themselves apart from other solvent wastes.

2.13.5 Why weren't others chosen?

All of the other chemicals in this group are all pesticides that currently have relatively limited use. They do not tend to show up in wastes unless they are discarded as pesticide products. While there are a few specific listed RCRA wastes from the production of Disulfoton and Phorate, neither of these pesticides are being produced. In general, there is less of a need to develop exemption levels for the majority of these chemicals.

2.14 Cationic Metals

2.14.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	Primary Ionic Form	# of Waste Streams in NHWCS	# of TRI Forms in 1994
7440-39-3	Barium	yes	cationic	219	57
7440-41-7	Beryllium	yes	cationic	46	10
7440-43-9	Cadmium	yes	cationic	268	45
7440-50-8	Copper	no	cationic	57	2,537
7439-92-1	Lead*	yes	cationic	370	817
7440-02-0	Nickel	yes	cationic	171	1,739
7440-22-4	Silver*	yes	cationic	189	66
7440-66-6	Zinc	yes	cationic	73	410
7439-97-6	Mercury**	yes	cationic	174	21
62-38-4	Phenyl mercury acetate**	no	cationic	none	none

* - Lead and Silver were chosen to be examined even though the benchmarks for these two metals were still under investigation during the development of this document. They were not included in the total number of 188 chemicals.

** - While benchmarks exist for Phenyl mercury acetate, the model was expected to only address Mercury on a "total" basis.

2.14.2 What was the basis for creating the group?

All of the chemicals in this group are metals that when in aqueous systems tend to be present as dissolved cationic species (i.e., positively charged). They are typically found together with other metals in varying concentrations in a very large portion of the hazardous waste universe.

2.14.3 What chemicals were selected for the first round of constituents?

Barium, Beryllium, Cadmium, Lead, Nickel, Silver, Zinc and Mercury.

2.14.4 Why were they chosen?

Almost all of the cationic metals were chosen because they are typically found together in a wide variety of wastes from a wide variety of industries. Lead and Silver were added to the list of cationic metals, in order to enhance the coverage of metals by the model.

2.14.5 Why weren't others chosen?

Copper was not selected because only ecological benchmarks were available for it. While it is present in a vast number of wastes, it was added to the HWIR Master List of chemicals primarily because it is a chemical "of concern" to RCRA with respect to groundwater monitoring (40 CFR 264 Appendix IX). Phenyl mercury acetate was not selected, even though it had separate toxicity benchmarks for it, because the model currently handles all metals on a "total" basis. The inclusion of "Total Mercury" for testing the model will therefore cover this chemical.

2.15 Anionic Metals

2.15.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	Primary Ionic Form	# of Waste Streams in NHWCS	# of TRI Forms in 1994
7440-36-0	Antimony	yes	oxoanionic	71	120
7440-38-2	Arsenic	yes	oxoanionic	214	89
7440-47-3	Chromium*	yes	oxoanionic	400	???
7782-49-2	Selenium	yes	oxoanionic	129	12
7440-28-0	Thallium	yes	oxoanionic	38	1
7440-62-2	Vanadium	yes	oxoanionic	11	12

* - Based on benchmarks for Hexavalent Chromium.

2.15.2 What was the basis for creating the group?

All of the chemicals in this group are metals that when in aqueous systems tend to be present primarily as dissolved oxoanionic species (i.e., negatively charged). While the metal within the oxoanionic species maintains an internal positive charge, when surrounded by oxygen the solublized metallic species acts like an anion. These metals are typically found together with other cationic metals in varying concentrations in a very large portion of the hazardous waste universe.

2.15.3 What chemicals were selected for the first round of constituents?

Antimony, Arsenic, Chromium, Selenium, Thallium, and Vanadium.

2.15.4 Why were they chosen?

All of the metals were chosen because they are typically found together in a wide variety of wastes from a wide variety of industries. Toxicity benchmarks for Chromium are based on Hexavalent chromium. The model partitions the distribution of different ionic states of all of these

metals, so it is less important that individual ionic species be selected for testing the model. These anionic metals, when combined with the list of selected cationic metals, ensure that all of the eight metals covered by the Toxicity Characteristic will be tested in the model.

2.15.5 Why weren't others chosen?

No other oxoanionic metals were considered under HWIR.

2.16 Cyanides and Inorganics

2.16.1 What chemicals are represented by this group?

CASRN	Chemical Name	Chosen	Form When Dissolved	# of Waste Streams in NHWCS	# of TRI Forms in 1994
57-12-5	Cyanide	NA	anion	under reported	247
18496-25-8	Sulfide	NA	anion	under reported	not covered
16984-48-8	Fluoride	NA	anion	under reported	not covered

NA - Not Applicable. Benchmarks were not investigated for this document.

2.16.2 What was the basis for creating the group?

This group represents the key dissolved anionic species of various salts and chemicals on the HWIR Master List. When dissolved in aqueous systems, these salts and chemicals dissolve to form either cyanide, sulfide or fluoride. Benchmarks were not investigated for these three ionic species and were not included in the total number of 188 chemicals with benchmarks. They have been included in this document because they are known to be present in many RCRA listed wastes. The Land Disposal Treatment Standards regulate these chemical species for many high volume listed wastes. The NHWCS data for these chemicals is believed to be severely under reported and is not reported above. There are several hundred electroplating facilities that use cyanides which should end up in their F006, F007, F008 and F009 listed wastes.

2.16.3 What chemicals were selected for the first round of constituents?

None.

2.16.4 Why were none selected?

For the first round of constituents, EPA decided not to model sulfide, fluoride or cyanide. The reasons for not modeling cyanide, in particular, are discussed in the preamble to the proposed rule.

3.0 Composite list of the 42 Selected Chemicals

A composite list of the 42 selected chemicals and the group from which they were selected is presented in the following Table. The chemicals are presented alphabetically. For convenience of the reader, the table provides a crosswalk back to the section of this document where that group is discussed .

Initial Chemicals for HWIR 99 Exit Levels			
Chemical Name [Alternate Name]	**CASRN**	**Representative Class**	**Section**
Acetonitrile	75-05-8	Organonitrogens	2.11
Acrylonitrile	107-13-1	Organonitrogens	2.11
Aniline	62-53-3	Organonitrogens	2.11
Antimony	7440-36-0	Anionic Metals	2.15
Arsenic	7440-38-2	Anionic Metals	2.15
Barium	7440-39-3	Cationic Metals	2.14
Benzene	71-43-2	Aromatic Hydrocarbons	2.1
Benzo[a]pyrene	50-32-8	Polynuclear Aromatics	2.2
Beryllium	7440-41-7	Cationic Metals	2.14
Bis-(2-ethylhexyl)phthalate [Di-(2-ethylhexyl)phthalate]	117-81-7	Oxygen, Hydrogen and Carbon Chemicals	2.10
Cadmium	7440-43-9	Cationic Metals	2.14
Carbon disulfide	75-15-0	Sulfur and/or Phosphorus Containing Chemicals	2.13
Chlorobenzene	108-90-7	Chlorinated Aromatics	2.5
Chloroform	67-66-3	Chlorinated Hydrocarbons	2.4
Chromium	7440-47-3[1]	Anionic Metals	2.15
Dibenz[a,h]anthracene	53-70-3	Polynuclear Aromatics	2.2
2,4-Dichlorophenoxyacetic acid	94-75-7	Chlorinated Pesticides	2.6
Ethylene dibromide [1,2-Dibromoethane]	106-93-4	Brominated Hydrocarbons	2.3
Hexachloro-1,3-butadiene	87-68-3	Miscellaneous Chlorinated Organics	2.9
Lead	7439-92-1	Cationic Metals	2.14
Mercury	7439-97-6	Cationic Metals	2.14
Methoxychlor	72-43-5	Chlorinated Pesticides	2.6
Methyl ethyl ketone	78-93-3	Oxygen, Hydrogen and Carbon Chemicals	2.10

[1] The CASRN listed above for chromium is for the elemental form of chromium. The model can differentiate and predict different species of the metal. The CASRN number for the trivalent state is 16065-83-1 and the CASRN for the hexavalent state is 18540-29-9.

Initial Chemicals for HWIR 99 Exit Levels			
Chemical Name [Alternate Name]	**CASRN**	**Representative Class**	**Section**
Methylene chloride [Dichloromethane]	75-09-2	Chlorinated Hydrocarbons	2.4
Methyl methacrylate	80-62-6	Oxygen, Hydrogen and Carbon Chemicals	2.10
Nickel	7440-02-0	Cationic Metals	2.14
Nitrobenzene	98-95-3	Organonitrogen	2.11
Pentachlorophenol	87-86-5	Chlorinated Phenolics	2.7
Phenol	108-95-2	Oxygen, Hydrogen and Carbon Chemicals	2.10
Pyridine	110-86-1	Organonitrogen	2.11
Selenium	7782-49-2	Anionic Metals	2.15
Silver	7440-22-4	Cationic Metals	2.14
2,3,7,8-Tetrachlorodibenzo-p-dioxin	1746-01-6	Halogenated Dioxins and Furans	2.8
Tetrachloroethylene	127-18-4	Chlorinated Hydrocarbons	2.4
Thallium	7440-28-0	Anionic Metals	2.15
Thiram	137-26-8	Carbamates and Related Structures	2.12
Toluene	108-88-3	Aromatic Hydrocarbons	2.1
1,1,1-Trichloroethane	71-55-6	Chlorinated Hydrocarbons	2.4
Trichloroethylene	79-01-6	Chlorinated Hydrocarbons	2.4
Vanadium	7440-62-2	Anionic Metals	2.15
Vinyl chloride	75-01-4	Chlorinated Hydrocarbons	2.4
Zinc	7440-66-6	Cationic Metals	2.14