



# TOXICS RELEASE INVENTORY

## List of Toxic Chemicals within the Polychlorinated Alkanes Category and Guidance for Reporting

Section 313 of the Emergency Planning and Community Right-to-Know Act of 1986 (EPCRA) requires certain facilities manufacturing, processing, or otherwise using listed toxic chemicals to report their environmental releases of such chemicals annually. Beginning with the 1991 reporting year, such facilities also must report pollution prevention and recycling data for such chemicals, pursuant to section 6607 of the Pollution Prevention Act, 42 U.S.C. 13106. When enacted, EPCRA section 313 established an initial list of toxic chemicals that was comprised of more than 300 chemicals and 20 chemical categories. EPCRA section 313(d) authorizes EPA to add chemicals to or delete chemicals from the list, and sets forth criteria for these actions. EPCRA section 313 is also known as the Toxics Release Inventory (TRI).

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## Section 1. Introduction

On November 30, 1994 EPA added nearly 300 chemicals and chemical categories to the list of toxic chemicals subject to reporting under EPCRA section 313, 42 U.S.C 11001. These additions are described at 59 FR 61432, and were effective January 1, 1995 for reports due July 1, 1996. The polychlorinated alkanes category was included in these additions. At the time of the addition, EPA indicated that the Agency would develop, as appropriate, interpretations and guidance that the Agency determines are necessary to facilitate accurate reporting for these categories. This document constitutes such guidance for the polychlorinated alkanes category.

### Section 1.1 Who Must Report

A plant, factory, or other facility is subject to the provisions of EPCRA section 313, if it meets all three of the following criteria:

1. It is included in the following North American Industrial Classification System (NAICS) manufacturing codes (corresponding to Standard Industrial Classification (SIC) codes 20 through 39): 311\*, 312\*, 313\*, 314\*, 315\*, 316, 321, 322, 323\*, 324, 325\*, 326\*, 327, 331, 332, 333, 334\*, 335\*, 336, 337\*, 339\*, 111998\*, 113310, 211130\*, 212324\*, 212325\*, 212393\*, 212399\*, 488390\*, 511110, 511120, 511130, 511140\*, 511191, 511199, 512230\*, 512250\*, 519130\*, 541713\*, 541715\* or 811490\*. \*Exceptions and/or limitations exist for these NAICS codes.

Facilities included in the following NAICS codes (corresponding to SIC codes other than SIC codes 20 through 39): 212111, 212112, 212113 (corresponds to SIC code 12, Coal Mining (except 1241)); or 212221, 212222, 212230, 212299 (corresponds to SIC code 10, Metal Mining (except 1011, 1081, and 1094)); or 221111, 221112, 221113, 221118, 221121, 221122, 221330 (limited to facilities that combust coal and/or oil for the purpose of generating power for distribution in commerce) (corresponds to SIC codes 4911, 4931, and 4939, Electric Utilities); or 424690, 425110, 425120 (limited to facilities previously classified in SIC code 5169, Chemicals and Allied Products, Not Elsewhere Classified); or 424710 (corresponds to SIC code 5171, Petroleum Bulk Terminals and Plants); or 562112 (limited to facilities primarily engaged in solvent recovery services on a contract or fee basis (previously classified under SIC code 7389, Business Services, NEC)); or 562211, 562212, 562213, 562219, 562920 (limited to facilities regulated under the Resource Conservation and Recovery Act, subtitle C, 42 U.S.C. 6921 et seq.) (corresponds to SIC code 4953, Refuse Systems); and

2. It has 10 or more full-time employees (or the equivalent 20,000 hours per year); and
3. It manufactures (includes imports), processes or otherwise uses any of the toxic chemicals listed on the EPCRA section 313 list in amounts greater than the established threshold quantities.

In addition, beginning with Executive Order 13148 signed in 1993, federal facilities are required to comply with the reporting requirements of EPCRA section 313 starting with calendar year 1994. This requirement is mandated regardless of the facility's NAICS or SIC code. The most recent Executive Order that continues this requirement is "Planning for Federal Sustainability in the Next Decade" (EO 13693, March 19, 2015).

## Section 1.2 Thresholds

Thresholds are specified amounts of toxic chemicals used during the calendar year that trigger reporting requirements.

If a facility *manufactures* or *imports* any of the listed toxic chemicals, the threshold quantity will be:

- 25,000 pounds per toxic chemical or category over the calendar year.

If a facility *processes* any of the listed toxic chemicals, the threshold quantity will be:

- 25,000 pounds per toxic chemical or category over the calendar year.

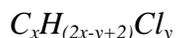
If a facility *otherwise uses* any of the listed toxic chemicals (without incorporating it into any product or producing it at the facility), the threshold quantity is:

- 10,000 pounds per toxic chemical or category over the calendar year.

EPCRA section 313 requires threshold determinations for chemical categories to be based on the total of all chemicals in the category manufactured, processed, or otherwise used. For example, a facility that manufactures three members of a chemical category would count the total amount of all three chemicals manufactured towards the manufacturing threshold for that category. When filing reports for chemical categories, the releases are determined in the same manner as the thresholds. One report is filed for the category and all releases are reported on this form.

## Section 1.3 Polychlorinated Alkanes Category Definition

The polychlorinated alkanes category is defined by the following formula and description:



where:

x = 10-13;

y = 3-12;

and the average chlorine content ranges from 40 to 70 percent with the limiting molecular formulas set at C<sub>10</sub>H<sub>19</sub>Cl<sub>3</sub> and C<sub>13</sub>H<sub>16</sub>Cl<sub>12</sub>

Chemicals that meet this category definition are reportable.

EPA is providing two lists of CAS numbers and chemical names to aid the regulated community in determining whether they need to report for the polychlorinated alkanes category. The first list includes individual chemicals that meet the polychlorinated alkanes category definition. If a facility is manufacturing, processing, or otherwise using a chemical which is on this list, they must report this chemical. However, this list is not exhaustive. If a facility is manufacturing, processing, or otherwise using a polychlorinated alkane that meets the category definition, they must report this chemical, even if it does not appear on the list. The second list includes chemical mixtures which might contain polychlorinated alkanes that meet the category definition. If a facility is manufacturing, processing, or otherwise using a mixture which is on this list and contains a polychlorinated alkane that meets the category definition, they must report the polychlorinated alkane component. However, this list is not exhaustive. If a facility is manufacturing, processing, or otherwise using a mixture that contains a polychlorinated alkane that meets the category definition, they must report the polychlorinated alkane component, even if the mixture does not appear on the list.

#### **Section 1.4 *De Minimis* Concentrations**

Polychlorinated alkanes and mixtures of polychlorinated alkanes that have an average chain length of 12 carbons and contain an average chlorine content of 60 percent by weight are subject to the 0.1 percent *de minimis* concentration. All other members of the polychlorinated alkanes category are subject to the one percent *de minimis* concentration. Thus, mixtures that contain members of this category equal to or in excess of the *de minimis* should be factored into threshold and release determinations.

## Section 2. Guidance for Reporting Chemicals within the Polychlorinated Alkanes Category

Polychlorinated alkanes represent a large class of compounds that are typically classified according to structural characteristics such as carbon chain length and degree of chlorination. Polychlorinated alkanes are also classified according to the variety of feedstocks from which they are manufactured (polychlorinated paraffins and polychlorinated  $\alpha$ -olefins, for example, are two such categories). Factors dictating whether a chemical is included in the polychlorinated alkanes category and reportable under EPCRA section 313 are based strictly on structural properties and are independent of the feedstock used in the manufacture of the chemical.

The polychlorinated alkanes category in general includes all  $C_{10}$  to  $C_{13}$  saturated hydrocarbons that are 40-70% chlorinated. A more specific description of the category is given below.

### Section 2.1 Feedstocks Used in the Manufacture of Polychlorinated Alkanes

Polychlorinated alkanes are synthesized industrially by chlorination of a variety of hydrocarbon feedstocks that include:

- paraffins and other alkanes;
- olefins and other alkenes;
- alkynes.

The feedstocks most commonly used in the manufacture of polychlorinated alkanes are normal paraffins and to a lesser degree, normal  $\alpha$ -olefins.

Paraffins are saturated hydrocarbons that are natural components in crude petroleum. Because they are typically obtained as fractions from petroleum distillation, paraffins are usually mixtures of components that vary in carbon chain length. The normal paraffin fractions that are most commonly used in the manufacture of polychlorinated alkanes are short chain ( $C_{10}$  to  $C_{13}$ , average  $C_{12}$ ), intermediate chain ( $C_{14}$  to  $C_{19}$ , average  $C_{15}$ ), and long chain ( $C_{20}$  to  $C_{30}$ , average  $C_{24}$ ) fractions.

Olefins are mono-unsaturated hydrocarbons that are also natural components in crude petroleum. In  $\alpha$ -olefin structures, the site of unsaturation or double bond is terminal in position on the carbon chain. Olefins in general are often found in the same petroleum distillation fractions from which paraffins and other alkenes are obtained. Because the separation of discrete olefins and even olefin mixtures from these usually complex hydrocarbon mixtures is physically very difficult, olefins are more commonly obtained from a variety of synthetic methods that include:

- ethylene oligomerization;
- paraffin steam cracking;

- dehydrogenation of paraffins;
- chlorination/dehydrochlorination of paraffins.

Ethylene oligomerization typically affords high purity C<sub>6</sub>-C<sub>20</sub> linear  $\alpha$ -olefins with an even number of carbons. Paraffin steam cracking affords up to 90% of primarily linear  $\alpha$ -olefins with an even or odd number of carbons. Dehydrogenation of paraffins and chlorination/dehydrochlorination of paraffins both yield primarily linear internal olefins.

Although normal paraffins obtained from petroleum distillation and normal  $\alpha$ -olefins obtained from various petroleum-based synthetic methods are the feedstocks that are most commonly used in the industrial manufacture of polychlorinated alkanes, any hydrocarbon species can be used, regardless of its source. Feedstocks can be branched or linear in structure and can be mixtures or discrete species. Alkene feedstocks can include species with more than one double bond. Alkynes are an additional class of compounds suitable for use as feedstocks in the manufacture of polychlorinated alkanes, although they are not nearly as commonly used.

## Section 2.2 Chlorination of Hydrocarbons

The chlorination of hydrocarbons using general reagents (such as Cl<sub>2</sub>) is a particularly non-selective chemical reaction that invariably yields a product mixture that is comprised of various structural isomers as well as species with different molecular weights. The reaction is synthetically useful only if a mixture either is required for or has no consequences on the intended use of the product. In the monochlorination of alkanes, for example, every monochlorinated structural isomer is anticipated in which the position of the chlorine atom varies from component to component in the product mixture. In addition, components that are di-, tri-, and polychlorinated are likely, although they are expected to be formed in relatively small quantities. In the polychlorination of hydrocarbons, product mixtures even more complex in number and type of components are expected. Since the degree of chlorination usually cannot be strictly controlled in these types of reactions (particularly if polychlorination is intended), the percent chlorination is typically described by either an average or range of the values observed among the components that constitute the polychlorinated alkane.

If a hydrocarbon mixture rather than a discrete species is used as the feedstock in the manufacture of a polychlorinated alkane, carbon chain length will also vary from component to component in the product mixture. Unlike the variations that are possible with respect to the degree of chlorination and the positions of the chlorine atoms, variations in carbon chain length are not a result of the poor selectivity of polychlorination reactions but are a consequence of the source of the feedstock used in the reaction.

The type of feedstock (alkane or alkene) used in polychlorination reactions is not expected to have a significant effect on the type of structural isomers formed, as long as carbon chain length (or for mixtures, average carbon chain length) and the degree of chlorination are constant, since polychlorination reactions can result in the formation of every possible structural isomer. The variations

in chlorine positions observed *between* polychlorinated paraffins and polychlorinated  $\alpha$ -olefins, for example, are not expected to differ significantly compared to the variations observed *within* these two polychlorinated alkanes. The relative amounts of the different structural isomers that are formed may differ, however, depending on the type of feedstock used. 1,2-Chlorinated isomers, for example, are expected to be formed in significant quantities from the polychlorination of  $\alpha$ -olefins regardless of the degree of chlorination. 1,2-Chlorinated isomers are also expected to be formed from the polychlorination of alkanes, however, they will most likely will be formed in smaller quantities as the degree of chlorination decreases.

Although chlorination reactions in general are highly non-selective, it is possible when using controlled reaction conditions, specific halogenating reagents, and certain catalysts to selectively chlorinate a discreet hydrocarbon species such that only one chlorinated or polychlorinated structural isomer is formed.

### **Section 2.3 Properties and Uses of Polychlorinated Alkanes**

Polychlorinated alkanes in general have high boiling points, low vapor pressures, low water solubilities, and high chemical and thermal stability. Although these physical properties will vary from component to component in complex polychlorinated alkane mixtures, they are not expected to vary between polychlorinated alkanes with the same carbon chain length (or for mixtures, the same average carbon chain length) and the same degree of chlorination, even though the polychlorinated alkanes may be manufactured from different feedstocks.

Because of their high stability in a variety of conditions, polychlorinated alkanes are widely used in numerous applications. Currently, the most common use for polychlorinated alkanes is as an extreme-pressure, anti-wear additive in lubricants used for metal machinery (particularly cutting oils). Polychlorinated alkanes are frequently used as plasticizers in plastics (including vinyls, resins, and foams) and paints (including enamels, polyurethanes, and vinyl), and to a lesser degree in adhesives, caulks and sealants. Polychlorinated alkanes are also used as flame retardants in rubber and plastic. A miscellaneous use for polychlorinated alkanes is as a water repellent.

### **Section 2.4 Structural Requirements for Chemicals within the Polychlorinated Alkanes Category**

Polychlorinated alkanes are saturated, chlorinated hydrocarbons that can be represented by the general formula  $C_xH_{(2x-y+2)}Cl_y$ . Polychlorinated alkanes are classified structurally by carbon chain length and percent chlorination. The most common industrial classes based on chain length include the same short chain ( $C_{10}$  to  $C_{13}$ , average  $C_{12}$ ), intermediate chain ( $C_{14}$  to  $C_{19}$ , average  $C_{15}$ ), and long chain ( $C_{20}$  to  $C_{30}$ , average  $C_{24}$ ) designations that are used to describe straight chain paraffin fractions. The most common classes based on the degree of chlorination (by weight) are 40-50% chlorinated, 50-60% chlorinated, and 60-70% chlorinated.

The polychlorinated alkanes category includes all saturated C<sub>10</sub> to C<sub>13</sub> species that have an average chlorine content of 40-70%. The category can be more specifically defined using the general polychlorinated alkanes formula (C<sub>x</sub>H<sub>(2x-y+2)</sub>Cl<sub>y</sub>) in which x equals 10 to 13 and y, depending on the value of x, ranges from 3 to 12. Using this formula and description, the specific molecular formulas that define the boundaries of the category are C<sub>10</sub>H<sub>19</sub>Cl<sub>3</sub> and C<sub>13</sub>H<sub>16</sub>Cl<sub>12</sub>. Specific molecular formulas for all individual chemicals that meet the category definition can be similarly derived and are tabulated in matrix form below.

The polychlorinated alkanes category includes linear and branched chain compounds as well as chemicals manufactured as discrete species or mixtures (for mixtures, only those components that meet the category definition are reportable). Straight chain hydrocarbons are used almost exclusively as feedstocks in the industrial manufacture of polychlorinated alkanes. However, branched chain species are common impurities in otherwise linear alkane and alkene feedstocks. The polychlorinated branched alkanes that result from the polychlorination of branched chain impurities therefore may be components in industrially manufactured polychlorinated alkanes and are included in the polychlorinated alkanes category provided that they meet the category definition.

Molecular Formulas for Individual Chemicals within the Polychlorinated Alkanes Category				
C <sub>x</sub> H <sub>(2x-y+2)</sub> Cl <sub>y</sub>	x = 10	x = 11	x = 12	x = 13
y = 3	C <sub>10</sub> H <sub>19</sub> Cl <sub>3</sub>	C <sub>11</sub> H <sub>21</sub> Cl <sub>3</sub>	C <sub>12</sub> H <sub>23</sub> Cl <sub>3</sub>	
y = 4	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	C <sub>11</sub> H <sub>20</sub> Cl <sub>4</sub>	C <sub>12</sub> H <sub>22</sub> Cl <sub>4</sub>	C <sub>13</sub> H <sub>24</sub> Cl <sub>4</sub>
y = 5	C <sub>10</sub> H <sub>17</sub> Cl <sub>5</sub>	C <sub>11</sub> H <sub>19</sub> Cl <sub>5</sub>	C <sub>12</sub> H <sub>21</sub> Cl <sub>5</sub>	C <sub>13</sub> H <sub>23</sub> Cl <sub>5</sub>
y = 6	C <sub>10</sub> H <sub>16</sub> Cl <sub>6</sub>	C <sub>11</sub> H <sub>18</sub> Cl <sub>6</sub>	C <sub>12</sub> H <sub>20</sub> Cl <sub>6</sub>	C <sub>13</sub> H <sub>22</sub> Cl <sub>6</sub>
y = 7	C <sub>10</sub> H <sub>15</sub> Cl <sub>7</sub>	C <sub>11</sub> H <sub>17</sub> Cl <sub>7</sub>	C <sub>12</sub> H <sub>19</sub> Cl <sub>7</sub>	C <sub>13</sub> H <sub>21</sub> Cl <sub>7</sub>
y = 8	C <sub>10</sub> H <sub>14</sub> Cl <sub>8</sub>	C <sub>11</sub> H <sub>16</sub> Cl <sub>8</sub>	C <sub>12</sub> H <sub>18</sub> Cl <sub>8</sub>	C <sub>13</sub> H <sub>20</sub> Cl <sub>8</sub>
y = 9	C <sub>10</sub> H <sub>13</sub> Cl <sub>9</sub>	C <sub>11</sub> H <sub>15</sub> Cl <sub>9</sub>	C <sub>12</sub> H <sub>17</sub> Cl <sub>9</sub>	C <sub>13</sub> H <sub>19</sub> Cl <sub>9</sub>
y = 10		C <sub>11</sub> H <sub>14</sub> Cl <sub>10</sub>	C <sub>12</sub> H <sub>16</sub> Cl <sub>10</sub>	C <sub>13</sub> H <sub>18</sub> Cl <sub>10</sub>
y = 11			C <sub>12</sub> H <sub>15</sub> Cl <sub>11</sub>	C <sub>13</sub> H <sub>17</sub> Cl <sub>11</sub>
y = 12				C <sub>13</sub> H <sub>16</sub> Cl <sub>12</sub>

### Section 3. CAS Number List of Some of the Individual Chemicals within the Polychlorinated Alkanes Category

EPA is providing the following list of CAS numbers, chemical names, and molecular formulas to aid the regulated community in determining whether they need to report for the polychlorinated alkanes category. If a facility is manufacturing, processing, or otherwise using a chemical which is listed below, they must report this chemical. However, this list is not exhaustive. If a facility is manufacturing, processing, or otherwise using a polychlorinated alkane that meets the category definition, they must report this chemical, even if it does not appear on the following list.

Listing by CAS Number of Some of the Individual Chemicals within the Polychlorinated Alkanes Category		
Chemical Name	Molecular Formula	CAS Number
Octane, 1,1,1-trichloro-3,5-dimethyl-	$C_{10}H_{19}Cl_3$	13275-21-3
Octane, 1,3,7-trichloro-3,7-dimethyl-, ( $\pm$ )-	$C_{10}H_{19}Cl_3$	17081-64-0
Decane, 2,2,4-trichloro-	$C_{10}H_{19}Cl_3$	39185-78-9
Decane, 1,1,1-trichloro-	$C_{10}H_{19}Cl_3$	62108-56-9
Decane, trichloro-	$C_{10}H_{19}Cl_3$	64554-71-8
Octane, 1,3,7-trichloro-3,7-dimethyl-	$C_{10}H_{19}Cl_3$	64961-16-6
Decane, 1,1,3-trichloro-	$C_{10}H_{19}Cl_3$	66651-36-3
Octane, 1,3,5-trichloro-7,7-dimethyl-(R*,R*)-	$C_{10}H_{19}Cl_3$	87147-86-2
Octane, 1,3,5-trichloro-7,7-dimethyl-(R*,S*)-	$C_{10}H_{19}Cl_3$	87147-87-3
Octane, 1,3,5-trichloro-7,7-dimethyl-	$C_{10}H_{19}Cl_3$	87260-59-1
Octane, 1,2,7-trichloro-3,7-dimethyl-	$C_{10}H_{19}Cl_3$	99175-28-7
Decane, 1,3,5-trichloro-	$C_{10}H_{19}Cl_3$	108140-20-1
Heptane, 1,7-dichloro-4-(3-chloropropyl)-	$C_{10}H_{19}Cl_3$	154120-66-8
Not yet assigned	$C_{10}H_{19}Cl_3$	159715-71-6
Decane, 1,1,1,10-tetrachloro-	$C_{10}H_{18}Cl_4$	10311-15-6
Octane, 1,1,1,7-tetrachloro-3,5-dimethyl-	$C_{10}H_{18}Cl_4$	17977-23-0
Octane, 1,1,1,7-tetrachloro-3,5-dimethyl-, D,D,L-	$C_{10}H_{18}Cl_4$	29293-15-0
Octane, 1,1,1,7-tetrachloro-3,5-dimethyl-, -D,D,D-	$C_{10}H_{18}Cl_4$	29293-20-7
Octane, 1,1,1,7-tetrachloro-3,5-dimethyl-, D,L,D-	$C_{10}H_{18}Cl_4$	29293-21-8
Octane, 1,1,1,7-tetrachloro-3,5-dimethyl-, D,L,L-	$C_{10}H_{18}Cl_4$	29293-22-9
Octane, 1,1,1,7-tetrachloro-3,5-dimethyl-(3R*,5R*,7R*)	$C_{10}H_{18}Cl_4$	31031-25-1

Listing by CAS Number of Some of the Individual Chemicals within the Polychlorinated Alkanes Category		
Chemical Name	Molecular Formula	CAS Number
Octane, 1,1,1,7-tetrachloro-3,5-dimethyl-, heterotactic	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	31031-26-2
Octane, 1,1,1,7-tetrachloro-3,5-dimethyl-, (3R*,5S*,7R*)	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	31107-32-1
Decane, 1,1,10,10-tetrachloro-	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	33025-70-6
Nonane, 2,4,4,8-tetrachloro-6-methyl	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	51500-53-9
Decane, 1,1,1,3-tetrachloro-	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	51755-60-3
Decane, 5,5,6,6-tetrachloro-	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	91087-09-1
Decane, 1,5,6,10-tetrachloro-	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	102880-00-2
Decane, 1,3,3,5-tetrachloro-	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	108140-19-8
Heptane, 1,1,1,6-tetrachloro-3,3,6-trimethyl-	C <sub>10</sub> H <sub>18</sub> Cl <sub>4</sub>	109749-69-1
Decane, 1,5,5,6,6,10-hexachloro-	C <sub>10</sub> H <sub>16</sub> Cl <sub>6</sub>	90943-97-8
Octane, 2,4,4,5,5,7-hexachloro-2,7-dimethyl-	C <sub>10</sub> H <sub>16</sub> Cl <sub>6</sub>	99192-48-0
Decane, heptachloro-	C <sub>10</sub> H <sub>15</sub> Cl <sub>7</sub>	32534-78-4
Heptane, 2,2,4,6,6-pentachloro-4-(2,2-dichloropropyl)-	C <sub>10</sub> H <sub>15</sub> Cl <sub>7</sub>	69537-72-0
Undecane, 1,1,1-trichloro	C <sub>11</sub> H <sub>21</sub> Cl <sub>3</sub>	3922-25-6
Undecane, 1,1,3-trichloro	C <sub>11</sub> H <sub>21</sub> Cl <sub>3</sub>	56686-58-9
Undecane, 1,1,5-trichloro	C <sub>11</sub> H <sub>21</sub> Cl <sub>3</sub>	80365-36-2
Undecane, 1,1,6-trichloro	C <sub>11</sub> H <sub>21</sub> Cl <sub>3</sub>	80365-37-3
Undecane, 1,1,8-trichloro	C <sub>11</sub> H <sub>21</sub> Cl <sub>3</sub>	80365-38-4
Undecane, 1,1,9-trichloro	C <sub>11</sub> H <sub>21</sub> Cl <sub>3</sub>	80365-39-5
Undecane, 1,1,10-trichloro	C <sub>11</sub> H <sub>21</sub> Cl <sub>3</sub>	80365-40-8
Nonane, 4-(2,2,2-trichloroethyl)-	C <sub>11</sub> H <sub>21</sub> Cl <sub>3</sub>	86405-89-2
Undecane, 1,1,1,11-tetrachloro	C <sub>11</sub> H <sub>20</sub> Cl <sub>4</sub>	3922-34-7
Pentane, 1,1,1,3-tetrachloro-3-(1,1-dimethylethyl)-4,4-dimethyl-	C <sub>11</sub> H <sub>20</sub> Cl <sub>4</sub>	39580-89-7
Undecane, 1,1,1,3-tetrachloro-	C <sub>11</sub> H <sub>20</sub> Cl <sub>4</sub>	56686-55-6
Undecane, 1,1,1,2-tetrachloro-	C <sub>11</sub> H <sub>20</sub> Cl <sub>4</sub>	63981-28-2
Undecane, tetrachloro-	C <sub>11</sub> H <sub>20</sub> Cl <sub>4</sub>	63988-32-9
Heptane, 1,1,7,7-tetrachloro-3,3,5,5-tetramethyl-	C <sub>11</sub> H <sub>20</sub> Cl <sub>4</sub>	105278-95-3
Undecane, 2,4,6,8,10-pentachloro-	C <sub>11</sub> H <sub>19</sub> Cl <sub>5</sub>	140899-23-6

Listing by CAS Number of Some of the Individual Chemicals within the Polychlorinated Alkanes Category		
Chemical Name	Molecular Formula	CAS Number
Undecane, octachloro-	C <sub>11</sub> H <sub>16</sub> Cl <sub>8</sub>	36312-81-9
Undecane, 1,1,1,3,5,7,9,11-11-nonachloro	C <sub>11</sub> H <sub>15</sub> Cl <sub>9</sub>	18993-26-5
Dodecane, 1,1,1-trichloro-	C <sub>12</sub> H <sub>23</sub> Cl <sub>3</sub>	62108-57-0
Dodecane, 1,1,1,12-tetrachloro-	C <sub>12</sub> H <sub>22</sub> Cl <sub>4</sub>	10311-16-7
Dodecane, 1,1,1,3-tetrachloro-	C <sub>12</sub> H <sub>22</sub> Cl <sub>4</sub>	14983-60-9
Dodecane, 1,1,12,12-tetrachloro-	C <sub>12</sub> H <sub>22</sub> Cl <sub>4</sub>	60836-00-2
Decane, 1,3,5,7-tetrachloro-9,9-dimethyl-(3R*,5S*,7S*)	C <sub>12</sub> H <sub>22</sub> Cl <sub>4</sub>	87562-53-6
Decane, 1,3,5,7-tetrachloro-9,9-dimethyl-(3R*,5R*,7S*)	C <sub>12</sub> H <sub>22</sub> Cl <sub>4</sub>	87585-26-0
Decane, 1,3,5,7-tetrachloro-9,9-dimethyl-(3R*,5R*,7R*)	C <sub>12</sub> H <sub>22</sub> Cl <sub>4</sub>	87585-27-1
Decane, 1,3,5,7-tetrachloro-9,9-dimethyl-(3R*,5S*,7R*)	C <sub>12</sub> H <sub>22</sub> Cl <sub>4</sub>	87585-28-2
Dodecane, 1,1,1,2,2,12-hexachloro-	C <sub>12</sub> H <sub>20</sub> Cl <sub>6</sub>	100525-30-2
Octane, 1,1,1,8,8,8-hexachloro-3,3,6,6-tetramethyl-	C <sub>12</sub> H <sub>20</sub> Cl <sub>6</sub>	128600-85-1
Dodecane, 1,3,5,7,9,11-hexachloro-	C <sub>12</sub> H <sub>20</sub> Cl <sub>6</sub>	136671-00-6
Tridecane, 1,1,1,13-tetrachloro-	C <sub>13</sub> H <sub>24</sub> Cl <sub>4</sub>	3922-33-6
Tridecane, 1,1,1,3-tetrachloro	C <sub>13</sub> H <sub>24</sub> Cl <sub>4</sub>	67095-50-5
Undecane, 5-chloro-7-(2,2,2-trichloroethyl)-	C <sub>13</sub> H <sub>24</sub> Cl <sub>4</sub>	88938-19-6
Tridecane, tetrachloro-	C <sub>13</sub> H <sub>24</sub> Cl <sub>4</sub>	96621-01-1
Tridecane, pentachloro-	C <sub>13</sub> H <sub>23</sub> Cl <sub>5</sub>	57437-54-4
Tridecane, 2,4,6,8,10,12-hexachloro-	C <sub>13</sub> H <sub>22</sub> Cl <sub>6</sub>	141600-29-5

#### Section 4. CAS Number List of Some Mixtures That Might Contain Chemicals within the Polychlorinated Alkanes Category

EPA is providing the following list of CAS numbers and chemical names for mixtures which might contain polychlorinated alkanes within the category. This list will aid the regulated community in determining whether they need to report for the polychlorinated alkanes category. If a facility is manufacturing, processing, or otherwise using a mixture which is listed below and contains a polychlorinated alkane that meets the category definition, they must report the polychlorinated alkane component. However, this list is not exhaustive. If a facility is manufacturing, processing, or otherwise using a mixture that contains a polychlorinated alkane that meets the category definition, they must report the polychlorinated alkane component, even if the mixture does not appear on the following list. Threshold calculations for the polychlorinated alkanes category should account only for the percentage of the polychlorinated alkane(s) contained in the mixture.

Listing by CAS Number of Some Mixtures That Might Contain Polychlorinated Alkanes within the Category <sup>1</sup>	
Mixture Name	CAS Number
AK 243 (chloroparaffin)	37207-94-6
WK 30 (chloroparaffin)	39443-51-1
Alkanes, chloro	61788-76-9
Paraffin oils, chloro	85422-92-0
Paraffins (petroleum), normal C>10, chloro	97553-43-0
Alkanes, C10-12, chloro	108171-26-2
Alkanes, C10-13, chloro	85535-84-8
Alkanes, C10-14, chloro	85681-73-8
Alkanes, C10-21, chloro	84082-38-2
Alkanes, C10-22, chloro	104948-36-9
Alkanes, C10-26, chloro	97659-46-6
Alkanes, C10-32, chloro	84776-06-7
Alkanes, C12-13, chloro	71011-12-6
Alkanes, C12-14, chloro	85536-22-7
Paraffin waxes and hydrocarbon waxes, chloro	63449-39-8
Paraffin waxes and hydrocarbon waxes, mixed with polypropylene chlorinated	68553-93-5
Paraffin waxes and hydrocarbon waxes, chloro, reaction products with naphthalene	68938-42-1
Hydrocarbon waxes (petroleum), microcryst., chlorinated	68938-43-2

<sup>1</sup> It cannot be determined from the mixture name if a chemical that meets the category definition is actually contained in the mixture.

Listing by CAS Number of Some Mixtures That Might Contain Polychlorinated Alkanes within the Category <sup>1</sup>	
Mixture Name	CAS Number
Hydrocarbon waxes (petroleum), microcryst., chlorinated, reaction products with naphthalene	68938-44-3
Hydrocarbons, chloro, chlorine manuf. diaphragm cell wastes	70514-07-7
Hydrocarbons, C2-unsatd., chlorinated, distn. residues	91053-07-5
Antimony oxide (Sb <sub>2</sub> O <sub>3</sub> ), mixture with chloro paraffin waxes	148709-58-4
Phenol, pentachloro-, mixture with chloro paraffin oils and 1-chloronaphthalene	70645-04-4
Benzene, 1,1'-oxybis[2,3,4,5,6-pentabromo-, mixture with antimony oxide (Sb <sub>2</sub> O <sub>3</sub> ) and chloro paraffin waxes	148709-59-5
Sulfonic acids, C13-17-alkane, mixed with C13-17-alkanes, chlorinated, sodium salts	94167-10-9

<sup>1</sup> It cannot be determined from the mixture name if a chemical that meets the category definition is actually contained in the mixture.

## References

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3. J. March, *Advanced Organic Chemistry*, 3<sup>rd</sup> edition, John Wiley & Sons, New York, 1985, pages 620-624.
4. *Chlorinated Paraffins: A Status Report*, CPIA 1990.