The Transport and Deposition of Persistent Toxic Substances to the Great Lakes

I. The Capability of Specific Persistent Toxic Substances to be Subjected to Long Range Atmospheric Transport

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by

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Preface

This report was commissioned by the IJC International Air Quality Advisory Board. It is the first in a series of five closely related reports prepared for the Board which examine a set of persistent toxic substances identified in the Binational Virtual Elimination Strategy (BVES). The second report deals with the status and capabilities of available emissions inventories for BVES compounds. The third and fourth reports deal with modeling the atmospheric transport and deposition of BVES compounds to the Great Lakes and monitoring of these compounds in the Great Lakes region, respectively. The fifth report is a summary of the first four reports.

These reports were prepared as background documents for the IJC-sponsored Joint International Air Quality Board and Great Lakes Water Quality Board Workshop on Significant Sources, Pathways and Reduction/Elimination of Persistent Toxic Substances, held May 21-22, in Romulus Michigan.

The material presented here was collected and analyzed during the period from October 1996 through May 1997.

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Executive Summary

This report examines the potential for long range atmospheric transport and the status of emissions inventories of a group of persistent toxic substances identified by the Binational Virtual Elimination Strategy (BVES) for pollutants of concern in the Great Lakes Basin:

Alkylated lead
Mercury
Cadmium
Tributyltin
Aldrin
Dieldrin
DDT
DDD
DDE
Mirex
Toxaphene
Endrin
Heptachlor
Heptachlor Epoxide
Hexachlorocyclohexanes
Methoxychlor
Pentachlorophenol
Octachlorostyrene
3,3'-Dichlorobenzidene
4,4'-Methylene bis (2-Chloroaniline)
4-Bromophenyl Phenyl Ether
Hexachloro-1,3-Butadiene
1,4-Dichlorobenzene
Tetrachlorobenzenes
Pentachlorobenzene
Hexachlorobenzene
PCDD/F's
PCB's
Dinitropyrenes
Benzo[a]Pyrene
Phenanthrene
Anthracene
Benz[a]Anthracene
Perylene
Benzo[g,h,i]Perylene
PAH's (as a group)

The analysis is based on the characteristics of these compounds/groups that are likely to influence their potential for long-range air transport. The following analytical strategy was adopted.

First, it was determined whether the substances are in fact emitted into the atmosphere and actually detected in the atmosphere.

Second, an assessment was made, based on a consideration of the phase in which each compound is likely to occur in the atmosphere, of the degree to which each substance will respond to a group of factors that influence its fate in the atmosphere. These factors are:

- resistance to destructive chemical reactions in atmosphere;
- resistance to photolytic degradation;
- resistance to gas-phase rainfall washout;
- if and/or when the substance is associated with particles in the atmosphere, whether the substance is associated with *small* particles.

Third, the influences of these factors were used to estimate the substances' approximate lifetime in the atmosphere. Thus, for example, hexachlorobenzene is extremely resistant to all of the factors that tend to remove it from the atmosphere;

hence it has an atmospheric lifetime measured in years and moves over global distances. In contrast, a substance very susceptible to photolytic degradation while airborne may have a lifetime measured in minutes. The approximate overall lifetime is essentially based on the factor(s) which exerts the greatest influence on the removal of the substance from the atmosphere.

Fourth, evidence that the substances have been found at distances remote from their points of emission (for example, the occurrence of DDT in the Arctic) is considered, together with the estimated overall lifetime, to arrive at an overall Long-range Transport Rating.

Based on this procedure, it has been possible to classify the compounds/groups into four rough categories. Four overall LRT ratings are employed:

Rating 1: Atmospheric half-life, one year or more
Geographic distribution from sources: global

Rating 2: Atmospheric half-life, one week to a few months
Geographic distribution: 1,000-10,000 km (possibly global)

Rating 3: Atmospheric half-life, a few hours to a few days
Geographic distribution: 100-1,000 km

Rating 4: Atmospheric half-life, seconds to minutes
Geographic distribution: local

Table ES-1 lists the compounds/groups that fall into these categories. Four of them are in Rating 1 and are likely to be distributed globally. Three appear to be removed from the atmosphere so quickly as to fall into Rating 4 (although as noted, the evidence is not reliable). The remaining substances fall into the intermediate Ratings, 2 and 3, and are subject to transport over distances ranging from 100-10,000 km (with some possibly globally distributed), depending on their specific properties.

The grasshopper effect may be important for several of these compounds, and will probably serve to lengthen the effective scale of atmospheric transport; thus, for some of the compounds, the estimates of atmospheric lifetime and transport scale may represent lower bounds. Moreover, the rates of destruction in the atmosphere may be significantly slower in remote northern climates (due to lower concentrations of reactive species such as hydroxyl radical and lower temperatures), and so, the long range transport potential may again be underestimated for compounds traveling in these regions.

Table ES-1: Summary of Long-Range Air Transport Potential of Considered Compounds

Rating			
1	2	3	4
Atmospheric Half Life			
1 year or more	1 week-few mos.	few hrs-few days	seconds-minutes
Geographic Distribution			
global	1,000-10,000 km (possibly global)	100-1,000 km	local
mercury hexachloro-1,3-butadiene tetrachlorobenzenes pentachlorobenzene hexachlorobenzene	alkylated lead cadmium DDT/DDD/DDE mirex toxaphene hexachloro-cyclohexanes (HCH's) pentachlorophenol octachlorostyrene 3,3'-dichloro-benzidene 1,4-dichlorobenzene PCDD/F's PCBs dinitropyrenes benzo[a]pyrene benz[a]anthracene perylene benzo[g,h,i]perylene PAHs (as a group)	aldrin(?) heptachlor(?) 4,4'-methylene bis (2-chloroaniline) (?) tributyltin (?) heptachlor epoxide methoxychlor dieldrin endrin 4-bromophenyl phenyl ether phenanthrene anthracene	aldrin (?) heptachlor (?) 4,4'-methylene bis (2-chloroaniline) (?)

The Capability of Specific Persistent Toxic Substances to be Subjected to Long Range Atmospheric Transport

A. Introduction

Atmospheric deposition of pollutants is a major pathway for the entry of pollutants to the Great Lakes. Some of the pollution deposited from the air above the lakes originated from local sources, i.e., sources in the region immediately surrounding the lakes. However, some of the pollution that is deposited may have come from far away, transported in the atmosphere to the Great Lakes over long distances. For pollutants for which atmospheric deposition is an important contamination pathway, it is important to unravel the origin of the material that is deposited. If the bulk of it comes from local sources, then efforts to prevent deposition can be concentrated on reducing local emissions of the compound. On the other hand, if a significant portion of the pollutant comes from more distant sources, then efforts to lessen its impact must include a consideration of such long-range sources.

The Binational Virtual Elimination Strategy (BVES) identified a target list of 27 chemicals or chemical groups, including twelve Level I substances or groups and fifteen Level II substances or groups.

> Level I substances are the 11 Critical Pollutants identified by the IJC's Great Lakes Water Quality Board, plus one additional Critical Pollutant identified by the Lake Superior LaMP and the Lake Ontario Toxics Management Plan (Octachlorostyrene).[1]
>
> Level II Substances are those substances identified by the Canada-Ontario Agreement respecting the Great Lakes Basin Ecosystem (COA) as "Tier II" chemicals, plus additional substances of concern identified by LaMP and RAP processes and the Great Lakes Water Quality Guidance in the U.S.
>
> A list of the BVES compounds or groups is given in the following table.

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[1] Note: Chlordane was also an additional Critical Pollutant identified on the BVES list, but it was inadvertently omitted from work scope for this analysis.

Table 1. Summary of Chemicals and Chemical Groups Considered in this Evaluation

Chemical or Group	Level	Notes
METALS / ORGANOMETALLICS		
Alkylated Lead	I	There are a range of compounds of environmental interest, including tetra-alkyl, tri-alkyl, and di-alkyl lead compounds, with methyl and ethyl alkyl groups alone and in combination.
Mercury	I	There are a range of inorganic and organic compounds containing mercury of environmental interest. These include elemental mercury, mercuric chloride, mercuric oxide, methyl mercury, dimethyl mercury, and possibly other compounds.
Cadmium	II	There are a range of inorganic cadmium compounds (including CdO, CdCl2, and others) and organic cadmium compounds of potential environmental interest.
Tributyltin	II	There are a range of tributyltin compounds of environmental interest.
ORGANOCHLORINE BIOCIDES		
Aldrin / Dieldrin	I	Dieldrin has been used as a biocide in its own right, and is also an environmental breakdown product of Aldrin
Chlordane	I	(inadvertently omitted and not included in this particular analysis)
DDT / DDD / DDE	I	DDD and DDE are breakdown products of DDT
Mirex	I	
Toxaphene	I	Toxaphene is a complex mixture of polychlorinated camphenes. There are over 30,000 theoretically possible congeners, with about 300 that may be likely to be present in the environment.
Endrin	II	
Heptachlor / Heptachlor Epoxide	II	Heptachlor Epoxide is an environmental breakdown product of Heptachlor
Hexachlorocyclohexane	II	There are five isomers: α-HCH, β-HCH, δ-HCH, ϵ-HCH and γ-HCH (lindane).
Methoxychlor	II	
Pentachlorophenol	II	
INDUSTRIAL / MISCELLANEOUS		
Octachlorostyrene	I	
3,3'-Dichlorobenzidene	II	
4,4'-Methylene bis (2-Chloroaniline)	II	
4-Bromophenyl Phenyl Ether	II	
Hexachloro-1,3-Butadiene	II	

Table 1. Summary of Chemicals and Chemical Groups Considered in this Evaluation

Chemical or Group	Level	Notes
CHLOROBENZENES		
1,4-dichlorobenzene	II	
Tetrachlorobenzene	II	There are three isomers: 1,2,3,4-tetrachlorobenzene and 1,2,3,5-tetrachlorobenzene are classified as Level II substances; 1,2,4,5-tetrachlorobenzene is not classified.
Pentachlorobenzene	II	
Hexachlorobenzene	I	
POLYCHLORINATED DIBENZO-P-DIOXINS AND DIBENZOFURANS (PCDD/F'S)		
2,3,7,8-TCDD	I	In addition to 2,3,7,8-TCDD/F, there are fifteen other penta-Cl through octa-Cl chlorinated dibenzo-p-dioxins and dibenzofurans that are 2,3,7,8-Cl-substituted that should be considered. In all, There are a total of 210 CDD/F's. In this analysis, all 17 toxic PCDD/F congeners were considered separately, although results are frequently presented for them as an entire group or as homologue groups (e.g, groups of PCDD/F with the same number of chlorine atoms)
2,3,7,8-TCDF	I	
POLYCHLORINATED BIPHENYLS (PCB'S)		
PCB's as a group	I	In all, there are a total of 209 possible PCB congeners. Many of these are commonly found in environmental samples. In this analysis, an attempt was made to consider the full set of PCB congeners, although results are frequently presented for them as an entire group or as homologue groups (e.g, groups of PCB's with the same number of chlorine atoms)
POLYCYCLIC AROMATIC HYDROCARBONS		
Benzo [a] Pyrene	I	
Dinitropyrenes	II	There are at least four isomers: 1,3-dinitropyrene; 1,6-dinitropyrene; 1,8-dinitropyrene; and 2,7-dinitropyrene. These may be emitted directly by sources, and, they may be formed by chemical reactions of pyrene with nitrogen species in the atmosphere.
PAH's as a group	II	There are many thousands of possible PAH compounds and derivatives. The target list specifies that the analysis of PAH's as group include (but not be limited to) the following specific PAH's: Phenanthrene Anthracene Benz[a]Anthracene Perylene Benzo[g,h,i]Perylene To create a group of PAH's for this analysis, the following PAH's were added, consisting of the universe of compounds considered in the EPA's 16-PAH list and the ATSDR 17-PAH list: Naphthalene Acenaphthene Acenaphthylene Fluorene Pyrene Fluoranthene Chrysene Benzo[b]Fluoranthene Benzo[j]Fluoranthene Benzo[k]Fluoranthene Benzo[e]Pyrene Dibenz[a,h]Anthracene Indeno[1,2,3-c,d]Pyrene

In order for a pollutant emitted to the atmosphere to be transported long distances in the atmosphere and be deposited in the Great Lakes, several conditions must be met:

- The pollutant must be emitted into the air;
- The atmospheric lifetime of the pollutant must be sufficient to allow it to be transported in the air over long distances;
- The pollutant must be capable of being deposited to the Lakes.

Emissions to the air will be considered in the second section of this report. This first section will consider the fate and transport of pollutants, if they were emitted to the air.

First, an attempt was made to assemble the physical/chemical properties for the substances of this study. For some of substances, there were no reported data for some or all of the relevant properties, and for some of the others, there were often conflicting data, where fairly widely diverse values for a given property were reported. It was beyond the scope of this study to attempt to evaluate the relative accuracy of different property values. Whenever possible, tabulations of “selected values” were used, in which the it is presumed that the authors selected the most likely value for a given property from among the available data.

Tables of physical and chemical properties assembled in Appendix A of this draft, and additional information is included as well, e.g., some of the methods used to estimate properties when no data were available.

B. Atmospheric Loss Mechanisms and Atmospheric Lifetimes

B.1. Introduction

1. Vapor/Particle Partitioning. Compounds may exist in vapor or particulate phase; vapor particle partitioning will depend on the compound's physical-chemical characteristics, the detailed nature of the local airborne particulate, and the detailed local meteorological conditions — thus, V/P partitioning is not a static phenomenon; the V/P partitioning characteristics of a given compound will vary with location and time. The atmospheric fate of the compound will depend intimately on the vapor/particle partitioning characteristics.

2. Chemical Reactions. Transformation reactions can occur in the gas phase, on particle surfaces, in liquid droplets or liquid shells around solid particles; different reactions may be important in different phases. Note: in some cases, the compound may be transformed to a more toxic species.

   A. Direct photolysis reactions can occur, in which a compound absorbs ultraviolet light of a particular wavelength and is broken down.

   B. Reactions with reactive species in the atmosphere can occur, such as reaction with hydroxyl radical, ozone, nitrate, hydrogen peroxide, chlorine, and others. For most species, reaction with hydroxyl radical is typically considered to be the most important chemical transformation reaction in the atmosphere.

3. Deposition.

   A. Dry deposition. Both particles and vapors can be dry-deposited. By definition, dry deposition includes all atmospheric deposition of compounds to the earth's surface when there is no precipitation.

   B. Wet deposition. Again, both particle-phase and vapor-phase material can be transported from the atmosphere to the ground through wet deposition processes.

B.2. Vapor/Particle Partitioning

In order to understand and predict the fate and transport of atmospheric pollutants, their vapor/particle partitioning must be characterized (Bidleman, 1988).

As described in Appendix C, estimates were made using the adsorption-based theory of Junge (1977), with the subcooled liquid-phase vapor pressure substituted for the solid phase vapor pressure, as recommended by Bidleman (1988). The physical properties values used to make these estimates are given in Appendix A. A discussion of the theory and some of its limitations is presented in Appendix C-1. The calculation details are presented in Appendix C-2. The estimates are summarized in Appendix C-3, and comparisons are made to examples of vapor/particle partitioning measurements and/or estimates from the literature. In Appendix C-4, a detailed comparison of vapor/particle partitioning theoretical predictions and recent experimental measurements is presented.

In general, even though a relatively simple theoretical framework was used here to estimate the vapor/particle partitioning characteristics of BVES compounds in the atmosphere, the predictions appear to be reasonably consistent with the available experimental data.

An overall summary of the vapor/particle partitioning estimates is provided in Table 2, below. As mentioned above, details of the calculation procedure are provided in Appendix C.

Table 2. Overall Summary of Vapor/Particle Partitioning Estimates

Compounds which are predicted to exist almost entirely in the particle phase in the atmosphere (fraction adsorbed ≥ 98% under most conditions)	Compounds which are predicted to exist mostly in the particle phase in the atmosphere (fraction adsorbed ≥ 90% under most conditions)	Compounds which are predicted to exist in significant proportions in both the particle phase and the vapor phase as conditions vary	Compounds which are predicted to exist mostly in the vapor phase in the atmosphere (fraction adsorbed ≤ 10% under most conditions)	Compounds which are predicted to exist almost entirely in the vapor phase in the atmosphere (fraction adsorbed ≤ 2% under most conditions)
• Cadmium • OCDD/F • Dibenz(a,h)Anthracene	• HpCDD/F's • HxCDD/F's • Indeno(1,2,3-cd)Pyrene • Benzo(j)Fluoranthene (h) • Benzo(b)Fluoranthene (h) • Benzo(k)Fluoranthene (h) • Perylene (h) • Benzo(g,h,i)Perylene (h) • Benzo(a)Pyrene (h) • Benzo(e)Pyrene (h)	• Tributyltin oxide • DDT / DDD / DDE • Toxaphene • Methoxychlor • 3,3'-Dichlorobenzidene (b) • 2,3,7,8-TCDD/F • PeCDD/F's • PCB's (c) • Dinitropyrenes • Pyrene • Fluoranthene • Chrysene • Benz(a)Anthracene	• Mercury (e) • γ-HCH (Lindane) (a) • Octachlorostyrene • 4,4' Methylene bis-(2-chloroaniline) (b)	• Tetraethyl Lead (f) • Tetramethyl Lead (f) • Aldrin / Dieldrin • Mirex • Endrin • Heptachlor • Heptachlor Epoxide • α-HCH / β-HCH / δ-HCH • Pentachlorophenol (b) • Hexachloro-1,3-Butadiene • 4-Bromophenyl Phenyl Ether • Chlorobenzenes (d) • Naphthalene • Acenaphthene • Acenaphthylene • Fluorene (?) (g) • Phenanthrene (?) (g) • Anthracene

(a) γ-HCH (Lindane) is predicted to exist generally in the vapor phase but, under very cold conditions with high atmospheric particle surface area, as much as 3% of the atmospheric content may be associated with particles

(b) Compound is relatively water soluble (solubility may be pH dependent, e.g., Pentachlorophenol). Under high humidity conditions where the atmospheric aerosol might be expected to consist (in part) of liquid droplets, higher fractions of compound may be adsorbed into such liquid droplets.

(c) Different PCB congeners have different predicted behavior; monochloro-PCB's are predicted to be predominantly in the vapor phase under most conditions; dichloro- through decachloro-PCB's show increasing particle affinity, generally as the number of chlorines in the molecule increase.

(d) 1,4-Dichlorobenzene; Tetrachlorobenzenes; Pentachlorobenzene; Hexachlorobenzene

(e) The total fraction of atmospheric mercury associated with particles is uncertain, but is believed to be on the order a few, perhaps five, percent. Mercuric chloride is very soluble in water; if it is emitted then it could partition significantly to atmospheric water droplets.

(f) Atmospheric breakdown products of tetra-alkyl-lead compounds (e.g., trialkyl- and dialkyl- lead compounds) are very soluble in water; after they are formed, they may partition significantly to atmospheric water droplets.

(g) Evidence for less than fullvapor/particle exchangeability exists; thus, compound may exist more on particles than predicted by theory which assumes full exchangeability.

(h) Simple adsorption theory suggests this compound may exist significantly in the vapor phase under some conditions, but, field measurements show that the compound exists primarily in the particulate phase in almost all measurements; therefore, the compound has been placed in this column.

B.3. Destruction and Transformation of Atmospheric Pollutants by Chemical Reactions and Photochemical Processes

Pollutants in the atmosphere can undergo a number of processes which lead to chemical transformation, i.e., processes in which in which the chemical identity of the compound is changed. The two potentially most important of these processes are generally considered to be chemical reaction (e.g., with hydroxyl radical or ozone) and direct photochemical transformation (e.g, as a result of absorption of uv light), although there can be other important processes for certain compounds in certain situations. Chemical reactions and photolytic processes can occur in both the vapor and particle phases in the atmosphere.

Reactions with hydroxyl radical — considered to be the most significant reaction for many atmospheric compounds — are generally considered to occur only in the vapor phase.[2] Other reactions, however, can occur in condensed phases. Reactions can occur, for example, in atmospheric water droplets. Many of the BVES compounds are relatively insoluble in water — with a few exceptions — and so atmospheric aqueous phase reactions, e.g., with hydrogen peroxide, will probably be relatively insignificant. Reactions can also occur in organic liquid-layer shells which may exist around atmospheric particles. For example, substituted phenols abundant in wood smoke particles react rapidly with PAH's (Odum *et al.* 1994); these reactions appear to be faster than those of PAH's with hexadecane in particles, representative of aliphatic hydrocarbons found in diesel exhaust (McDow *et al.*, 1994).

Like chemical reactions, photolysis can occur in the gas phase and in condensed phases. In addition to differences in photolytic rates of transformation between compounds based on chemical structures, substrate and solvent effects are frequently found in condensed phases.

Thus, for example, photodegradation rates of PAH's adsorbed to flyash are generally found to depend on the nature of the flyash, with rates on carbon-rich particles frequently lower than those on particles with less carbon [e.g., Baek et al. 1991 (review); Behymer and Hites, 1988 (example of a particular experiment)]. The protective effect may have to do with the light-absorbing nature of carbon-rich particles.

In a smog-chamber experiment, Pennise and Kamens (1996) found that PAH's and PCDD/F's were more stable on particles generated under high-temperature combustion of wood chips and PVC (and other chlorinated compounds) than on particles generated by low-temperature combustion of the same materials. On the high-temperature combustion, half-lives of particle-phase PAH's were on the order of 5-10 hours in an experiment in the summer (in North Carolina) and in the winter, some of the PAH's degraded with half-lives of between 6 -12 hours, with others showing no decay over a 6-hour daylight exposure. With the same high-temperature-combustion-

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[2]. Little or no information could be found regarding hydroxyl radical reactions in condensed phases, e.g., on the surface of particles. If this is an important phenomenon, then it is not well understood at the present.

generated particles, half-lives of particle-phase PCDD/F's were generally longer than those of the PAH's measured: particle-phase TCDD's half-life was estimated to be 6.8 hours in the summer and 68 hours in the winter, and OCDD's half-life was estimated to be 36 hours in the summer and 257 hours in the winter.[3]

As another example, particle-phase PCDD/F appears to be relatively invulnerable to photodegradation, based on measurements of PCDD/F adsorbed to flyash (Koester and Hites, 1992). This may serve to explain the observation that higher chlorinated PCDD/F congeners, which tend to be associated with the particle phase in the atmosphere, appear to be longer-lived in the atmosphere than lower chlorinated congeners, which exist significantly in the vapor phase. The difference in PCDD/PCDF congener profiles between atmospheric <u>sources</u> (where the distribution among congners is more uniform) and <u>sinks</u> (where the higher chlorinated congeners are disproportionately present) is consistent with this phenomenon.

Destruction/Transformation by Chemical Reaction

As mentioned above, the most important reaction for many <u>gas phase</u> atmospheric organic compounds is generally considered to be the reaction with hydroxyl radical (OH·) (e.g., Seinfeld, 1986; Finlayson-Pitts and Pitts, 1986). Reactions with other species — e.g. ozone, singlet oxygen, nitrogen oxides, chlorine — can be important under some conditions and with some compounds. In general, much less is known about the atmospheric reactions of these other reactive species in the atmosphere. Attention has been largely focused on hydroxyl radical attack because it is generally considered to be the most important.

Reaction rates with hydroxyl radical have been experimentally determined for a number of compounds, including a few of the compounds considered in this analysis. A summary of the data availability (for this project's compounds) for experimentally determined reaction rates with hydroxyl radical is summarized in Table 3. It can be seen that while data exist for some of the compounds considered, data for hydroxyl radical reaction rate are not available for most of the compounds considered in this analysis.

Because of the high cost of experimental measurements of the rate of hydroxyl radical reaction, it is common to attempt to estimate the reaction rate of a particular compound using structure-activity correlations. In such an approach, available data are analyzed for patterns which suggest how the rate is influenced by various aspects of the molecular structure. Atkinson and coworkers have made a number of the experimental measurements of hydroxyl radical rate constants (a list of many of their

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[3]. As is often the case, there were a number of factors in these experiments which complicate their extrapolation to the ambient atmosphere. Only particle-phase measurements were made, while some of the compounds may have existed to a certain extent in the vapor phase. As in any smog chamber experiment, wall losses can be significant. In addition, the particle concentrations in these experiments, 1000 - 7000 µg/m3 (10 - 100 times that found in the ambient atmosphere), and, the chlorine content of the particle-generating fuel was very high.

papers is given in Appendix D-5) and they have developed and refined a structure-activity model for organic compound reaction with hydroxyl radical.

Table 3. Summary of Experimentally Determined Hydroxyl Radical Rate Constants Available for Compounds Considered in this Evaluation

category	**specific species for which hydroxyl radical rate constant has been experimentally determined**	**notes**
Mercury Compounds	• dimethyl mercury	
Alkyl-Lead Compounds	• tetraethyl lead • tetramethyl lead	
Chlorobenzenes	• 1,4-dichlorobenzene	
PCB's	• PCB 0: biphenyl • PCB 1: 2-monochloro-biphenyl • PCB 2: 3-monochloro-biphenyl • PCB 3: 4-monochloro-biphenyl • PCB 4: 2,2'-dichloro-biphenyl • PCB 7: 2,4-dichloro-biphenyl • PCB 11: 3,3'-dichloro-biphenyl • PCB 14: 3,5-dichloro-biphenyl • PCB 15: 4,4'-dichloro-biphenyl • PCB 28: 2,4,4'-trichloro-biphenyl • PCB 29: 2,4,5-trichloro-biphenyl • PCB 31: 2,4',5-trichloro-biphenyl • PCB 33: 2',3,4-trichloro-biphenyl • PCB 44: 2,2',3,5'-tetrachloro-biphenyl • PCB 47: 2,2',4,4'-tetrachloro-biphenyl • PCB 95: 2,2',3,5,6-pentachloro-biphenyl • PCB 110: 2,3,3',4',6-pentachloro-biphenyl • PCB 116: 2,3,4,5,6-pentachloro-biphenyl	• upper bound on reaction rate of biphenyl (PCB 0) with ozone is available
PAH's specifically identified on target list	• phenanthrene • anthracene	
PAH's added to list to create a "PAH group" for overall analysis	• naphthalene • acenaphthene • acenaphthylene • fluorene • pyrene • fluoranthene	• reaction rate of naphthalene with NO_3 has been determined • upper bound on reaction rate of naphthalene with ozone is available

The structure-activity model of Atkinson and coworkers has been presented in the following series of papers:

- Atkinson, R. (1987). “A Structure-Activity Relationship For the Estimation Of Rate Constants For the Gas-Phase Reactions Of OH Radicals With Organic-Compounds.” International Journal Of Chemical Kinetics **19**(9): 799-828.
- Atkinson, R. (1988). “Estimation Of Gas-Phase Hydroxyl Radical Rate Constants For Organic Chemicals.” Environmental Toxicology and Chemistry **7**(6): 435-442.
- Atkinson, R. and S. M. Aschmann (1992). “OH Radical Reaction-Rate Constants For Polycyclic Alkanes - Effects Of Ring Strain and Consequences For Estimation Methods.” International Journal Of Chemical Kinetics **24**(11): 983-989.
- Kwok, E. S. C., R. Atkinson, et al. (1995). “Rate Constants For the Gas-Phase Reactions Of the OH Radical With Dichlorobiphenyls, 1-Chlorodibenzo-P-Dioxin, 1,2-Dimethoxybenzene, and Diphenyl Ether - Estimation Of OH Radical Reaction-Rate Constants For PCBs, PCDDs, and PCDFs.” Environmental Science & Technology **29**(6): 1591-1598.
- Kwok, E. S. C. and R. Atkinson (1995). “Estimation Of Hydroxyl Radical Reaction-Rate Constants For Gas-Phase Organic-Compounds Using a Structure-Reactivity Relationship - an Update.” Atmospheric Environment **29**(14): 1685-1695.

Meylan and Howard of the Syracuse Research Corporation (SRC: Syracuse, New York) have utilized the structure-activity relationships of Atkinson and colleagues — including the latest update (Kwok and Atkinson, 1995) — to create the Atmospheric Oxidation Rate Program. A few changes to Atkinson’s methodology were made which are believed to improve the accuracy of the estimates (Meylan and Howard, 1996). The latest version of this program was obtained from SRC (AOPWIN Version 1.82 (for Windows), 1996) and was used to make estimates for each of the compounds considered in this study.

A summary of the results of these estimates — including the estimated atmospheric half-life for reaction with hydroxyl radical — are presented in Appendix D-2 and D-3.

Appendix D-2 contains the a summary of the basic output from the program, including experimentally determined and estimated rate constants of the reaction with hydroxyl radical, experimental and estimated reaction rates and half-lives for reaction with ozone, and available data regarding reaction with NO_3.

Appendix D-3 contains estimates of an “adjusted” atmospheric half-life which factors in the effect of vapor/particle partitioning. To adjust the half-life, the values in Appendix D-2 were divided by the fraction of the compound predicted to exist in the vapor phase in the atmosphere. For example, for a compound which is predicted to exist 99% in the particle phase and 1% in the vapor phase, the vapor fraction equals 0.01, and, when the gas-phase half-life is divided by this fraction, it is increased by a factor of 100. In essence, the half-life is adjusted for the fact that the hydroxyl radical reaction is assumed to only proceed effectively in the vapor phase. Thus, compounds that don't exist significantly in the vapor phase will not react quickly with hydroxyl radical, even if their "theoretically" predicted gas-phase reaction rate — based on structure activity relationships — would indicate a rapid reaction.

The screening level calculations performed here have been based on an average hydroxyl radical concentration of 1.5×10^6 molecules per cm^3, 12 hours of reaction per day, and reaction rates estimated generally at 25 °C. These assumed screening level conditions may overestimate rate of destruction in northern climates, where temperatures may be substantially lower, and, in remote areas, where the hydroxyl radical concentrations may be lower. Thus, for pollutants being transported to the arctic — experiencing cooler temperatures and lower hydroxyl radical concentrations — the rate of chemical reaction may be substantially less than the screening level estimates given here. Thus, the extent of transport to the arctic may be increased.

Photolytic Destruction in the Atmosphere

As mentioned above, another pathway for the chemical transformation of compounds in the atmosphere is direct photolysis. In this phenomenon, a molecule absorbs a photon of ultraviolet (uv) radiation and is raised to a photochemically excited state. This state may be relatively unstable, and a chemical transformation process may occur. In such processes, the chemical nature of the molecule changes: bonds between one or more pairs of atoms in the molecule are broken or changed, and the new molecule may be slightly or radically different from the starting molecule.

Ultraviolet radiation with wavelengths below 290 nm is generally prevented from reaching the troposphere because it is absorbed in the upper levels of the atmosphere. Thus, for a compound to potentially undergo a photochemical transformation, it must be able to effectively absorb at electromagnetic radiation at at least some wavelengths greater than 290 nm.

Very few gas-phase measurements of photolysis have been attempted. Generally, measurements are made in the solution phase, i.e., the compound is dissolved in water or in some other solvent, or an adsorbed phase, i.e., on the surface of particles of a certain type.

Photolysis in the solution phase can be "direct" or "indirect". Indirect photolysis refers to the situation in which another species in the solution undergoes a photochemical transformation, and the product of this transformation subsequently reacts with the compound of interest. Sometimes the solvent itself participates in this process. In these cases, solution-phase photolysis rates can vary dramatically depending on which solvent is used. Thus, solution-phase photolysis rates cannot necessarily be applied to the atmosphere.

Photolysis measurements with compounds adsorbed to different substrates are also frequently made. For example, Freitag *et al.* (1985) report photodegradation rates for 100 compounds — including many of the BVES compounds — adsorbed to silica gel. As mentioned above, experiments measuring the photodegradation of particle-associated materials have been made, for example, for PAH's (e.g., Behymer and Hites, 1988) and PCDD/F's (Koester and Hites, 1992). In the laboratory experiments of Koester and Hites (1992), essentially no photodegradation was observed for PCDD/F associated with flyash. This suggests that particle-associated PCDD/F in the atmosphere may be similarly resistant to photodegradation. However, as with the solution phase measurements above, it is difficult to directly extrapolate adsorbed-phase experimental results to ambient atmospheric conditions.

A very brief summary of available information about the possible importance of photolysis is given in the following table. Additional information about photolysis is presented in Appendix D-4.

Table 4. Summary of Information about Photolysis Rates
(values in parentheses indicate a higher degree of uncertainty;
values with question marks are even more uncertain)

Chemical or Group	Level	Information About Photolysis Rates	photolytic resistance (0=vulnerable; 1=relatively invulnerable)
METALS / ORGANOMETALLICS			
Alkylated Lead	I		
Mercury	I	• Photolysis may be very important for organomercurials in the atmosphere (4) • However, elemental mercury will not be affected (5)	1
Cadmium	II		(1)
Tributyltin	II	• Slow photolysis observed in water; half-life estimated to be about 3 months (4)	1
ORGANOCHLORINE BIOCIDES			
Aldrin	I	• Aldrin does not absorb uv light at wavelengths greater than 260 nm in hexane; absorption maximum at 211 nm (6) • Vapor-phase photolysis reportedly significant in some tests, but reportedly not significant in others (4) • Photolysis can be important (11)	(½)
Dieldrin	I	• Dieldrin reportedly does not absorb uv light at wavelengths greater than 290 nm in hexane; absorption maximum at 218 nm (6) • However, photolysis can be important (11)	(½)
DDT	I	• Not expected to be significant based on lack of degradation in 7 days in one experiment and very slow rate of decay in another experiment (6)	1
DDD	I		(½)
DDE	I	• in water, photolysis half-life ranges from 1-6 days (4); • this same estimate applied to atmospheric DDE (6) • (reaction with OH probably more important)	½
Mirex	I	• direct photolysis half-life in sunlight in water determined experimentally to be on the order of 1 year (2); thus atmospheric photolysis should be relatively unimportant	1
Toxaphene	I	• Not expected to undergo direct photolysis (4)	1
Endrin	II	• Half-life estimated to be on the order of 5 - 9 days in intense summer sunlight; atmospheric information not available (4)	½
Heptachlor	II	• Half life measured in natural water to be 3.5 days (4) • Has absorption peaks above 290 nm (6) • Photolysis can form photo-heptachlor, a stable and toxic photo-product (11)	½
Heptachlor Epoxide	II	• Experimental evidence suggests that direct photolysis not very important, although indirect, i.e., sensitized, photolysis can be important in condensed phases	1

Table 4. Summary of Information about Photolysis Rates
(values in parentheses indicate a higher degree of uncertainty;
values with question marks are even more uncertain)

Chemical or Group	Level	Information About Photolysis Rates	photolytic resistance (0=vulnerable; 1=relatively invulnerable)
α-Hexachlorocyclohexane	II		
β-Hexachlorocyclohexane	II	• less stable to uv than lindane, but not dramatically so (3)	¾ - 1
δ-Hexachlorocyclohexane	II		
γ-Hexachlorocyclohexane (Lindane)	II	• relatively stable to uv light (3) • photolysis not expected to be important because chemical structure suggests very little absorption above 290 nm	1
Methoxychlor	II	• direct photolysis half-life in sunlight in water determined experimentally to be on the order of 1 month (2); thus atmospheric photolysis should be relatively unimportant	1
Pentachlorophenol	II	• fairly rapid photolysis when absorbed onto silica gel (3) • photolysis important in aqueous solution (e.g., half-life on the order of hours) (4). • photolysis estimated to be much more important than hydoxyl radical attack; half-life estimated to be on the order of <1 day (summer) to about 9 days (winter) at the latitude of Toronto, Canada (8).	¼
INDUSTRIAL / MISCELLANEOUS			
Octachlorostyrene	I		(1) ?
3,3'-Dichloro-benzidene	II	• Relatively unstable to uv light exposure when adsorbed to silica gel (similar to pentachlorophenol) (3) • Found to be very unstable to photolysis in water (4) • Exists in vapor and particle phase and so may be protected some of the time	¼ - ½
4,4'-Methylene bis (2-Chloroaniline)	II	• Absorption peak above 290 nm exists	?
4-Bromophenyl Phenyl Ether	II		?
Hexachloro-1,3-Butadiene	II		**?**
CHLOROBENZENES			
1,4-dichlorobenzene	II	• photolysis not expected to be significant (4) • relatively stable against ultraviolet light (3)	1
Tetrachlorobenzenes	II	• (reasoning by analogy with other chlorobenzenes)	(1)
Pentachlorobenzene	II	• particularly stable against ultraviolet light (3)	1
Hexachlorobenzene	I	• photolysis not expected to be significant, based on experimental evidence (4) • particularly stable against ultraviolet light (3)	1
POLYCHLORINATED DIBENZO-P-DIOXINS AND DIBENZOFURANS (PCDD/F'S)			

Table 4. Summary of Information about Photolysis Rates

(values in parentheses indicate a higher degree of uncertainty;
values with question marks are even more uncertain)

Chemical or Group	Level	**Information About Photolysis Rates**	**photolytic resistance** (0=vulnerable; 1=relatively invulnerable)
PCDD/F's (as a group)	I	• Atkinson compared sunlight-water photolysis rates with estimated hydroxyl radical attack, and estimated that hydroxyl radical reaction would be faster, but not overwhelmingly so (7) • Photolysis in natural waters in sunlight estimated to be on the order of 1 - 7 days for 2,3,7,8-TCDD (data cited in 7) • All tetra- through octa CDD/F's exist to a certain extent (or almost completely) in the particle phase; thus, they will be somewhat protected against photolysis • In a smog-chamber experiment, it was found that PCDD/F's were more stable on particles generated under high-temperature combustion of wood chips and PVC (and other chlorinated compounds) than on particles generated by low-temperature combustion of the same materials. On the high-temperature combustion, half-lives of particle-phase, half-lives of particle-phase PCDD/F's were generally longer than those of the PAH's measured: particle-phase TCDD's half-life was estimated to be 6.8 hours in the summer and 68 hours in the winter, and OCDD's half-life was estimated to be 36 hours in the summer and 257 hours in the winter (10)	½
POLYCHLORINATED BIPHENYLS (PCB'S)			
PCB's (as a group)	I	• For PCB's with up to 6 chlorines, there does not appear to be any uv absorption (6) • For PCB's with 6 or more chlorines, there may be absorption bands above 290 nm (6); • However, portions of these heavier PCB's will be associated with particles; thus they *may* be somewhat protected, although particle-associated photolysis can occur.	¾ - 1

Table 4. Summary of Information about Photolysis Rates
(values in parentheses indicate a higher degree of uncertainty;
values with question marks are even more uncertain)

Chemical or Group	Level	Information About Photolysis Rates	photolytic resistance (0=vulnerable; 1=relatively invulnerable)
POLYCYCLIC AROMATIC HYDROCARBONS			
Dinitropyrenes	II	• Photolytic degradation of particle-phase nitropyrenes occured with a half-life on the order of 0.5 to 2 hours in a smog chamber experiment, with degradation faster on wood smoke particles than on diesel exhaust particles (possibly because of the promotion of photodecay by methoxyphenols and methoxybenzaldehydes associated with wood smoke) (9)	¼
Benzo (a) Pyrene	I	• Direct photolysis half-life exposed to sunlight in water determined experimentally to be on the order of 1 hour (2); thus atmospheric photolysis may be relatively important • This compound had one of the shortest particle-phase photodegradation half-lives of nine PAH's investigated in a smog chamber experiment — 4 hours under summer conditions and 6 hours under winter conditions (10); however, the conditions were very different from ambient, and extrapolation of these results to the natural atmosphere is difficult.	½
Phenanthrene	II	• Direct photolysis half-life exposed to 313nm light in water determined experimentally to be on the order of 8.4 hours (2); thus atmospheric photolysis may be relatively important • This compound exists largely in the vapor phase	¼
Anthracene	II	• Has somewhat significant absorption peak at 360 nm (2) • Direct photolysis half-life in water determined experimentally to be on the order of 45 minutes for irradiation at 366 nm (2); thus atmospheric photolysis may be relatively important • This compound exists largely in the vapor phase	0 - ¼
Benz (a) Anthracene	II	• Direct photolysis half-life exposed to sunlight in water determined experimentally to be on the order of 3.3 hours (2); thus atmospheric photolysis may be relatively important • This compound had particle-associate photodegradation half-lives approximately twice as long as Benzo(a)Pyrene in smog chamber experiments (10).	½
Perylene	II		½
Benzo (g,h,i) Perylene	II	• This compound had some of the longest particle-phase photodegradation half-lives of nine PAH's investigated in a smog chamber experiment — 10 hours under summer conditions and essentially no decay under winter conditions (10); however, the conditions were very different from ambient, and extrapolation of these results to the natural atmosphere is difficult.	¾
Naphthalene	see note (1)	• Direct photolysis half-life exposed to 313 nm light in water determined experimentally to be on the order of 3 days (2); thus atmospheric photolysis may be somewhat important • This compound exists in the vapor phase	½

Table 4. Summary of Information about Photolysis Rates
(values in parentheses indicate a higher degree of uncertainty;
values with question marks are even more uncertain)

Chemical or Group	Level	Information About Photolysis Rates	photolytic resistance (0=vulnerable; 1=relatively invulnerable)
Chrysene		● Direct photolysis half-life exposed to 313 nm light in water determined experimentally to be on the order of 4.4 hours (2); thus atmospheric photolysis may be relatively important ● This compound (measured together with Benz(a)Anthracene) had mid-range particle-phase photodegradation half-lives in a study of nine PAH's in a series of smog chamber experiments — 6 hours under summer conditions and 12 hours under winter conditions (10); however, the conditions were very different from ambient, and extrapolation of these results to the natural atmosphere is difficult.	¾
Pyrene		● Has a significant absorption peak at 295 nm (2) ● Direct photolysis half-life exposed to 313 and 366 nm light in water determined experimentally to be on the order of 0.68 hours (2); thus atmospheric photolysis may be relatively important ● This compound had mid-range particle-phase photodegradation half-lives in a study of nine PAH's in a series of smog chamber experiments — 6 hours under summer conditions and 8 hours under winter conditions (10); however, the conditions were very different from ambient, and extrapolation of these results to the natural atmosphere is difficult.	½
Dibenz(a,h)anthacene		● Found to have one of the most rapid photodegradation rates of all PAH's tested in an experiment with compounds adsorbed to silica gel (3) ● This compound had mid-to-long particle-phase photodegradation half-lives in a study of nine PAH's in a series of smog chamber experiments — 6 hours under summer conditions and 8 hours under winter conditions (10); however, the conditions were very different from ambient, and extrapolation of these results to the natural atmosphere is difficult.	½
PAH's (as a group)	II		

Table 4. Summary of Information about Photolysis Rates
(values in parentheses indicate a higher degree of uncertainty;
values with question marks are even more uncertain)

Chemical or Group	Level	**Information About Photolysis Rates**	**photolytic resistance** (0=vulnerable; 1=relatively invulnerable)

References and Notes for above Table

(1) Individual compounds added to consider PAH's as a group include: Naphthalene: Acenaphthene; Acenaphthylene; Fluorene; Indeno(1,2,3-c,d)Pyrene; Dibenz (a,h) Anthracene; Benzo(b)Fluoranthene; Benzo (j) Fluoranthene; Benzo(k)Fluoranthene; Benzo(e)Pyrene; Pyrene; Fluoranthene; and Chrysene

(2) Harris, J., 1982: "Aqueous Photolysis," in Handbook of Chemical Property Estimation Methods, edited by Lyman, W., et al. Washington D.C.: American Chemical Society. pp 8-1 to 8-43.

(3) Freitag et al., 1985: "Environmental Hazard Profile of Organic Chemicals," Chemosphere 14(10): 1589-1616.

(4) Information summarized from Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profile for the substance (documents released over several different years; most in 1993-1995)

(5) Schroeder et al., 1991: "Transformation Processes Involving Mercury Species in the Atmosphere — Results from a Literature Survey," Water, Air and Soil Pollution 56: 653-666.

(6) Howard, P.J., et al., 1991: Handbook of Environmental Degradation Rates, Boca Raton FL: CRC Lewis Press

(7) Atkinson, R.,1991: "Atmospheric Lifetimes of Dibenzo-*p*-dioxins and Dibenzofurans," Science of the Total Environment 104: 17-33.

(8) Bunce, N.J., et al., 1991: "A Model for Estimating the Rate of Chemical Transformation of a VOC in the Troposphere by two Pathways: Photolysis by Sunlight and Hydroxyl Radical Attack," Chemosphere 22(3-4):305-315.

(9) Fan, Z, R.M. Kamens, et al. (1996). "Photostability of Nitro-Polycyclic Aromatic Hydrocarbons on Combustion Soot Particles in Sunlight." Environmental Science and Technology **30**(4): 1358-1364.

(10) Pennise, D. M. and R. M. Kamens (1996). "Atmospheric Behavior Of Polychlorinated Dibenzo-P-Dioxins and Dibenzofurans and the Effect Of Combustion Temperature." Environmental Science & Technology **30**(9): 2832-2842. [Note: the high temperature combustion results of this paper were used in providing input to the above table.]

(11) Bidleman (1997) (personal communication)

B.4. Removal of Vapor-Phase Pollutants from the Atmosphere by Wet and Dry Deposition

Vapor-phase pollutants can be removed from the atmosphere by wet or dry deposition.

Wet Deposition of Vapor Phase Material

Unless the compound is relatively water soluble, the removal of vapor-phase material by wet deposition will generally be relatively insignificant, although there may be some exceptions (see below). A qualitative analysis of the "gas-phase washout" phenomenon is presented in Appendix D-1. Estimates were made of the relative importance of this phenomenon for each of the compounds considered in this analysis, based on each compound's estimated Henry's Law constant (a measure of the partitioning between the air and water phases) and the extent to which the compound is expected to exist in the gas phase.

For most of the considered compounds, gas-phase washout is expected to be an insignificant atmospheric removal process (the details are given in Appendix D-1). For one of the compounds -- 4,4'-methylene bis(2-chloroaniline, "MBOCA") — the qualitative analysis suggests that suggests very rapid removal from the atmosphere by rainfall. The analysis also indicated that mercuric chloride ($HgCl_2$), 3,3'-Dichlorobenzidene, pentachlorophenol, and at least some of the hexachlorocyclohexane isomers might be removed relatively rapidly from the atmosphere by rainfall. Interestingly, mercury in precipitation has been found to be correlated with concentrations of chloride ion, suggesting that an important form of mercury in precipitation is $HgCl_2$ (Keeler, Glinsorn, and Pirrono, 1995).

It is likely that the situation regarding gas-phase washout may be more complicated than the simplified screening analysis used here.

For example, this analysis suggested that alpha-HCH and gamma-HCH — predicted by the simplified vapor/particle partitioning theory used here to exist largely in the vapor phase — would not be appreciably washed out by precipitation. However, they are found in significant concentrations in precipitation (e.g., Chan *et al.*, 1994; Hoff *et al.*, 1996). With these compounds, it is not clear if the vapor/particle characterization of this analysis is in error, or, if other factors are contributing to the larger-than-anticipated washout.

Similarly, Ligocki *et al.* (1985ab) found significant apparent gas-phase washout for many somewhat volatile PAH's in experimental measurements, in some cases greater than the measured particle-phase washout efficiencies for the same compounds. While interpretation of these measurements is somewhat difficult[4], they suggest an apparently higher degree of precipitation washout of these compounds than anticipated in this screening analysis.

Finally, chemical reactions may influence the degree to which a pollutant is absorbed into precipitation. For example, elemental mercury — which is believed to be relatively insoluble in water — may be slowly absorbed but then subsequently oxidized (by dissolved ozone or other oxidants) to the more soluble divalent Hg^{+2} in aqueous droplets. This process may result in a relatively significant amount of mercury being incorporated into atmospheric water droplets (which may fall to the earth's surface as precipitation). Alkylated lead compounds may also be affected in this way. Tetraethyl lead and tetramethyl lead are relativlely insoluble, but their atmospheric breakdown products (e.g., triethyl lead^{+1}, trimethyl lead^{+1}) may be highly soluble.

Dry Deposition of Vapor Phase Material

Dry deposition of vapor-phase material can be a relatively significant removal mechanism of pollutants from the atmosphere. At the surface of the earth, substantial quantities of atmospheric pollutants can be adsorbed into soil, vegetation (e.g., Calamari et al., 1991), and surface water. There are many interesting consequences of this phenomenon.

First, gas exchange of some pollutants with lakes can be important to the overall mass balance of the pollutant in the lake. Gas exchange of semivolatile pollutants with the Great Lakes may be a very significant phenomenon, although data to assess its relative importance are scarce (e.g. Hoff et al., 1996). Even if a pollutant is relatively insoluble in water, partitioning to suspended sediment and other organic matter in the water column can allow the transfer of vapor-phase atmospheric pollutants to be thermodynamically possible under certain conditions. There have been several studies that have attempted to estimate the direction and rate of gas exchange of different pollutants with one or more of the Great Lakes. Examples are given in the following table.

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[4]. In these measurements, vapor and particle phase concentrations were measured near the ground, and compared with operationally dissolved and particulate concentrations of the same pollutant in precipitation samples. Since the ground-level concentration of pollutant in the vapor and particle phases is not necessarily the same as that at higher elevations, the significance of washout ratios estimated from such measurements is an issue.

Table 5. Examples and Reviews of Analyses of Gas Exchange with Lakes	
Hoff *et al.* (1996)	a range of compounds measured in the Great Lakes region
Bidleman and McConnell (1995)	review of measurements and analyses
Hoff, Bidleman, & Eisenreich (1993)	toxaphene
Achman, Hornbuckle, & Eisenreich (1993) Jeremiason, Hornbuckle, & Eisenreich (1994) Hornbuckle *et al.* (1995) Honrath, Sweet, & Plouff (1997)	PCB's
Baker & Eisenreich (1990)	PAH's and PCB's
McConnell, Cotham, & Bidleman (1993) Ridal *et al.* (1996)	α-HCH and γ-HCH

Second, the gas-phase adsorption of pollutants into vegetation can be an extremely significant pathway of the pollutant into terrestrial food chains. A significant proportion of the overall exposure of the general population to PCDD/F, for example, is thought to arise largely from consumption of contaminated meat and milk products. The contamination in the meat and milk is believed to be present because of adsorption of vapor-phase PCDD/F into vegetation which is later consumed, for example, by dairy cows and beef cattle.

Third, material adsorbed to soil at the earth's surface may be resuspended as dust particles and contribute to — at least — the ground level atmospheric concentrations of pollution and the apparent ground level deposition of pollution. This phenomenon may at least partly serve to explain the recent findings that dry deposition of PCB's is apparently dominated by very large particles (e.g. Holsen et al., 1991; Lee et al., 1996). A theoretical analysis of this phenomenon in relation to dioxins and furans was recently presented by Kao and Venkataraman (1995). They concluded that while the re-entrainment of dioxin-laden dust particles would probably not contribute more than about 4% of ambient, ground level atmospheric dioxin concentrations, the particles could account for as much as 70 - 90% of the apparent dry deposition in urban areas and as much as 20 - 40% of the apparent dry deposition in rural areas (where the soil concentrations of PCDD/F are lower).

Finally, it has recently been hypothesized that certain compounds might be adsorbed at the earth's surface at a particular location and then re-emitted to the atmosphere at a later time (e.g., when the temperature has increased). This so-called "grasshopper effect" is thought to contribute to a global fractionation of semivolatile compounds, in which some compounds may be (over time) preferentially partitioned to colder climates. The strong, apparent correlation of certain compounds in the atmosphere with ambient temperature (e.g., Hoff et al., 1992a,b) provides evidence that this phenomenon can be important. Discussions and reviews of this phenomenon are given in a series of articles by Wania and Mackay (1993ab, 1995, 1996).

This grasshopper effect is an area of current research, and it is difficult to make quantitative estimates at this time. In the following, a brief discussion will be given, and is considered to be only a preliminary consideration of this phenomenon.

The tendency of a given compound to be subject to this phenomenon will depend, of course, on the detailed nature of the various physical and chemical interactions between the pollutant and different surfaces to which it initially deposits, and on a variety of additional factors (e.g., meteorological conditions, the ability of the compound to survive in the atmosphere during each hop, etc.) The grasshopper effect is believed to be most important for persistent compounds of intermediate volatility. Compounds that are very volatile will not deposit readily, and compounds with very low volatility will be less likely to be revolatilized once they are deposited. It appears that the grasshopper effect may be important for many of the BVES compounds, particularly for many of the compounds in the right-most three columns of Table 2, i.e., the compounds which exist with significant — or predominant — proportions in the vapor phase in the atmosphere.

As discussed by Bidleman et al (1997), some compounds might be considered to be subjected to only a single "hop", in which they are emitted and then deposited, and then are not revolatilized significantly. These compounds would be said not to exhibit the grasshopper phenomenon. Other compounds — which do exhibit the phenomenon — might be considered to be able to undergo multiple hops.

Wania and McKay (1996) have classified compounds into 4 qualitative classes, based on their tendency to be subjected to the grasshopper effect. A first class of compounds are least likely to be subject to the phenomenon, and these include compounds such as PCB's with eight or more chlorines, PCDD/F's with 4 to 8 chlorines, PAH's with 4 or more rings, and mirex. These compounds and those similar to them are believed to only undergo one hop — i.e., once they are deposited, they are not significantly re-emitted. A second class of compounds is capable of several hops, especially in somewhat warm climates, but, ultimately may tend to preferentially deposit in mid-latitude regions. Compounds in this class include PCB's with four to eight chlorines, PCDD/F's with 2 to 4 chlorines, PAH's with 4 rings, toxaphene, DDT's, and chlordanes.[5] A third class of compounds — including penta- and hexachlorobenzene, mono- through tetra-chloro PCB's, 3-ring PAH's, HCH's, and dieldrin — may undergo many hops and ultimately be preferentially deposited in polar regions. A last class of compounds — including chlorobenzenes with 1 to 4 chlorines, monochloro-PCB's, and two-ring PAH's (e.g., naphthalene) — are so volatile that they may not be deposited significantly from the atmosphere. These classes would seem to be a very useful start towards classifying the various BVES compounds with respect to the grasshopper

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[5]. As can be seen, the categories appear to overlap somewhat, with certain classes of compounds. For example, PCDD/F's with 4-8 chlorines are in the first category, and PCDD/F's with 2-4 chlorines are in the second category; thus, it would appear that PCDD/F's with 4 chlorines are in both categories. In fact, different compounds within a given homologue group can exhibit different properties — in this case, for example, different tetrachlorodibenzo-p-dioxin congeners will have different physical-chemical properties, and so, it is possible that group spans two different classes.

phenomenon.

One question that arises is the length of time and distance traveled between hops, or in the case of a single hop-compound, the atmospheric lifetime characteristic of a single hop.

In an attempt to model the long-range transport of PCDD/F's in the U.S. and southern portions of Canada, the dry deposition of vapor phase material was found to be approximately as significant a removal pathway as particle-phase deposition (wet + dry) for 2,3,7,8-TCDD, a compound which exists about equally in the vapor and particle phases in the atmosphere (Cohen et al., 1995). In this example, the atmospheric lifetime of 2,3,7,8-TCDD relative to vapor phase dry deposition can be estimated (very approximately) to have been on the order of one week based on its comparability to particle phase (wet + dry) deposition.[6] That is, the time-scale for a single hop for vapor-phase 2,3,7,8-TCDD appears to have been on the order of one week (for the calculations done in this study).

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[6] **.** As discussed below, a rough estimate of the atmospheric lifetime for particle phase deposition processes (wet + dry) is on the order of 7 - 10 days.

B.5. Removal of Particle-Phase Pollutants from the Atmosphere by Wet and Dry Deposition

Particles in the atmosphere are generally classified into three separate size ranges: the "nucleation range", comprising particles with diameters less than approximately 0.05 µm (1 µm = 1×10^{-6} meters); the "accumulation range", comprising particles with diameters roughly between 0.05 µm and about 2 µm; and the "coarse particle range", consisting of particles with diameters greater than about 2 µm in diameter (e.g., Lodge, 1981; Prospero et al., 1983; Seinfeld, 1986; Pacyna, 1995). Particles in the two smallest ranges are sometimes grouped together in a "fine particle" category.

Particles in the nucleation range are subject to coagulation and incorporation into larger particles; thus, the material contained in them is generally transferred to larger particles, generally in the accumulation range. The time scale for such processes is on the order of hours (Pacyna, 1995). Particles greater than about 10 µm -- generated primarily by mechanical actions and wind erosion -- have relatively fast sedimentation rates, and can be removed relatively quickly by dry deposition from the atmosphere. Typical residence times for such large particles are on the order of a few hours. Particles in the accumulation range, on the order of 1 µm in size, do not efficiently coagulate into larger particles, and do not have large sedimentation velocities. They can be removed by wet and dry deposition processes, but, have atmospheric lifetimes on the order of 7 - 10 days (Pacyna, 1995; Prospero, 1983). Since the fate of nucleation range particles is often to end up quickly incorporated into the accumulation range, the atmospheric lifetime of the *pollutants* associated with these small particles is also on the order of 7-10 days.

Windblown soil particles are often relatively large, and fall into the coarse particle range. However, a fraction of such aerosols are fine particles (e.g., Pacyna, 1995).

Manchester-Neesvig and Andren (1989) used an average residence time for atmospheric particles in the Northern Hemisphere of 6 days in their estimation of the particle-mediated atmospheric lifetime of particle-bound PCB's.

Particles emitted from combustion and incineration processes will generally fall into the fine-particle category. Vapor/particle partitioning is often considered a surface phenomenon, and partitioning to particles is often assumed to scale with particle surface area.[7] That is, when vapor-phase material condenses onto particles, it is considered to do so relatively equally onto each available surface, on a per-area basis. The most significant portion of the surface area available for adsorption is with the fine particles. Thus, for exchangeable, semivolatile compounds that partition between the particle and vapor phases, a significant fraction of their particle-associated mass will lie in the fine-particle range.

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[7] Compounds can also be *absorbed into* semi-liquid organic surface layers around atmospheric particles, and thus vapor/particle partitioning is not strictly a surface phenomenon.

Measurements of the size of particles to which semivolatile compounds in the atmosphere are absorbed are difficult, and many factors can bias the results (e.g., Poster et al., 1995). Examples of attempted measurements of the average particle size in which specific pollutants are found in the atmosphere are summarized in Table 6.

In summary, to the extent that they are associated with particles, the pollutants of this analysis are estimated — on the basis of theoretical and experimental considerations — to exist predominantly in the fine particle range, with sizes less than approximately 2 µm. The atmospheric lifetime of pollution associated with such particles will be highly variable depending on meteorological conditions, source characteristics, and particle characteristics, but, perhaps the average atmospheric lifetime of such particle-associated pollution will be on the order of 1 week. Depending on the meteorological conditions, such particles could travel hundreds to thousands of kilometers in the atmosphere before they are removed by wet or dry deposition processes.

Table 6. Examples of Measured Average Atmospheric Particle Sizes of Selected Pollutants

Note: for pollutants which exist both in the vapor and particle phase,
the measurements generally refer to the particle phase only

Pollutant	**Atmospheric Particle Size Information**	**References Notes**
Metals and Metallic Compounds		
Cadmium	• The mass-weighted average particle size in the atmosphere was estimated to be approximately **0.84 µm**, based on a number of ambient measurement studies.	(1)
Organic Biocides		
DDT / DDE	• At ambient temperatures between 267 and 275 °K, 73-88% of atmospheric DDT and 18-41% of atmospheric DDE was found in the particle phase in measurements at the University of Bayreuth, Germany (Kaupp and Umlauf, 1990). The concentration of DDT and DDE in the atmosphere ranged from 24-74 and 6.2-11 pg/m3, respectively. **Particulate-associated DDT and DDE was largely found on particles less than 1 µm in diameter.**	(3)
Polychlorinated Dibenzo-*p*-Dioxins and Dibenzofurans (PCDD/F's)		
PCDD/F's	• Three samples collected in a rural area • PCDD/F found in both vapor-phase and particle-phase • Approximately 90% of particle-phase PCDD/F's found on particles less than 1.35 µm in diameter; • Approximately 50 - 60% of the particle-phase PCDD/F's found on particles less than 0.45 µm in diameter; • Smaller particles tended to have higher concentrations of PCDD/F's than bigger particles, consistent with a surface-area-related partitioning phenomena.	(4)
Polychlorinated Biphenyls (PCB's)		
PCB's	• five samples collected; • average results given in paper for dichloro-, trichloro-, tetrachloro-, pentachloro-, hexachloro-, heptachloro-, and octachloro-PCB's, and for total PCB's; • there were differences among the different homologue groups, but, the results can be summarized as follows: • approx. 38 - 52% of particle-phase PCB's found on particles < 1 µm diameter; • approx. 46 - 67% of particle-phase PCB's found on particles < 2.5 µm diameter; • approx. 80 - 93% of particle-phase PCB's found on particles < 10 µm diameter; • approx. 98 - 99.9% of particle-phase PCB's found on particles < 25 µm diameter; • The particle size distribution of particle-associated PCB's in the atmosphere appeared to be bimodal, with a peak in the fine mode at particle diameters	(5)

Table 6. Examples of Measured Average Atmospheric Particle Sizes of Selected Pollutants

Note: for pollutants which exist both in the vapor and particle phase,
the measurements generally refer to the particle phase only

Pollutant	Atmospheric Particle Size Information	References Notes
Polycyclic Aromatic Hydrocarbons (PAH's)		
Fluoranthene	• 95% of particle-phase material found on particles ≤ 1.7 μm • 55% of particle-phase material found on particles ≤ 0.49 μm	(2)
Pyrene	• 96% of particle-phase material found on particles ≤ 1.7 μm • 61% of particle-phase material found on particles ≤ 0.49 μm	(2)
Benz(a)Anthracene	• 97% of particle-phase material found on particles ≤ 1.7 μm • 58% of particle-phase material found on particles ≤ 0.49 μm	(2)
Chrysene	• 96% of particle-phase material found on particles ≤ 1.7 μm • 57% of particle-phase material found on particles ≤ 0.49 μm	(2)
Benzo(b) Fluoranthene	• 96% of particle-phase material found on particles ≤ 1.7 μm • 50% of particle-phase material found on particles ≤ 0.49 μm	(2)
Benzo(k) Fluoranthene	• 97% of particle-phase material found on particles ≤ 1.7 μm • 56% of particle-phase material found on particles ≤ 0.49 μm	(2)
Benzo(e)pyrene	• 96% of particle-phase material found on particles ≤ 1.7 μm • 55% of particle-phase material found on particles ≤ 0.49 μm	(2)
Benzo(a)pyrene	• 95% of particle-phase material found on particles ≤ 1.7 μm • 23% of particle-phase material found on particles ≤ 0.49 μm	(2)
Indeno(1,2,3-cd) pyrene	• 98% of particle-phase material found on particles ≤ 1.7 μm • 61% of particle-phase material found on particles ≤ 0.49 μm	(2)
Benzo(g,h,i) perylene	• 97% of particle-phase material found on particles ≤ 1.7 μm • 59% of particle-phase material found on particles ≤ 0.49 μm	(2)

References:

(1) Milford and Davidson (1985)

(2) Poster, Hoff, and Baker (1995) ... Ambient size-segregated sample at Egbert, Ontario, February 8, 1993; rural location. Similar results found in an urban-area sample in Chicago, Illinois, in the same study.

(3) Kaupp and Umlauf (1990) ... At ambient temperatures between 267 and 275 °K, 73-88% of atmospheric DDT and 18-41% of atmospheric DDE was found in the particle phase in measurements at the University of Bayreuth, Germany (considered to be a rural location by the authors). The concentration of DDT and DDE in the atmosphere ranged from 24-74 and 6.2-11 pg/m3, respectively.

(4) Kaupp, Towara, and McLachlan (1994) ... Three samples with mean ambient temperatures from 17.4 - 21.9 °C. Samples taken at the University of Bayreuth, Germany (a rural location).

(5) Lee et al., 1996 ... Tainan City, Taiwan

C. Empirical Evidence of Long Range Transport

There are many uncertainties in our understanding of the fate and transport of pollutants in the atmosphere. Even for compounds that have been the subject of numerous investigations (e.g., PCB's), there are numerous uncertainties that make an extremely accurate estimate of their atmospheric behavior difficult. For many of the compounds considered in this analysis, the lack of data on physical-chemical properties and/or the lack of extensive measurement in the atmosphere make such estimates even more difficult.

Given this situation, another approach to evaluating the long range atmospheric transport of a given compound is to consider various types of empirical evidence.

Perhaps the most straightforward measure of a substance's potential to be transported long distances in the atmosphere is the extent to which it is found in remote locations, far removed from any sources. If the pollutant is found at such remote sites at significant levels in the atmosphere, in atmospheric deposition (e.g., precipitation), or in vegetation, then it can be generally concluded that the pollutant in question reached these sites as a result of long-range atmospheric transport. Measured concentrations in fish, terrestrial animals and humans can be more difficult to interpret, as other (non-atmospheric) exposure pathways may be important (e.g., ocean circulation). Recent reviews of this phenomenon include those by Barrie et al. (1992), Wania and Mackay (1996), and Kurtz (1990).

Another, perhaps less straightforward, type of empirical evidence is the relative concentrations of a given compound in places which are very distant from one another. If the concentration in the air, in precipitation, or in vegetation is very similar in several widely separated locations, or, follows consistent patterns (e.g., a latitudinal pattern in which temperature effects appear to play a significant role), then this is evidence that there is a widespread distribution of the compound in the atmosphere. Thus, for example, the fact that the level of hexachlorobenzene in the air is relatively constant — at concentrations on the order of 100 pg/m^3 — from location to location in ambient air measurements around the world (e.g., Wania and Mackay, 1993; Risebrough, 1990; Gatz et al., 1994; Oehme, 1991) suggest that the distribution of HCB is essentially global.

The fact that similar concentrations might be found in diverse locations does not necessarily mean that long range air transport is occurring, however. Such a finding might simply be an indication that the source strengths are similar in each area. Such a situation might be the case, for example, for pentachlorophenol (PCP). It is widely used as a wood preservative, and can volatilize to the air from treated wood. PCP was recently measured in pine needles[8] at seventeen different locations in Saskatchewan,

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[8]. The dominant pathway by which PCP enters pine needles is through the air. Thus, measurements of the concentrations of PCP in pine needles gives information about the levels in the atmosphere.

Canada (Thompson and Treble, 1995). Fifteen of the samples were taken in various locations in the city of Regina, and two samples were taken sites relatively far away (Saskatoon, a city 250 km northwest of Regina, and Yellowgrass, a rural community 80 km southeast of Regina). Similar concentrations of PCP were found in pine needles at all locations. The similarity of the samples *could* be indicative of widespread PCP distribution resulting from long-range atmospheric transport. However, the similarity could also simply be the result of widespread emissions of PCP resulting from its ubiquitous use a wood preservative.

By the same token, when there *are* large spatial variations in environmental concentrations, this does not prove that long range atmospheric transport is *not* occurring. One can imagine a case where relatively strong local sources create moderate or even intense local concentration gradients, and these local contributions are superimposed onto a regional, continental, or global “background” resulting from widespread atmospheric dispersal. This may well be the case, for example, for polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/F’s). There are many sources of these compounds, including many strong point sources. Certainly, in the vicinity of a strong source, the environmental concentrations may be found to be relatively high. However, if the source did not exist, the concentrations would not be “zero” — long range transport from other locations will almost certainly contribute to environmental levels at the given site.

In sum, the interpretation of the degree of spatial variability as providing evidence for or against long-range atmospheric transport of a given pollutant depends on spatial variability of the pollutant’s sources.

Examples of empirical evidence supporting (or not supporting) long range atmospheric transport for compounds considered in this analysis are given in Table 7. For some of the compounds, empirical evidence was not found.

Table 7. Examples of Empirical Evidence for Long Range Atmospheric Transport

Chemical or Group	Level (b)	Examples of studies which have found compound in remote areas, i.e., areas believed to be distant from any source of the particular compound
METALS / ORGANOMETALLICS		
Alkylated Lead	I	• Lobinski et al. (1994a) found diethyl, triethyl, dimethyl, and trimethyl lead compounds in fresh Greenland snow. Tetraethyl and tetramethyl lead were at or below detection limits. The authors suggest that the atmospheric lifetime of diethyl and triethyl lead compounds may be longer than predicted based on laboratory experiments. Organolead is enriched over inorganic lead in long range atmospheric transport, suggesting that organolead compounds are longer-lived in the atmosphere than inorganic lead compounds. • Lobinski et al. (1994b) found diethyl and triethyl lead compounds in Greenland snow cores; these are atmospheric breakdown products of tetraethyl lead, and may be longer- lived in the atmosphere. The levels of diethyl and triethyl lead compounds found appeared to account for the total amount of organolead in the samples, which was also measured. This suggests that significant quantities of tetraethyl were not present. No methyl-lead compounds were found.
Mercury	I	• Landers et al., 1995 (U.S. Arctic)
Cadmium	II	• Davidson et al., 1981(Greenland) cadmium found in wet deposition • Cheam et al., 1996 (Canadian Arctic snow) • Boutron et al., 1995, measured the trends of Cd in Greenland snow and ice cores, for the period from 1750 to the present. The concentration of Cadmium rose by a factor of about 5 between 1750 and the mid-1960's. Between the mid-1960's and the early 1990's, the concentration of Cd in the snow had decreased by a factor of about 2.5 • Ford et al., 1995, measured cadmium levels in vegetation (moss) in the U.S. Arctic. They found highly variable levels between different sites. The authors stated an opinion that long-range atmospheric transport of cadmium was not important.
Tributyltin	II	
ORGANOCHLORINE BIOCIDES		
Aldrin	I	
Dieldrin	I	• Atlas & Giam, 1981; Atlas & Schauffler, 1990 (atmosphere above the North Pacific Ocean) • Bidleman et al., 1990a (Canadian Arctic)
DDT	I	• Calamari et al, 1991 (Antarctic, etc.) • Bidleman et al., 1990a (Canadian Arctic)
DDD	I	
DDE	I	• Atlas & Giam, 1981 (atmosphere above the North Pacific Ocean) • Calamari et al., 1991 (Antarctic, etc.)
Mirex	I	
Toxaphene	I	• Bidleman et al., 1990a (Canadian Arctic)
Endrin	II	
Heptachlor	II	
Heptachlor Epoxide	II	• Welch et al., 1991 (Canadian Arctic)

Table 7. Examples of Empirical Evidence for Long Range Atmospheric Transport

Chemical or Group	Level (b)	Examples of studies which have found compound in remote areas, i.e., areas believed to be distant from any source of the particular compound
α-Hexachlorocyclohexane	II	● Atlas & Giam, 1981 (atmosphere above the North Pacific Ocean) ● Calamari et al., 1991 (Antarctic, etc.) ● Bidleman et al., 1990a (Canadian Arctic)
β-Hexachlorocyclohexane	II	
δ-Hexachlorocyclohexane	II	
γ-Hexachlorocyclohexane (Lindane)	II	● Atlas & Giam, 1981 (atmosphere above the North Pacific Ocean) ● Calamari et al., 1991 (Antarctic, etc.) ● Bidleman et al., 1990a (Canadian Arctic)
Methoxychlor	II	● Welch et al, 1991 (Canadian Arctic)
Pentachlorophenol	II	
INDUSTRIAL / MISCELLANEOUS		
Octachlorostyrene	I	
3,3'-Dichloro-benzidene	II	
4,4'-Methylene bis (2-Chloroaniline)	II	
4-Bromophenyl Phenyl Ether	II	
Hexachloro-1,3-Butadiene	II	● Class & Ballschmiter, 1986
CHLOROBENZENES		
1,4-dichlorobenzene	II	
Tetrachlorobenzenes	II	● Atlas & Schauffler, 1990 (atmosphere above the North Pacific Ocean) (1234 & 1245 TCB measured)
Pentachlorobenzene	II	● Atlas & Schauffler, 1990 (atmosphere above the North Pacific Ocean)
Hexachlorobenzene	I	● Atlas & Giam, 1981; Atlas & Schauffler, 1990 (atmosphere above the North Pacific Ocean) ● Calamari et al., 1991 (Antarctic, elsewhere) ● Bidleman et al., 1990a (Canadian Arctic)
POLYCHLORINATED DIBENZO-P-DIOXINS AND DIBENZOFURANS (PCDD/F'S)		
PCDD/F's (as a group)	I	● Rappe et al. (1989) and Tysklind et al. (1993) compared measured atmospheric concentrations of PCDD/F at locations in Sweden to modeled back-trajectories of the air masses sampled, and found evidence that long-range atmospheric transport of these compounds was occurring. ● Grundy et al. (1995) found relatively high levels of PCCD/F in soils around military installations in the Canadian arctic, and found lower, but detectable concentrations in "pristine" areas, at least 20 km away from any human activity
POLYCHLORINATED BIPHENYLS (PCB'S)		

Table 7. Examples of Empirical Evidence for Long Range Atmospheric Transport		
Chemical or Group	**Level (b)**	**Examples of studies which have found compound in remote areas, i.e., areas believed to be distant from any source of the particular compound**
PCB's (as a group)	I	● Barrie et al., 1992 ● Bidleman et al., 1990a (Canadian Arctic) ● Atlas & Giam, 1981; Atlas & Schauffler, 1990 (atmosphere above the North Pacific Ocean) ● Bright et al. (1995) found relatively high levels of PCB's in soils around military installations in the Canadian arctic, and found lower, but detectable concentrations in "pristine" areas, at least 20 km away from any human activity; the pristine samples were enriched in lower chlorinated congeners, consistent with long-range transport considerations
POLYCYCLIC AROMATIC HYDROCARBONS		
Dinitropyrenes	II	● Gibson et al. (1986) found nitro-PAH's in remote areas (as cited in Bidleman et al., 1990b)
Benzo (a) Pyrene	I	● Daisey et al., 1981 (U.S. Arctic) ● Jaffrezo et al., 1994 (Greenland snow) ● Knulst et al., 1995, did find this PAH in about half of the samples of humus and moss analyzed from background sites in Sweden; in the other half, the levels were below the detection limit
Phenanthrene	II	● Daisey et al., 1981 (U.S. Arctic) ● Jaffrezo et al., 1994 (Greenland snow) ● Knulst et al., 1995, did find this PAH in humus and moss in background sites in Sweden
Anthracene	II	● Daisey et al., 1981 (U.S. Arctic) ● Knulst et al., 1995, did not, however, find this PAH in humus and moss at background sites in Sweden
Benz (a) Anthracene	II	● Jaffrezo et al., 1994 (Greenland snow) ● Knulst et al., 1995, did find this PAH in humus and moss in background sites in Sweden
Perylene	II	● Daisey et al., 1981 (U.S. Arctic) ● Knulst et al., 1995, did not, however, generally find this PAH in humus and moss in background sites in Sweden; it was not detected in any of 11 humus samples, and was only detected in 1 of 11 moss samples.
Benzo (g,h,i) Perylene	II	● Daisey et al., 1981 (U.S. Arctic) ● Jaffrezo et al., 1994 (Greenland snow) ● Knulst et al., 1995, did find this PAH in humus and moss at most background sites in Sweden
PAH's added to ANALYZE as a GROUP(see note a)		● Daisey et al., 1981 (U.S. Arctic): fluoranthene, pyrene, chrysene, benzo(e)pyrene ● Jaffrezo et al., 1994 (Greenland snow): naphthalene, fluoranthene, pyrene, chrysene, benzo(b)fluoranthene, benzo(k)fluoranthene ● Knulst et al., 1995, found the following PAH's in humus and moss in background sites in Sweden: Indeno(1,2,3-c,d)Pyrene, Dibenz (a,h) Anthracene; Benzo (bjk) Fluoranthenes (b+j+k combined), Fluoranthene, Benzo (e) Pyrene, Pyrene, and Chrysene ● Knulst et al., 1995, did **not** find the following PAH's in humus and moss in background sites in Sweden: Naphthalene, Acenaphthene, Acenaphthylene, Fluorene

Table 7. Examples of Empirical Evidence for Long Range Atmospheric Transport

Chemical or Group	Level (b)	Examples of studies which have found compound in remote areas, i.e., areas believed to be distant from any source of the particular compound
PAH's (as a group)	II	• Daisey et al., 1981, found PAH's in the Arctic aerosol at Barrow, Alaska and attributed their presence to long range atmospheric transport (and, for some PAH's, possibly to local sources as well) • Bidleman et al., 1990b cite several studies which have demonstrated the long range atmospheric transport of PAH's. • Welch et al., 1991, found elevated levels of high molecular weight PAH's in lake sediments in the Canadian Arctic, and concluded that the source was probably long-range atmospheric transport. • Atlas & Schauffler (1990) found only very low concentrations of PAH's in the atmosphere above the North Pacific Ocean, and cite other examples in the literature suggesting a rapid fall off in atmospheric concentration with distance from the source. Nevertheless, differences in concentrations observed could be at least partially explained by a consideration of air-mass back trajectories, with the highest concentrations of PAH's found when the air mass had traversed source regions. While organochlorine levels generally had similar values to other studies over marine sites in the Northern Hemisphere, the PAH concentrations found by Atlas & Schauffler were much lower than found in other studies. This led the authors to suggest that the atmospheric stability of PAH's is less than that of most organochlorines. • Jaffrezo et al., 1994, found PAH's in ice cores in Greenland • Knulst et al., 1995, found relatively non-volatile PAH's in humus and moss in background sites in Sweden; relatively volatile PAH's were **not** found (e.g., Naphthalene, Acenaphthene, Acenaphthylene, Fluorene, Anthracene) • Aamot et al., 1996, found the geographical pattern of 4 and 5 ring PAH's in Norwegian forest soils to be consistent with long range atmospheric transport

Abbreviations and Notes for above Table

(a) Individual compounds added to consider PAH's as a group included: Naphthalene (Naph): Acenaphthene (Acn); Acenaphthylene (Acl); Fluorene (Flr); Indeno(1,2,3-c,d)Pyrene (IPyr); Dibenz (a,h) Anthracene (dBA); Benzo (b) Fluoranthene (BbF); Benzo (j) Fluoranthene (BjF); Benzo (k) Fluoranthene (BkF); Benzo (e) Pyrene (BeP); Pyrene (Pyr); Fluoranthene (Fln); and Chrysene (Chr)

(b) "Level" refers to the compounds assignment in the Binational Virtual Elimination Strategy as a Level I or Level II compound; it does not refer to its capability or evidence for long-range air transport [see Table 1]

D. Synthesis and Summary of Information Regarding the Potential for Long Range Atmospheric Transport of Substances

For each compound or group of compounds considered in this analysis, the various atmospheric removal mechanisms discussed above will play a greater or lesser role, depending on the physical-chemical properties of the pollutant in the atmosphere. In the real world, all of the processes are happening simultaneously, and the pollutants are subjected to movement in the atmosphere due to convective and diffusive processes. For a given parcel of air containing a given pollutant, the factors governing atmospheric fate and transport will vary from moment to moment, i.e., temperature, concentration of reactive species, atmospheric aerosol, humidity, precipitation intensity, intensity of solar radiation and other factors will change continuously throughout a pollutant's atmospheric lifetime. The changing factors are frequently interrelated. For example, during a warm summer day, the temperature may favor a particular compound (e.g., 2,3,7,8-TCDD) existing more in the vapor phase, where it is more vulnerable to chemical reaction and photolytic breakdown. During the winter, the same pollutant might be more associated with particles and somewhat protected from such destruction.

Because of the complicated interrelationships, these various factors generally combine in non-linear ways. In this analysis, the various fate and transport mechanisms have been treated, more or less, in isolation, although, in a crude way, an attempt was made to include the effect of vapor/particle partitioning in the consideration of various removal mechanisms. Ultimately, a useful exercise is to combine a mathematical description of all of the fate and transport processes together, and attempt to *model* the fate of pollutants emitted to the atmosphere. To the extent that the relevant physical and chemical processes are understood and have been adequately characterized, modeling can be a useful way to develop more accurate estimates of atmospheric fate and transport. Models need to be connected, of course, to experimental, real-world data in at least two ways. First, a wide range of experimental data will generally need to be considered in the formation of the basic theoretical and/or empirical characterizations of environmental phenomena. Second, to the greatest extent possible, validation tests of the model components and of the overall model — based on real-world measurements — should be carried out.

This analysis has not included quantitative, integrated modeling in its scope, due to time limitations. Instead, a qualitative approach to the assessment of long-range atmospheric transport has been taken. In this approach, pollutants have been generally categorized as to the relative importance of various fate mechanisms.

It must be stated that for some compounds, the grasshopper effect may substantially increase the ultimate distance that the pollutant can travel in the atmosphere. Secondly, the rates of reaction with hydroxyl radical used in this screening level approach may underestimate the atmospheric lifetime for transport to remote northern regions. Thus, it is likely that for some compounds, the rough estimates made here represent a lower-bound estimate of the potential extent of atmospheric transport.

A basic question arises regarding the extent of transport that might be expected in a particular atmospheric lifetime. That is, if a compound is expected to have a lifetime of approximately 1 week, how far will it typically be able to travel in that time? Obviously, the travel length will depend on the time and location of the pollutant emission, as the meteorological parameters that influence atmospheric transport vary substantially in space and time. One estimate of mean atmospheric transport velocities gives a value of 480 km/day for one day, and 310 km/day for five days (Summers and Young, 1987). Dennis *et al.* (1996) use an average transport velocity of 4 meters/sec (~ 350 km/day) to provide an overall estimate of the spatial scale of transport of atmospheric pollutants. Using the "average" value of 4 meters/sec, the following transport distances are estimated:

Table 8. Approximate Atmospheric Transport Distances Associated with Given Atmospheric Transport Times

transport time	transport distance (km) assuming 4 meters/sec average atmospheric transport velocity
1 minute	0.24
10 minutes	2.4
1 hour	14
10 hours	140
1 day	350
2 days	700
1 week	2,400
2 weeks	4,800
1 month	10,500
3 months	31,000
1 year	125,000
2 years	250,000

The numbers in the above table are obviously just rough, average estimates, and the behavior at any given time and location for a particular pollutant might be much different from these values. For example, under conditions of very calm, stagnant meteorological conditions, a pollutant may stay in the same general location for days. Under very windy conditions, a pollutant might be moved much greater distances than shown in the above table.

Based on these considerations, an attempt has been made to qualitatively estimate the atmospheric lifetimes of each of the pollutants considered in this analysis. A "Long Range Air Transport Potential" rating scale of 1-4 is defined as follows:

- Rating = 1 The pollutant is extemely long-lived in the atmosphere, with an atmospheric lifetime of on the order of a year or longer; distribution of the pollutant will be global. With the rough distance estimates above, a compound being transported at an average velocity of 4 meters per second for one year will travel on the order of 125,000 km, about three times the circumference of the earth. *Some* of the compounds in this class will likely be experience the grasshopper effect, and undergo many hops, while *some* may be so volatile that they are not significantly deposited.

- Rating = 2 The pollutant is relatively long-lived in the atmosphere, with atmospheric residence times on the order of at least a week to perhaps several months; long range transport can definitely occur over 1000's to 10,000's of kilometers. Using the above rough transport distance estimates, this class of compound could travel on the order of 2,000 - 20,000 km from the source, on average. At the high end of this range, a transport distance of 20,000 km means the distribution will be virtually global. *Some* of the compounds in this class will likely be experience the grasshopper effect, and undergo many hops, while *some* may be so volatile that they are not significantly deposited.

- Rating = 3 The pollutant is relatively short-lived in the atmosphere, with atmospheric residence times on the order of several hours to a few days; atmospheric transport may occur on regional, mesoscale distances. Using the above rough transport distance estimates, this class of compound could travel on the order of 30 - 1000 km from the source, on average. Since the atmospheric lifetime for these compounds may be shorter than the characteristic time of a grasshopper effect "hop", many of these compounds may not exhibit this phenomenon — i.e., they may not survive long enough (on average) in the atmosphere to make it through even their "first" hop.

- Rating = 4 The pollutant is extremely short-lived in the atmosphere, with atmospheric residence times on the order of seconds to minutes to at most an hour or so; with such pollutants, atmospheric transport of emissions will be limited to the local region around the source. Using the above rough transport distances, one could say that compounds in this class would be limited, on average, to transport within a local area within 0.1 - 10 km from the source. Certainly for these compounds, it is unlikely that any will survive long enough (on average) in the atmosphere to make it through even one hop and so, it is unlikely that any of them will participate in the grasshopper effect.

This qualitative categorization and rating scheme is summarized in Table 9.

In Table 10, the information relevant to the Long Range Air Transport Potential is summarized for each compound or group of compounds considered, and an estimate of the overall rating is made for each.

Table 9. Types of Atmospheric Pollutants, With Particular Attention to the Properties that Influence Long Range Transport and Potential Deposition

L.R.T. Rating	Phase	Volatility	Reactivity and/or Photolytic Degradability	Henry's Law Rainout Potential	Particle Size	Atmospheric Fate	Approximate Atmospheric Lifetime	Examples
1	vapor	very volatile	minimally reactive	minimally soluble		may not be deposited significantly from the atmosphere to the Great Lakes because compound is relatively volatile	~ months to years	Hexachloro-1,3-butadiene
4			very reactive			atmospheric lifetime on the order of seconds, minutes, or hours; thus, unlikely to be transported long distances	~ minutes to hours	Aldrin
3				very soluble		vulnerable to rain washout, but since rain is sporadic, will probably have lifetime on the order of a week — capable of being transported moderately long distances	~ 1-2 weeks	3,3'-Dichlorobenzidene
1		semi-volatile	minimally reactive	minimally soluble		capable of being transported extremely long distances in the atmosphere; may undergo the grass-hopper effect.	~ 1 year or longer	Hexachlorobenzene
2	vapor/ particle: exchangeable	semi-volatile	minimally reactive		full range	capable of being transported long distances in the atmosphere; grass-hopper effect will likely extend transport distances considerably.	~ weeks to months	PCB's (esp. with, e.g., 4-8 chlorines)
3			moderately reactive		full range	may be somewhat protected from reaction and photolytic degradation when on particles; when in vapor phase, more vulnerable; capable of being transported moderately long distances; grass-hopper effect may extend transport distances, but compounds may undergo substantial degradation during each hop.	~ days	2,3,7,8-TCDD
4	particle				large	large particle lifetimes relatively short; thus potential for long range atmospheric transport is generally low	~ minutes to hours	pollutants associated with *portions* of windblown dust
2					small	small particle lifetimes are moderately long, on the order of 1-2 weeks; thus, there is a potential for long range atmospheric transport	~ 1-2 weeks	Cadmium emissions from incineration
3-4			reactive			particle phase reactions degrade compounds relatively quickly; reduced potential for long range transport, even on small particles	~ hours to days	PAH's on wood smoke particles

Table 10. Overall Summary of Compounds Considered in this Evaluation

(See Notes Following Table for Column Descriptions, Codes Used, and Other Information)

Chemical or Group ↓	Level	Is the Atmosphere a Potentially Important Transport Pathway?		Long Range Atmospheric Transport Potential							
				Assessment of Factors Influencing Fate and Transport in the Atmosphere						L.R.T. Evi-dence	Overall L.R.T. Rating
		Emitted to the Air?	Measured / Found in Atm?	Phase in Atm	Resistant to Gas Rxn?	Photolytic Resistance	Gas Washout Resistance?	[2] Small Particles in Atm?	Avg Atm Lifetime	Measured / Found in Remote Areas?	LRT Potential (Rating)
COLUMN # --> (1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)
METALS / ORGANOMETALLICS											
Alkylated Lead	I	1	1	(V V)	(½)	?	(½)	(1)	(1 wk)	1	2
Mercury	I	1	1	v	1	1	¾ (?)	(1)	(1 yr)	1	1
Cadmium	II	1	1	P P	1	1	1 (?)	1	(1 wk)	1	2
Tributyltin	II	?	?	v/p	0	1	1	~ 1 (?)	?	?	(3 ?)
ORGANOCHLORINE BIOCIDES											
Aldrin Dieldrin	I I	1 1	1 1	V V V V	0 ¼	(½) (½)	1 1	- -	<1 day 1 day	? 1	3 - 4 3
DDT DDD DDE	I I I	1 1 1	1 1 1	v/p v/p v/p	½ ½ ¼	1 (½) ½	1 1 1	1 1 1	(1 wk) (1 wk) (1 wk)	1 ? 1	2 2 2
Mirex	I	1	½	(V V)	1	1	1	-	>1wk?	?	2
Toxaphene	I	1	1	v/p	½	1	1	½ - 1	1 wk	1	2
Endrin	II	1	1	V V	0	½	1	-	1 day	?	3
Heptachlor Heptachlor Epoxide	II II	1	1	V V V V	0 ½	½ 1	1 1	- -	<1 day 3 days	? 1	3 - 4 3
α-Hexachlorocyclohexane β-Hexachlorocyclohexane δ-Hexachlorocyclohexane (Lindane) γ-Hexachlorocyclohexane	II II II II	1 1 1 1	1 1 1 1	V V V V V V v	1 1 1 1	(¾ -1) ¾ -1 (¾ -1) 1	(½-¾) (½-¾) (½-¾) (½-¾)	- - - (1)	1 mo? 1 mo? 1 mo? 1 mo?	1 ? ? 1	2 2 2 2
Methoxychlor	II	1	1	v/p	¼	1	1	(1)	2 days	1	3
Pentachlorophenol	II	1	1	V V	1	¼	¾ -1	-	1 wk	?	2
INDUSTRIAL / MISCELLANEOUS											
Octachlorostyrene	I	1	1	v	¾	(1) ?	1	(1)	>1wk?	?	2
3,3'-Dichlorobenzidene	II	½	?	v/p	½	¼ - ½	½	(1) (?)	1 wk	?	2
4,4'-Methylene bis (2-Chloroaniline)	II	1	1	v	0	?	0	(1) (?)	<1 day	?	3 - 4
4-Bromophenyl Phenyl Ether	II	~ 1	?	V V	¼	?	1	-	2 days	?	3
Hexachloro-1,3-Butadiene	II	1	1	V V	1	(1)	1	-	1 yr	1	1

Table 10. Overall Summary of Compounds Considered in this Evaluation

(See Notes Following Table for Column Descriptions, Codes Used, and Other Information)

		Is the Atmosphere a Potentially Important Transport Pathway?		**Long Range Atmospheric Transport Potential**							
				Assessment of Factors Influencing Fate and Transport in the Atmosphere						L.R.T. Evidence	**Overall L.R.T. Rating**
Chemical or Group ↓	Level	Emitted to the Air?	Measured / Found in Atm?	Phase in Atm	Resistant to Gas Rxn?	Photolytic Resistance	Gas Washout Resistance?	~Small Particles in Atm?	Avg Atm Lifetime	Measured / Found in Remote Areas?	LRT Potential (Rating)
COLUMN # --> (1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)
CHLOROBENZENES											
1,4-dichlorobenzene	II	1	1	V V	1	1	1	-	1 mo	?	2
Tetrachlorobenzenes	II	1	1	V V	1	1	1	-	4 mo	1	1
Pentachlorobenzene	II	1	1	V V	1	1	1	-	6 mo	1	1
Hexachlorobenzene	I	1	1	V V	1	1	1	-	2 yrs	1	1
POLYCHLORINATED DIBENZO-*p*-DIOXINS & DIBENZOFURANS (PCDD/F'S)											
PCDD/F's	I	1	1	v/p	1	½	1	1	(1 wk)	(½)	2
POLYCHLORINATED BIPHENYLS (PCB'S)											
PCB's	I	1	1	v/p	½ - 1	¾ -1	1	½	(1 wk)	1	2
POLYCYCLIC AROMATIC HYDROCARBONS											
Dinitropyrenes	II	1	1	v/p	?	½	1	(1)	(1 wk)	(1)	2
Benzo [a] Pyrene	I	1	1	p	½	½	1	(1)	(1 wk)	(1)	2
Phenanthrene	II	1	1	(V V)	¼	¼	½	(1)	(1day)	1	3
Anthracene	II	1	1	V V	0	0 - ¼	½	(1)	(1day)	½	3
Benz [a] Anthracene	II	1	1	v/p	¼	½	½	(1)	(1 wk)	1	2
Perylene	II	1	1	p	½	(½)	1	(1)	(1 wk)	(½)	2
Benzo [g,h,i] Perylene	II	1	1	p	½	(¾)	1	(1)	(1 wk)	1	2
PAH's (as a group)	II	1	1	v/p	0 - 1	½	1	(1)	(1 wk)	(½ - 1)	2

Codes and Notes for Table 10

A. Some General Features of the Table, common to some or all columns

- In columns 3 through 9, and column 11, as described in detail below, an entry of "1" indicates that, all things being equal, the compound or group is expected to be capable of being transported for long distances in the atmosphere; in other words, *this particular factor does not appear to rule out long range atmospheric transport.*

- In these same columns, as described below, an entry of "0" indicates that the particular factor significantly limits the atmospheric lifetime of the compound in the atmosphere, making long range atmospheric transport unlikely. *Thus, if there is a "0" in any of the columns 3 - 9 or 11, then this suggests that long range atmospheric transport is not expected to be significant for the compound or compound group.*

- Again, in these same columns, as described below, an entry of "¼" or "½" or "¾" suggests that the particular factor has an intermediate significance, placed between the two extremes of "1" and "0"

- a dash, "-", indicates that the factor is not applicable.

- an entry in parentheses -- e.g., "(1)" -- indicates that an educated guess is being made and that the estimate is *relatively* uncertain.

- a question mark — "?" — as an entry means that the piece of information might be relevant, but, no information could be found. If an estimate is provided, it is *very* uncertain

B. Descriptions of Columns in Table 1

(1) **Chemical or Group:**

Many of the "chemicals" on this list are really groups of chemicals. In these cases, an overall evaluation of the group was attempted.

(2) **Level:**

Level I Substances are the 11 Critical Pollutants identified by the IJC's Great Lakes Water Quality Board, plus one additional Critical Pollutant identified by the Lake Superior LaMP and the Lake Ontario Toxics Management Plan (Octachlorostyrene). Note: Chlordane was also an additional Critical Pollutant identified, but it was not included on the target list for this analysis.

Level II Substances are those substances identified by the Canada-Ontario Agreement respecting the Great Lakes Basin Ecosystem (COA) as "Tier II" chemicals, plus additional substances of concern identified by LaMP and RAP processes and the Great Lakes Water Quality Guidance in the U.S.

(3) **Emitted to the Air?:**

0 = Pollutant is not considered be emitted to the air in potentially significant quantities.

1 = Pollutant is considered to be emitted to the air in potentially significant quantities.

(4) Measured / Found in Atm?:

1 = Attempt(s) have been made to measure the compound in the atmosphere, and it has been found in at least some of the measurements

0 = Attempt(s) have been made to measure the compound in the atmosphere, and it is never or rarely found

(5) Phase in Atm:

P P = Compound is expected to exist almost entirely in the particle phase in the atmosphere (fraction adsorbed ≥ 98% under all conditions)

p = Compound is expected to exist mostly in the particle phase in the atmosphere (fraction adsorbed ≥ 90% under all conditions)

v/p = Compound is expected to exist in significant proportions in both the particle phase and the vapor phase as conditions vary

v = Compound is expected to exist mostly in the vapor phase in the atmosphere (fraction adsorbed ≤ 10% under all conditions)

V V = Compound is expected to exist almost entirely in the vapor phase in the atmosphere (fraction adsorbed ≤ 2% under all conditions)

(6) Resistant to Gas Rxn?:

1 = Compound is predicted to be relatively resistant to gas-phase reaction in the atmosphere with hydroxyl radical (in some cases, reaction with ozone was also considered), either because it exists largely in the particle phase, or, because its predicted reaction rate with hydroxyl radical is relatively low

0 = Compound is predicted to be very susceptible to gas-phase reaction in the atmosphere with hydroxyl radical (in some cases, reaction with ozone was also considered), because the compound exists to a significant extent in the gas phase, and, because its reaction with hydroxyl radical (or, in some cases, ozone) is relatively rapid

(7) Photolytic Resistance?:

1 = Compound is predicted to be relatively resistant to photolysis by ultraviolet light in the atmosphere, either because it does not appear to have significant absorption peaks at uv wavelengths greater than 290 nm, or, because it exists largely in the particle phase.

0 = Compound is predicted to be very susceptible to photolysis by ultraviolet light in the atmosphere, because it exists in the gas phase, and, it either appears to have very strong absorption peaks at uv wavelengths greater than 290 nm, or, other strong evidence for atmospheric photolysis exists.

(8) Gas Washout Resistance?:

1 = Compound is predicted to be relatively resistant to gas phase wet deposition by precipitation, either because it does not exist to a great extent in the vapor phase, or, because its Henry's Law constant (atm-m3/mol) is relatively large (i.e., the compound is not particularly water soluble and, when given a choice between the water and vapor phase in the atmosphere, does not significantly partition to the aqueous phase).

0	=	Compound is predicted to be relatively vulnerable to gas phase wet deposition by precipitation, because it exists to a great extent in the vapor phase, and, because its Henry's Law constant (atm-m3/mol) is relatively small (i.e., the compound is relatively water soluble and, when given a choice between the water and vapor phase in the atmosphere, it will partition significantly to the aqueous phase).

(9) Small Particles in Atm?:

1	=	When or if the compound is associated with particles in the atmosphere, a substantial fraction is associated with small particles, generally less than about 1 - 2 µm in diameter.
0	=	The bulk of the compound in the atmosphere is associated with large particles -- i.e., greater than about 5 - 10 µm in diameter. Such particles have a relatively short atmospheric lifetime and thus, the potential for long range atmospheric transport would be limited.
½	=	Significant fractions have been found (or are estimated) to exist in fine *and* coarse particles, or, with particles of intermediate size (i.e., on the order of 2 - 5 µm in diameter).

(10) <u>Avg Atm Lifetime (days, unless otherwise noted)</u>

Based on the preceding columns, information contained in this analysis, or information from the literature, a very rough estimate of the mean atmospheric lifetime of the pollutant is given. There are many uncertainties in these estimates, and these are regarded — at best — as only very rough order-of-magnitude estimates. Various limitations of these estimates are discussed throughout the text. *Note that some of the more volatile or mid-range volatile compounds probably are involved in the grasshopper effect. For these compounds with atmospheric lifetimes of ~ 1 week (or longer), they probably survive long enough in the atmosphere to experience multiple hops. For such compounds with very long lifetimes, e.g, hexachlorobenzene, they probably experience many, many such hops, with very little degradation while airborne during each hop.*

(11) <u>Measured / Found in Remote Areas?</u>

1	=	Attempt(s) have been made to measure the compound in remote areas — far from any sources -- in the atmosphere, atmospheric deposition (e.g., precipitation), vegetation, or other environmental media with relatively direct links to atmospheric pollutants.
0	=	Attempt(s) have been made to measure the compound in remote areas, as described above, and it is never or rarely found

(12) L.R.T. (Long Range Transport) Potential (Rating)

(see text in section D).

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Appendix A.

Physical-Chemical Properties

NAME			**Molecular Formula and Weight**				**PHYSICAL STATE**
common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd molecular weight	rept'd molecular weight	"physical state" (probably at room temperature)	reference
octachlorostyrene		029082-74-4	C8 Cl8	379.7	379.68		
4-bromophenyl phenyl ether		000101-55-3	C6H5-O-C6H4Br	249.1	249.11	varies; Tm ~ 18 deg C	considering Tm
3,3'-dichlorobenzidene		000091-94-1	C12 H10 Cl2 N2	253.1	253.13	solid	considering Tm; also stated by ATSDR citing HSDB
1,3-dinitropyrene		075321-20-9	C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
1,6-dinitropyrene		042397-64-8	C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
1,8-dinitropyrene		042397-65-9	C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
2,7-dinitropyrene		117929-15-4	C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
dinitropyrenes (mixed)		078432-19-6	C16 H8 N2 O4	292.3	292.25	probably solid	considering Tm of 1,6 DNP
hexachloro-1,3-butadiene		000087-68-3	C4 Cl6	260.7	260.76	liquid	99; consistent with Tm
4,4'-methylene bis(2-chloroaniline)		000101-14-4	C13 H12 Cl2 N2	267.2	267	solid	considering Tm
pentachlorophenol		000087-86-5	C6 H Cl5 O	266.3	266.34	flakes or crystalline solid	42; also consistent with Tm
aldrin		000309-00-2	C12 H8 Cl6	364.9	364.93	crystalline solid	47; also consistent with Tm
dieldrin		000060-57-1	C12 H8 Cl6 O	380.9	380.93	crystalline solid	47; also consistent with Tm
p,p'-DDT		000050-29-3	(ClC6H4)2CHCCl3	354.5	354.49	crystalline solid	59; also consistent with Tm
p,p'-DDD		000072-54-8	(ClC6H4)2CHCHCl2	320.0	320.05	crystalline solid	60; also consistent with Tm
p,p'-DDE		000072-55-9	(ClC6H4)2C=CCl2	318.0	318.03	crystalline solid	60; also consistent with Tm
heptachlor		000076-44-8	C10 H5 Cl7	373.3	373.35	crystalline solid	53; also consistent with Tm
heptachlor epoxide		001024-57-3	C10 H5 Cl7 O	389.3	389.4	crystalline solid	**53; note: ref 52 says that its liquid...; but if melti**
methoxychlor		000072-43-5	C16 H15 Cl3 O2	345.6	345.65	solid	considering Tm
mirex		002385-85-5	C10 Cl12	545.5	545.59	crystalline solid	65; also consistent with Tm
toxaphene		008001-35-2	approx C10 H10 Cl8	413.8	414 (avg)	waxy solid	42; also consistent with Tm
endrin		000072-20-8	C12 H8 Cl6 O	380.9	380.92	crystalline solid	42; also consistent with Tm
alpha-hexachlorocyclohexane		000319-84-6	C6 H6 Cl6	290.8	290.83	crystalline solid	32; also consistent with Tm
beta-hexachlorocyclohexane		000319-85-7	C6 H6 Cl6	290.8	290.83	crystalline solid	33; also consistent with Tm
delta-hexachlorocyclohexane		000319-86-8	C6 H6 Cl6	290.8	290.83	fine plates	29; also consistent with Tm
gamma-hexachlorocyclohexane		000058-89-9	C6 H6 Cl6	290.8	290.83	crystalline solid	33; also consistent with Tm
mixed hexachlorocyclohexanes		000319-84-6	C6 H6 Cl6	290.8	290.83		

NAME			Molecular Formula and Weight			PHYSICAL STATE	
common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd molecular weight	rept'd molecular weight	"physical state" (probably at room temperature)	reference
cadmium		007440-43-9	Cd	112.4	112.4	solid	71; also consistent with Tm
cadmium carbonate		000513-78-0	CdCO3	172.4	172.42	solid	71; also consistent with Tm
cadmium chloride		010108-64-2	CdCl2	183.3	183.32	solid	71; also consistent with Tm
cadmium oxide		001306-19-0	CdO	128.4	128.41	solid	71; also consistent with Tm
cadmium sulfate		010124-36-4	CdSO4	208.5	208.47	solid	71; also consistent with Tm
cadmium sulfide		001306-23-6	CdS	144.5	144.47	solid	71; also consistent with Tm
elemental mercury		007439-97-6	Hg	200.59	200.59	liquid	94
mercury oxide		021908-53-2	HgO				
mercuric chloride		007487-94-7	Hg Cl2	271.49		solid	94
monomethyl mercury chloride		000115-09-3	CH3 Hg Cl	251.08	251.08	solid	95; also consistent with Tm
dimethyl mercury		000593-74-8	CH3 Hg CH3				
tetraethyl lead		000078-00-2	C8 H20 Pb	323.4	323.44	probably liquid	melting point is -136 deg C; boiling point is ~ 215 C
tetramethyl lead		000075-74-1	C4 H12 Pb	267.3		liquid	hsdb
triethyl lead radical (1+ cation)		014570-15-1	C6 H15 Pb (1+)	294.4			
triethyl lead hydride		005224-23-7	C6 H16 Pb	295.4			
triethyl lead chloride		001067-14-7	C6 H15 Cl Pb	329.8			
diethyl lead radical (2+ cation)		024952-65-6	C4 H10 Pb (2+)	265.3			
diethyl lead dihydride		081494-11-3	C4 H12 Pb	267.3			
diethyl lead dichloride		013231-90-8	C4 H10 Cl2 Pb	336.2			
trimethyl lead radical (1+ cation)		014570-16-2	C3 H9 Pb (1+)	252.3			
trimethyl lead hydride		007442-13-9	C3 H10 Pb	253.3			
trimethyl lead chloride		001520-78-1	C3 H9 Cl Pb	287.8			
dimethyl lead radical (2+ cation)		021774-13-0	C2 H6 Pb (2+)	237.3			
dimethyl lead dihydride		030691-92-0	C2 H8 Pb	239.3			
dimethyl lead dichloride		001520-77-0	C2 H6 Cl2 Pb	308.2			
bis (tributyltin) oxide		000056-35-9	C24 H54 O Sn2		595.62	liquid	97
tributyl tin		000688-75-3					
tributyltin fluoride		001983-10-4	C12 H27 F Sn				
tributyltin chloride		001461-22-9	C12 H27 Cl Sn				
tributyltin hydroxide		001067-97-6	C12 H28 O Sn				
tributyltin naphthenate							
tris(tributylstannyl) phosphate		013435-05-7					

NAME			Molecular Formula and Weight				PHYSICAL STATE
						"physical state"	
				calc'd	rept'd	(probably	
			molecular	molecular	molecular	at room	
common chemical name	IUPAC #	cas # (1)	formula	weight	weight	temperature)	reference
1,4-dichlorobenzene		000106-46-7	C6 H4 Cl2	147.0	147.01	solid	considering Tm
1,2,3,4-tetrachlorobenzene		000634-66-2	C6 H2 Cl4	215.9	215.89	solid	considering Tm
1,2,4,5-tetrachlorobenzene		000095-94-3	C6 H2 Cl4	215.9	215.89	solid	considering Tm
1,2,3,5-tetrachlorobenzene		000634-90-2	C6 H2 Cl4	215.9	215.89	solid	considering Tm
pentachlorobenzene		000608-93-5	C6 H Cl5	250.3	250.34	solid	considering Tm
hexachlorobenzene		000118-74-1	C6 Cl6	284.8	284.78	solid	considering Tm
naphthalene		000091-20-3	C8 H10	106.2	128.19	solid	considering Tm
acenaphthene		000083-32-9	C12 H10	154.2	154.21	solid	considering Tm
acenaphthylene		000208-96-8	C12 H8	152.2	150.2	solid	considering Tm
fluorene		000086-73-7	C13 H10	166.2	166.2	solid	considering Tm
phenanthrene		000085-01-8	C14 H10	178.2	178.2	solid	considering Tm
anthracene		000120-12-7	C14 H10	178.2	178.2	solid	considering Tm
pyrene		000129-00-0	C16 H10	202.3	202.3	solid	considering Tm
fluoranthene		000206-44-0	C16 H10	202.3	202.3	solid	considering Tm
chrysene		000218-01-9	C18 H12	228.3	228.3	solid	considering Tm
benz [a] anthracene		000056-55-3	C18 H12	228.3	228.3	solid ???	considering Tm from ref 6; but ref 85 gives Tm of -1
benzo [b] fluoranthene		000205-99-2	C20 H12	252.3	252.3	solid	considering Tm
benzo [j] fluoranthene		000205-82-3	C20 H12	252.3	252.3	solid	considering Tm
benzo [k] fluoranthene		000207-08-9	C20 H12	252.3	252.3	solid	considering Tm
benzo [a] pyrene		000050-32-8	C20 H12	252.3	252.3	solid	considering Tm
benzo [e] pyrene		000192-97-2	C20 H12	252.3	252.3	solid	considering Tm
perylene		000198-55-0	C20 H12	252.3	252.3	solid	considering Tm
benzo [g,h,i] perylene		000191-24-2	C21 H16	268.4	268.36	solid	considering Tm
dibenz [a,h] anthracene		000053-70-3	C22 H14	278.4	278.35	solid	considering Tm
indeno [1,2,3-c,d] pyrene		000193-39-5	C22 H12	276.3	276.3	solid	considering Tm

NAME			Molecular Formula and Weight			PHYSICAL STATE	
common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd molecular weight	rept'd molecular weight	"physical state" (probably at room temperature)	reference
2,3,7,8-TCDD		001746-01-6	C12 H4 O2 Cl4	322.0	322	solid	considering Tm
1,2,3,7,8-PeCDD		040321-76-4	C12 H3 O2 Cl5	356.4	356.4	solid	considering Tm
1,2,3,4,7,8-HxCDD		039227-28-6	C12 H2 O2 Cl6	390.8	391	solid	considering Tm
1,2,3,6,7,8-HxCDD		057653-85-7	C12 H2 O2 Cl6	390.8	391	solid	considering Tm
1,2,3,7,8,9-HxCDD		019408-74-3	C12 H2 O2 Cl6	390.8	391	solid	considering Tm
1,2,3,4,6,7,8-HpCDD		035822-46-9	C12 H1 O2 Cl7	425.3	425.2	solid	considering Tm
OCDD		003268-87-9	C12 H0 O2 Cl8	459.7	460	solid	considering Tm
2,3,7,8-TCDF		051207-31-9	C12 H4 O Cl4	306.0	306	solid	considering Tm
2,3,4,7,8-PeCDF		057117-31-4	C12 H3 O Cl5	340.4	340.42	solid	considering Tm
1,2,3,7,8-PeCDF		057117-41-6	C12 H3 O Cl5	340.4	340.42	solid	considering Tm
1,2,3,4,7,8-HxCDF		070648-26-9	C12 H2 O Cl6	374.8	374.87	solid	considering Tm
1,2,3,6,7,8-HxCDF		057117-44-9	C12 H2 O Cl6	374.8	374.87	solid	considering Tm
1,2,3,7,8,9-HxCDF		072918-21-9	C12 H2 O Cl6	374.8	374.87	solid	considering Tm
2,3,4,6,7,8-HxCDF		060851-34-5	C12 H2 O Cl6	374.8	374.87	solid	considering Tm
1,2,3,4,6,7,8-HpCDF		067562-39-4	C12 H1 O Cl7	409.3	409.31	solid	considering Tm
1,2,3,4,7,8,9-HpCDF		055673-89-7	C12 H1 O Cl7	409.3	409.31	solid	considering Tm
OCDF		039001-02-0	C12 H0 O Cl8	443.7	443.8	solid	considering Tm

NAME			Molecular Formula and Weight				PHYSICAL STATE
common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd molecular weight	rept'd molecular weight	"physical state" (probably at room temperature)	reference
biphenyl	0	000092-52-4	C12 H10	154.2	154.2	solid	considering Tm
2-PCB	1	002051-60-7	C12 H9 Cl	188.7	188.7	varies	Tm near room temp
3-PCB	2	002051-61-8	C12 H9 Cl	188.7	188.7	varies	Tm near room temp
4-PCB	3	002051-62-9	C12 H9 Cl	188.7	188.7	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2'-PCB	4	013029-08-8	C12 H8 Cl2	223.1	223.1	solid	considering Tm
2,3-PCB	5	016605-91-7	C12 H8 Cl2	223.1	223.1	oil	96
2,4-PCB	7	033284-50-3	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
2,4'-PCB	8	034883-43-7	C12 H8 Cl2	223.1	223.1	solid	considering Tm
2,5-PCB	9	034883-39-1	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
2,6-PCB	10	033146-45-1	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
3,3'-PCB	11	002050-67-1	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
3,4-PCB	12	002974-92-7	C12 H8 Cl2	223.1	223.1	solid	considering Tm
3,5-PCB	14	034883-41-5	C12 H8 Cl2	223.1	223.1	varies	Tm near room temp
4,4'-PCB	15	002050-68-2	C12 H8 Cl2	223.1	223.1	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							

NAME			Molecular Formula and Weight				PHYSICAL STATE
common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd molecular weight	rept'd molecular weight	"physical state" (probably at room temperature)	reference
2,2',3-PCB	16	038444-78-9	$C_{12}H_7Cl_3$	257.5	257.5	varies	Tm near room temp
2,2',5-PCB	18	037680-65-2	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
2,3,3'-PCB	20	038444-84-7	$C_{12}H_7Cl_3$	257.5	257.5	solid	solid, considering Tm
2,3,4-PCB	21	055702-46-0	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
2,3',5-PCB	26	038444-85-8	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
2,4,4'-PCB	28	007012-37-5	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
2,4,5-PCB	29	015862-07-4	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
2,4,6-PCB	30	035693-92-6	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
2,4',5,-PCB	31	016606-02-3	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
2',3,4-PCB	33	038444-86-9	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
3,3',4-PCB	35	037680-69-6	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
3,4,4'-PCB	37	038444-90-5	$C_{12}H_7Cl_3$	257.5	257.5	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3'-PCB	40	038444-93-8	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,2',3,5'-PCB	44	041464-39-5	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,2',4,4'-PCB	47	002437-79-8	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,2',4,5'-PCB	49	041464-40-8	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,2',4,6-PCB	50	062796-65-0	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,2',4,6'-PCB	51	068194-04-7	$C_{12}H_6Cl_4$	292.0	292.0	oil	95
2,2,5,5'-PCB	52	035693-99-3	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,2,5,6'-PCB	53	041464-41-9	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,2,6,6'-PCB	54	015968-05-5	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,3,4,4'-PCB	60	033025-41-1	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,3,4,5-PCB	61	033284-53-6	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,3,5,6-PCB	65	033284-54-7	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,3,4,4'-PCB	66	032598-10-0	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,3',4',5-PCB	70	032598-11-1	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
2,4,4',6-PCB	75	032598-12-2	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
3,3',4,4'-PCB	77	032598-13-3	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
3,3',5,5'-PCB	80	033284-52-5	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
3,4,4',5-PCB	81	070362-50-4	$C_{12}H_6Cl_4$	292.0	292.0	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							

NAME			**Molecular Formula and Weight**				**PHYSICAL STATE**
common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd molecular weight	rept'd molecular weight	"physical state" (probably at room temperature)	reference
2,2',3,3',5-PCB	83	060145-20-2	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,2',3,4,5-PCB	86	065510-45-4	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,2',3,4,5'-PCB	87	038380-02-8	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,2',3,4,6-PCB	88	055215-17-3	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,2',3,5,6-PCB	95	038379-99-6	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,2',4,4',5-PCB	99	038380-01-7	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,2',4,4',6-PCB	100	039485-83-1	C12 H5 Cl5	326.4	326.4	oil	95
2,2',4,5,5'-PCB	101	037680-73-2	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,2',4,6,6'-PCB	104	056558-16-8	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,3,3',4,4'-PCB	105	032598-14-4	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,3,3',4',6-PCB	110	038380-03-9	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,3,4,4',5-PCB	114	074472-37-0	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,3,4,5,6-PCB	116	018259-05-7	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2,3',4,4',5-PCB	118	031508-00-6	C12 H5 Cl5	326.4	326.4	solid	considering Tm
2',3,4,5,5'-PCB	124	070424-70-3	C12 H5 Cl5	326.4	326.4	solid	considering Tm
3,3',4,4',5-PCB	126	057465-28-8	C12 H5 Cl5	326.4	326.4	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4'-PCB	128	038380-07-3	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,2',3,3',4,5-PCB	129	055215-18-4	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,2',3,3',5,6-PCB	134	052704-70-8	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,2',3,3',6,6'-PCB	136	038411-22-2	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,2',3,4,4',5'-PCB	138	035065-28-2	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,2',3,4',5',6-PCB	149	038380-04-0	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,2',4,4',5,5'-PCB	153	035065-27-1	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,2',4,4',6,6'-PCB	155	033979-03-2	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,3,3',4,4',5-PCB	156	038380-08-4	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,3,3',4,4',5'-PCB	157	069782-90-7	C12 H4 Cl6	360.9	360.9	solid	considering Tm
2,3',4,4',5,5'-PCB	167	052663-72-6	C12 H4 Cl6	360.9	360.9	solid	considering Tm
3,3',4,4',5,5'-PCB	169	032774-16-6	C12 H4 Cl6	360.9	360.9	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							

NAME			Molecular Formula and Weight				PHYSICAL STATE
common chemical name	IUPAC #	cas # (1)	molecular formula	calc'd molecular weight	rept'd molecular weight	"physical state" (probably at room temperature)	reference
2,2',3,3',4,4',5-PCB	170	035065-30-6	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,2',3,3',4,4',6-PCB	171	052663-71-5	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,2',3,4,4',5,5'-PCB	180	035065-29-3	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,2',3,4,5,5',6-PCB	185	052712-05-7	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,2',3,4',5,5',6-PCB	187	052663-68-0	C12 H3 Cl7	395.3	395.3	solid	considering Tm
2,3,3',4,4',5,5'-PCB	189	039635-31-9	C12 H3 Cl7	395.3	395.3	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	C12 H2 Cl8	429.7	429.7	solid	considering Tm
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	C12 H2 Cl8	429.7	429.7	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	C12 H Cl9	464.2	464.2	solid	considering Tm
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	C12 H Cl9	464.2	464.2	solid	considering Tm
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	C12 H Cl9	464.2	464.2	solid	considering Tm
count							
average							
standard deviation							
minimum							
maximum							
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	C12 Cl10	498.6	498.6	solid	considering Tm

NAME

MELTING POINT

common chemical name	IUPAC #	cas # (1)	melting point range	melting point average	melting point units	melting point ref	for V/P melting point deg K	data notes
octachlorostyrene		029082-74-4		150	deg C	89	423	estimated using linear regression; not in SRC database
4-bromophenyl phenyl ether		000101-55-3		18	deg C	7	291.15	
3,3'-dichlorobenzidene		000091-94-1	132-133	132.5	deg C	Howard, Volume 1	405.65	same in ref 8; & ATSDR
1,3-dinitropyrene		075321-20-9					479.15	crude: pyrene+50 C
1,6-dinitropyrene		042397-64-8	> 300		deg C	aldrich catalog, pag	479.15	crude: pyrene+50 C
1,8-dinitropyrene		042397-65-9					479.15	crude: pyrene+50 C
2,7-dinitropyrene		117929-15-4					479.15	crude: pyrene+50 C
dinitropyrenes (mixed)		078432-19-6					479.15	crude: pyrene+50 C
hexachloro-1,3-butadiene		000087-68-3		-21	deg C	7; 99	252.15	
4,4'-methylene bis(2-chloroaniline)		000101-14-4		110	deg C	15	383.15	
pentachlorophenol		000087-86-5		174	deg C	8	447.15	
aldrin		000309-00-2		104	deg C	25	377.15	
dieldrin		000060-57-1	175-176	175.5	deg C	25	448.65	
p,p'-DDT		000050-29-3	107-110	108.5	deg C?	aldrich catalog, pag	381.65	same in ref 61
p,p'-DDD		000072-54-8	109-111	110	deg C?	aldrich catalog, pag	383.15	same in ref 61
p,p'-DDE		000072-55-9	88-90	89	deg C?	aldrich catalog, pag	362.15	same in ref 61 and SRC data set
heptachlor		000076-44-8	95-96	95.5	deg C	25	368.65	same in ref 85
heptachlor epoxide		001024-57-3	160-161.5	160.75	deg C	25	433.9	same in ref 85
methoxychlor		000072-43-5		89	deg C	24; 85	362.15	
mirex		002385-85-5		485	deg C	65	758.15	decomposes
toxaphene		008001-35-2	65 - 90	77.5	deg C	25	350.65	
endrin		000072-20-8	226-230	228	deg C	25	501.15	decomposes when melted
alpha-hexachlorocyclohexane		000319-84-6		159.5	deg C	29	432.65	
beta-hexachlorocyclohexane		000319-85-7		314.5	deg C	29	587.65	
delta-hexachlorocyclohexane		000319-86-8		141.5	deg C	29	414.65	
gamma-hexachlorocyclohexane		000058-89-9		112.5	deg C	29, 30	385.65	
mixed hexachlorocyclohexanes		000319-84-6						

NAME			MELTING POINT					
							for V/P	
			melting point range	melting point average	melting point units	melting point ref	**melting point deg K**	data notes
common chemical name	IUPAC #	cas # (1)						
cadmium		007440-43-9		320.9	deg C		594.05	71
cadmium carbonate		000513-78-0	decomposes	at less than 500 deg C				72
cadmium chloride		010108-64-2		568	deg C		841.15	71
cadmium oxide		001306-19-0	less than 1426 deg C					73
cadmium sulfate		010124-36-4		1000	deg C		1273.15	71
cadmium sulfide		001306-23-6		1475	deg C		1748.15	74
elemental mercury		007439-97-6		-38.87	deg C	94	234.28	
mercury oxide		021908-53-2						
mercuric chloride		007487-94-7		276	deg C	94	549.15	
monomethyl mercury chloride		000115-09-3		170	deg C	95	443.15	
dimethyl mercury		000593-74-8						
tetraethyl lead		000078-00-2		-136	deg C	85	137.15	
tetramethyl lead		000075-74-1		-27.5	deg C	97	245.65	
triethyl lead radical (1+ cation)		014570-15-1						
triethyl lead hydride		005224-23-7						
triethyl lead chloride		001067-14-7						
diethyl lead radical (2+ cation)		024952-65-6						
diethyl lead dihydride		081494-11-3						
diethyl lead dichloride		013231-90-8						
trimethyl lead radical (1+ cation)		014570-16-2						
trimethyl lead hydride		007442-13-9						
trimethyl lead chloride		001520-78-1						
dimethyl lead radical (2+ cation)		021774-13-0						
dimethyl lead dihydride		030691-92-0						
dimethyl lead dichloride		001520-77-0						
bis (tributyltin) oxide		000056-35-9		-45	deg C	97	228.15	ref says "solidifies below -45 C"
tributyl tin		000688-75-3						
tributyltin fluoride		001983-10-4						
tributyltin chloride		001461-22-9						
tributyltin hydroxide		001067-97-6						
tributyltin naphthenate								
tris(tributylstannyl) phosphate		013435-05-7						

NAME			**MELTING POINT**					
							for V/P	
			melting	melting	melting	melting	**melting**	
			point	point	point	point	**point**	data
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	**deg K**	notes
1,4-dichlorobenzene		000106-46-7		53.1	deg C	5	326.25	similar in Aldrich catalog
1,2,3,4-tetrachlorobenzene		000634-66-2		47.5	deg C	5	320.65	similar in Aldrich catalog
1,2,4,5-tetrachlorobenzene		000095-94-3		140	deg C	5	413.15	similar in Aldrich catalog
1,2,3,5-tetrachlorobenzene		000634-90-2		54.5	deg C	5	327.65	
pentachlorobenzene		000608-93-5		86	deg C	5	359.15	similar in Aldrich catalog
hexachlorobenzene		000118-74-1		230	deg C	5	503.15	similar in Aldrich catalog
naphthalene		000091-20-3		80.5	deg C	6	353.65	
acenaphthene		000083-32-9		96.2	deg C	6	369.35	
acenaphthylene		000208-96-8		92	deg C	6	365.15	
fluorene		000086-73-7		116	deg C	6	389.15	
phenanthrene		000085-01-8		101	deg C	6	374.15	
anthracene		000120-12-7		216.2	deg C	6	489.35	
pyrene		000129-00-0		156	deg C	6	429.15	
fluoranthene		000206-44-0		111	deg C	6	384.15	
chrysene		000218-01-9		255	deg C	6	528.15	
benz [a] anthracene		000056-55-3		160	deg C	6	433.15	
benzo [b] fluoranthene		000205-99-2		168	deg C	6	441.15	
benzo [j] fluoranthene		000205-82-3		166	deg C	6	439.15	
benzo [k] fluoranthene		000207-08-9		217	deg C	6	490.15	
benzo [a] pyrene		000050-32-8		175	deg C	6	448.15	
benzo [e] pyrene		000192-97-2		178	deg C	6	451.15	
perylene		000198-55-0		277	deg C	6	550.15	
benzo [g,h,i] perylene		000191-24-2		277	deg C	6	550.15	
dibenz [a,h] anthracene		000053-70-3		267	deg C	6	540.15	
indeno [1,2,3-c,d] pyrene		000193-39-5		163.6	deg C	9	436.75	

NAME			MELTING POINT					
							for V/P	
			melting point	melting point	melting point	melting point	**melting point**	data
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	**deg K**	notes
2,3,7,8-TCDD		001746-01-6		305	deg C	6	578.15	
1,2,3,7,8-PeCDD		040321-76-4		195	deg C	6	468.15	using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD		039227-28-6		273	deg C	6	546.15	
1,2,3,6,7,8-HxCDD		057653-85-7		273	deg C	6	546.15	using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD		019408-74-3		273	deg C	6	546.15	using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD		035822-46-9		265	deg C	6	538.15	
OCDD		003268-87-9		322	deg C	6	595.15	
2,3,7,8-TCDF		051207-31-9		227	deg C	6	500.15	
2,3,4,7,8-PeCDF		057117-31-4		196	deg C	6	469.15	
1,2,3,7,8-PeCDF		057117-41-6		196	deg C	6	469.15	using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF		070648-26-9		225.5	deg C	6	498.65	
1,2,3,6,7,8-HxCDF		057117-44-9		232	deg C	6	505.15	
1,2,3,7,8,9-HxCDF		072918-21-9		228.75	deg C	6	501.9	using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF		060851-34-5		228.75	deg C	6	501.9	using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF		067562-39-4		236	deg C	6	509.15	
1,2,3,4,7,8,9-HpCDF		055673-89-7		221	deg C	6	494.15	
OCDF		039001-02-0		258	deg C	6	531.15	

NAME						MELTING POINT		
							for V/P	
common chemical name	IUPAC #	cas # (1)	melting point range	melting point average	melting point units	melting point ref	**melting point deg K**	data notes
biphenyl	0	000092-52-4		71	deg C	5	344.15	
2-PCB	1	002051-60-7		34	deg C	5	307.15	
3-PCB	2	002051-61-8		25.1	deg C	5	298.25	
4-PCB	3	002051-62-9		77.9	deg C	5	351.05	
count								
average								
standard deviation								
minimum								
maximum								
2,2'-PCB	4	013029-08-8		61	deg C	5	334.15	
2,3-PCB	5	016605-91-7		***not in ref 5, 85, or 95***			**273.15**	**guess; since oil at room temp, must be less than room temp**
2,4-PCB	7	033284-50-3		24.4	deg C	5	297.55	
2,4'-PCB	8	034883-43-7		43	deg C	5	316.15	
2,5-PCB	9	034883-39-1		25.1	deg C	5	298.25	
2,6-PCB	10	033146-45-1		34.9	deg C	5	308.05	
3,3'-PCB	11	002050-67-1		29	deg C	5	302.15	
3,4-PCB	12	002974-92-7		49	deg C	5	322.15	
3,5-PCB	14	034883-41-5		31	deg C	5	304.15	
4,4'-PCB	15	002050-68-2		149	deg C	5	422.15	
count								
average								
standard deviation								
minimum								
maximum								

NAME

MELTING POINT

common chemical name	IUPAC #	cas # (1)	melting point range	melting point average	melting point units	melting point ref	for V/P **melting point deg K**	data notes
2,2',3-PCB	16	038444-78-9		28	deg C	5	301.15	
2,2',5-PCB	18	037680-65-2		44	deg C	5	317.15	
2,3,3'-PCB	20	038444-84-7	43 - 44.5	43.75	deg C	95	316.9	
2,3,4-PCB	21	055702-46-0		102	deg C	5	375.15	
2,3',5-PCB	26	038444-85-8		40.5	deg C	5	313.65	
2,4,4'-PCB	28	007012-37-5		57	deg C	5	330.15	
2,4,5-PCB	29	015862-07-4		78	deg C	5	351.15	
2,4,6-PCB	30	035693-92-6		62.5	deg C	5	335.65	
2,4',5,-PCB	31	016606-02-3		67	deg C	5	340.15	
2',3,4-PCB	33	038444-86-9		60	deg C	5	333.15	
3,3',4-PCB	35	037680-69-6		87	deg C	5	360.15	
3,4,4'-PCB	37	038444-90-5		87	deg C	5	360.15	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3'-PCB	40	038444-93-8		121	deg C	5	394.15	
2,2',3,5'-PCB	44	041464-39-5		47	deg C	5	320.15	
2,2',4,4'-PCB	47	002437-79-8		83	deg C	5	356.15	
2,2',4,5'-PCB	49	041464-40-8		64	deg C	5	337.15	
2,2',4,6-PCB	50	062796-65-0	47 - 48	47.5	deg C	95	320.65	
2,2',4,6'-PCB	51	068194-04-7		***not in ref 5, 85, or 95***			**273.15**	**guess; since oil at room temp, must be less than room temp**
2,2,5,5'-PCB	52	035693-99-3		87	deg C	5	360.15	
2,2,5,6'-PCB	53	041464-41-9		104	deg C	5	377.15	
2,2,6,6'-PCB	54	015968-05-5		198	deg C	5	471.15	
2,3,4,4'-PCB	60	033025-41-1		142	deg C	5	415.15	
2,3,4,5-PCB	61	033284-53-6		92	deg C	5	365.15	
2,3,5,6-PCB	65	033284-54-7		79	deg C	5	352.15	
2,3,4,4'-PCB	66	032598-10-0		124	deg C	5	397.15	
2,3',4',5-PCB	70	032598-11-1		104	deg C	5	377.15	
2,4,4',6-PCB	75	032598-12-2	62 - 63	62.5	deg C	95	335.65	
3,3',4,4'-PCB	77	032598-13-3		180	deg C	5	453.15	
3,3',5,5'-PCB	80	033284-52-5		164	deg C	5	437.15	
3,4,4',5-PCB	81	070362-50-4	160 - 163	161.5	deg C	95	434.65	
count								
average								
standard deviation								
minimum								
maximum								

NAME			MELTING POINT					
							for V/P	
common chemical name	IUPAC #	cas # (1)	melting point range	melting point average	melting point units	melting point ref	**melting point deg K**	data notes
2,2',3,3',5-PCB	83	060145-20-2	83 - 84	83.5	deg C	95	356.65	
2,2',3,4,5-PCB	86	065510-45-4		100	deg C	5	373.15	
2,2',3,4,5'-PCB	87	038380-02-8		114	deg C	5	387.15	
2,2',3,4,6-PCB	88	055215-17-3		100	deg C	5	373.15	
2,2',3,5,6-PCB	95	038379-99-6		100	deg C	5	373.15	
2,2',4,4',5-PCB	99	038380-01-7	59 - 60	59.5	deg C	95	332.65	
2,2',4,4',6-PCB	100	039485-83-1		***not in ref 5, 85, or 95***			**273.15**	**guess; since oil at room temp, must be less than room temp**
2,2',4,5,5'-PCB	101	037680-73-2		76.5	deg C	5	349.65	
2,2',4,6,6'-PCB	104	056558-16-8	87 - 88	87.5	deg C	95	360.65	
2,3,3',4,4'-PCB	105	032598-14-4		105	deg C	5	378.15	
2,3,3',4',6-PCB	110	038380-03-9	53 - 55	54	deg C	95	327.15	
2,3,4,4',5-PCB	114	074472-37-0	111 - 113	112	deg C	95	385.15	
2,3,4,5,6-PCB	116	018259-05-7		124	deg C	5	397.15	
2,3',4,4',5-PCB	118	031508-00-6		107	deg C	5	380.15	
2',3,4,5,5'-PCB	124	070424-70-3	116 - 117	116.5	deg C	95	389.65	
3,3',4,4',5-PCB	126	057465-28-8	160 - 161	160.5	deg C	95	433.65	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4'-PCB	128	038380-07-3		150	deg C	5	423.15	
2,2',3,3',4,5-PCB	129	055215-18-4		85	deg C	5	358.15	
2,2',3,3',5,6-PCB	134	052704-70-8		100	deg C	5	373.15	
2,2',3,3',6,6'-PCB	136	038411-22-2		112.2	deg C	5	385.35	
2,2',3,4,4',5'-PCB	138	035065-28-2		80	deg C	5	353.15	
2,2',3,4',5',6-PCB	149	038380-04-0	78-79	78.5	deg C	95	351.65	reported as oil in ref 5
2,2',4,4',5,5'-PCB	153	035065-27-1		103	deg C	5	376.15	
2,2',4,4',6,6'-PCB	155	033979-03-2		114	deg C	5	387.15	
2,3,3',4,4',5-PCB	156	038380-08-4	129.5 - 131	130.25	deg C	95	403.4	
2,3,3',4,4',5'-PCB	157	069782-90-7	161 - 162	161.5	deg C	95	434.65	
2,3',4,4',5,5'-PCB	167	052663-72-6	125 - 127	126	deg C	95	399.15	
3,3',4,4',5,5'-PCB	169	032774-16-6		202	deg C	5	475.15	
count								
average								
standard deviation								
minimum								
maximum								

NAME			MELTING POINT					
							for V/P	
common chemical name	IUPAC #	cas # (1)	melting point range	melting point average	melting point units	melting point ref	**melting point deg K**	data notes
2,2',3,3',4,4',5-PCB	170	035065-30-6	136.5 - 138.5	137.5	deg C	95	410.65	
2,2',3,3',4,4',6-PCB	171	052663-71-5		122.4	deg C	5	395.55	
2,2',3,4,4',5,5'-PCB	180	035065-29-3		110	deg C	5	383.15	
2,2',3,4,5,5',6-PCB	185	052712-05-7		149	deg C	5	422.15	
2,2',3,4',5,5',6-PCB	187	052663-68-0	104 - 105	104.5	deg C	95	377.65	
2,3,3',4,4',5,5'-PCB	189	039635-31-9	162 - 163	162.5	deg C	95	435.65	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7		159	deg C	5	432.15	
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4		162	deg C	5	435.15	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9		206	deg C	5	479.15	
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	213 - 215	214	deg C	95	487.15	
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1		182.8	deg C	5	455.95	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3		305.9	deg C	5	579.05	

NAME							BOILING POINT	
							for V/P	
common chemical name	IUPAC #	cas # (1)	boiling point range	boiling point average	boiling point units	boiling point ref	**boiling point deg K**	boiling point data notes
octachlorostyrene		029082-74-4		379	deg C	89	652	estimated using linear regression; not in SRC database
4-bromophenyl phenyl ether		000101-55-3		310	deg C	7	583.15	
3,3'-dichlorobenzidene		000091-94-1		420	deg C	18	693.15	368 deg C value given in ATSDR as an estimate, citing PCGEMS 1988 as a re
1,3-dinitropyrene		075321-20-9					683.15	crude: pyrene + 50 C
1,6-dinitropyrene		042397-64-8					683.15	crude: pyrene + 50 C
1,8-dinitropyrene		042397-65-9					683.15	crude: pyrene + 50 C
2,7-dinitropyrene		117929-15-4					683.15	crude: pyrene + 50 C
dinitropyrenes (mixed)		078432-19-6					683.15	crude: pyrene + 50 C
hexachloro-1,3-butadiene		000087-68-3		215	deg C	19; 99	488.15	
4,4'-methylene bis(2-chloroaniline)		000101-14-4		378.9	deg C	83	652.05	
pentachlorophenol		000087-86-5		309.5	deg C	25	582.65	decomposes
aldrin		000309-00-2		664	deg K	87	664.01	estimated using Clausius Clapyron equation
dieldrin		000060-57-1		330	deg C	48	603.15	estm'd?; same data given in SRC data set
p,p'-DDT		000050-29-3		260	deg C	60	533.15	not given in ref 85
p,p'-DDD		000072-54-8		350	deg C	85	623.15	
p,p'-DDE		000072-55-9		336	deg C	85	609.15	
heptachlor		000076-44-8		310	deg C	85	583.15	
heptachlor epoxide		001024-57-3		no data			583.15	**No data available; use value for heptachlor for now**
methoxychlor		000072-43-5		346	deg C	85	619.15	one ref says that it decomposes when heated, so no data...; however SRC dat
mirex		002385-85-5		no data		65	960	**hypothetical estm based on Tb vs. Tm regression**
toxaphene		008001-35-2					580	**decomposes; hypothetical Tb estimated using Tb vs Tm regression**
endrin		000072-20-8					720	**decomposes at 245 deg C when heated, ref 22; estimate for hypothetical**
alpha-hexachlorocyclohexane		000319-84-6		288	deg C	31	561.15	
beta-hexachlorocyclohexane		000319-85-7		301.59	deg C	estm-29-92	574.74	based on 60 deg C @ 0.5 mm Hg
delta-hexachlorocyclohexane		000319-86-8		312.43	deg C	estm-29-92	585.58	based on 60 deg C @ 0.36 mm Hg
gamma-hexachlorocyclohexane		000058-89-9		323.4	deg C	31	596.55	
mixed hexachlorocyclohexanes		000319-84-6						

NAME

BOILING POINT

common chemical name	IUPAC #	cas # (1)	boiling point range	boiling point average	boiling point units	boiling point ref	**for V/P boiling point deg K**	boiling point data notes
cadmium		007440-43-9		767	deg C	71	1040.15	
cadmium carbonate		000513-78-0		no data		71		
cadmium chloride		010108-64-2		960	deg C	71	1233.15	
cadmium oxide		001306-19-0	decomposes at 900 C			71		
cadmium sulfate		010124-36-4		no data		71		
cadmium sulfide		001306-23-6	sublimes in N2 at 980 C			71		
elemental mercury		007439-97-6		356.58	deg C	94	629.73	
mercury oxide		021908-53-2						
mercuric chloride		007487-94-7		302	deg C	94	575.15	
monomethyl mercury chloride		000115-09-3		no data		95	**666**	**hypothetical estm using Tb vs Tm correlation**
dimethyl mercury		000593-74-8						
tetraethyl lead		000078-00-2	200 - 227.2	213.6	deg C	85	486.75	
tetramethyl lead		000075-74-1		274.24	deg C	estm	547.39	based on Bp of 110 deg C at 10 mm Hg, reported in HSDB from IARC volume
triethyl lead radical (1+ cation)		014570-15-1						
triethyl lead hydride		005224-23-7						
triethyl lead chloride		001067-14-7						
diethyl lead radical (2+ cation)		024952-65-6						
diethyl lead dihydride		081494-11-3						
diethyl lead dichloride		013231-90-8						
trimethyl lead radical (1+ cation)		014570-16-2						
trimethyl lead hydride		007442-13-9						
trimethyl lead chloride		001520-78-1						
dimethyl lead radical (2+ cation)		021774-13-0						
dimethyl lead dihydride		030691-92-0						
dimethyl lead dichloride		001520-77-0						
bis (tributyltin) oxide		000056-35-9		669.14	deg K	estm	669.14	based on 254 deg C at 50 mmHg from ref 97
tributyl tin		000688-75-3						
tributyltin fluoride		001983-10-4						
tributyltin chloride		001461-22-9						
tributyltin hydroxide		001067-97-6						
tributyltin naphthenate								
tris(tributylstannyl) phosphate		013435-05-7						

NAME

BOILING POINT

common chemical name	IUPAC #	cas # (1)	boiling point range	boiling point average	boiling point units	boiling point ref	for V/P boiling point deg K	boiling point data notes
1,4-dichlorobenzene		000106-46-7		174.6	deg C	5	447.75	
1,2,3,4-tetrachlorobenzene		000634-66-2		254	deg C	5	527.15	similar in Aldrich catalog
1,2,4,5-tetrachlorobenzene		000095-94-3		243	deg C	5	516.15	similar in Aldrich catalog
1,2,3,5-tetrachlorobenzene		000634-90-2		246	deg C	5	519.15	
pentachlorobenzene		000608-93-5		277	deg C	5	550.15	similar in Aldrich catalog
hexachlorobenzene		000118-74-1		322	deg C	5	595.15	similar in Aldrich catalog
naphthalene		000091-20-3		218	deg C	6	491.15	
acenaphthene		000083-32-9		277.5	deg C	6	550.65	
acenaphthylene		000208-96-8	265-275	270	deg C	6	543.15	
fluorene		000086-73-7		295	deg C	6	568.15	
phenanthrene		000085-01-8		339	deg C	6	612.15	
anthracene		000120-12-7		340	deg C	6	613.15	
pyrene		000129-00-0		360	deg C	6	633.15	
fluoranthene		000206-44-0		375	deg C	6	648.15	
chrysene		000218-01-9		448	deg C	6	721.15	
benz [a] anthracene		000056-55-3		435	deg C	6	708.15	
benzo [b] fluoranthene		000205-99-2		481	deg C	6	754.15	
benzo [j] fluoranthene		000205-82-3		480	deg C	6	753.15	
benzo [k] fluoranthene		000207-08-9		481	deg C	6	754.15	
benzo [a] pyrene		000050-32-8		495	deg C	6	768.15	
benzo [e] pyrene		000192-97-2		561	deg C	79	834.55	Estimated using calculation; value not given in Ref 6; 310-312 deg C at 10 mm
perylene		000198-55-0		495	deg C	6	768.15	
benzo [g,h,i] perylene		000191-24-2		550	deg C	11	823.15	
dibenz [a,h] anthracene		000053-70-3		524	deg C	6	797.15	
indeno [1,2,3-c,d] pyrene		000193-39-5		530	deg C	11	803.15	

NAME			BOILING POINT					
							for V/P	
common chemical name	IUPAC #	cas # (1)	boiling point range	boiling point average	boiling point units	boiling point ref	**boiling point deg K**	boiling point data notes
2,3,7,8-TCDD		001746-01-6		446.5	deg C	6	719.65	
1,2,3,7,8-PeCDD		040321-76-4		464.7	deg C	6	737.85	using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD		039227-28-6		487.7	deg C	6	760.85	
1,2,3,6,7,8-HxCDD		057653-85-7		487.7	deg C	6	760.85	using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD		019408-74-3		487.7	deg C	6	760.85	using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD		035822-46-9		507.2	deg C	6	780.35	
OCDD		003268-87-9		510	deg C	6	783.15	
2,3,7,8-TCDF		051207-31-9		438.3	deg C	6	711.45	
2,3,4,7,8-PeCDF		057117-31-4		464.7	deg C	6	737.85	
1,2,3,7,8-PeCDF		057117-41-6		464.7	deg C	6	737.85	using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF		070648-26-9		487.7	deg C	6	760.85	
1,2,3,6,7,8-HxCDF		057117-44-9		487.7	deg C	6	760.85	
1,2,3,7,8,9-HxCDF		072918-21-9		487.7	deg C	6	760.85	using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF		060851-34-5		487.7	deg C	6	760.85	using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF		067562-39-4		507.2	deg C	6	780.35	
1,2,3,4,7,8,9-HpCDF		055673-89-7		507.2	deg C	6	780.35	
OCDF		039001-02-0		537	deg C	6	810.15	

NAME							BOILING POINT	
							for V/P	
								boiling
			boiling	boiling	boiling	boiling	**boiling**	point
			point	point	point	point	**point**	data
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	**deg K**	notes
biphenyl	0	000092-52-4		255	deg C	5	528.15	
2-PCB	1	002051-60-7		274	deg C	5	547.15	
3-PCB	2	002051-61-8		284	deg C	5	557.15	
4-PCB	3	002051-62-9		291	deg C	5	564.15	
count								
average								
standard deviation								
minimum								
maximum								
2,2'-PCB	4	013029-08-8		***not in ref 5***			**565**	**estimated using Tb vs Tm regression**
2,3-PCB	5	016605-91-7		***not in ref 5***			**508**	**estimated using Tb vs Tm regression**
2,4-PCB	7	033284-50-3		***not in ref 5***			**531**	**estimated using Tb vs Tm regression**
2,4'-PCB	8	034883-43-7		***not in ref 5***			**548**	**estimated using Tb vs Tm regression**
2,5-PCB	9	034883-39-1		***not in ref 5***			**532**	**estimated using Tb vs Tm regression**
2,6-PCB	10	033146-45-1		***not in ref 5***			**541**	**estimated using Tb vs Tm regression**
3,3'-PCB	11	002050-67-1		322	deg C	5	595.15	
3,4-PCB	12	002974-92-7		***not in ref 5***			**554**	**estimated using Tb vs Tm regression**
3,5-PCB	14	034883-41-5		***not in ref 5***			**537**	**estimated using Tb vs Tm regression**
4,4'-PCB	15	002050-68-2		315	deg C	5	588.15	
count								
average								
standard deviation								
minimum								
maximum								

NAME							BOILING POINT	
common chemical name	IUPAC #	cas # (1)	boiling point range	boiling point average	boiling point units	boiling point ref	**for V/P boiling point deg K**	boiling point data notes
2,2',3-PCB	16	038444-78-9		***not in ref 5***			**534**	**estimated using Tb vs Tm regression**
2,2',5-PCB	18	037680-65-2		***not in ref 5***			**549**	**estimated using Tb vs Tm regression**
2,3,3'-PCB	20	038444-84-7		***not in ref 5***			**549**	**estimated using Tb vs Tm regression**
2,3,4-PCB	21	055702-46-0		***not in ref 5***			**603**	**estimated using Tb vs Tm regression**
2,3',5-PCB	26	038444-85-8		***not in ref 5***			**546**	**estimated using Tb vs Tm regression**
2,4,4'-PCB	28	007012-37-5		***not in ref 5***			**561**	**estimated using Tb vs Tm regression**
2,4,5-PCB	29	015862-07-4		***not in ref 5***			**581**	**estimated using Tb vs Tm regression**
2,4,6-PCB	30	035693-92-6		***not in ref 5***			**566**	**estimated using Tb vs Tm regression**
2,4',5,-PCB	31	016606-02-3		***not in ref 5***			**571**	**estimated using Tb vs Tm regression**
2',3,4-PCB	33	038444-86-9		***not in ref 5***			**564**	**estimated using Tb vs Tm regression**
3,3',4-PCB	35	037680-69-6		***not in ref 5***			**589**	**estimated using Tb vs Tm regression**
3,4,4'-PCB	37	038444-90-5		***not in ref 5***			**589**	**estimated using Tb vs Tm regression**
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3'-PCB	40	038444-93-8		***not in ref 5***			**621**	**estimated using Tb vs Tm regression**
2,2',3,5'-PCB	44	041464-39-5		***not in ref 5***			**552**	**estimated using Tb vs Tm regression**
2,2',4,4'-PCB	47	002437-79-8		***not in ref 5***			**585**	**estimated using Tb vs Tm regression**
2,2',4,5'-PCB	49	041464-40-8		***not in ref 5***			**568**	**estimated using Tb vs Tm regression**
2,2',4,6-PCB	50	062796-65-0		***not in ref 5***			**552**	**estimated using Tb vs Tm regression**
2,2',4,6'-PCB	51	068194-04-7		***not in ref 5***			**508**	**estimated using Tb vs Tm regression**
2,2,5,5'-PCB	52	035693-99-3		***not in ref 5***			**589**	**estimated using Tb vs Tm regression**
2,2,5,6'-PCB	53	041464-41-9		***not in ref 5***			**605**	**estimated using Tb vs Tm regression**
2,2,6,6'-PCB	54	015968-05-5		***not in ref 5***			**693**	**estimated using Tb vs Tm regression**
2,3,4,4'-PCB	60	033025-41-1		***not in ref 5***			**640**	**estimated using Tb vs Tm regression**
2,3,4,5-PCB	61	033284-53-6		***not in ref 5***			**594**	**estimated using Tb vs Tm regression**
2,3,5,6-PCB	65	033284-54-7		***not in ref 5***			**582**	**estimated using Tb vs Tm regression**
2,3,4,4'-PCB	66	032598-10-0		***not in ref 5***			**624**	**estimated using Tb vs Tm regression**
2,3',4',5-PCB	70	032598-11-1		***not in ref 5***			**605**	**estimated using Tb vs Tm regression**
2,4,4',6-PCB	75	032598-12-2		***not in ref 5***			**566**	**estimated using Tb vs Tm regression**
3,3',4,4'-PCB	77	032598-13-3		***not in ref 5***			**676**	**estimated using Tb vs Tm regression**
3,3',5,5'-PCB	80	033284-52-5		***not in ref 5***			**661**	**estimated using Tb vs Tm regression**
3,4,4',5-PCB	81	070362-50-4		***not in ref 5***			**659**	**estimated using Tb vs Tm regression**
count								
average								
standard deviation								
minimum								
maximum								

NAME							**BOILING POINT**	
							for V/P	
common chemical name	IUPAC #	cas # (1)	boiling point range	boiling point average	boiling point units	boiling point ref	**boiling point deg K**	boiling point data notes
2,2',3,3',5-PCB	83	060145-20-2		***not in ref 5***			**586**	**estimated using Tb vs Tm regression**
2,2',3,4,5-PCB	86	065510-45-4		***not in ref 5***			**601**	**estimated using Tb vs Tm regression**
2,2',3,4,5'-PCB	87	038380-02-8		***not in ref 5***			**614**	**estimated using Tb vs Tm regression**
2,2',3,4,6-PCB	88	055215-17-3		***not in ref 5***			**601**	**estimated using Tb vs Tm regression**
2,2',3,5,6-PCB	95	038379-99-6		***not in ref 5***			**601**	**estimated using Tb vs Tm regression**
2,2',4,4',5-PCB	99	038380-01-7		***not in ref 5***			**564**	**estimated using Tb vs Tm regression**
2,2',4,4',6-PCB	100	039485-83-1		***not in ref 5***			**508**	**estimated using Tb vs Tm regression**
2,2',4,5,5'-PCB	101	037680-73-2		***not in ref 5***			**579**	**estimated using Tb vs Tm regression**
2,2',4,6,6'-PCB	104	056558-16-8		***not in ref 5***			**590**	**estimated using Tb vs Tm regression**
2,3,3',4,4'-PCB	105	032598-14-4		***not in ref 5***			**606**	**estimated using Tb vs Tm regression**
2,3,3',4',6-PCB	110	038380-03-9		***not in ref 5***			**558**	**estimated using Tb vs Tm regression**
2,3,4,4',5-PCB	114	074472-37-0		***not in ref 5***			**612**	**estimated using Tb vs Tm regression**
2,3,4,5,6-PCB	116	018259-05-7		***not in ref 5***			**624**	**estimated using Tb vs Tm regression**
2,3',4,4',5-PCB	118	031508-00-6		***not in ref 5***			**608**	**estimated using Tb vs Tm regression**
2',3,4,5,5'-PCB	124	070424-70-3		***not in ref 5***			**617**	**estimated using Tb vs Tm regression**
3,3',4,4',5-PCB	126	057465-28-8		***not in ref 5***			**658**	**estimated using Tb vs Tm regression**
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4'-PCB	128	038380-07-3		***not in ref 5***			**648**	**estimated using Tb vs Tm regression**
2,2',3,3',4,5-PCB	129	055215-18-4		***not in ref 5***			**587**	**estimated using Tb vs Tm regression**
2,2',3,3',5,6-PCB	134	052704-70-8		***not in ref 5***			**601**	**estimated using Tb vs Tm regression**
2,2',3,3',6,6'-PCB	136	038411-22-2		***not in ref 5***			**613**	**estimated using Tb vs Tm regression**
2,2',3,4,4',5'-PCB	138	035065-28-2		***not in ref 5***			**583**	**estimated using Tb vs Tm regression**
2,2',3,4',5',6-PCB	149	038380-04-0		***not in ref 5***			**581**	**estimated using Tb vs Tm regression**
2,2',4,4',5,5'-PCB	153	035065-27-1		***not in ref 5***			**604**	**estimated using Tb vs Tm regression**
2,2',4,4',6,6'-PCB	155	033979-03-2		***not in ref 5***			**614**	**estimated using Tb vs Tm regression**
2,3,3',4,4',5-PCB	156	038380-08-4		***not in ref 5***			**629**	**estimated using Tb vs Tm regression**
2,3,3',4,4',5'-PCB	157	069782-90-7		***not in ref 5***			**659**	**estimated using Tb vs Tm regression**
2,3',4,4',5,5'-PCB	167	052663-72-6		***not in ref 5***			**625**	**estimated using Tb vs Tm regression**
3,3',4,4',5,5'-PCB	169	032774-16-6		***not in ref 5***			**696**	**estimated using Tb vs Tm regression**
count								
average								
standard deviation								
minimum								
maximum								

NAME							BOILING POINT	
							for V/P	boiling
			boiling	boiling	boiling	boiling	**boiling**	point
			point	point	point	point	**point**	data
common chemical name	IUPAC #	cas # (1)	range	average	units	ref	**deg K**	notes
2,2',3,3',4,4',5-PCB	170	035065-30-6		***not in ref 5***			**636**	**estimated using Tb vs Tm regression**
2,2',3,3',4,4',6-PCB	171	052663-71-5		***not in ref 5***			**622**	**estimated using Tb vs Tm regression**
2,2',3,4,4',5,5'-PCB	180	035065-29-3		***not in ref 5***			**611**	**estimated using Tb vs Tm regression**
2,2',3,4,5,5',6-PCB	185	052712-05-7		***not in ref 5***			**647**	**estimated using Tb vs Tm regression**
2,2',3,4',5,5',6-PCB	187	052663-68-0		***not in ref 5***			**605**	**estimated using Tb vs Tm regression**
2,3,3',4,4',5,5'-PCB	189	039635-31-9		***not in ref 5***			**659**	**estimated using Tb vs Tm regression**
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7		***not in ref 5***			**656**	**estimated using Tb vs Tm regression**
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4		***not in ref 5***			**659**	**estimated using Tb vs Tm regression**
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9		***not in ref 5***			**700**	**estimated using Tb vs Tm regression**
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3		***not in ref 5***			**707**	**estimated using Tb vs Tm regression**
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1		***not in ref 5***			**678**	**estimated using Tb vs Tm regression**
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3		***not in ref 5***			**793**	**estimated using Tb vs Tm regression**

NAME

VAPOR PRESSURE - solid phase

common chemical name	IUPAC #	cas # (1)	P sub s solid phase vapor pressure	units	at what temp?	temp units	refer	for V/P calculation solid Vp atm	T(Vp) deg K	data notes
octachlorostyrene		029082-74-4	1.32E-005	mm Hg	25	deg C	85	1.7E-008	298.15	SRC data set cites estimate by Neely and Blau, 1985
4-bromophenyl phenyl ether		000101-55-3								
3,3'-dichlorobenzidene		000091-94-1	4.5E-009	mm Hg	20	deg C	ATSI	5.9E-012	293.15	this is much lower than the value in MacKay's compilation, which came from M
1,3-dinitropyrene		075321-20-9	1.93E-008	mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
1,6-dinitropyrene		042397-64-8	1.93E-008	mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
1,8-dinitropyrene		042397-65-9	1.93E-008	mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
2,7-dinitropyrene		117929-15-4	1.93E-008	mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
dinitropyrenes (mixed)		078432-19-6	1.93E-008	mm Hg	25	deg	91	2.5E-011	298.15	estimated: see ref 91
hexachloro-1,3-butadiene		000087-68-3								
4,4'-methylene bis(2-chloroaniline)		000101-14-4	1E-005	mm Hg	25	deg C	16	1.3E-008	298.15	data for other temperatures also reported; note that SRC reports a much lower
pentachlorophenol		000087-86-5	0.00415	Pa	25	deg C	8	4.1E-008	298.15	
aldrin		000309-00-2	3.75E-005	mm Hg	20	deg C	49	1.6E-007	298.15	use data from ref 84 for V/P calc; ATSDR much different.
dieldrin		000060-57-1	3.75E-006	mm Hg	20	deg C	49	7.8E-009	298.15	use data from ref 84 for V/P calc; ATSDR much different.
p,p'-DDT		000050-29-3	1.6E-007	mm Hg	20	deg C	85	2.1E-010	293.15	
p,p'-DDD		000072-54-8	6.70E-007	mm Hg	20	deg C	85	8.8E-010	293.15	
p,p'-DDE		000072-55-9	6.0E-006	mm Hg	25	deg C	85	7.9E-009	298.15	
heptachlor		000076-44-8	4E-004	mm Hg	25	deg C	9; 85	5.3E-007	298.15	expt'l
heptachlor epoxide		001024-57-3	1.95E-005	mm Hg	30	deg C	3; 85	2.6E-008	303.15	ref 43 lists as estimated; ref 85 lists as expt'l, and gives reference
methoxychlor		000072-43-5	1.4E-006	mm Hg	25	deg C	25	1.9E-009	298.15	estimated based on EPA P-Chem Program; SRC data set gives a value of 2.5
mirex		002385-85-5	8E-007	mm Hg	25	deg C	85	1.1E-009	298.15	
toxaphene		008001-35-2								
endrin		000072-20-8	3E-006	mm Hg	20	deg C	43	3.9E-009	293.15	
alpha-hexachlorocyclohexane		000319-84-6	4.5E-005	mm Hg	25	deg C	85	5.9E-008	298.15	Schwabe and Legler 1960; extrapolated
beta-hexachlorocyclohexane		000319-85-7	4.66E-007	mm Hg	25	deg C	85	6.1E-010	298.15	Schwabe and Legler 1960; extrapolated
delta-hexachlorocyclohexane		000319-86-8	3.52E-005	mm Hg	25	deg C	85	4.6E-008	298.15	Schwabe and Legler 1960; extrapolated
gamma-hexachlorocyclohexane		000058-89-9	4.0E-008	atm	25	deg C	93	4.0E-008	298.15	see note 93
mixed hexachlorocyclohexanes		000319-84-6								

NAME

VAPOR PRESSURE - solid phase

common chemical name	IUPAC #	cas # (1)	P sub s solid phase vapor pressure	units	at what temp?	temp units	refer	**for V/P calculation** **solid** **Vp** **atm**	**T(Vp)** **deg K**	data notes
cadmium		007440-43-9								
cadmium carbonate		000513-78-0								
cadmium chloride		010108-64-2								
cadmium oxide		001306-19-0	1	mm Hg	1000	deg C	75	1.3E-003	1273.15	
cadmium sulfate		010124-36-4								
cadmium sulfide		001306-23-6								
elemental mercury		007439-97-6								
mercury oxide		021908-53-2								
mercuric chloride		007487-94-7	1	mm Hg	136.2	deg C	94	1.3E-003	409.35	
monomethyl mercury chloride		000115-09-3	0.0085	mm Hg	25	deg C	95	1.1E-005	298.15	note: HSDB gives much higher vapor pressure
dimethyl mercury		000593-74-8								
tetraethyl lead		000078-00-2								
tetramethyl lead		000075-74-1								
triethyl lead radical (1+ cation)		014570-15-1								
triethyl lead hydride		005224-23-7								
triethyl lead chloride		001067-14-7								
diethyl lead radical (2+ cation)		024952-65-6								
diethyl lead dihydride		081494-11-3								
diethyl lead dichloride		013231-90-8								
trimethyl lead radical (1+ cation)		014570-16-2								
trimethyl lead hydride		007442-13-9								
trimethyl lead chloride		001520-78-1								
dimethyl lead radical (2+ cation)		021774-13-0								
dimethyl lead dihydride		030691-92-0								
dimethyl lead dichloride		001520-77-0								
bis (tributyltin) oxide		000056-35-9								
tributyl tin		000688-75-3								
tributyltin fluoride		001983-10-4								
tributyltin chloride		001461-22-9								
tributyltin hydroxide		001067-97-6								
tributyltin naphthenate										
tris(tributylstannyl) phosphate		013435-05-7								

NAME

VAPOR PRESSURE - solid phase

common chemical name	IUPAC #	cas # (1)	P sub s solid phase vapor pressure	units	at what temp?	temp units	refer	for V/P calculation solid Vp atm	T(Vp) deg K	data notes
1,4-dichlorobenzene		000106-46-7	90.2	Pa	25	deg C	5	8.9E-004	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,4-tetrachlorobenzene		000634-66-2	5.2	Pa	25	deg C	5	5.1E-005	298.15	since a solid at room temp; used saturated Vp for this
1,2,4,5-tetrachlorobenzene		000095-94-3	0.72	Pa	25	deg C	5	7.1E-006	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,5-tetrachlorobenzene		000634-90-2	9.8	Pa	25	deg C	5	9.7E-005	298.15	since a solid at room temp; used saturated Vp for this
pentachlorobenzene		000608-93-5	0.22	Pa	25	deg C	5	2.2E-006	298.15	since a solid at room temp; used saturated Vp for this
hexachlorobenzene		000118-74-1	0.0023	Pa	25	deg C	5	2.3E-008	298.15	since a solid at room temp; used saturated Vp for this
naphthalene		000091-20-3	10.4	Pa	25	deg C	6	1.0E-004	298.15	
acenaphthene		000083-32-9	0.3	Pa	25	deg C	6	3.0E-006	298.15	
acenaphthylene		000208-96-8	0.9	Pa	25	deg C	6	8.9E-006	298.15	
fluorene		000086-73-7	0.09	Pa	25	deg C	6	8.9E-007	298.15	
phenanthrene		000085-01-8	0.02	Pa	25	deg C	6	2.0E-007	298.15	
anthracene		000120-12-7	0.001	Pa	25	deg C	6	9.9E-009	298.15	
pyrene		000129-00-0	0.0006	Pa	25	deg C	6	5.9E-009	298.15	
fluoranthene		000206-44-0	0.00123	Pa	25	deg C	6	1.2E-008	298.15	
chrysene		000218-01-9	5.7E-007	Pa	25	deg C	6	5.6E-012	298.15	
benz [a] anthracene		000056-55-3	3.1E-008	mm Hg	25	deg C	85	4.0E-011	298.15	from SRC data set; a "new" - presumably better - value to use, to see if V/P e
benzo [b] fluoranthene		000205-99-2	5.0E-007	mm Hg	25	deg C	80	6.6E-010	298.15	SRC data set
benzo [j] fluoranthene		000205-82-3	1.5E-008	mm Hg	25	deg C	81	2.0E-011	298.15	HSDB 1994, cited in ATSDR PAH
benzo [k] fluoranthene		000207-08-9	5.2E-008	Pa	25	deg C	6	5.1E-013	298.15	
benzo [a] pyrene		000050-32-8	7.0E-007	Pa	25	deg C	6	6.9E-012	298.15	
benzo [e] pyrene		000192-97-2	7.4E-007	Pa	25	deg C	6	7.3E-012	298.15	
perylene		000198-55-0	1.4E-008	Pa	25	deg C	6	1.4E-013	298.15	
benzo [g,h,i] perylene		000191-24-2	1.0E-010	mm Hg	25	deg C	10	1.4E-013	298.15	ref 10 cited in ATSDR-PAH
dibenz [a,h] anthracene		000053-70-3	3.7E-010	Pa	25	deg C	6	3.7E-015	298.15	
indeno [1,2,3-c,d] pyrene		000193-39-5	1.0E-010	mm Hg	**20**	deg C	82	1.4E-013	293.15	20 deg C; cited in SRC data set

NAME								VAPOR PRESSURE - solid phase		
			P sub s					for V/P calculation		
			solid					----------------	------------	
			phase					**solid**		
			vapor		at what	temp		**Vp**	**T(Vp)**	data
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	refer	**atm**	**deg K**	notes
2,3,7,8-TCDD		001746-01-6	7.4E-010	mmHg	25	deg C	78	9.7E-013	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,7,8-PeCDD		040321-76-4	8.8E-008	Pa	25	deg C	6	8.7E-013	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,4,7,8-HxCDD		039227-28-6	5.1E-009	Pa	25	deg C	6	5.0E-014	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,6,7,8-HxCDD		057653-85-7	5.1E-009	Pa	25	deg C	6	5.0E-014	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,7,8,9-HxCDD		019408-74-3	5.1E-009	Pa	25	deg C	6	5.0E-014	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,4,6,7,8-HpCDD		035822-46-9	7.5E-010	Pa	25	deg C	6	7.4E-015	298.15	since a solid at room temp; used saturated Vp for this
OCDD		003268-87-9	1.1E-010	Pa	25	deg C	6	1.1E-015	298.15	since a solid at room temp; used saturated Vp for this
2,3,7,8-TCDF		051207-31-9	2.0E-006	Pa	25	deg C	6	2.0E-011	298.15	since a solid at room temp; used saturated Vp for this
2,3,4,7,8-PeCDF		057117-31-4	3.5E-007	Pa	25	deg C	6	3.5E-012	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,7,8-PeCDF		057117-41-6	3.5E-007	Pa	25	deg C	6	3.5E-012	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,4,7,8-HxCDF		070648-26-9	3.2E-008	Pa	25	deg C	6	3.2E-013	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,6,7,8-HxCDF		057117-44-9	3.5E-008	Pa	25	deg C	6	3.5E-013	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,7,8,9-HxCDF		072918-21-9	3.35E-008	Pa	25	deg C	6	3.3E-013	298.15	since a solid at room temp; used saturated Vp for this
2,3,4,6,7,8-HxCDF		060851-34-5	3.35E-008	Pa	25	deg C	6	3.3E-013	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,4,6,7,8-HpCDF		067562-39-4	4.7E-009	Pa	25	deg C	6	4.6E-014	298.15	since a solid at room temp; used saturated Vp for this
1,2,3,4,7,8,9-HpCDF		055673-89-7	6.2E-009	Pa	25	deg C	6	6.1E-014	298.15	since a solid at room temp; used saturated Vp for this
OCDF		039001-02-0	5.0E-010	Pa	25	deg C	6	4.9E-015	298.15	since a solid at room temp; used saturated Vp for this

NAME			**VAPOR PRESSURE - solid phase**							
			P sub s solid phase vapor					**for V/P calculation** **solid**		
					at what	temp		**Vp**	**T(Vp)**	data
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	refer	**atm**	**deg K**	notes
biphenyl	0	000092-52-4	1.3	Pa	25	deg C	5	1.3E-005	298.15	
2-PCB	1	002051-60-7	2.04	Pa	25	deg C	5			
3-PCB	2	002051-61-8	1	Pa	25	deg C	5			
4-PCB	3	002051-62-9	0.279	Pa	25	deg C	5			
count										
average										
standard deviation										
minimum										
maximum										
2,2'-PCB	4	013029-08-8	0.265	Pa	25	deg C	5			
2,3-PCB	5	016605-91-7	***not in ref 5; see liquid estm at right***							
2,4-PCB	7	033284-50-3	0.254	Pa	25	deg C	5			
2,4'-PCB	8	034883-43-7	**2.09E-003**	**mm Hg**	**25**	**deg C**	**85**	2.8E-006	298.15	
2,5-PCB	9	034883-39-1	0.18	Pa	25	deg C	5			
2,6-PCB	10	033146-45-1	**1.91E-004**	**mm Hg**	**25**	**deg C**	**85**	2.5E-007	298.15	
3,3'-PCB	11	002050-67-1	0.027	Pa	25	deg C	5			
3,4-PCB	12	002974-92-7	**1.91E-004**	**mm Hg**	**25**	**deg C**	**85**	2.5E-007	298.15	
3,5-PCB	14	034883-41-5	0.105	Pa	25	deg C	5			
4,4'-PCB	15	002050-68-2	0.0048	Pa	25	deg C	5			
count										
average										
standard deviation										
minimum										
maximum										

NAME								**VAPOR PRESSURE - solid phase**		
			P sub s					**for V/P calculation**		
			solid							
			phase					**solid**		
			vapor		at what	temp		**Vp**	**T(Vp)**	data
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	refer	**atm**	**deg K**	notes
2,2',3-PCB	16	038444-78-9	***not in ref 5 or 85***							
2,2',5-PCB	18	037680-65-2	0.143	Pa	25	deg C	5			
2,3,3'-PCB	20	038444-84-7	**4E-005**	**mm Hg**	**25**	**deg C**	**85**	5.3E-008	298.15	
2,3,4-PCB	21	055702-46-0	**4E-005**	**mm Hg**	**25**	**deg C**	**85**	5.3E-008	298.15	
2,3',5-PCB	26	038444-85-8	***not in ref 5 or 85***							
2,4,4'-PCB	28	007012-37-5	**1.95E-004**	**mm Hg**	**25**	**deg C**	**85**	2.6E-007	298.15	
2,4,5-PCB	29	015862-07-4	0.132	Pa	25	deg C	5			
2,4,6-PCB	30	035693-92-6	0.0384	Pa	25	deg C	5			
2,4',5,-PCB	31	016606-02-3	***not in ref 5 or 85***							
2',3,4-PCB	33	038444-86-9	0.0136	Pa	25	deg C	5			
3,3',4-PCB	35	037680-69-6	***not in ref 5 or 85***							
3,4,4'-PCB	37	038444-90-5	***not in ref 5 or 85***							
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3'-PCB	40	038444-93-8	0.00225	Pa	25	deg C	5			
2,2',3,5'-PCB	44	041464-39-5	**8.45E-006**	**mm Hg**	**25**	**deg C**	**85**	1.1E-008	298.15	
2,2',4,4'-PCB	47	002437-79-8	0.0054	Pa	25	deg C	5			
2,2',4,5'-PCB	49	041464-40-8	**8.48E-006**	**mm Hg**	**25**	**deg C**	**85**	1.1E-008	298.15	
2,2',4,6-PCB	50	062796-65-0	**8.45E-006**	**mm Hg**	**25**	**deg C**	**85**	1.1E-008	298.15	
2,2',4,6'-PCB	51	068194-04-7	***not in ref 5; a liquid at room temp***							
2,2,5,5'-PCB	52	035693-99-3	0.0049	Pa	25	deg C	5			
2,2,5,6'-PCB	53	041464-41-9	**2.05E-004**	**mm Hg**	**25**	**deg C**	**85**	2.7E-007	298.15	
2,2,6,6'-PCB	54	015968-05-5	**8.45E-006**	**mm Hg**	**25**	**deg C**	**85**	1.1E-008	298.15	
2,3,4,4'-PCB	60	033025-41-1	**8.45E-006**	**mm Hg**	**25**	**deg C**	**85**	1.1E-008	298.15	
2,3,4,5-PCB	61	033284-53-6	**3.75E-005**	**mm Hg**	**25**	**deg C**	**85**	4.9E-008	298.15	
2,3,5,6-PCB	65	033284-54-7	***not in ref 5 or 85***							
2,3,4,4'-PCB	66	032598-10-0	**8.45E-006**	**mm Hg**	**25**	**deg C**	**85**	1.1E-008	298.15	
2,3',4',5-PCB	70	032598-11-1	**4.08E-005**	**mm Hg**	**25**	**deg C**	**85**	5.4E-008	298.15	
2,4,4',6-PCB	75	032598-12-2	***not in ref 5 or 85***							
3,3',4,4'-PCB	77	032598-13-3	0.0000588	Pa	25	deg C	5			
3,3',5,5'-PCB	80	033284-52-5	**8.45E-006**	**mm Hg**	**25**	**deg C**	**85**	1.1E-008	298.15	
3,4,4',5-PCB	81	070362-50-4	***not in ref 5 or 85***							
count										
average										
standard deviation										
minimum										
maximum										

NAME

VAPOR PRESSURE - solid phase

			P sub s					**for V/P calculation**		
			solid					----------------	------------	
			phase					**solid**		
			vapor		at what	temp		**Vp**	**T(Vp)**	data
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	refer	**atm**	**deg K**	notes
2,2',3,3',5-PCB	83	060145-20-2	***not in ref 5 or 85***							
2,2',3,4,5-PCB	86	065510-45-4	0.00927	Pa	25	deg C	5			
2,2',3,4,5'-PCB	87	038380-02-8	0.000304	Pa	25	deg C	5			
2,2',3,4,6-PCB	88	055215-17-3	**2.22E-006**	**mm Hg**	**25**	**deg C**	**85**	2.9E-009	298.15	
2,2',3,5,6-PCB	95	038379-99-6	***not in ref 5 or 85***							
2,2',4,4',5-PCB	99	038380-01-7	**2.2E-005**	**mm Hg**	**25**	**deg C**	**85**	2.9E-008	298.15	
2,2',4,4',6-PCB	100	039485-83-1	**liquid at room temperature**							
2,2',4,5,5'-PCB	101	037680-73-2	0.00109	Pa	25	deg C	5			
2,2',4,6,6'-PCB	104	056558-16-8	***not in ref 5 or 85***							
2,3,3',4,4'-PCB	105	032598-14-4	**6.53E-006**	**mm Hg**	**25**	**deg C**	**85**	8.6E-009	298.15	
2,3,3',4',6-PCB	110	038380-03-9	**2.22E-006**	**mm Hg**	**25**	**deg C**	**85**	2.9E-009	298.15	
2,3,4,4',5-PCB	114	074472-37-0	***not in ref 5 or 85***							
2,3,4,5,6-PCB	116	018259-05-7	**2.22E-006**	**mm Hg**	**25**	**deg C**	**85**	2.9E-009	298.15	
2,3',4,4',5-PCB	118	031508-00-6	***not in ref 5 or 85***							
2',3,4,5,5'-PCB	124	070424-70-3	***not in ref 5 or 85***							
3,3',4,4',5-PCB	126	057465-28-8	***not in ref 5 or 85***							
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4'-PCB	128	038380-07-3	0.0000198	Pa	25	deg C	5			
2,2',3,3',4,5-PCB	129	055215-18-4	**5.81E-007**	**mm Hg**	**25**	**deg C**	**85**	7.6E-010	298.15	
2,2',3,3',5,6-PCB	134	052704-70-8	**1.10E-006**	**mm Hg**	**25**	**deg C**	**85**	1.4E-009	298.15	
2,2',3,3',6,6'-PCB	136	038411-22-2	**5.81E-007**	**mm Hg**	**25**	**deg C**	**85**	7.6E-010	298.15	
2,2',3,4,4',5'-PCB	138	035065-28-2	**3.79E-006**	**mm Hg**	**25**	**deg C**	**85**	5.0E-009	298.15	
2,2',3,4',5',6-PCB	149	038380-04-0	**8.43E-006**	**mm Hg**	**25**	**deg C**	**85**	1.1E-008	298.15	
2,2',4,4',5,5'-PCB	153	035065-27-1	0.000119	Pa	25	deg C	5			
2,2',4,4',6,6'-PCB	155	033979-03-2	0.00048	Pa	25	deg C	5			
2,3,3',4,4',5-PCB	156	038380-08-4	**1.61E-006**	**mm Hg**	**25**	**deg C**	**85**	2.1E-009	298.15	
2,3,3',4,4',5'-PCB	157	069782-90-7	***not in ref 5 or 85***							
2,3',4,4',5,5'-PCB	167	052663-72-6	**5.81E-007**	**mm Hg**	**25**	**deg C**	**85**	7.6E-010	298.15	
3,3',4,4',5,5'-PCB	169	032774-16-6	**5.81E-007**	**mm Hg**	**25**	**deg C**	**85**	7.6E-010	298.15	
count										
average										
standard deviation										
minimum										
maximum										

NAME								**VAPOR PRESSURE - solid phase**		
			P sub s solid phase vapor pressure	units	at what temp?	temp units	refer	**for V/P calculation** **solid** **Vp** **atm**	**T(Vp)** **deg K**	data notes
common chemical name	IUPAC #	cas # (1)								
2,2',3,3',4,4',5-PCB	170	035065-30-6	**6.28E-007**	**mm Hg**	**25**	**deg C**	**85**	8.3E-010	298.15	
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.0000273	Pa	25	deg C	5			
2,2',3,4,4',5,5'-PCB	180	035065-29-3	**9.77E-007**	**mm Hg**	**25**	**deg C**	**85**	1.3E-009	298.15	
2,2',3,4,5,5',6-PCB	185	052712-05-7	**1.3E-007**	**mm Hg**	**25**	**deg C**	**85**	1.7E-010	298.15	
2,2',3,4',5,5',6-PCB	187	052663-68-0	**1.3E-007**	**mm Hg**	**25**	**deg C**	**85**	1.7E-010	298.15	
2,3,3',4,4',5,5'-PCB	189	039635-31-9	***not in ref 5 or 85***							
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	**2.87E-008**	**mm Hg**	**25**	**deg C**	**85**	3.8E-011	298.15	
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0000266	Pa	25	deg C	5			
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	1.96E-007	Pa	25	deg C	5			
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	***not in ref 5 or 85***							
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	**7.6E-009**	**mm Hg**	**25**	**deg C**	**85**	1.0E-011	298.15	
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	5.02E-008	Pa	25	deg C	5			

			||||	**Vapor Pressure Estimation for**				||||
NAME			||||	**PCB's Using Correlation of**				||||
			||||	**Falconer and Bidleman, 1994**				||||
			||||			liq Vp		||||
			||||			at temp =		||||
			||||			**298.15**		||||
			||||			deg K		||||
common chemical name	IUPAC #	cas # (1)	||||	-mL	bL	Pa	NOTES	||||
octachlorostyrene		029082-74-4	||||					||||
4-bromophenyl phenyl ether		000101-55-3	||||					||||
3,3'-dichlorobenzidene		000091-94-1	||||					||||
1,3-dinitropyrene		075321-20-9	||||					||||
1,6-dinitropyrene		042397-64-8	||||					||||
1,8-dinitropyrene		042397-65-9	||||					||||
2,7-dinitropyrene		117929-15-4	||||					||||
dinitropyrenes (mixed)		078432-19-6	||||					||||
hexachloro-1,3-butadiene		000087-68-3	||||					||||
4,4'-methylene bis(2-chloroaniline)		000101-14-4	||||					||||
pentachlorophenol		000087-86-5	||||					||||
aldrin		000309-00-2	||||					||||
dieldrin		000060-57-1	||||					||||
p,p'-DDT		000050-29-3	||||					||||
p,p'-DDD		000072-54-8	||||					||||
p,p'-DDE		000072-55-9	||||					||||
heptachlor		000076-44-8	||||					||||
heptachlor epoxide		001024-57-3	||||					||||
methoxychlor		000072-43-5	||||					||||
mirex		002385-85-5	||||					||||
toxaphene		008001-35-2	||||					||||
endrin		000072-20-8	||||					||||
alpha-hexachlorocyclohexane		000319-84-6	||||					||||
beta-hexachlorocyclohexane		000319-85-7	||||					||||
delta-hexachlorocyclohexane		000319-86-8	||||					||||
gamma-hexachlorocyclohexane		000058-89-9	||||					||||
mixed hexachlorocyclohexanes		000319-84-6	||||					||||

NAME

Vapor Pressure Estimation for PCB's Using Correlation of Falconer and Bidleman, 1994

common chemical name	IUPAC #	cas # (1)	-mL	bL	liq Vp at temp = **298.15** deg K Pa	NOTES
cadmium		007440-43-9				
cadmium carbonate		000513-78-0				
cadmium chloride		010108-64-2				
cadmium oxide		001306-19-0				
cadmium sulfate		010124-36-4				
cadmium sulfide		001306-23-6				
elemental mercury		007439-97-6				
mercury oxide		021908-53-2				
mercuric chloride		007487-94-7				
monomethyl mercury chloride		000115-09-3				
dimethyl mercury		000593-74-8				
tetraethyl lead		000078-00-2				
tetramethyl lead		000075-74-1				
triethyl lead radical (1+ cation)		014570-15-1				
triethyl lead hydride		005224-23-7				
triethyl lead chloride		001067-14-7				
diethyl lead radical (2+ cation)		024952-65-6				
diethyl lead dihydride		081494-11-3				
diethyl lead dichloride		013231-90-8				
trimethyl lead radical (1+ cation)		014570-16-2				
trimethyl lead hydride		007442-13-9				
trimethyl lead chloride		001520-78-1				
dimethyl lead radical (2+ cation)		021774-13-0				
dimethyl lead dihydride		030691-92-0				
dimethyl lead dichloride		001520-77-0				
bis (tributyltin) oxide		000056-35-9				
tributyl tin		000688-75-3				
tributyltin fluoride		001983-10-4				
tributyltin chloride		001461-22-9				
tributyltin hydroxide		001067-97-6				
tributyltin naphthenate						
tris(tributylstannyl) phosphate		013435-05-7				

NAME

Vapor Pressure Estimation for PCB's Using Correlation of Falconer and Bidleman, 1994

common chemical name	IUPAC #	cas # (1)	-mL	bL	liq Vp at temp = **298.15** deg K Pa	NOTES
1,4-dichlorobenzene		000106-46-7				
1,2,3,4-tetrachlorobenzene		000634-66-2				
1,2,4,5-tetrachlorobenzene		000095-94-3				
1,2,3,5-tetrachlorobenzene		000634-90-2				
pentachlorobenzene		000608-93-5				
hexachlorobenzene		000118-74-1				
naphthalene		000091-20-3				
acenaphthene		000083-32-9				
acenaphthylene		000208-96-8				
fluorene		000086-73-7				
phenanthrene		000085-01-8				
anthracene		000120-12-7				
pyrene		000129-00-0				
fluoranthene		000206-44-0				
chrysene		000218-01-9				
benz [a] anthracene		000056-55-3				
benzo [b] fluoranthene		000205-99-2				
benzo [j] fluoranthene		000205-82-3				
benzo [k] fluoranthene		000207-08-9				
benzo [a] pyrene		000050-32-8				
benzo [e] pyrene		000192-97-2				
perylene		000198-55-0				
benzo [g,h,i] perylene		000191-24-2				
dibenz [a,h] anthracene		000053-70-3				
indeno [1,2,3-c,d] pyrene		000193-39-5				

			Vapor Pressure Estimation for			
NAME			**PCB's Using Correlation of**			
			Falconer and Bidleman, 1994			
					liq Vp	
					at temp =	
					298.15	
					deg K	
common chemical name	IUPAC #	cas # (1)	-mL	bL	Pa	NOTES
2,3,7,8-TCDD		001746-01-6				
1,2,3,7,8-PeCDD		040321-76-4				
1,2,3,4,7,8-HxCDD		039227-28-6				
1,2,3,6,7,8-HxCDD		057653-85-7				
1,2,3,7,8,9-HxCDD		019408-74-3				
1,2,3,4,6,7,8-HpCDD		035822-46-9				
OCDD		003268-87-9				
2,3,7,8-TCDF		051207-31-9				
2,3,4,7,8-PeCDF		057117-31-4				
1,2,3,7,8-PeCDF		057117-41-6				
1,2,3,4,7,8-HxCDF		070648-26-9				
1,2,3,6,7,8-HxCDF		057117-44-9				
1,2,3,7,8,9-HxCDF		072918-21-9				
2,3,4,6,7,8-HxCDF		060851-34-5				
1,2,3,4,6,7,8-HpCDF		067562-39-4				
1,2,3,4,7,8,9-HpCDF		055673-89-7				
OCDF		039001-02-0				

NAME

Vapor Pressure Estimation for PCB's Using Correlation of Falconer and Bidleman, 1994

common chemical name	IUPAC #	cas # (1)	-mL	bL	liq Vp at temp = **298.15** deg K Pa	NOTES
biphenyl	0	000092-52-4				
2-PCB	1	002051-60-7	3366	11.57	1.9E+000	
3-PCB	2	002051-61-8	3476	11.65	9.8E-001	
4-PCB	3	002051-62-9	3488	11.67	9.4E-001	
count						
average						
standard deviation						
minimum						
maximum						
2,2'-PCB	4	013029-08-8	3642	11.73	3.3E-001	
2,3-PCB	5	016605-91-7	3769	11.81	1.5E-001	
2,4-PCB	7	033284-50-3	3841	12.15	1.9E-001	
2,4'-PCB	8	034883-43-7	3769	11.84	1.6E-001	
2,5-PCB	9	034883-39-1	3862	12.22	1.8E-001	
2,6-PCB	10	033146-45-1	3642	11.74	3.3E-001	
3,3'-PCB	11	002050-67-1	3936	12.14	8.7E-002	
3,4-PCB	12	002974-92-7	3885	11.92	7.8E-002	
3,5-PCB	14	034883-41-5	3885	12.13	1.3E-001	
4,4'-PCB	15	002050-68-2	3971	12.18	7.3E-002	
count						
average						
standard deviation						
minimum						
maximum						

NAME

Vapor Pressure Estimation for PCB's Using Correlation of Falconer and Bidleman, 1994

common chemical name	IUPAC #	cas # (1)	-mL	bL	liq Vp at temp = **298.15** deg K Pa	NOTES
2,2',3-PCB	16	038444-78-9	3935	11.93	5.4E-002	
2,2',5-PCB	18	037680-65-2	3935	12.09	7.8E-002	
2,3,3'-PCB	20	038444-84-7	4075	12.12	2.8E-002	
2,3,4-PCB	21	055702-46-0	4075	12.11	2.8E-002	
2,3',5-PCB	26	038444-85-8	4075	12.28	4.1E-002	
2,4,4'-PCB	28	007012-37-5	4075	12.2	3.4E-002	
2,4,5-PCB	29	015862-07-4	4007	12.09	4.5E-002	
2,4,6-PCB	30	035693-92-6	3886	12.02	9.7E-002	
2,4',5,-PCB	31	016606-02-3	4058	12.05	2.8E-002	
2',3,4-PCB	33	038444-86-9	4075	12.09	2.6E-002	
3,3',4-PCB	35	037680-69-6	4242	12.37	1.4E-002	
3,4,4'-PCB	37	038444-90-5	4242	12.33	1.3E-002	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3'-PCB	40	038444-93-8	4271	12.32	9.9E-003	
2,2',3,5'-PCB	44	041464-39-5	4229	12.29	1.3E-002	
2,2',4,4'-PCB	47	002437-79-8	4229	12.37	1.5E-002	
2,2',4,5'-PCB	49	041464-40-8	4229	12.41	1.7E-002	
2,2',4,6-PCB	50	062796-65-0	**not given by Falconer & Bidleman**			
2,2',4,6'-PCB	51	068194-04-7	4117	12.2	2.5E-002	
2,2,5,5'-PCB	52	035693-99-3	4220	12.36	1.6E-002	
2,2,5,6'-PCB	53	041464-41-9	4114	12.24	2.8E-002	
2,2,6,6'-PCB	54	015968-05-5	3751	11.17	3.9E-002	
2,3,4,4'-PCB	60	033025-41-1	4382	12.42	5.3E-003	
2,3,4,5-PCB	61	033284-53-6	4382	12.78	1.2E-002	
2,3,5,6-PCB	65	033284-54-7	4229	12.33	1.4E-002	
2,3,4,4'-PCB	66	032598-10-0	4349	12.38	6.2E-003	
2,3',4',5-PCB	70	032598-11-1	4431	12.6	5.5E-003	
2,4,4',6-PCB	75	032598-12-2	4229	12.44	1.8E-002	
3,3',4,4'-PCB	77	032598-13-3	4552	12.61	2.2E-003	
3,3',5,5'-PCB	80	033284-52-5	4598	13.16	5.5E-003	
3,4,4',5-PCB	81	070362-50-4	4598	12.88	2.9E-003	
count						
average						
standard deviation						
minimum						
maximum						

			Vapor Pressure Estimation for			
NAME			**PCB's Using Correlation of**			
			Falconer and Bidleman, 1994			
					liq Vp	
					at temp =	
					298.15	
					deg K	
common chemical name	IUPAC #	cas # (1)	-mL	bL	Pa	NOTES
2,2',3,3',5-PCB	83	060145-20-2	4522	12.6	2.7E-003	
2,2',3,4,5-PCB	86	065510-45-4	4522	12.61	2.8E-003	
2,2',3,4,5'-PCB	87	038380-02-8	4562	12.66	2.3E-003	
2,2',3,4,6-PCB	88	055215-17-3	4399	12.53	6.0E-003	
2,2',3,5,6-PCB	95	038379-99-6	4399	12.48	5.3E-003	
2,2',4,4',5-PCB	99	038380-01-7	4533	12.68	3.0E-003	
2,2',4,4',6-PCB	100	039485-83-1	**not given by Falconer & Bidleman**			
2,2',4,5,5'-PCB	101	037680-73-2	4514	12.67	3.4E-003	
2,2',4,6,6'-PCB	104	056558-16-8	**4522**	**12.6**	**2.7E-003**	**use coefficients for IUPAC #83, which has a similar melting point**
2,3,3',4,4'-PCB	105	032598-14-4	4758	12.9	8.7E-004	
2,3,3',4',6-PCB	110	038380-03-9	4522	12.43	1.8E-003	
2,3,4,4',5-PCB	114	074472-37-0	4688	12.82	1.2E-003	
2,3,4,5,6-PCB	116	018259-05-7	4522	12.53	2.3E-003	
2,3',4,4',5-PCB	118	031508-00-6	4664	12.72	1.2E-003	
2',3,4,5,5'-PCB	124	070424-70-3	4688	12.62	7.9E-004	
3,3',4,4',5-PCB	126	057465-28-8	4956	13.31	4.9E-004	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4'-PCB	128	038380-07-3	4881	12.91	3.5E-004	
2,2',3,3',4,5-PCB	129	055215-18-4	4816	12.8	4.4E-004	
2,2',3,3',5,6-PCB	134	052704-70-8	4681	12.79	1.2E-003	
2,2',3,3',6,6'-PCB	136	038411-22-2	4303	11.63	1.6E-003	
2,2',3,4,4',5'-PCB	138	035065-28-2	4800	12.81	5.1E-004	
2,2',3,4',5',6-PCB	149	038380-04-0	4689	12.78	1.1E-003	
2,2',4,4',5,5'-PCB	153	035065-27-1	4775	12.85	6.8E-004	
2,2',4,4',6,6'-PCB	155	033979-03-2	4303	12.02	3.9E-003	
2,3,3',4,4',5-PCB	156	038380-08-4	4949	12.94	2.2E-004	
2,3,3',4,4',5'-PCB	157	069782-90-7	4994	13.05	2.0E-004	
2,3',4,4',5,5'-PCB	167	052663-72-6	4994	13.2	2.8E-004	
3,3',4,4',5,5'-PCB	169	032774-16-6	5313	13.64	6.6E-005	
count						
average						
standard deviation						
minimum						
maximum						

NAME

Vapor Pressure Estimation for PCB's Using Correlation of Falconer and Bidleman, 1994

common chemical name	IUPAC #	cas # (1)	-mL	bL	liq Vp at temp = **298.15** deg K Pa	NOTES
2,2',3,3',4,4',5-PCB	170	035065-30-6	5139	13.17	8.6E-005	
2,2',3,3',4,4',6-PCB	171	052663-71-5	5008	13.07	1.9E-004	
2,2',3,4,4',5,5'-PCB	180	035065-29-3	5042	13.03	1.3E-004	
2,2',3,4,5,5',6-PCB	185	052712-05-7	4962	13.15	3.2E-004	
2,2',3,4',5,5',6-PCB	187	052663-68-0	4911	12.96	3.1E-004	
2,3,3',4,4',5,5'-PCB	189	039635-31-9	5300	13.46	4.8E-005	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	5402	13.43	2.0E-005	
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	4851	12.99	5.2E-004	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	5526	13.57	1.1E-005	
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	5127	12.7	3.2E-005	
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	5127	12.68	3.0E-005	
count						
average						
standard deviation						
minimum						
maximum						
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	5402	13.27	1.4E-005	

NAME			VAPOR PRESSURE - liquid phase							
								for V/P calculation		
common chemical name	IUPAC #	cas # (1)	liquid phase vapor pressure	units	at wha temp?	temp units	referenc	liquid Vp atm	T(Vp) deg K	data notes
octachlorostyrene		029082-74-4								
4-bromophenyl phenyl ether		000101-55-3	0.2	Pa	25	deg C	7	2.0E-006	298.15	
3,3'-dichlorobenzidene		000091-94-1	6.41E-004	Pa	25	deg C	8			
1,3-dinitropyrene		075321-20-9								
1,6-dinitropyrene		042397-64-8								
1,8-dinitropyrene		042397-65-9								
2,7-dinitropyrene		117929-15-4								
dinitropyrenes (mixed)		078432-19-6								
hexachloro-1,3-butadiene		000087-68-3	20	Pa	25	deg C	7	2.0E-004	298.15	ref 99 gives same
4,4'-methylene bis(2-chloroaniline)		000101-14-4								
pentachlorophenol		000087-86-5	0.12	Pa	25	deg C	8			
aldrin		000309-00-2								
dieldrin		000060-57-1								
p,p'-DDT		000050-29-3								
p,p'-DDD		000072-54-8								
p,p'-DDE		000072-55-9								
heptachlor		000076-44-8								
heptachlor epoxide		001024-57-3								
methoxychlor		000072-43-5								
mirex		002385-85-5								
toxaphene		008001-35-2	6.69E-006	mm Hg	25	deg C	57	8.8E-009	298.15	Murphy paper says that its a subcooled liquid value...
endrin		000072-20-8								
alpha-hexachlorocyclohexane		000319-84-6								
beta-hexachlorocyclohexane		000319-85-7								
delta-hexachlorocyclohexane		000319-86-8								
gamma-hexachlorocyclohexane		000058-89-9								
mixed hexachlorocyclohexanes		000319-84-6								

NAME

VAPOR PRESSURE - liquid phase

common chemical name	IUPAC #	cas # (1)	liquid phase vapor pressure	units	at wha temp?	temp units	referenc	**for V/P calculation** **liquid Vp atm**	**T(Vp) deg K**	data notes
cadmium		007440-43-9	1	mm Hg	394	deg C	75, 94	1.3E-003	667.15	
cadmium carbonate		000513-78-0								
cadmium chloride		010108-64-2	10	mm Hg	656	deg C	75, 94	1.3E-002	929.15	
cadmium oxide		001306-19-0								
cadmium sulfate		010124-36-4								
cadmium sulfide		001306-23-6								
elemental mercury		007439-97-6	0.001201	mm Hg	20	deg C	94	1.6E-006	293.15	data at other temperatures also given
mercury oxide		021908-53-2								
mercuric chloride		007487-94-7								
monomethyl mercury chloride		000115-09-3								
dimethyl mercury		000593-74-8								
tetraethyl lead		000078-00-2	3.9E-001	mm Hg	25	deg C	85	5.1E-004	298.15	expt'l data
tetramethyl lead		000075-74-1	22.5	mm Hg	20	deg C	97	3.0E-002	293.15	
triethyl lead radical (1+ cation)		014570-15-1								
triethyl lead hydride		005224-23-7								
triethyl lead chloride		001067-14-7								
diethyl lead radical (2+ cation)		024952-65-6								
diethyl lead dihydride		081494-11-3								
diethyl lead dichloride		013231-90-8								
trimethyl lead radical (1+ cation)		014570-16-2								
trimethyl lead hydride		007442-13-9								
trimethyl lead chloride		001520-78-1								
dimethyl lead radical (2+ cation)		021774-13-0								
dimethyl lead dihydride		030691-92-0								
dimethyl lead dichloride		001520-77-0								
bis (tributyltin) oxide		000056-35-9	6.4E-007	mm Hg	20	deg C	97 (atm	8.4E-010	293.15	assuming liquid at this temp
tributyl tin		000688-75-3								
tributyltin fluoride		001983-10-4								
tributyltin chloride		001461-22-9								
tributyltin hydroxide		001067-97-6								
tributyltin naphthenate										
tris(tributylstannyl) phosphate		013435-05-7								

NAME

VAPOR PRESSURE - liquid phase

common chemical name	IUPAC #	cas # (1)	liquid phase vapor pressure	units	at wha temp?	temp units	referenc	for V/P calculation liquid Vp atm	T(Vp) deg K	data notes
1,4-dichlorobenzene		000106-46-7	170.19	Pa	25	deg C	5			
1,2,3,4-tetrachlorobenzene		000634-66-2	8.67	Pa	25	deg C	5			
1,2,4,5-tetrachlorobenzene		000095-94-3	9.6	Pa	25	deg C	5			
1,2,3,5-tetrachlorobenzene		000634-90-2	19.22	Pa	25	deg C	5			
pentachlorobenzene		000608-93-5	0.9565	Pa	25	deg C	5			
hexachlorobenzene		000118-74-1	0.2447	Pa	25	deg C	5			
naphthalene		000091-20-3	36.81	Pa	25	deg C	6			
acenaphthene		000083-32-9	1.52	Pa	25	deg C	6			
acenaphthylene		000208-96-8	4.14	Pa	25	deg C	6			
fluorene		000086-73-7	0.715	Pa	25	deg C	6			
phenanthrene		000085-01-8	0.113	Pa	25	deg C	6			
anthracene		000120-12-7	0.0778	Pa	25	deg C	6			
pyrene		000129-00-0	0.0119	Pa	25	deg C	6			
fluoranthene		000206-44-0	8.72E-003	Pa	25	deg C	6			
chrysene		000218-01-9	1.07E-004	Pa	25	deg C	6			
benz [a] anthracene		000056-55-3	6.06E-004	Pa	25	deg C	6			
benzo [b] fluoranthene		000205-99-2	***not given in reference 6***							
benzo [j] fluoranthene		000205-82-3	***not given in reference 6***							
benzo [k] fluoranthene		000207-08-9	4.12E-006	Pa	25	deg C	6			
benzo [a] pyrene		000050-32-8	2.13E-005	Pa	25	deg C	6			
benzo [e] pyrene		000192-97-2	2.41E-005	Pa	25	deg C	6			
perylene		000198-55-0	***not given in reference 6***							
benzo [g,h,i] perylene		000191-24-2	2.25E-005	Pa	25	deg C	6			
dibenz [a,h] anthracene		000053-70-3	9.16E-008	Pa	25	deg C	6			
indeno [1,2,3-c,d] pyrene		000193-39-5	***not given in reference 6***							

NAME

VAPOR PRESSURE - liquid phase

								for V/P calculation		
common chemical name	IUPAC #	cas # (1)	liquid phase vapor pressure	units	at wha temp?	temp units	referenc	**liquid Vp atm**	**T(Vp) deg K**	data notes
2,3,7,8-TCDD		001746-01-6	1.18E-004	Pa	25	deg C	6			
1,2,3,7,8-PeCDD		040321-76-4	4.23E-006	Pa	25	deg C	6			using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD		039227-28-6	1.45E-006	Pa	25	deg C	6			
1,2,3,6,7,8-HxCDD		057653-85-7	1.45E-006	Pa	25	deg C	6			using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD		019408-74-3	1.45E-006	Pa	25	deg C	6			using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD		035822-46-9	1.77E-007	Pa	25	deg C	6			
OCDD		003268-87-9	9.53E-007	Pa	25	deg C	6			
2,3,7,8-TCDF		051207-31-9	1.99E-004	Pa	25	deg C	6			
2,3,4,7,8-PeCDF		057117-31-4	1.72E-005	Pa	25	deg C	6			
1,2,3,7,8-PeCDF		057117-41-6	1.72E-005	Pa	25	deg C	6			using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF		070648-26-9	3.08E-006	Pa	25	deg C	6			
1,2,3,6,7,8-HxCDF		057117-44-9	3.61E-006	Pa	25	deg C	6			
1,2,3,7,8,9-HxCDF		072918-21-9	3.35E-006	Pa	25	deg C	6			using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF		060851-34-5	3.35E-006	Pa	25	deg C	6			using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF		067562-39-4	5.74E-007	Pa	25	deg C	6			
1,2,3,4,7,8,9-HpCDF		055673-89-7	5.39E-007	Pa	25	deg C	6			
OCDF		039001-02-0	1.01E-007	Pa	25	deg C	6			

NAME								**VAPOR PRESSURE - liquid phase**		
								for V/P calculation		
common chemical name	IUPAC #	cas # (1)	liquid phase vapor pressure	units	at wha temp?	temp units	referenc	**liquid Vp atm**	**T(Vp) deg K**	data notes
biphenyl	0	000092-52-4	3.69	Pa	25	deg C	5	3.6E-005	298.15	
2-PCB	1	002051-60-7	2.5	Pa	25	deg C	5	2.5E-005	298.15	
3-PCB	2	002051-61-8	1	Pa	25	deg C	5	9.9E-006	298.15	
4-PCB	3	002051-62-9	0.9	Pa	25	deg C	5	8.9E-006	298.15	
count										
average										
standard deviation										
minimum										
maximum										
2,2'-PCB	4	013029-08-8	0.6	Pa	25	deg C	5	5.9E-006	298.15	
2,3-PCB	5	016605-91-7	**1.91E-004**	**mm Hg**	**25**	**deg C**	**85**	2.5E-007	298.15	
2,4-PCB	7	033284-50-3	0.25	Pa	25	deg C	5	2.5E-006	298.15	
2,4'-PCB	8	034883-43-7	**not in ref 5; see solid estm at left**							
2,5-PCB	9	034883-39-1	0.18	Pa	25	deg C	5	1.8E-006	298.15	
2,6-PCB	10	033146-45-1	**not in ref 5; see solid estm at left**							
3,3'-PCB	11	002050-67-1	0.03	Pa	25	deg C	5	3.0E-007	298.15	
3,4-PCB	12	002974-92-7	**not in ref 5; see solid estm at left**							
3,5-PCB	14	034883-41-5	0.12	Pa	25	deg C	5	1.2E-006	298.15	
4,4'-PCB	15	002050-68-2	0.08	Pa	25	deg C	5	7.9E-007	298.15	
count										
average										
standard deviation										
minimum										
maximum										

NAME								VAPOR PRESSURE - liquid phase		
								for V/P calculation		
			liquid							
			phase					**liquid**		
			vapor		at wha	temp		**Vp**	**T(Vp)**	data
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	referenc	**atm**	**deg K**	notes
2,2',3-PCB	16	038444-78-9	***not in ref***	***5 or 85***						
2,2',5-PCB	18	037680-65-2	0.22	Pa	25	deg C	5			
2,3,3'-PCB	20	038444-84-7	**not in ref**	**5; see solid estm at left**						
2,3,4-PCB	21	055702-46-0	**not in ref**	**5; see solid estm at left**						
2,3',5-PCB	26	038444-85-8	***not in ref***	***5 or 85***						
2,4,4'-PCB	28	007012-37-5	**not in ref**	**5; see solid estm at left**						
2,4,5-PCB	29	015862-07-4	0.044	Pa	25	deg C	5			
2,4,6-PCB	30	035693-92-6	0.09	Pa	25	deg C	5			
2,4',5,-PCB	31	016606-02-3	***not in ref***	***5 or 85***						
2',3,4-PCB	33	038444-86-9	0.003	Pa	25	deg C	5			
3,3',4-PCB	35	037680-69-6	***not in ref***	***5 or 85***						
3,4,4'-PCB	37	038444-90-5	***not in ref***	***5 or 85***						
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3'-PCB	40	038444-93-8	0.002	Pa	25	deg C	5			
2,2',3,5'-PCB	44	041464-39-5	**not in ref**	**5; see solid estm at left**						
2,2',4,4'-PCB	47	002437-79-8	0.002	Pa	25	deg C	5			
2,2',4,5'-PCB	49	041464-40-8	**not in ref**	**5; see solid estm at left**						
2,2',4,6-PCB	50	062796-65-0	**not in ref**	**5; see solid estm at left**						
2,2',4,6'-PCB	51	068194-04-7	***not in ref***	***5 or 85***						
2,2,5,5'-PCB	52	035693-99-3	0.002	Pa	25	deg C	5			
2,2,5,6'-PCB	53	041464-41-9	**not in ref**	**5; see solid estm at left**						
2,2,6,6'-PCB	54	015968-05-5	**not in ref**	**5; see solid estm at left**						
2,3,4,4'-PCB	60	033025-41-1	**not in ref**	**5; see solid estm at left**						
2,3,4,5-PCB	61	033284-53-6	**not in ref**	**5; see solid estm at left**						
2,3,5,6-PCB	65	033284-54-7	***not in ref***	***5 or 85***						
2,3,4,4'-PCB	66	032598-10-0	**not in ref**	**5; see solid estm at left**						
2,3',4',5-PCB	70	032598-11-1	**not in ref**	**5; see solid estm at left**						
2,4,4',6-PCB	75	032598-12-2	***not in ref***	***5 or 85***						
3,3',4,4'-PCB	77	032598-13-3	0.002	Pa	25	deg C	5			
3,3',5,5'-PCB	80	033284-52-5	**not in ref**	**5; see solid estm at left**						
3,4,4',5-PCB	81	070362-50-4	***not in ref***	***5 or 85***						
count										
average										
standard deviation										
minimum										
maximum										

NAME								VAPOR PRESSURE - liquid phase		
								for V/P calculation		
			liquid					**liquid**		
			phase							
			vapor		at wha	temp		**Vp**	**T(Vp)**	data
common chemical name	IUPAC #	cas # (1)	pressure	units	temp?	units	referenc	**atm**	**deg K**	notes
2,2',3,3',5-PCB	83	060145-20-2	***not in ref***	***5 or 85***						
2,2',3,4,5-PCB	86	065510-45-4	0.051	Pa	25	deg C	5			
2,2',3,4,5'-PCB	87	038380-02-8	0.0023	Pa	25	deg C	5			
2,2',3,4,6-PCB	88	055215-17-3	**not in ref**	**5; see solid estm at left**						
2,2',3,5,6-PCB	95	038379-99-6	***not in ref***	***5 or 85***						
2,2',4,4',5-PCB	99	038380-01-7	**not in ref**	**5; see solid estm at left**						
2,2',4,4',6-PCB	100	039485-83-1	**2.22E-006**	**mm Hg**	**25**	**deg C**	**85**	2.9E-009	298.15	
2,2',4,5,5'-PCB	101	037680-73-2	0.0035	Pa	25	deg C	5			
2,2',4,6,6'-PCB	104	056558-16-8	***not in ref***	***5 or 85***						
2,3,3',4,4'-PCB	105	032598-14-4	**not in ref**	**5; see solid estm at left**						
2,3,3',4',6-PCB	110	038380-03-9	**not in ref**	**5; see solid estm at left**						
2,3,4,4',5-PCB	114	074472-37-0	***not in ref***	***5 or 85***						
2,3,4,5,6-PCB	116	018259-05-7	**not in ref**	**5; see solid estm at left**						
2,3',4,4',5-PCB	118	031508-00-6	***not in ref***	***5 or 85***						
2',3,4,5,5'-PCB	124	070424-70-3	***not in ref***	***5 or 85***						
3,3',4,4',5-PCB	126	057465-28-8	***not in ref***	***5 or 85***						
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4'-PCB	128	038380-07-3	0.00034	Pa	25	deg C	5			
2,2',3,3',4,5-PCB	129	055215-18-4	**not in ref**	**5; see solid estm at left**						
2,2',3,3',5,6-PCB	134	052704-70-8	**not in ref**	**5; see solid estm at left**						
2,2',3,3',6,6'-PCB	136	038411-22-2	**not in ref**	**5; see solid estm at left**						
2,2',3,4,4',5'-PCB	138	035065-28-2	**not in ref**	**5; see solid estm at left**						
2,2',3,4',5',6-PCB	149	038380-04-0	**not in ref**	**5; see solid estm at left**						
2,2',4,4',5,5'-PCB	153	035065-27-1	0.0007	Pa	25	deg C	5			
2,2',4,4',6,6'-PCB	155	033979-03-2	0.00363	Pa	25	deg C	5			
2,3,3',4,4',5-PCB	156	038380-08-4	**not in ref**	**5; see solid estm at left**						
2,3,3',4,4',5'-PCB	157	069782-90-7	***not in ref***	***5 or 85***						
2,3',4,4',5,5'-PCB	167	052663-72-6	**not in ref**	**5; see solid estm at left**						
3,3',4,4',5,5'-PCB	169	032774-16-6	**not in ref**	**5; see solid estm at left**						
count										
average										
standard deviation										
minimum										
maximum										

NAME

VAPOR PRESSURE - liquid phase

common chemical name	IUPAC #	cas # (1)	liquid phase vapor pressure	units	at wha temp?	temp units	referenc	for V/P calculation liquid Vp atm	T(Vp) deg K	data notes
2,2',3,3',4,4',5-PCB	170	035065-30-6	**not in ref**	**5; see solid estm at eft**						
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.00025	Pa	25	deg C	5			
2,2',3,4,4',5,5'-PCB	180	035065-29-3	**not in ref**	**5; see solid estm at eft**						
2,2',3,4,5,5',6-PCB	185	052712-05-7	**not in ref**	**5; see solid estm at eft**						
2,2',3,4',5,5',6-PCB	187	052663-68-0	**not in ref**	**5; see solid estm at eft**						
2,3,3',4,4',5,5'-PCB	189	039635-31-9	***not in ref***	***5 or 85***						
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	**not in ref**	**5; see solid estm at eft**						
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0006	Pa	25	deg C	5			
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	1.2E-005	Pa	25	deg C	5			
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	***not in ref***	***5 or 85***						
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	**not in ref**	**5; see solid estm at eft**						
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	0.00003	Pa	25	deg C	5			

NAME

WATER SOLUBILITY- 1

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
octachlorostyrene		029082-74-4						
4-bromophenyl phenyl ether		000101-55-3	4.8	g/m3	25	deg C	7	
3,3'-dichlorobenzidene		000091-94-1	3.1	mg/lit	25	deg C	Banerjee et	same in ref 8
1,3-dinitropyrene		075321-20-9	0.0132	g/m3	25	deg C	crude estm	=pyrene / 10
1,6-dinitropyrene		042397-64-8	0.0132	g/m3	25	deg C	crude estm	=pyrene / 10
1,8-dinitropyrene		042397-65-9	0.0132	g/m3	25	deg C	crude estm	=pyrene / 10
2,7-dinitropyrene		117929-15-4	0.0132	g/m3	25	deg C	crude estm	=pyrene / 10
dinitropyrenes (mixed)		078432-19-6						
hexachloro-1,3-butadiene		000087-68-3	3.2	g/m3	25	deg C	7	
4,4'-methylene bis(2-chloroaniline)		000101-14-4	13.9	mg/liter	24	deg C	17	
pentachlorophenol		000087-86-5	14	g/m3	25	deg C	8	
aldrin		000309-00-2	0.02	mg/liter	20	deg C	49	
dieldrin		000060-57-1	0.17	mg/liter	20	deg C	49	
p,p'-DDT		000050-29-3	5.4	ug/liter	24	deg C	63	a lot of conflicting data
p,p'-DDD		000072-54-8	90	ppb	25	deg C	64	other data as well
p,p'-DDE		000072-55-9	120	ppb	25	deg C	64	other data as well
heptachlor		000076-44-8	0.18	mg/lit	temp not stated		26	
heptachlor epoxide		001024-57-3	0.2	mg/lit	temp not stated		26	
methoxychlor		000072-43-5	0.045	mg/lit	25	deg C	26	
mirex		002385-85-5	0.6	mg/lit	temp not stated		67	other data presented
toxaphene		008001-35-2						
endrin		000072-20-8	0.25	ug/liter	25	deg C	26	
alpha-hexachlorocyclohexane		000319-84-6	10	ppm	temp not reported		34	
beta-hexachlorocyclohexane		000319-85-7	5	ppm	temp not reported		34	
delta-hexachlorocyclohexane		000319-86-8	10	ppm	temp not reported		34	
gamma-hexachlorocyclohexane		000058-89-9	17	ppm	temp not reported		35	
mixed hexachlorocyclohexanes		000319-84-6						

NAME

WATER SOLUBILITY- 1

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
cadmium		007440-43-9	"insoluble"				76	
cadmium carbonate		000513-78-0	"practically	insoluble"			74	
cadmium chloride		010108-64-2	1400	g/liter	20	deg C	72	other data at other temps
cadmium oxide		001306-19-0	5	mg/liter	temp not stated		74	
cadmium sulfate		010124-36-4	750	g/liter	0	deg C	72	other data at other temps
cadmium sulfide		001306-23-6	1.3	mg/lit	18	deg C	74	
elemental mercury		007439-97-6	0.00000006	g/mL	25	deg C	95	
mercury oxide		021908-53-2						ref 95: no data
mercuric chloride		007487-94-7	7.4E+004	mg/lit	25	deg C	95	
monomethyl mercury chloride		000115-09-3						ref 95: no data
dimethyl mercury		000593-74-8						ref 95: no data
tetraethyl lead		000078-00-2	0.21	mg/lit	26	deg C	85	
tetramethyl lead		000075-74-1	9	mg/lit	not stated		97 citing 98	estm?
triethyl lead radical (1+ cation)		014570-15-1						
triethyl lead hydride		005224-23-7						
triethyl lead chloride		001067-14-7						
diethyl lead radical (2+ cation)		024952-65-6						
diethyl lead dihydride		081494-11-3						
diethyl lead dichloride		013231-90-8						
trimethyl lead radical (1+ cation)		014570-16-2						
trimethyl lead hydride		007442-13-9						
trimethyl lead chloride		001520-78-1						
dimethyl lead radical (2+ cation)		021774-13-0						
dimethyl lead dihydride		030691-92-0						
dimethyl lead dichloride		001520-77-0						
bis (tributyltin) oxide		000056-35-9	4	mg/lit	20	deg C	97	expt'l
tributyl tin		000688-75-3						
tributyltin fluoride		001983-10-4						
tributyltin chloride		001461-22-9						
tributyltin hydroxide		001067-97-6						
tributyltin naphthenate								
tris(tributylstannyl) phosphate		013435-05-7						

NAME

WATER SOLUBILITY- 1

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	||||	water solubility	units	at what temp?	temp units	reference	data notes	||||
1,4-dichlorobenzene		000106-46-7	||||	83	g/m3	25	deg C	5		||||
1,2,3,4-tetrachlorobenzene		000634-66-2	||||	7.8	g/m3	25	deg C	5		||||
1,2,4,5-tetrachlorobenzene		000095-94-3	||||	1.27	g/m3	25	deg C	5		||||
1,2,3,5-tetrachlorobenzene		000634-90-2	||||	3.6	g/m3	25	deg C	5		||||
pentachlorobenzene		000608-93-5	||||	0.65	g/m3	25	deg C	5		||||
hexachlorobenzene		000118-74-1	||||	0.005	g/m3	25	deg C	5		||||
naphthalene		000091-20-3	||||	31	g/m3	25	deg C	6		||||
acenaphthene		000083-32-9	||||	3.8	g/m3	25	deg C	6		||||
acenaphthylene		000208-96-8	||||	16.1	g/m3	25	deg C	6		||||
fluorene		000086-73-7	||||	1.9	g/m3	25	deg C	6		||||
phenanthrene		000085-01-8	||||	1.1	g/m3	25	deg C	6		||||
anthracene		000120-12-7	||||	0.045	g/m3	25	deg C	6		||||
pyrene		000129-00-0	||||	0.132	g/m3	25	deg C	6		||||
fluoranthene		000206-44-0	||||	0.26	g/m3	25	deg C	6		||||
chrysene		000218-01-9	||||	2.8E-003	mg/lit	temp not reported		14		||||
benz [a] anthracene		000056-55-3	||||	0.011	g/m3	25	deg C	6		||||
benzo [b] fluoranthene		000205-99-2	||||	0.0015	g/m3	25	deg C	6		||||
benzo [j] fluoranthene		000205-82-3	||||	0.0025	g/m3	25	deg C	6		||||
benzo [k] fluoranthene		000207-08-9	||||	0.0008	g/m3	25	deg C	6		||||
benzo [a] pyrene		000050-32-8	||||	0.0038	g/m3	25	deg C	6		||||
benzo [e] pyrene		000192-97-2	||||	0.004	g/m3	25	deg C	6		||||
perylene		000198-55-0	||||	0.0004	g/m3	25	deg C	6		||||
benzo [g,h,i] perylene		000191-24-2	||||	0.00026	g/m3	25	deg C	6		||||
dibenz [a,h] anthracene		000053-70-3	||||	0.0006	g/m3	25	deg C	6		||||
indeno [1,2,3-c,d] pyrene		000193-39-5	||||	0.062	mg/lit	temp not reported		9		||||

NAME

WATER SOLUBILITY- 1

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,3,7,8-TCDD		001746-01-6	0.0193	mg/m3	25	deg C	6	
1,2,3,7,8-PeCDD		040321-76-4	0.118	mg/m3	25	deg C	6	using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD		039227-28-6	0.00442	mg/m3	25	deg C	6	
1,2,3,6,7,8-HxCDD		057653-85-7	0.00442	mg/m3	25	deg C	6	using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD		019408-74-3	0.00442	mg/m3	25	deg C	6	using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD		035822-46-9	0.0024	mg/m3	25	deg C	6	
OCDD		003268-87-9	0.000074	mg/m3	25	deg C	6	
2,3,7,8-TCDF		051207-31-9	0.419	mg/m3	25	deg C	6	
2,3,4,7,8-PeCDF		057117-31-4	0.236	mg/m3	25	deg C	6	
1,2,3,7,8-PeCDF		057117-41-6	0.236	mg/m3	25	deg C	6	using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF		070648-26-9	0.00825	mg/m3	25	deg C	6	
1,2,3,6,7,8-HxCDF		057117-44-9	0.0177	mg/m3	25	deg C	6	
1,2,3,7,8,9-HxCDF		072918-21-9	0.012975	mg/m3	25	deg C	6	using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF		060851-34-5	0.012975	mg/m3	25	deg C	6	using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF		067562-39-4	0.00135	mg/m3	25	deg C	6	
1,2,3,4,7,8,9-HpCDF		055673-89-7	0.00135	mg/m3	25	deg C	6	using value for 1234678 HpCDF
OCDF		039001-02-0	0.00116	mg/m3	25	deg C	6	

NAME

WATER SOLUBILITY- 1

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
biphenyl	0	000092-52-4	7	g/m3	25	deg C	5	
2-PCB	1	002051-60-7	5.5	g/m3	25	deg C	5	
3-PCB	2	002051-61-8	2.5	g/m3	25	deg C	5	
4-PCB	3	002051-62-9	1.2	g/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2'-PCB	4	013029-08-8	1	g/m3	25	deg C	5	
2,3-PCB	5	016605-91-7	-------------------- ***not in reference 5*** --------------------					
2,4-PCB	7	033284-50-3	1.25	g/m3	25	deg C	5	
2,4'-PCB	8	034883-43-7	1	g/m3	25	deg C	5	
2,5-PCB	9	034883-39-1	2	g/m3	25	deg C	5	
2,6-PCB	10	033146-45-1	1.4	g/m3	25	deg C	5	
3,3'-PCB	11	002050-67-1	0.354	g/m3	25	deg C	5	
3,4-PCB	12	002974-92-7	0.008	g/m3	25	deg C	5	
3,5-PCB	14	034883-41-5	-------------------- ***not in reference 5*** --------------------					
4,4'-PCB	15	002050-68-2	0.06	g/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								

NAME

WATER SOLUBILITY- 1

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,2',3-PCB	16	038444-78-9	-------------------- ***not in reference 5*** --------------------					
2,2',5-PCB	18	037680-65-2	0.4	g/m3	25	deg C	5	
2,3,3'-PCB	20	038444-84-7	-------------------- ***not in reference 5*** --------------------					
2,3,4-PCB	21	055702-46-0	-------------------- ***not in reference 5*** --------------------					
2,3',5-PCB	26	038444-85-8	0.251	g/m3	25	deg C	5	
2,4,4'-PCB	28	007012-37-5	0.16	g/m3	25	deg C	5	
2,4,5-PCB	29	015862-07-4	0.14	g/m3	25	deg C	5	
2,4,6-PCB	30	035693-92-6	0.2	g/m3	25	deg C	5	
2,4',5,-PCB	31	016606-02-3	-------------------- ***not in reference 5*** --------------------					
2',3,4-PCB	33	038444-86-9	0.08	g/m3	25	deg C	5	
3,3',4-PCB	35	037680-69-6	-------------------- ***not in reference 5*** --------------------					
3,4,4'-PCB	37	038444-90-5	0.015	g/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3'-PCB	40	038444-93-8	0.03	g/m3	25	deg C	5	
2,2',3,5'-PCB	44	041464-39-5	0.1	g/m3	25	deg C	5	
2,2',4,4'-PCB	47	002437-79-8	0.09	g/m3	25	deg C	5	
2,2',4,5'-PCB	49	041464-40-8	0.016	g/m3	25	deg C	5	
2,2',4,6-PCB	50	062796-65-0	-------------------- ***not in reference 5*** --------------------					
2,2',4,6'-PCB	51	068194-04-7	-------------------- ***not in reference 5*** --------------------					
2,2,5,5'-PCB	52	035693-99-3	0.03	g/m3	25	deg C	5	
2,2,5,6'-PCB	53	041464-41-9	-------------------- ***not in reference 5*** --------------------					
2,2,6,6'-PCB	54	015968-05-5	-------------------- ***not in reference 5*** --------------------					
2,3,4,4'-PCB	60	033025-41-1	-------------------- ***not in reference 5*** --------------------					
2,3,4,5-PCB	61	033284-53-6	0.02	g/m3	25	deg C	5	
2,3,5,6-PCB	65	033284-54-7	-------------------- ***not in reference 5*** --------------------					
2,3,4,4'-PCB	66	032598-10-0	0.04	g/m3	25	deg C	5	
2,3',4',5-PCB	70	032598-11-1	-------------------- ***not in reference 5*** --------------------					
2,4,4',6-PCB	75	032598-12-2	0.091	g/m3	25	deg C	5	
3,3',4,4'-PCB	77	032598-13-3	0.001	g/m3	25	deg C	5	
3,3',5,5'-PCB	80	033284-52-5	0.0012	g/m3	25	deg C	5	
3,4,4',5-PCB	81	070362-50-4	-------------------- ***not in reference 5*** --------------------					
count								
average								
standard deviation								
minimum								
maximum								

NAME

WATER SOLUBILITY- 1

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,2',3,3',5-PCB	83	060145-20-2	***-------------------- not in reference 5 --------------------***					
2,2',3,4,5-PCB	86	065510-45-4	0.02	g/m3	25	deg C	5	
2,2',3,4,5'-PCB	87	038380-02-8	0.004	g/m3	25	deg C	5	
2,2',3,4,6-PCB	88	055215-17-3	0.012	g/m3	25	deg C	5	
2,2',3,5,6-PCB	95	038379-99-6	***-------------------- not in reference 5 --------------------***					
2,2',4,4',5-PCB	99	038380-01-7	***-------------------- not in reference 5 --------------------***					
2,2',4,4',6-PCB	100	039485-83-1	***-------------------- not in reference 5 --------------------***					
2,2',4,5,5'-PCB	101	037680-73-2	0.01	g/m3	25	deg C	5	
2,2',4,6,6'-PCB	104	056558-16-8	0.0156	g/m3	25	deg C	5	
2,3,3',4,4'-PCB	105	032598-14-4	***-------------------- not in reference 5 --------------------***					
2,3,3',4',6-PCB	110	038380-03-9	0.004	g/m3	25	deg C	5	
2,3,4,4',5-PCB	114	074472-37-0	***-------------------- not in reference 5 --------------------***					
2,3,4,5,6-PCB	116	018259-05-7	0.008	g/m3	25	deg C	5	
2,3',4,4',5-PCB	118	031508-00-6	***-------------------- not in reference 5 --------------------***					
2',3,4,5,5'-PCB	124	070424-70-3	***-------------------- not in reference 5 --------------------***					
3,3',4,4',5-PCB	126	057465-28-8	***-------------------- not in reference 5 --------------------***					
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4'-PCB	128	038380-07-3	0.0006	g/m3	25	deg C	5	
2,2',3,3',4,5-PCB	129	055215-18-4	0.0006	g/m3	25	deg C	5	
2,2',3,3',5,6-PCB	134	052704-70-8	0.0004	g/m3	25	deg C	5	
2,2',3,3',6,6'-PCB	136	038411-22-2	0.0008	g/m3	25	deg C	5	
2,2',3,4,4',5'-PCB	138	035065-28-2	***-------------------- not in reference 5 --------------------***					
2,2',3,4',5',6-PCB	149	038380-04-0	***-------------------- not in reference 5 --------------------***					
2,2',4,4',5,5'-PCB	153	035065-27-1	0.001	g/m3	25	deg C	5	
2,2',4,4',6,6'-PCB	155	033979-03-2	0.002	g/m3	25	deg C	5	
2,3,3',4,4',5-PCB	156	038380-08-4	***-------------------- not in reference 5 --------------------***					
2,3,3',4,4',5'-PCB	157	069782-90-7	***-------------------- not in reference 5 --------------------***					
2,3',4,4',5,5'-PCB	167	052663-72-6	***-------------------- not in reference 5 --------------------***					
3,3',4,4',5,5'-PCB	169	032774-16-6	***-------------------- not in reference 5 --------------------***					
count								
average								
standard deviation								
minimum								
maximum								

NAME

WATER SOLUBILITY- 1

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,2',3,3',4,4',5-PCB	170	035065-30-6	-------------------- ***not in reference 5*** --------------------					
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.002	g/m3	25	deg C	5	
2,2',3,4,4',5,5'-PCB	180	035065-29-3	-------------------- ***not in reference 5*** --------------------					
2,2',3,4,5,5',6-PCB	185	052712-05-7	0.00045	g/m3	25	deg C	5	
2,2',3,4',5,5',6-PCB	187	052663-68-0	-------------------- ***not in reference 5*** --------------------					
2,3,3',4,4',5,5'-PCB	189	039635-31-9	-------------------- ***not in reference 5*** --------------------					
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	0.0002	g/m3	25	deg C	5	
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0003	g/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	0.00011	g/m3	25	deg C	5	
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	-------------------- ***not in reference 5*** --------------------					
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	0.000018	g/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	0.000001	g/m3	25	deg C	5	

NAME

WATER SOLUBILITY- 2

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
octachlorostyrene		029082-74-4						
4-bromophenyl phenyl ether		000101-55-3	0.0193	mol/m3	25	deg C	7	
3,3'-dichlorobenzidene		000091-94-1	0.0122	mol/m3	25	deg C	8	
1,3-dinitropyrene		075321-20-9	0.132	g/m3	25	deg C	crude estm	= pyrene
1,6-dinitropyrene		042397-64-8	0.132	g/m3	25	deg C	crude estm	= pyrene
1,8-dinitropyrene		042397-65-9	0.132	g/m3	25	deg C	crude estm	= pyrene
2,7-dinitropyrene		117929-15-4	0.132	g/m3	25	deg C	crude estm	= pyrene
dinitropyrenes (mixed)		078432-19-6						
hexachloro-1,3-butadiene		000087-68-3	0.013	mol/m3	25	deg C	7	
4,4'-methylene bis(2-chloroaniline)		000101-14-4						
pentachlorophenol		000087-86-5	0.053	mol/m3	25	deg C	8	
aldrin		000309-00-2						
dieldrin		000060-57-1						
p,p'-DDT		000050-29-3						
p,p'-DDD		000072-54-8						
p,p'-DDE		000072-55-9						
heptachlor		000076-44-8						
heptachlor epoxide		001024-57-3						
methoxychlor		000072-43-5						
mirex		002385-85-5						
toxaphene		008001-35-2						
endrin		000072-20-8						
alpha-hexachlorocyclohexane		000319-84-6						
beta-hexachlorocyclohexane		000319-85-7						
delta-hexachlorocyclohexane		000319-86-8						
gamma-hexachlorocyclohexane		000058-89-9						
mixed hexachlorocyclohexanes		000319-84-6						

NAME

WATER SOLUBILITY- 2

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
cadmium		007440-43-9						
cadmium carbonate		000513-78-0						
cadmium chloride		010108-64-2						
cadmium oxide		001306-19-0						
cadmium sulfate		010124-36-4						
cadmium sulfide		001306-23-6						
elemental mercury		007439-97-6						
mercury oxide		021908-53-2						
mercuric chloride		007487-94-7						
monomethyl mercury chloride		000115-09-3						
dimethyl mercury		000593-74-8						
tetraethyl lead		000078-00-2						
tetramethyl lead		000075-74-1						
triethyl lead radical (1+ cation)		014570-15-1						
triethyl lead hydride		005224-23-7						
triethyl lead chloride		001067-14-7						
diethyl lead radical (2+ cation)		024952-65-6						
diethyl lead dihydride		081494-11-3						
diethyl lead dichloride		013231-90-8						
trimethyl lead radical (1+ cation)		014570-16-2						
trimethyl lead hydride		007442-13-9						
trimethyl lead chloride		001520-78-1						
dimethyl lead radical (2+ cation)		021774-13-0						
dimethyl lead dihydride		030691-92-0						
dimethyl lead dichloride		001520-77-0						
bis (tributyltin) oxide		000056-35-9						
tributyl tin		000688-75-3						
tributyltin fluoride		001983-10-4						
tributyltin chloride		001461-22-9						
tributyltin hydroxide		001067-97-6						
tributyltin naphthenate								
tris(tributylstannyl) phosphate		013435-05-7						

NAME

WATER SOLUBILITY- 2

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
1,4-dichlorobenzene		000106-46-7	0.5646	mol/m3	25	deg C	5	
1,2,3,4-tetrachlorobenzene		000634-66-2	0.0361	mol/m3	25	deg C	5	
1,2,4,5-tetrachlorobenzene		000095-94-3	0.00588	mol/m3	25	deg C	5	
1,2,3,5-tetrachlorobenzene		000634-90-2	0.0167	mol/m3	25	deg C	5	
pentachlorobenzene		000608-93-5	0.0026	mol/m3	25	deg C	5	
hexachlorobenzene		000118-74-1	0.0000176	mol/m3	25	deg C	5	
naphthalene		000091-20-3	241.83	mmol/m3	25	deg C	6	
acenaphthene		000083-32-9	24.642	mmol/m3	25	deg C	6	
acenaphthylene		000208-96-8	107.19	mmol/m3	25	deg C	6	
fluorene		000086-73-7	11.43	mmol/m3	25	deg C	6	
phenanthrene		000085-01-8	6.173	mmol/m3	25	deg C	6	
anthracene		000120-12-7	0.253	mmol/m3	25	deg C	6	
pyrene		000129-00-0	0.652	mmol/m3	25	deg C	6	
fluoranthene		000206-44-0	1.186	mmol/m3	25	deg C	6	
chrysene		000218-01-9		***not given in reference 6***				
benz [a] anthracene		000056-55-3	0.0482	mmol/m3	25	deg C	6	
benzo [b] fluoranthene		000205-99-2	0.00595	mmol/m3	25	deg C	6	
benzo [j] fluoranthene		000205-82-3	0.0099	mmol/m3	25	deg C	6	
benzo [k] fluoranthene		000207-08-9	0.00317	mmol/m3	25	deg C	6	
benzo [a] pyrene		000050-32-8	0.0151	mmol/m3	25	deg C	6	
benzo [e] pyrene		000192-97-2	0.0159	mmol/m3	25	deg C	6	
perylene		000198-55-0	0.00159	mmol/m3	25	deg C	6	
benzo [g,h,i] perylene		000191-24-2	0.000968	mmol/m3	25	deg C	6	
dibenz [a,h] anthracene		000053-70-3	0.00216	mmol/m3	25	deg C	6	
indeno [1,2,3-c,d] pyrene		000193-39-5		***not given in reference 6***				

NAME

WATER SOLUBILITY- 2

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	||||	water solubility	units	at what temp?	temp units	reference	data notes	||||
2,3,7,8-TCDD		001746-01-6	||||	6.00E-005	mmol/m3	25	deg C	6		||||
1,2,3,7,8-PeCDD		040321-76-4	||||	3.31E-004	mmol/m3	25	deg C	6	using value for 12347 PeCDD	||||
1,2,3,4,7,8-HxCDD		039227-28-6	||||	1.13E-005	mmol/m3	25	deg C	6		||||
1,2,3,6,7,8-HxCDD		057653-85-7	||||	1.13E-005	mmol/m3	25	deg C	6	using value for 123478 HxCDD	||||
1,2,3,7,8,9-HxCDD		019408-74-3	||||	1.13E-005	mmol/m3	25	deg C	6	using value for 123478 HxCDD	||||
1,2,3,4,6,7,8-HpCDD		035822-46-9	||||	5.64E-006	mmol/m3	25	deg C	6		||||
OCDD		003268-87-9	||||	1.61E-007	mmol/m3	25	deg C	6		||||
2,3,7,8-TCDF		051207-31-9	||||	1.37E-003	mmol/m3	25	deg C	6		||||
2,3,4,7,8-PeCDF		057117-31-4	||||	6.93E-004	mmol/m3	25	deg C	6		||||
1,2,3,7,8-PeCDF		057117-41-6	||||	6.93E-004	mmol/m3	25	deg C	6	using value for 23478 PeCDF	||||
1,2,3,4,7,8-HxCDF		070648-26-9	||||	2.20E-005	mmol/m3	25	deg C	6		||||
1,2,3,6,7,8-HxCDF		057117-44-9	||||	4.72E-005	mmol/m3	25	deg C	6		||||
1,2,3,7,8,9-HxCDF		072918-21-9	||||	3.46E-005	mmol/m3	25	deg C	6	using avg of values for 123478 HxCDF and 123678 HxCDF	||||
2,3,4,6,7,8-HxCDF		060851-34-5	||||	3.46E-005	mmol/m3	25	deg C	6	using avg of values for 123478 HxCDF and 123678 HxCDF	||||
1,2,3,4,6,7,8-HpCDF		067562-39-4	||||	3.3E-006	mmol/m3	25	deg C	6		||||
1,2,3,4,7,8,9-HpCDF		055673-89-7	||||	3.3E-006	mmol/m3	25	deg C	6	using value for 1234678 HpCDF	||||
OCDF		039001-02-0	||||	2.61E-006	mmol/m3	25	deg C	6		||||

NAME

WATER SOLUBILITY- 2

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
biphenyl	0	000092-52-4	45.39	mmol/m3	25	deg C	5	
2-PCB	1	002051-60-7	29.15	mmol/m3	25	deg C	5	
3-PCB	2	002051-61-8	13.25	mmol/m3	25	deg C	5	
4-PCB	3	002051-62-9	6.36	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2'-PCB	4	013029-08-8	4.48	mmol/m3	25	deg C	5	
2,3-PCB	5	016605-91-7	***-------------------- not in reference 5 --------------------***					
2,4-PCB	7	033284-50-3	5.6	mmol/m3	25	deg C	5	
2,4'-PCB	8	034883-43-7	4.48	mmol/m3	25	deg C	5	
2,5-PCB	9	034883-39-1	8.96	mmol/m3	25	deg C	5	
2,6-PCB	10	033146-45-1	6.28	mmol/m3	25	deg C	5	
3,3'-PCB	11	002050-67-1	1.587	mmol/m3	25	deg C	5	
3,4-PCB	12	002974-92-7	***-------------------- not in reference 5 --------------------***					
3,5-PCB	14	034883-41-5	***-------------------- not in reference 5 --------------------***					
4,4'-PCB	15	002050-68-2	0.269	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								

NAME

WATER SOLUBILITY- 2

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,2',3-PCB	16	038444-78-9	-------------------- ***not in reference 5*** --------------------					
2,2',5-PCB	18	037680-65-2	1.55	mmol/m3	25	deg C	5	
2,3,3'-PCB	20	038444-84-7	-------------------- ***not in reference 5*** --------------------					
2,3,4-PCB	21	055702-46-0	-------------------- ***not in reference 5*** --------------------					
2,3',5-PCB	26	038444-85-8	0.975	mmol/m3	25	deg C	5	
2,4,4'-PCB	28	007012-37-5	0.621	mmol/m3	25	deg C	5	
2,4,5-PCB	29	015862-07-4	0.544	mmol/m3	25	deg C	5	
2,4,6-PCB	30	035693-92-6	0.777	mmol/m3	25	deg C	5	
2,4',5,-PCB	31	016606-02-3	-------------------- ***not in reference 5*** --------------------					
2',3,4-PCB	33	038444-86-9	0.311	mmol/m3	25	deg C	5	
3,3',4-PCB	35	037680-69-6	-------------------- ***not in reference 5*** --------------------					
3,4,4'-PCB	37	038444-90-5	0.0582	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3'-PCB	40	038444-93-8	0.103	mmol/m3	25	deg C	5	
2,2',3,5'-PCB	44	041464-39-5	0.342	mmol/m3	25	deg C	5	
2,2',4,4'-PCB	47	002437-79-8	0.308	mmol/m3	25	deg C	5	
2,2',4,5'-PCB	49	041464-40-8	0.0548	mmol/m3	25	deg C	5	
2,2',4,6-PCB	50	062796-65-0	-------------------- ***not in reference 5*** --------------------					
2,2',4,6'-PCB	51	068194-04-7	-------------------- ***not in reference 5*** --------------------					
2,2,5,5'-PCB	52	035693-99-3	0.103	mmol/m3	25	deg C	5	
2,2,5,6'-PCB	53	041464-41-9	-------------------- ***not in reference 5*** --------------------					
2,2,6,6'-PCB	54	015968-05-5	-------------------- ***not in reference 5*** --------------------					
2,3,4,4'-PCB	60	033025-41-1	-------------------- ***not in reference 5*** --------------------					
2,3,4,5-PCB	61	033284-53-6	0.0685	mmol/m3	25	deg C	5	
2,3,5,6-PCB	65	033284-54-7	-------------------- ***not in reference 5*** --------------------					
2,3,4,4'-PCB	66	032598-10-0	0.0147	mmol/m3	25	deg C	5	
2,3',4',5-PCB	70	032598-11-1	-------------------- ***not in reference 5*** --------------------					
2,4,4',6-PCB	75	032598-12-2	-------------------- ***not in reference 5*** --------------------					
3,3',4,4'-PCB	77	032598-13-3	0.0342	mmol/m3	25	deg C	5	
3,3',5,5'-PCB	80	033284-52-5	0.0041	mmol/m3	25	deg C	5	
3,4,4',5-PCB	81	070362-50-4	-------------------- ***not in reference 5*** --------------------					
count								
average								
standard deviation								
minimum								
maximum								

NAME

WATER SOLUBILITY- 2

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,2',3,3',5-PCB	83	060145-20-2	-------------------- ***not in reference 5*** --------------------					
2,2',3,4,5-PCB	86	065510-45-4	0.0613	mmol/m3	25	deg C	5	
2,2',3,4,5'-PCB	87	038380-02-8	0.0123	mmol/m3	25	deg C	5	
2,2',3,4,6-PCB	88	055215-17-3	0.0368	mmol/m3	25	deg C	5	
2,2',3,5,6-PCB	95	038379-99-6	-------------------- ***not in reference 5*** --------------------					
2,2',4,4',5-PCB	99	038380-01-7	-------------------- ***not in reference 5*** --------------------					
2,2',4,4',6-PCB	100	039485-83-1	-------------------- ***not in reference 5*** --------------------					
2,2',4,5,5'-PCB	101	037680-73-2	0.0306	mmol/m3	25	deg C	5	
2,2',4,6,6'-PCB	104	056558-16-8	0.0306	mmol/m3	25	deg C	5	
2,3,3',4,4'-PCB	105	032598-14-4	-------------------- ***not in reference 5*** --------------------					
2,3,3',4',6-PCB	110	038380-03-9	-------------------- ***not in reference 5*** --------------------					
2,3,4,4',5-PCB	114	074472-37-0	-------------------- ***not in reference 5*** --------------------					
2,3,4,5,6-PCB	116	018259-05-7	0.0145	mmol/m3	25	deg C	5	
2,3',4,4',5-PCB	118	031508-00-6	-------------------- ***not in reference 5*** --------------------					
2',3,4,5,5'-PCB	124	070424-70-3	-------------------- ***not in reference 5*** --------------------					
3,3',4,4',5-PCB	126	057465-28-8	-------------------- ***not in reference 5*** --------------------					
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4'-PCB	128	038380-07-3	0.00166	mmol/m3	25	deg C	5	
2,2',3,3',4,5-PCB	129	055215-18-4	0.00166	mmol/m3	25	deg C	5	
2,2',3,3',5,6-PCB	134	052704-70-8	0.00111	mmol/m3	25	deg C	5	
2,2',3,3',6,6'-PCB	136	038411-22-2	0.00222	mmol/m3	25	deg C	5	
2,2',3,4,4',5'-PCB	138	035065-28-2	-------------------- ***not in reference 5*** --------------------					
2,2',3,4',5',6-PCB	149	038380-04-0	-------------------- ***not in reference 5*** --------------------					
2,2',4,4',5,5'-PCB	153	035065-27-1	0.00277	mmol/m3	25	deg C	5	
2,2',4,4',6,6'-PCB	155	033979-03-2	0.0055	mmol/m3	25	deg C	5	
2,3,3',4,4',5-PCB	156	038380-08-4	-------------------- ***not in reference 5*** --------------------					
2,3,3',4,4',5'-PCB	157	069782-90-7	-------------------- ***not in reference 5*** --------------------					
2,3',4,4',5,5'-PCB	167	052663-72-6	-------------------- ***not in reference 5*** --------------------					
3,3',4,4',5,5'-PCB	169	032774-16-6	-------------------- ***not in reference 5*** --------------------					
count								
average								
standard deviation								
minimum								
maximum								

NAME

WATER SOLUBILITY- 2

relative to most stable condensed phase

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,2',3,3',4,4',5-PCB	170	035065-30-6	***-------------------- not in reference 5 --------------------***					
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.00506	mmol/m3	25	deg C	5	
2,2',3,4,4',5,5'-PCB	180	035065-29-3	***-------------------- not in reference 5 --------------------***					
2,2',3,4,5,5',6-PCB	185	052712-05-7	0.00114	mmol/m3	25	deg C	5	
2,2',3,4',5,5',6-PCB	187	052663-68-0	***-------------------- not in reference 5 --------------------***					
2,3,3',4,4',5,5'-PCB	189	039635-31-9	***-------------------- not in reference 5 --------------------***					
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	0.00047	mmol/m3	25	deg C	5	
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0007	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	0.000237	mmol/m3	25	deg C	5	
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	***-------------------- not in reference 5 --------------------***					
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	0.000038	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	0.000002	mmol/m3	25	deg C	5	

NAME

WATER SOLUBILITY- 3

relative to subcooled liquid

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
octachlorostyrene		029082-74-4						
4-bromophenyl phenyl ether		000101-55-3	0.0193	mol/m3	25	deg C	7	
3,3'-dichlorobenzidene		000091-94-1	0.14	mol/m3	25	deg C	8	
1,3-dinitropyrene		075321-20-9						
1,6-dinitropyrene		042397-64-8						
1,8-dinitropyrene		042397-65-9						
2,7-dinitropyrene		117929-15-4						
dinitropyrenes (mixed)		078432-19-6						
hexachloro-1,3-butadiene		000087-68-3	0.013	mol/m3	25	deg C	7	
4,4'-methylene bis(2-chloroaniline)		000101-14-4						
pentachlorophenol		000087-86-5	1.565	mol/m3	25	deg C	8	
aldrin		000309-00-2						
dieldrin		000060-57-1						
p,p'-DDT		000050-29-3						
p,p'-DDD		000072-54-8						
p,p'-DDE		000072-55-9						
heptachlor		000076-44-8						
heptachlor epoxide		001024-57-3						
methoxychlor		000072-43-5						
mirex		002385-85-5						
toxaphene		008001-35-2	0.55	mg/lit	20	deg C	57	Murphy paper says that its a subcooled liquid value
endrin		000072-20-8						
alpha-hexachlorocyclohexane		000319-84-6						
beta-hexachlorocyclohexane		000319-85-7						
delta-hexachlorocyclohexane		000319-86-8						
gamma-hexachlorocyclohexane		000058-89-9						
mixed hexachlorocyclohexanes		000319-84-6						

NAME

WATER SOLUBILITY- 3

relative to subcooled liquid

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
cadmium		007440-43-9						
cadmium carbonate		000513-78-0						
cadmium chloride		010108-64-2						
cadmium oxide		001306-19-0						
cadmium sulfate		010124-36-4						
cadmium sulfide		001306-23-6						
elemental mercury		007439-97-6						
mercury oxide		021908-53-2						
mercuric chloride		007487-94-7						
monomethyl mercury chloride		000115-09-3						
dimethyl mercury		000593-74-8						
tetraethyl lead		000078-00-2						
tetramethyl lead		000075-74-1						
triethyl lead radical (1+ cation)		014570-15-1						
triethyl lead hydride		005224-23-7						
triethyl lead chloride		001067-14-7						
diethyl lead radical (2+ cation)		024952-65-6						
diethyl lead dihydride		081494-11-3						
diethyl lead dichloride		013231-90-8						
trimethyl lead radical (1+ cation)		014570-16-2						
trimethyl lead hydride		007442-13-9						
trimethyl lead chloride		001520-78-1						
dimethyl lead radical (2+ cation)		021774-13-0						
dimethyl lead dihydride		030691-92-0						
dimethyl lead dichloride		001520-77-0						
bis (tributyltin) oxide		000056-35-9						
tributyl tin		000688-75-3						
tributyltin fluoride		001983-10-4						
tributyltin chloride		001461-22-9						
tributyltin hydroxide		001067-97-6						
tributyltin naphthenate								
tris(tributylstannyl) phosphate		013435-05-7						

NAME								**WATER SOLUBILITY- 3**
								relative to subcooled liquid
common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
1,4-dichlorobenzene		000106-46-7	1.0653	mol/m3	25	deg C	5	
1,2,3,4-tetrachlorobenzene		000634-66-2	0.0602	mol/m3	25	deg C	5	
1,2,4,5-tetrachlorobenzene		000095-94-3	0.0784	mol/m3	25	deg C	5	
1,2,3,5-tetrachlorobenzene		000634-90-2	0.0327	mol/m3	25	deg C	5	
pentachlorobenzene		000608-93-5	0.0113	mol/m3	25	deg C	5	
hexachlorobenzene		000118-74-1	0.00187	mol/m3	25	deg C	5	
naphthalene		000091-20-3	855.92	mmol/m3	25	deg C	6	
acenaphthene		000083-32-9	124.7	mmol/m3	25	deg C	6	
acenaphthylene		000208-96-8	492.97	mmol/m3	25	deg C	6	
fluorene		000086-73-7	90.816	mmol/m3	25	deg C	6	
phenanthrene		000085-01-8	34.847	mmol/m3	25	deg C	6	
anthracene		000120-12-7	19.65	mmol/m3	25	deg C	6	
pyrene		000129-00-0	12.89	mmol/m3	25	deg C	6	
fluoranthene		000206-44-0	8.41	mmol/m3	25	deg C	6	
chrysene		000218-01-9	0.00876	mmol/m3	25	deg C	6	
benz [a] anthracene		000056-55-3	1.045	mmol/m3	25	deg C	6	
benzo [b] fluoranthene		000205-99-2	0.154	mmol/m3	25	deg C	6	
benzo [j] fluoranthene		000205-82-3	0.246	mmol/m3	25	deg C	6	
benzo [k] fluoranthene		000207-08-9	0.252	mmol/m3	25	deg C	6	
benzo [a] pyrene		000050-32-8	0.459	mmol/m3	25	deg C	6	
benzo [e] pyrene		000192-97-2	0.517	mmol/m3	25	deg C	6	
perylene		000198-55-0	0.493	mmol/m3	25	deg C	6	
benzo [g,h,i] perylene		000191-24-2	0.301	mmol/m3	25	deg C	6	
dibenz [a,h] anthracene		000053-70-3	0.533	mmol/m3	25	deg C	6	
indeno [1,2,3-c,d] pyrene		000193-39-5		***not given in reference 6***				

NAME

WATER SOLUBILITY- 3

relative to subcooled liquid

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,3,7,8-TCDD		001746-01-6	0.0352	mmol/m3	25	deg C	6	
1,2,3,7,8-PeCDD		040321-76-4	0.0159	mmol/m3	25	deg C	6	using value for 12347 PeCDD
1,2,3,4,7,8-HxCDD		039227-28-6	0.00321	mmol/m3	25	deg C	6	
1,2,3,6,7,8-HxCDD		057653-85-7	0.00321	mmol/m3	25	deg C	6	using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD		019408-74-3	0.00321	mmol/m3	25	deg C	6	using value for 123478 HxCDD
1,2,3,4,6,7,8-HpCDD		035822-46-9	0.00133	mmol/m3	25	deg C	6	
OCDD		003268-87-9	0.00014	mmol/m3	25	deg C	6	
2,3,7,8-TCDF		051207-31-9	0.136	mmol/m3	25	deg C	6	
2,3,4,7,8-PeCDF		057117-31-4	0.0341	mmol/m3	25	deg C	6	
1,2,3,7,8-PeCDF		057117-41-6	0.0341	mmol/m3	25	deg C	6	using value for 23478 PeCDF
1,2,3,4,7,8-HxCDF		070648-26-9	2.12E-003	mmol/m3	25	deg C	6	
1,2,3,6,7,8-HxCDF		057117-44-9	5.27E-003	mmol/m3	25	deg C	6	
1,2,3,7,8,9-HxCDF		072918-21-9	3.70E-003	mmol/m3	25	deg C	6	using avg of values for 123478 HxCDF and 123678 HxCDF
2,3,4,6,7,8-HxCDF		060851-34-5	3.70E-003	mmol/m3	25	deg C	6	using avg of values for 123478 HxCDF and 123678 HxCDF
1,2,3,4,6,7,8-HpCDF		067562-39-4	4.03E-004	mmol/m3	25	deg C	6	
1,2,3,4,7,8,9-HpCDF		055673-89-7	4.03E-004	mmol/m3	25	deg C	6	using value for 1234678 HpCDF
OCDF		039001-02-0	5.27E-005	mmol/m3	25	deg C	6	

NAME

WATER SOLUBILITY- 3

relative to subcooled liquid

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
biphenyl	0	000092-52-4	129.7	mmol/m3	25	deg C	5	
2-PCB	1	002051-60-7	35.66	mmol/m3	25	deg C	5	
3-PCB	2	002051-61-8	13.24	mmol/m3	25	deg C	5	
4-PCB	3	002051-62-9	21.15	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2'-PCB	4	013029-08-8	10.14	mmol/m3	25	deg C	5	
2,3-PCB	5	016605-91-7	------------------- ***not in reference 5*** -------------------					
2,4-PCB	7	033284-50-3	5.51	mmol/m3	25	deg C	5	
2,4'-PCB	8	034883-43-7	6.73	mmol/m3	25	deg C	5	
2,5-PCB	9	034883-39-1	8.95	mmol/m3	25	deg C	5	
2,6-PCB	10	033146-45-1	7.84	mmol/m3	25	deg C	5	
3,3'-PCB	11	002050-67-1	1.738	mmol/m3	25	deg C	5	
3,4-PCB	12	002974-92-7	------------------- ***not in reference 5*** -------------------					
3,5-PCB	14	034883-41-5	------------------- ***not in reference 5*** -------------------					
4,4'-PCB	15	002050-68-2	4.56	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								

NAME

WATER SOLUBILITY- 3

relative to subcooled liquid

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,2',3-PCB	16	038444-78-9	-------------------- ***not in reference 5*** --------------------					
2,2',5-PCB	18	037680-65-2	2.39	mmol/m3	25	deg C	5	
2,3,3'-PCB	20	038444-84-7	-------------------- ***not in reference 5*** --------------------					
2,3,4-PCB	21	055702-46-0	-------------------- ***not in reference 5*** --------------------					
2,3',5-PCB	26	038444-85-8	1.387	mmol/m3	25	deg C	5	
2,4,4'-PCB	28	007012-37-5	1.28	mmol/m3	25	deg C	5	
2,4,5-PCB	29	015862-07-4	1.81	mmol/m3	25	deg C	5	
2,4,6-PCB	30	035693-92-6	1.82	mmol/m3	25	deg C	5	
2,4',5,-PCB	31	016606-02-3	-------------------- ***not in reference 5*** --------------------					
2',3,4-PCB	33	038444-86-9	0.69	mmol/m3	25	deg C	5	
3,3',4-PCB	35	037680-69-6	-------------------- ***not in reference 5*** --------------------					
3,4,4'-PCB	37	038444-90-5	0.24	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3'-PCB	40	038444-93-8	0.91	mmol/m3	25	deg C	5	
2,2',3,5'-PCB	44	041464-39-5	0.565	mmol/m3	25	deg C	5	
2,2',4,4'-PCB	47	002437-79-8	1.15	mmol/m3	25	deg C	5	
2,2',4,5'-PCB	49	041464-40-8	0.133	mmol/m3	25	deg C	5	
2,2',4,6-PCB	50	062796-65-0	-------------------- ***not in reference 5*** --------------------					
2,2',4,6'-PCB	51	068194-04-7	-------------------- ***not in reference 5*** --------------------					
2,2,5,5'-PCB	52	035693-99-3	0.42	mmol/m3	25	deg C	5	
2,2,5,6'-PCB	53	041464-41-9	-------------------- ***not in reference 5*** --------------------					
2,2,6,6'-PCB	54	015968-05-5	-------------------- ***not in reference 5*** --------------------					
2,3,4,4'-PCB	60	033025-41-1	-------------------- ***not in reference 5*** --------------------					
2,3,4,5-PCB	61	033284-53-6	0.314	mmol/m3	25	deg C	5	
2,3,5,6-PCB	65	033284-54-7	-------------------- ***not in reference 5*** --------------------					
2,3,4,4'-PCB	66	032598-10-0	1.3	mmol/m3	25	deg C	5	
2,3',4',5-PCB	70	032598-11-1	-------------------- ***not in reference 5*** --------------------					
2,4,4',6-PCB	75	032598-12-2	-------------------- ***not in reference 5*** --------------------					
3,3',4,4'-PCB	77	032598-13-3	1.165	mmol/m3	25	deg C	5	
3,3',5,5'-PCB	80	033284-52-5	0.0974	mmol/m3	25	deg C	5	
3,4,4',5-PCB	81	070362-50-4	-------------------- ***not in reference 5*** --------------------					
count								
average								
standard deviation								
minimum								
maximum								

NAME

WATER SOLUBILITY- 3

relative to subcooled liquid

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,2',3,3',5-PCB	83	060145-20-2	-------------------- ***not in reference 5*** --------------------					
2,2',3,4,5-PCB	86	065510-45-4	0.337	mmol/m3	25	deg C	5	
2,2',3,4,5'-PCB	87	038380-02-8	0.0927	mmol/m3	25	deg C	5	
2,2',3,4,6-PCB	88	055215-17-3	0.202	mmol/m3	25	deg C	5	
2,2',3,5,6-PCB	95	038379-99-6	-------------------- ***not in reference 5*** --------------------					
2,2',4,4',5-PCB	99	038380-01-7	-------------------- ***not in reference 5*** --------------------					
2,2',4,4',6-PCB	100	039485-83-1	-------------------- ***not in reference 5*** --------------------					
2,2',4,5,5'-PCB	101	037680-73-2	0.0986	mmol/m3	25	deg C	5	
2,2',4,6,6'-PCB	104	056558-16-8	0.3103	mmol/m3	25	deg C	5	
2,3,3',4,4'-PCB	105	032598-14-4	-------------------- ***not in reference 5*** --------------------					
2,3,3',4',6-PCB	110	038380-03-9	-------------------- ***not in reference 5*** --------------------					
2,3,4,4',5-PCB	114	074472-37-0	-------------------- ***not in reference 5*** --------------------					
2,3,4,5,6-PCB	116	018259-05-7	0.233	mmol/m3	25	deg C	5	
2,3',4,4',5-PCB	118	031508-00-6	-------------------- ***not in reference 5*** --------------------					
2',3,4,5,5'-PCB	124	070424-70-3	-------------------- ***not in reference 5*** --------------------					
3,3',4,4',5-PCB	126	057465-28-8	-------------------- ***not in reference 5*** --------------------					
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4'-PCB	128	038380-07-3	0.0286	mmol/m3	25	deg C	5	
2,2',3,3',4,5-PCB	129	055215-18-4	0.0065	mmol/m3	25	deg C	5	
2,2',3,3',5,6-PCB	134	052704-70-8	0.0061	mmol/m3	25	deg C	5	
2,2',3,3',6,6'-PCB	136	038411-22-2	0.0161	mmol/m3	25	deg C	5	
2,2',3,4,4',5'-PCB	138	035065-28-2	-------------------- ***not in reference 5*** --------------------					
2,2',3,4',5',6-PCB	149	038380-04-0	-------------------- ***not in reference 5*** --------------------					
2,2',4,4',5,5'-PCB	153	035065-27-1	0.0163	mmol/m3	25	deg C	5	
2,2',4,4',6,6'-PCB	155	033979-03-2	0.042	mmol/m3	25	deg C	5	
2,3,3',4,4',5-PCB	156	038380-08-4	-------------------- ***not in reference 5*** --------------------					
2,3,3',4,4',5'-PCB	157	069782-90-7	-------------------- ***not in reference 5*** --------------------					
2,3',4,4',5,5'-PCB	167	052663-72-6	-------------------- ***not in reference 5*** --------------------					
3,3',4,4',5,5'-PCB	169	032774-16-6	-------------------- ***not in reference 5*** --------------------					
count								
average								
standard deviation								
minimum								
maximum								

NAME

WATER SOLUBILITY- 3

relative to subcooled liquid

common chemical name	IUPAC #	cas # (1)	water solubility	units	at what temp?	temp units	reference	data notes
2,2',3,3',4,4',5-PCB	170	035065-30-6	***-------------------- not in reference 5 --------------------***					
2,2',3,3',4,4',6-PCB	171	052663-71-5	0.046	mmol/m3	25	deg C	5	
2,2',3,4,4',5,5'-PCB	180	035065-29-3	***-------------------- not in reference 5 --------------------***					
2,2',3,4,5,5',6-PCB	185	052712-05-7	0.0191	mmol/m3	25	deg C	5	
2,2',3,4',5,5',6-PCB	187	052663-68-0	***-------------------- not in reference 5 --------------------***					
2,3,3',4,4',5,5'-PCB	189	039635-31-9	***-------------------- not in reference 5 --------------------***					
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	0.0098	mmol/m3	25	deg C	5	
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0.0158	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	0.0146	mmol/m3	25	deg C	5	
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	***-------------------- not in reference 5 --------------------***					
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	0.00141	mmol/m3	25	deg C	5	
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	0.0144	mmol/m3	25	deg C	5	

NAME — HENRY's LAW CONSTANT- 1

common chemical name	IUPAC #	cas # (1)	**Henry's Law Const for gas wet dep estm [atm m3/mol]**	**temp (K)**	Henry's Law Constant	units	at wha temp?	temp units	reference	how determined
octachlorostyrene		029082-74-4	1.30E-004	293.15	1.3E-004	atm m3/mo	20	deg C	58	experimental
4-bromophenyl phenyl ether		000101-55-3	1.02E-004	298.15	10.38	Pa m3/mol	25	deg C	7	calc'd from P/C
3,3'-dichlorobenzidene		000091-94-1	4.93E-008	298.15	5.0E-003	Pa m3/mol	25	deg C	8	calc'd from P/C
1,3-dinitropyrene		075321-20-9	5.62E-007	298.15						
1,6-dinitropyrene		042397-64-8	5.62E-007	298.15						
1,8-dinitropyrene		042397-65-9	5.62E-007	298.15						
2,7-dinitropyrene		117929-15-4	5.62E-007	298.15						
dinitropyrenes (mixed)		078432-19-6								
hexachloro-1,3-butadiene		000087-68-3	1.52E-002	298.15	1540	Pa m3/mol	25	deg C	7	calc'd P/C
4,4'-methylene bis(2-chloroaniline)		000101-14-4	4.00E-011	?	4.0E-011	atm m3/mo	temp	not report	15	
pentachlorophenol		000087-86-5	0.0000007797	298.15	0.079	Pa m3/mol	25	deg C	8	calc'd P/C
aldrin		000309-00-2	4.96E-004	?	4.960E-004	atm m3/mo	temp	not report	51	
dieldrin		000060-57-1	5.80E-005	?	5.8E-005	atm m3/mo	temp	not report	51	
p,p'-DDT		000050-29-3	5.13E-004	?	5.13E-004	atm m3/mo	temp	not stated	62	a lot of other conflicting data in ref 52
p,p'-DDD		000072-54-8	2.16E-005	?	2.16E-005	atm m3/mo	temp	not stated	62	a lot of other conflicting data in ref 52
p,p'-DDE		000072-55-9	6.80E-005	?	6.8E-005	atm m3/mo	temp	not stated	62	a lot of other conflicting data in ref 52
heptachlor		000076-44-8	1.48E-003	?	1.48E-003	atm m3/mo	temp	not stated	51	not stated
heptachlor epoxide		001024-57-3	3.20E-005	?	3.2E-005	atm m3/mo	temp	not stated	51	not stated
methoxychlor		000072-43-5	1.58E-005	298.15	1.58E-005	atm m3/mo	25	deg C	28	estimated
mirex		002385-85-5	8.28E-003	293.15	839.37	Pa m3/mole	20	deg C	69	
toxaphene		008001-35-2	6.00E-006	293.15	6.0E-006	atm m3/mo	20	deg C	57	experimental
endrin		000072-20-8	7.52E-006	?	7.52E-006	atm m3/mo	temp	not report	45	calculated
alpha-hexachlorocyclohexane		000319-84-6	5.40E-006	?	0.0000054	atm m3/mo	temp	not report	33, 37	
beta-hexachlorocyclohexane		000319-85-7	4.50E-007	?	4.5E-007	atm m3/mo	temp	not report	38, 39	
delta-hexachlorocyclohexane		000319-86-8	2.10E-007	?	2.1E-007	atm m3/mo	temp	not report	37, 40	
gamma-hexachlorocyclohexane		000058-89-9	5.50E-006	?	0.0000055	atm m3/mo	temp	not report	37, 41	
mixed hexachlorocyclohexanes		000319-84-6								

NAME

HENRY's LAW CONSTANT- 1

common chemical name	IUPAC #	cas # (1)	**Henry's Law Const for gas wet dep estm [atm m3/mol]**	**temp (K)**	Henry's Law Constant	units	at wha temp?	temp units	reference	how determined
cadmium		007440-43-9			no data				77	
cadmium carbonate		000513-78-0			no data				77	
cadmium chloride		010108-64-2			no data				77	
cadmium oxide		001306-19-0			no data				77	
cadmium sulfate		010124-36-4			no data				77	
cadmium sulfide		001306-23-6			no data				77	
elemental mercury		007439-97-6	5.66E-003							
mercury oxide		021908-53-2								
mercuric chloride		007487-94-7	1.40E-008							
monomethyl mercury chloride		000115-09-3								
dimethyl mercury		000593-74-8								
tetraethyl lead		000078-00-2	5.68E-001	297.15	5.68E-001	atm-m3/mo	24	deg C	85	experimental
tetramethyl lead		000075-74-1	8.79E-001	293.15	8.79E-001	atm-m3/mo	20	deg C	97	estimated based on expt'l Vp and estm'd Ws
triethyl lead radical (1+ cation)		014570-15-1								
triethyl lead hydride		005224-23-7								
triethyl lead chloride		001067-14-7								
diethyl lead radical (2+ cation)		024952-65-6								
diethyl lead dihydride		081494-11-3								
diethyl lead dichloride		013231-90-8								
trimethyl lead radical (1+ cation)		014570-16-2								
trimethyl lead hydride		007442-13-9								
trimethyl lead chloride		001520-78-1								
dimethyl lead radical (2+ cation)		021774-13-0								
dimethyl lead dihydride		030691-92-0								
dimethyl lead dichloride		001520-77-0								
bis (tributyltin) oxide		000056-35-9	1.25E-007	293.15						
tributyl tin		000688-75-3								
tributyltin fluoride		001983-10-4								
tributyltin chloride		001461-22-9								
tributyltin hydroxide		001067-97-6								
tributyltin naphthenate										
tris(tributylstannyl) phosphate		013435-05-7								

NAME **HENRY's LAW CONSTANT- 1**

common chemical name	IUPAC #	cas # (1)	**Henry's Law Const for gas wet dep estm [atm m3/mol]**	**temp (K)**	Henry's Law Constant	units	at wha temp?	temp units	reference	how determined
1,4-dichlorobenzene		000106-46-7	1.58E-003	298.15	160	Pa m3/mol	25	deg C	5	calc'd P/C
1,2,3,4-tetrachlorobenzene		000634-66-2	1.42E-003	298.15	144	Pa m3/mol	25	deg C	5	calc'd P/C
1,2,4,5-tetrachlorobenzene		000095-94-3	1.20E-003	298.15	122	Pa m3/mol	25	deg C	5	calc'd P/C
1,2,3,5-tetrachlorobenzene		000634-90-2	5.80E-003	298.15	588	Pa m3/mol	25	deg C	5	calc'd P/C
pentachlorobenzene		000608-93-5	8.39E-004	298.15	85	Pa m3/mol	25	deg C	5	calc'd P/C
hexachlorobenzene		000118-74-1	1.29E-003	298.15	131	Pa m3/mol	25	deg C	5	calc'd P/C
naphthalene		000091-20-3	4.24E-004	298.15	43.01	Pa m3/mol	25	deg C	6	calc'd P/C
acenaphthene		000083-32-9	1.20E-004	298.15	12.17	Pa m3/mol	25	deg C	6	calc'd P/C
acenaphthylene		000208-96-8	8.29E-005	298.15	8.40	Pa m3/mol	25	deg C	6	calc'd P/C
fluorene		000086-73-7	7.77E-005	298.15	7.87	Pa m3/mol	25	deg C	6	calc'd P/C
phenanthrene		000085-01-8	3.20E-005	298.15	3.24	Pa m3/mol	25	deg C	6	calc'd P/C
anthracene		000120-12-7	3.91E-005	298.15	3.96	Pa m3/mol	25	deg C	6	calc'd P/C
pyrene		000129-00-0	9.08E-006	298.15	0.92	Pa m3/mol	25	deg C	6	calc'd P/C
fluoranthene		000206-44-0	1.02E-005	298.15	1.04	Pa m3/mol	25	deg C	6	calc'd P/C
chrysene		000218-01-9	1.05E-006	?	1.05E-006	atm m3/mo	temp	not report	10	not reported
benz [a] anthracene		000056-55-3	5.73E-006	298.15	0.581	Pa m3/mol	25	deg C	6	calc'd P/C
benzo [b] fluoranthene		000205-99-2	1.22E-005	?	1.22E-005	atm m3/mo	temp	not report	10	not reported
benzo [j] fluoranthene		000205-82-3	1.00E-006	?	1.00E-006	atm m3/mo	temp	not report	13	not reported
benzo [k] fluoranthene		000207-08-9	1.58E-007	298.15	0.016	Pa m3/mol	25	deg C	6	calc'd P/C
benzo [a] pyrene		000050-32-8	4.54E-007	298.15	0.046	Pa m3/mol	25	deg C	6	calc'd P/C
benzo [e] pyrene		000192-97-2	1.97E-007	298.15	0.020	Pa m3/mol	25	deg C	6	calc'd P/C
perylene		000198-55-0	2.96E-008	298.15	0.003	Pa m3/mol	25	deg C	6	calc'd P/C
benzo [g,h,i] perylene		000191-24-2	7.40E-007	298.15	0.08	Pa m3/mol	25	deg C	6	calc'd P/C
dibenz [a,h] anthracene		000053-70-3	7.30E-008	?	7.30E-008	atm m3/mo	temp	not report	10	not reported
indeno [1,2,3-c,d] pyrene		000193-39-5	6.95E-008	?	6.95E-008	atm-m3/mo	temp	not report	10	not reported

NAME | **HENRY's LAW CONSTANT- 1**

common chemical name	IUPAC #	cas # (1)	**Henry's Law Const for gas wet dep estm [atm m3/mol]**	**temp (K)**	Henry's Law Constant	units	at wha temp?	temp units	reference	how determined
2,3,7,8-TCDD		001746-01-6	3.29E-005	298.15	3.337	Pa m3/mol	25	deg C	6	not stated
1,2,3,7,8-PeCDD		040321-76-4	2.63E-006	298.15	0.266	Pa m3/mol	25	deg C	6	not stated
1,2,3,4,7,8-HxCDD		039227-28-6	1.07E-005	298.15	1.084	Pa m3/mol	25	deg C	6	not stated
1,2,3,6,7,8-HxCDD		057653-85-7	1.07E-005	298.15	1.084	Pa m3/mol	25	deg C	6	not stated
1,2,3,7,8,9-HxCDD		019408-74-3	1.07E-005	298.15	1.084	Pa m3/mol	25	deg C	6	not stated
1,2,3,4,6,7,8-HpCDD		035822-46-9	1.26E-005	298.15	1.273	Pa m3/mol	25	deg C	6	not stated
OCDD		003268-87-9	6.75E-006	298.15	0.684	Pa m3/mol	25	deg C	6	not stated
2,3,7,8-TCDF		051207-31-9	1.44E-005	298.15	1.461	Pa m3/mol	25	deg C	6	not stated
2,3,4,7,8-PeCDF		057117-31-4	4.98E-006	298.15	0.505	Pa m3/mol	25	deg C	6	not stated
1,2,3,7,8-PeCDF		057117-41-6	4.98E-006	298.15	0.505	Pa m3/mol	25	deg C	6	not stated
1,2,3,4,7,8-HxCDF		070648-26-9	1.43E-005	298.15	1.454	Pa m3/mol	25	deg C	6	not stated
1,2,3,6,7,8-HxCDF		057117-44-9	7.31E-006	298.15	0.741	Pa m3/mol	25	deg C	6	not stated
1,2,3,7,8,9-HxCDF		072918-21-9	1.08E-005	298.15	1.098	Pa m3/mol	25	deg C	6	not stated
2,3,4,6,7,8-HxCDF		060851-34-5	1.08E-005	298.15	1.098	Pa m3/mol	25	deg C	6	not stated
1,2,3,4,6,7,8-HpCDF		067562-39-4	1.41E-005	298.15	1.425	Pa m3/mol	25	deg C	6	not stated
1,2,3,4,7,8,9-HpCDF		055673-89-7	1.41E-005	298.15	1.425	Pa m3/mol	25	deg C	6	not stated
OCDF		039001-02-0	1.89E-006	298.15	0.191	Pa m3/mol	25	deg C	6	not stated

NAME | **HENRY's LAW CONSTANT- 1**

common chemical name	IUPAC #	cas # (1)	**Henry's Law Const for gas wet dep estm [atm m3/mol]**	**temp (K)**	Henry's Law Constant	units	at wha temp?	temp units	reference	how determined
biphenyl	0	000092-52-4	5.28E-004	298.15	53.5	Pa m3/mol	25	deg	C	calc'd P/C
2-PCB	1	002051-60-7	6.92E-004	298.15	70.1	Pa m3/mol	25	deg	C	calc'd P/C
3-PCB	2	002051-61-8	7.46E-004	298.15	75.55	Pa m3/mol	25	deg	C	calc'd P/C
4-PCB	3	002051-62-9	4.20E-004	298.15	42.56	Pa m3/mol	25	deg	C	calc'd P/C
count										
average										
standard deviation										
minimum										
maximum										
2,2'-PCB	4	013029-08-8	5.84E-004	298.15	59.17	Pa m3/mol	25	deg	C	calc'd P/C
2,3-PCB	5	016605-91-7							***-------------------- not in reference 5 --------------------***	
2,4-PCB	7	033284-50-3	4.48E-004	298.15	45.39	Pa m3/mol	25	deg	C	calc'd P/C
2,4'-PCB	8	034883-43-7							***-------------------- not in reference 5 --------------------***	
2,5-PCB	9	034883-39-1	1.98E-004	298.15	20.1	Pa m3/mol	25	deg	C	calc'd P/C
2,6-PCB	10	033146-45-1			***-------------------- not in reference 5 --------------------***					calc'd P/C
3,3'-PCB	11	002050-67-1	1.70E-004	298.15	17.26	Pa m3/mol	25	deg	C	calc'd P/C
3,4-PCB	12	002974-92-7							***-------------------- not in reference 5 --------------------***	
3,5-PCB	14	034883-41-5							***-------------------- not in reference 5 --------------------***	
4,4'-PCB	15	002050-68-2	1.68E-004	298.15	17	Pa m3/mol	25	deg	C	calc'd P/C
count										
average										
standard deviation										
minimum										
maximum										

NAME

HENRY's LAW CONSTANT- 1

common chemical name	IUPAC #	cas # (1)	**Henry's Law Const for gas wet dep estm [atm m3/mol]**	**temp (K)**	Henry's Law Constant	units	at wha temp?	temp units	reference	how determined
2,2',3-PCB	16	038444-78-9					***-------------------- not in reference 5 --------------------***			
2,2',5-PCB	18	037680-65-2	9.10E-004	298.15	92.21	Pa m3/mole	25	deg	C	calc'd P/C
2,3,3'-PCB	20	038444-84-7					***-------------------- not in reference 5 --------------------***			
2,3,4-PCB	21	055702-46-0					***-------------------- not in reference 5 --------------------***			
2,3',5-PCB	26	038444-85-8					***-------------------- not in reference 5 --------------------***			
2,4,4'-PCB	28	007012-37-5					***-------------------- not in reference 5 --------------------***			
2,4,5-PCB	29	015862-07-4	2.40E-004	298.15	24.29	Pa m3/mole	25	deg	C	calc'd P/C
2,4,6-PCB	30	035693-92-6	4.89E-004	298.15	49.51	Pa m3/mole	25	deg	C	calc'd P/C
2,4',5,-PCB	31	016606-02-3					***-------------------- not in reference 5 --------------------***			
2',3,4-PCB	33	038444-86-9	4.31E-004	298.15	43.67	Pa m3/mole	25	deg	C	calc'd P/C
3,3',4-PCB	35	037680-69-6					***-------------------- not in reference 5 --------------------***			
3,4,4'-PCB	37	038444-90-5					***-------------------- not in reference 5 --------------------***			
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3'-PCB	40	038444-93-8	2.17E-004	298.15	21.94	Pa m3/mole	25	deg	C	calc'd P/C
2,2',3,5'-PCB	44	041464-39-5					***-------------------- not in reference 5 --------------------***			
2,2',4,4'-PCB	47	002437-79-8	1.72E-004	298.15	17.38	Pa m3/mole	25	deg	C	calc'd P/C
2,2',4,5'-PCB	49	041464-40-8					***-------------------- not in reference 5 --------------------***			
2,2',4,6-PCB	50	062796-65-0					***-------------------- not in reference 5 --------------------***			
2,2',4,6'-PCB	51	068194-04-7					***-------------------- not in reference 5 --------------------***			
2,2',5,5'-PCB	52	035693-99-3	4.70E-004	298.15	47.59	Pa m3/mole	25	deg	C	calc'd P/C
2,2,5,6'-PCB	53	041464-41-9					***-------------------- not in reference 5 --------------------***			
2,2,6,6'-PCB	54	015968-05-5					***-------------------- not in reference 5 --------------------***			
2,3,4,4'-PCB	60	033025-41-1					***-------------------- not in reference 5 --------------------***			
2,3,4,5-PCB	61	033284-53-6					***-------------------- not in reference 5 --------------------***			
2,3,5,6-PCB	65	033284-54-7					***-------------------- not in reference 5 --------------------***			
2,3,4,4'-PCB	66	032598-10-0					***-------------------- not in reference 5 --------------------***			
2,3',4',5-PCB	70	032598-11-1					***-------------------- not in reference 5 --------------------***			
2,4,4',6-PCB	75	032598-12-2					***-------------------- not in reference 5 --------------------***			
3,3',4,4'-PCB	77	032598-13-3	1.70E-005	298.15	1.72	Pa m3/mole	25	deg	C	calc'd P/C
3,3',5,5'-PCB	80	033284-52-5					***-------------------- not in reference 5 --------------------***			
3,4,4',5-PCB	81	070362-50-4					***-------------------- not in reference 5 --------------------***			
count										
average										
standard deviation										
minimum										
maximum										

NAME										**HENRY's LAW CONSTANT- 1**
			Henry's Law Const for gas wet dep estm		Henry's Law					
common chemical name	IUPAC #	cas # (1)	**[atm m3/mol]**	**temp (K)**	Constant	units	at wha temp?	temp units	reference	how determined
2,2',3,3',5-PCB	83	060145-20-2					***-------------------- not in reference 5 --------------------***			
2,2',3,4,5-PCB	86	065510-45-4	1.49E-003	298.15	151.4	Pa m3/mole	25	deg	C	calc'd P/C
2,2',3,4,5'-PCB	87	038380-02-8	2.45E-004	298.15	24.81	Pa m3/mole	25	deg	C	calc'd P/C
2,2',3,4,6-PCB	88	055215-17-3					***-------------------- not in reference 5 --------------------***			
2,2',3,5,6-PCB	95	038379-99-6					***-------------------- not in reference 5 --------------------***			
2,2',4,4',5-PCB	99	038380-01-7					***-------------------- not in reference 5 --------------------***			
2,2',4,4',6-PCB	100	039485-83-1					***-------------------- not in reference 5 --------------------***			
2,2',4,5,5'-PCB	101	037680-73-2	3.50E-004	298.15	35.48	Pa m3/mole	25	deg	C	calc'd P/C
2,2',4,6,6'-PCB	104	056558-16-8	1.38E-004	298.15	13.98	Pa m3/mole	25	deg	C	calc'd P/C
2,3,3',4,4'-PCB	105	032598-14-4					***-------------------- not in reference 5 --------------------***			
2,3,3',4',6-PCB	110	038380-03-9					***-------------------- not in reference 5 --------------------***			
2,3,4,4',5-PCB	114	074472-37-0					***-------------------- not in reference 5 --------------------***			
2,3,4,5,6-PCB	116	018259-05-7					***-------------------- not in reference 5 --------------------***			
2,3',4,4',5-PCB	118	031508-00-6					***-------------------- not in reference 5 --------------------***			
2',3,4,5,5'-PCB	124	070424-70-3					***-------------------- not in reference 5 --------------------***			
3,3',4,4',5-PCB	126	057465-28-8					***-------------------- not in reference 5 --------------------***			
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4'-PCB	128	038380-07-3	1.18E-004	298.15	11.91	Pa m3/mole	25	deg	C	calc'd P/C
2,2',3,3',4,5-PCB	129	055215-18-4					***-------------------- not in reference 5 --------------------***			
2,2',3,3',5,6-PCB	134	052704-70-8					***-------------------- not in reference 5 --------------------***			
2,2',3,3',6,6'-PCB	136	038411-22-2					***-------------------- not in reference 5 --------------------***			
2,2',3,4,4',5'-PCB	138	035065-28-2					***-------------------- not in reference 5 --------------------***			
2,2',3,4',5',6-PCB	149	038380-04-0					***-------------------- not in reference 5 --------------------***			
2,2',4,4',5,5'-PCB	153	035065-27-1	4.23E-004	298.15	42.9	Pa m3/mole	25	deg	C	calc'd P/C
2,2',4,4',6,6'-PCB	155	033979-03-2	8.55E-004	298.15	86.616	Pa m3/mole	25	deg	C	calc'd P/C
2,3,3',4,4',5-PCB	156	038380-08-4					***-------------------- not in reference 5 --------------------***			
2,3,3',4,4',5'-PCB	157	069782-90-7					***-------------------- not in reference 5 --------------------***			
2,3',4,4',5,5'-PCB	167	052663-72-6					***-------------------- not in reference 5 --------------------***			
3,3',4,4',5,5'-PCB	169	032774-16-6					***-------------------- not in reference 5 --------------------***			
count										
average										
standard deviation										
minimum										
maximum										

NAME

HENRY's LAW CONSTANT- 1

common chemical name	IUPAC #	cas # (1)	Henry's Law Const for gas wet dep estm [atm m3/mol]	temp (K)	Henry's Law Constant	units	at wha temp?	temp units	reference	how determined
2,2',3,3',4,4',5-PCB	170	035065-30-6					-------------------- ***not in reference 5*** --------------------			
2,2',3,3',4,4',6-PCB	171	052663-71-5	5.33E-005	298.15	5.4	Pa m3/mol	25	deg	C	calc'd P/C
2,2',3,4,4',5,5'-PCB	180	035065-29-3					-------------------- ***not in reference 5*** --------------------			
2,2',3,4,5,5',6-PCB	185	052712-05-7					-------------------- ***not in reference 5*** --------------------			
2,2',3,4',5,5',6-PCB	187	052663-68-0					-------------------- ***not in reference 5*** --------------------			
2,3,3',4,4',5,5'-PCB	189	039635-31-9					-------------------- ***not in reference 5*** --------------------			
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7					-------------------- ***not in reference 5*** --------------------			
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	3.76E-004	298.15	38.08	Pa m3/mol	25	deg	C	calc'd P/C
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	8.11E-004	298.15	82.2	Pa m3/mol	25	deg	C	calc'd P/C
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3					-------------------- ***not in reference 5*** --------------------			
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1					-------------------- ***not in reference 5*** --------------------			
count										
average										
standard deviation										
minimum										
maximum										
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	2.06E-004	298.15	20.84	Pa m3/mol	25	deg	C	calc'd P/C

NAME

HENRY's LAW CONSTANT- 1 (continued)

common chemical name	IUPAC #	cas # (1)	H calc'd from P-liquid/ C-liquid Pa m3/mol	pressure basis for calc	solubility basis for calc	percent diff of calc vs. stated value	calc notes	data notes
octachlorostyrene		029082-74-4						
4-bromophenyl phenyl ether		000101-55-3	10.4	liquid	liquid			
3,3'-dichlorobenzidene		000091-94-1	4.58E-003	liquid	liquid			same for solid basis
1,3-dinitropyrene		075321-20-9	5.70E-002	solid	solid			
1,6-dinitropyrene		042397-64-8	5.70E-002	solid	solid			
1,8-dinitropyrene		042397-65-9	5.70E-002	solid	solid			
2,7-dinitropyrene		117929-15-4	5.70E-002	solid	solid			
dinitropyrenes (mixed)		078432-19-6						
hexachloro-1,3-butadiene		000087-68-3	1538	saturated	saturated			
4,4'-methylene bis(2-chloroaniline)		000101-14-4						
pentachlorophenol		000087-86-5	0.078	solid	solid			
aldrin		000309-00-2						
dieldrin		000060-57-1						
p,p'-DDT		000050-29-3						
p,p'-DDD		000072-54-8						
p,p'-DDE		000072-55-9						
heptachlor		000076-44-8						
heptachlor epoxide		001024-57-3						
methoxychlor		000072-43-5						
mirex		002385-85-5						
toxaphene		008001-35-2						
endrin		000072-20-8						
alpha-hexachlorocyclohexane		000319-84-6						avg of two reported values
beta-hexachlorocyclohexane		000319-85-7						
delta-hexachlorocyclohexane		000319-86-8						
gamma-hexachlorocyclohexane		000058-89-9						avg of two reported values
mixed hexachlorocyclohexanes		000319-84-6						

NAME

HENRY's LAW CONSTANT- 1 (continued)

common chemical name	IUPAC #	cas # (1)	H calc'd from P-liquid/ C-liquid Pa m3/mol	pressure basis for calc	solubility basis for calc	percent diff of calc vs. stated value	calc notes	data notes
cadmium		007440-43-9						
cadmium carbonate		000513-78-0						
cadmium chloride		010108-64-2						
cadmium oxide		001306-19-0						
cadmium sulfate		010124-36-4						
cadmium sulfide		001306-23-6						
elemental mercury		007439-97-6	573.544711	liquid	liquid			
mercury oxide		021908-53-2						
mercuric chloride		007487-94-7	0.00142002	solid	solid		using estm	of Vp at 290 from V/P calc
monomethyl mercury chloride		000115-09-3						
dimethyl mercury		000593-74-8						
tetraethyl lead		000078-00-2						
tetramethyl lead		000075-74-1	89106.0049					
triethyl lead radical (1+ cation)		014570-15-1						
triethyl lead hydride		005224-23-7						
triethyl lead chloride		001067-14-7						
diethyl lead radical (2+ cation)		024952-65-6						
diethyl lead dihydride		081494-11-3						
diethyl lead dichloride		013231-90-8						
trimethyl lead radical (1+ cation)		014570-16-2						
trimethyl lead hydride		007442-13-9						
trimethyl lead chloride		001520-78-1						
dimethyl lead radical (2+ cation)		021774-13-0						
dimethyl lead dihydride		030691-92-0						
dimethyl lead dichloride		001520-77-0						
bis (tributyltin) oxide		000056-35-9	0.01270552				Pa (g/mol)	m3/g
tributyl tin		000688-75-3						
tributyltin fluoride		001983-10-4						
tributyltin chloride		001461-22-9						
tributyltin hydroxide		001067-97-6						
tributyltin naphthenate								
tris(tributylstannyl) phosphate		013435-05-7						

NAME					HENRY's LAW CONSTANT- 1 (continued)			
common chemical name	IUPAC #	cas # (1)	H calc'd from P-liquid/ C-liquid Pa m3/mol	pressure basis for calc	solubility basis for calc	percent diff of calc vs. stated value	calc notes	data notes
1,4-dichlorobenzene		000106-46-7	160	saturated	saturated			
1,2,3,4-tetrachlorobenzene		000634-66-2	144	saturated	saturated			
1,2,4,5-tetrachlorobenzene		000095-94-3	122	saturated	saturated			
1,2,3,5-tetrachlorobenzene		000634-90-2	587	saturated	saturated			
pentachlorobenzene		000608-93-5	85	saturated	saturated			
hexachlorobenzene		000118-74-1	131	saturated	saturated			
naphthalene		000091-20-3	4.30E+001	liquid	liquid			= solid basis
acenaphthene		000083-32-9	1.22E+001	liquid	liquid			= solid basis
acenaphthylene		000208-96-8	8.40E+000	liquid	liquid			= solid basis
fluorene		000086-73-7	7.87E+000	liquid	liquid			= solid basis
phenanthrene		000085-01-8	3.24E+000	liquid	liquid			= solid basis
anthracene		000120-12-7	3.96E+000	liquid	liquid			= solid basis
pyrene		000129-00-0	9.23E-001	liquid	liquid			= solid basis
fluoranthene		000206-44-0	1.04E+000	liquid	liquid			= solid basis
chrysene		000218-01-9	1.22E+001	liquid	liquid			no "solid" data
benz [a] anthracene		000056-55-3	5.80E-001	liquid	liquid			= solid basis
benzo [b] fluoranthene		000205-99-2						
benzo [j] fluoranthene		000205-82-3						
benzo [k] fluoranthene		000207-08-9	1.63E-002	liquid	liquid			= solid basis
benzo [a] pyrene		000050-32-8	4.64E-002	liquid	liquid			= solid basis
benzo [e] pyrene		000192-97-2	4.66E-002	liquid	liquid			= solid basis
perylene		000198-55-0	8.81E-003	solid	solid			
benzo [g,h,i] perylene		000191-24-2	7.48E-002	liquid	liquid			
dibenz [a,h] anthracene		000053-70-3	1.72E-004	liquid	liquid			= solid basis
indeno [1,2,3-c,d] pyrene		000193-39-5						

NAME

HENRY's LAW CONSTANT- 1 (continued)

common chemical name	IUPAC #	cas # (1)	||||	H calc'd from P-liquid/ C-liquid Pa m3/mol	pressure basis for calc	solubility basis for calc	percent diff of calc vs. stated value	calc notes	data notes	||||
2,3,7,8-TCDD		001746-01-6	||||	1.64430921	solid	solid	51%	different because using different solid vapor pressure than Mack		||||
1,2,3,7,8-PeCDD		040321-76-4	||||	0.26586103	solid	solid	0%		using value for 12347 PeCDD	||||
1,2,3,4,7,8-HxCDD		039227-28-6	||||	0.45132743	solid	solid	58%	**?? why different?**		||||
1,2,3,6,7,8-HxCDD		057653-85-7	||||	0.45132743	solid	solid	58%	**?? why dif**	using value for 123478 HxCDD	||||
1,2,3,7,8,9-HxCDD		019408-74-3	||||	0.45132743	solid	solid	58%	**?? why dif**	using value for 123478 HxCDD	||||
1,2,3,4,6,7,8-HpCDD		035822-46-9	||||	0.13297872	solid	solid	90%	**?? why different?**		||||
OCDD		003268-87-9	||||	0.68322981	solid	solid	0%	**?? different when calc with liquid**		||||
2,3,7,8-TCDF		051207-31-9	||||	1.45985401	solid	solid	0%			||||
2,3,4,7,8-PeCDF		057117-31-4	||||	0.50505051	solid	solid	0%			||||
1,2,3,7,8-PeCDF		057117-41-6	||||	0.50505051	solid	solid	0%		using value for 23478 PeCDF	||||
1,2,3,4,7,8-HxCDF		070648-26-9	||||	1.45454545	solid	solid	0%			||||
1,2,3,6,7,8-HxCDF		057117-44-9	||||	0.74152542	solid	solid	0%			||||
1,2,3,7,8,9-HxCDF		072918-21-9	||||	0.96820809	solid	solid	12%		using avg of values for 123478 HxCDF and 123678	||||
2,3,4,6,7,8-HxCDF		060851-34-5	||||	0.96820809	solid	solid	12%		using avg of values for 123478 HxCDF and 123678	||||
1,2,3,4,6,7,8-HpCDF		067562-39-4	||||	1.42424242	solid	solid	0%			||||
1,2,3,4,7,8,9-HpCDF		055673-89-7	||||	1.87878788	solid	solid	32%		using value for 1234678 HpCDF	||||
OCDF		039001-02-0	||||	0.19157088	solid	solid	0%			||||

NAME

HENRY's LAW CONSTANT- 1 (continued)

common chemical name	IUPAC #	cas # (1)	H calc'd from P-liquid/ C-liquid Pa m3/mol	pressure basis for calc	solubility basis for calc	percent diff of calc vs. stated value	calc notes	data notes
biphenyl	0	000092-52-4						
2-PCB	1	002051-60-7						
3-PCB	2	002051-61-8						
4-PCB	3	002051-62-9						
count								
average								
standard deviation								
minimum								
maximum								
2,2'-PCB	4	013029-08-8						
2,3-PCB	5	016605-91-7						
2,4-PCB	7	033284-50-3						
2,4'-PCB	8	034883-43-7						
2,5-PCB	9	034883-39-1						
2,6-PCB	10	033146-45-1						
3,3'-PCB	11	002050-67-1						
3,4-PCB	12	002974-92-7						
3,5-PCB	14	034883-41-5						
4,4'-PCB	15	002050-68-2						
count								
average								
standard deviation								
minimum								
maximum								

NAME | **HENRY's LAW CONSTANT- 1 (continued)**

common chemical name	IUPAC #	cas # (1)	H calc'd from P-liquid/ C-liquid Pa m3/mol	pressure basis for calc	solubility basis for calc	percent diff of calc vs. stated value	calc notes	data notes
2,2',3-PCB	16	038444-78-9						
2,2',5-PCB	18	037680-65-2						
2,3,3'-PCB	20	038444-84-7						
2,3,4-PCB	21	055702-46-0						
2,3',5-PCB	26	038444-85-8						
2,4,4'-PCB	28	007012-37-5						
2,4,5-PCB	29	015862-07-4						
2,4,6-PCB	30	035693-92-6						
2,4',5,-PCB	31	016606-02-3						
2',3,4-PCB	33	038444-86-9						
3,3',4-PCB	35	037680-69-6						
3,4,4'-PCB	37	038444-90-5						
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3'-PCB	40	038444-93-8						
2,2',3,5'-PCB	44	041464-39-5						
2,2',4,4'-PCB	47	002437-79-8						
2,2',4,5'-PCB	49	041464-40-8						
2,2',4,6-PCB	50	062796-65-0						
2,2',4,6'-PCB	51	068194-04-7						
2,2,5,5'-PCB	52	035693-99-3						
2,2,5,6'-PCB	53	041464-41-9						
2,2,6,6'-PCB	54	015968-05-5						
2,3,4,4'-PCB	60	033025-41-1						
2,3,4,5-PCB	61	033284-53-6						
2,3,5,6-PCB	65	033284-54-7						
2,3,4,4'-PCB	66	032598-10-0						
2,3',4',5-PCB	70	032598-11-1						
2,4,4',6-PCB	75	032598-12-2						
3,3',4,4'-PCB	77	032598-13-3						
3,3',5,5'-PCB	80	033284-52-5						
3,4,4',5-PCB	81	070362-50-4						
count								
average								
standard deviation								
minimum								
maximum								

NAME **HENRY's LAW CONSTANT- 1 (continued)**

common chemical name	IUPAC #	cas # (1)	H calc'd from P-liquid/ C-liquid Pa m3/mol	pressure basis for calc	solubility basis for calc	percent diff of calc vs. stated value	calc notes	data notes
2,2',3,3',5-PCB	83	060145-20-2						
2,2',3,4,5-PCB	86	065510-45-4						
2,2',3,4,5'-PCB	87	038380-02-8						
2,2',3,4,6-PCB	88	055215-17-3						
2,2',3,5,6-PCB	95	038379-99-6						
2,2',4,4',5-PCB	99	038380-01-7						
2,2',4,4',6-PCB	100	039485-83-1						
2,2',4,5,5'-PCB	101	037680-73-2						
2,2',4,6,6'-PCB	104	056558-16-8						
2,3,3',4,4'-PCB	105	032598-14-4						
2,3,3',4',6-PCB	110	038380-03-9						
2,3,4,4',5-PCB	114	074472-37-0						
2,3,4,5,6-PCB	116	018259-05-7						
2,3',4,4',5-PCB	118	031508-00-6						
2',3,4,5,5'-PCB	124	070424-70-3						
3,3',4,4',5-PCB	126	057465-28-8						
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4'-PCB	128	038380-07-3						
2,2',3,3',4,5-PCB	129	055215-18-4						
2,2',3,3',5,6-PCB	134	052704-70-8						
2,2',3,3',6,6'-PCB	136	038411-22-2						
2,2',3,4,4',5'-PCB	138	035065-28-2						
2,2',3,4',5',6-PCB	149	038380-04-0						
2,2',4,4',5,5'-PCB	153	035065-27-1						
2,2',4,4',6,6'-PCB	155	033979-03-2						
2,3,3',4,4',5-PCB	156	038380-08-4						
2,3,3',4,4',5'-PCB	157	069782-90-7						
2,3',4,4',5,5'-PCB	167	052663-72-6						
3,3',4,4',5,5'-PCB	169	032774-16-6						
count								
average								
standard deviation								
minimum								
maximum								

NAME			HENRY's LAW CONSTANT- 1 (continued)					
common chemical name	IUPAC #	cas # (1)	H calc'd from P-liquid/ C-liquid Pa m3/mol	pressure basis for calc	solubility basis for calc	percent diff of calc vs. stated value	calc notes	data notes
2,2',3,3',4,4',5-PCB	170	035065-30-6						
2,2',3,3',4,4',6-PCB	171	052663-71-5						
2,2',3,4,4',5,5'-PCB	180	035065-29-3						
2,2',3,4,5,5',6-PCB	185	052712-05-7						
2,2',3,4',5,5',6-PCB	187	052663-68-0						
2,3,3',4,4',5,5'-PCB	189	039635-31-9						
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7						
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4						
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9						
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3						
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1						
count								
average								
standard deviation								
minimum								
maximum								
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3						

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A value was not given in Ref 6. As a basis, used the 310-312 deg C at 10 mmHg boiling point, given in ATSDR-PAH
Note: this last 310C @ 10mmHg is not a "real" boiling point, e.g., at atmospheric pressure;
it is a boiling point at a much reduced pressure
However, this data was used to make an estimate of the "real" boiling point, i.e., the temperature at which
the liquid vapor pressure equals one atmosphere (detailed calc shown on another sheet)

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87 Estimated using calculation, including Clausius Clapyron equation and Trouton's Rule similar to V/P type calc.
As a basis, used the 145 deg C at 2 mmHg boiling point, given in ref 85 and ref 48
Note: this 145 C @ 2 mmHg is not a "real" boiling point, e.g., at atmospheric pressure;
it is a boiling point at a much reduced pressure
However, this data was used to make an estimate of the "real" boiling point, i.e., the temperature at which
the liquid vapor pressure equals one atmosphere (detailed calc shown on another sheet)
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92 Estimated; analogous method to note 87, etc.
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Ref 85 gives the Bidleman value ... this seems too high
For this analysis, used an average of data from: Balson, 1947; Klopffer et al, 1988; MacKay et al, 1986;
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Appendix B.

Estimation Methods Used for Physical Chemical Properties

B.1. Estimation of Boiling Temperature (T_b) at 1 atm pressure
(when T_b given at a pressure other than 1 atm)

B.2. Estimate of Boiling Temperature and Melting Temperature for Octachlorostyrene

B.3. Estimation of Physical Properties for Dinitropyrenes

B.4. Methodology Used to Estimate Boiling Temperature When No Data Were Available
(based on Regression Between Melting Temperature and Boiling Temperature for Other Compounds)

Appendix B.1.

Estimation of Boiling Temperature (T_b) at 1 atm pressure (when T_b given at a pressure other than 1 atm)

Zeroth Order Estimation Procedure for Boiling Temperature
When Tb given for a different pressure than Atmospheric

============================ : ==========   ============:   ==========   ==========

Basis of Calculation:

============================ : ==========   ============:   ==========   ==========

Suppose Tb' given at a different pressure than atmospheric
Suppose this pressure is Pb

What is the Tb at atmospheric pressure, i.e., the normal boiling point?

Use the Clausius Clapyron equation to estimate this...

$\mathrm{Ln}(Pb/Patm) = 84 * Tb / R\ (1/Tb - 1/Tb')$

This equation makes use of Troutons Rule, in which the enthalpy of vaporization can be approximately estimated by:

$$\text{delta } H / T_{boil} = 84 \text{ J/(mol deg K)}$$

Solving the above equation for Tb (in terms of Tb' and Pb), one gets:

$Tb = Tb' (K) * [\ 1 - (R / 84) \ln (Pb/ 1 \text{ atm})\ ]$

$$\text{where } R = 8.3144 \text{ J/(mol deg K)}$$

	Benz(e)Pyrene				Aldrin			
parameter	value	units	ref	notes	value	units	ref	notes
T boil at non std pres. = Tb'	584.15	deg K	86		418.15	deg K	85	
Non std pressure for Tb'	10	mm Hg	86		2	mm Hg	85	
R / 84	0.0990	dimensionless			0.0990	dimensionless		
ln (Pb / 1 atm)	-4.3307	dimensionless			-5.9402	dimensionless		
T-boil estimate at 1 atm	834.55	deg K			664.01	deg K		
ndependent Estm of T-boil at 1 atm								

	p,p'-DDD				**Heptachlor**			
parameter	value	units	ref	notes	value	units	ref	notes
T boil at non std pres. = Tb'	466.15	deg K	60		418.15	deg K	?	
Non std pressure for Tb'	1	mm Hg	60		1.5	mm Hg	?	
R / 84	0.0990	dimensionless			0.0990	dimensionless		
ln (Pb / 1 atm)	-6.6333	dimensionless			-6.2279	dimensionless		
T-boil estimate at 1 atm	772.21	deg K			675.91	deg K		
ndependent Estm of T-boil at 1 atm	623.15	deg K	85	not that close to the estima above (?) Use this new value in V/P calculation	583.15	deg K	85	not that close to the estima above (?) Use this new value in V/P calculation

parameter	Beta Hexachlorocyclohexane value	units	ref	notes	Delta Hexachlorocyclohexane value	units	ref	notes
T boil at non std pres. = Tb'	333.15	deg K			333.15	deg K		
Non std pressure for Tb'	0.5	mm Hg			0.36	mm Hg		
R / 84	0.0990	dimensionless			0.0990	dimensionless		
ln (Pb / 1 atm)	-7.3265	dimensionless			-7.6550	dimensionless		
T-boil estimate at 1 atm	574.74	deg K			585.58	deg K		
ndependent Estm of T-boil at 1 atm								

parameter	**Bis (Tributyltin) Oxide (TBTO)**				**Tetramethyl Lead (TML)**			
	value	units	ref	notes	value	units	ref	notes
T boil at non std pres. = Tb'	527.15	deg K			383.15	deg K		
Non std pressure for Tb'	50	mm Hg			10	mm Hg		
R / 84	0.0990	dimensionless			0.0990	dimensionless		
ln (Pb / 1 atm)	-2.7213	dimensionless			-4.3307	dimensionless		
T-boil estimate at 1 atm	669.14	deg K			547.39	deg K		
ndependent Estm of T-boil at 1 atm								

Appendix B.2.

Estimate of Boiling Temperature and Melting Temperature for Octachlorostyrene

Is there a relatively simple relationship between Parent Compounds and Fully Chlorinated Derivatives for Boiling Point and Melting Point?

parent compound	fully chlorinated compound	**boiling** temp of **parent** compound deg C	deg K	ref	**boiling** temp of **fully-Cl'd** compound deg C	deg K	ref	boiling temp of **fully-Cl'd** predicted by regression deg K	percent error	**melting** temp of **parent** compound deg C	deg K	ref	**melting** temp of **fully-Cl'd** compound deg C	deg K	ref	melting temp of **fully-Cl'd** predicted by regression deg K	percent error
styrene	octachlorostyrene	145	418	88	?	?		652		-31	242.15	88	?	?		423	
3-cyclohexanone	octachloro-3-cyclohexanone	155	429	88	?	?	88	663		-31	**242**	88	104	**377**	88	423	12%
propane	octachloropropane	-42	231	88	?	?	88	462		-188	**86**	88	160	**433**	88	276	-36%
1,5-hexadiene	decachloro-1,5-hexadiene	59	333	88	?	?	88	565		-141	**132**	88	49	**322**	88	320	-1%
biphenyl	decachloro-PCB	255	528	5	?	?		764		71	**344**	5	306	**579**	5	519	-10%
napthalene	octachloronapthalene	218	491	85	?	?		727		80	**353**	85	198	**471**	88	528	12%
styrene	octachlorostyrene	145	418	88				652		-31	242.15	88				423	
methane	carbon tetrachloride	-162	**112**	88	77	**350**	88	340	-3%	-182	**91**	88	-23	**250**	88	281	12%
ethylene	tetrachloroethylene	-104	**169**	88	121	**394**	88	399	1%	-169	**104**	88	-22	**251**	88	294	17%
1,3-butadiene	hexachlorobutadiene	-4	**269**	88	215	**488**	85	500	2%	-109	**164**	88	-21	**252**	85	350	39%
cyclopentene	octachlorocyclopentene	44	**317**	88	283	**556**	88	550	-1%	-135	**138**	88	40	**313**	88	325	4%
benzene	hexachlorobenzene	80	**353**	5	319	**592**	85	586	-1%	6	**279**	5	230	**503**	5	457	-9%
cyclohexane	avg for HCH's	81	**354**	88	306	**579**	85	587	1%	7	**280**	88	182	**455**	85	458	1%
dibenzo-p-dioxin	OCDD	284	**557**	6	510	**783**	6	793	1%	123	**396**	6	322	**595**	6	568	-5%
dibenzofuran	OCDF	287	**560**	6	537	**810**	6	797	-2%	87	**360**	6	258	**531**	6	533	0%
phenol	pentachlorophenol	182	455	88	310	583	85	690	18%	41	314	88	174	447	85	491	10%
cyclohexane	beta-HCH	81	354	88	?	?		587		7	280	88	315	588	85	458	-22%
cyclohexane	delta-HCH	81	354	88	?	?		587		7	280	88	142	415	85	458	10%
cyclohexane	alpha-HCH	81	354	88	288	561	85	587	5%	7	280	88	160	433	85	458	6%
cyclohexane	gamma-HCH	81	354	88	323	597	85	587	-2%	7	280	88	113	386	85	458	19%
	average for HCH's	81	354	88	306	579	85	587	1%	7	280	88	182	455	85	458	1%

Regression Output for Boiling Temperature

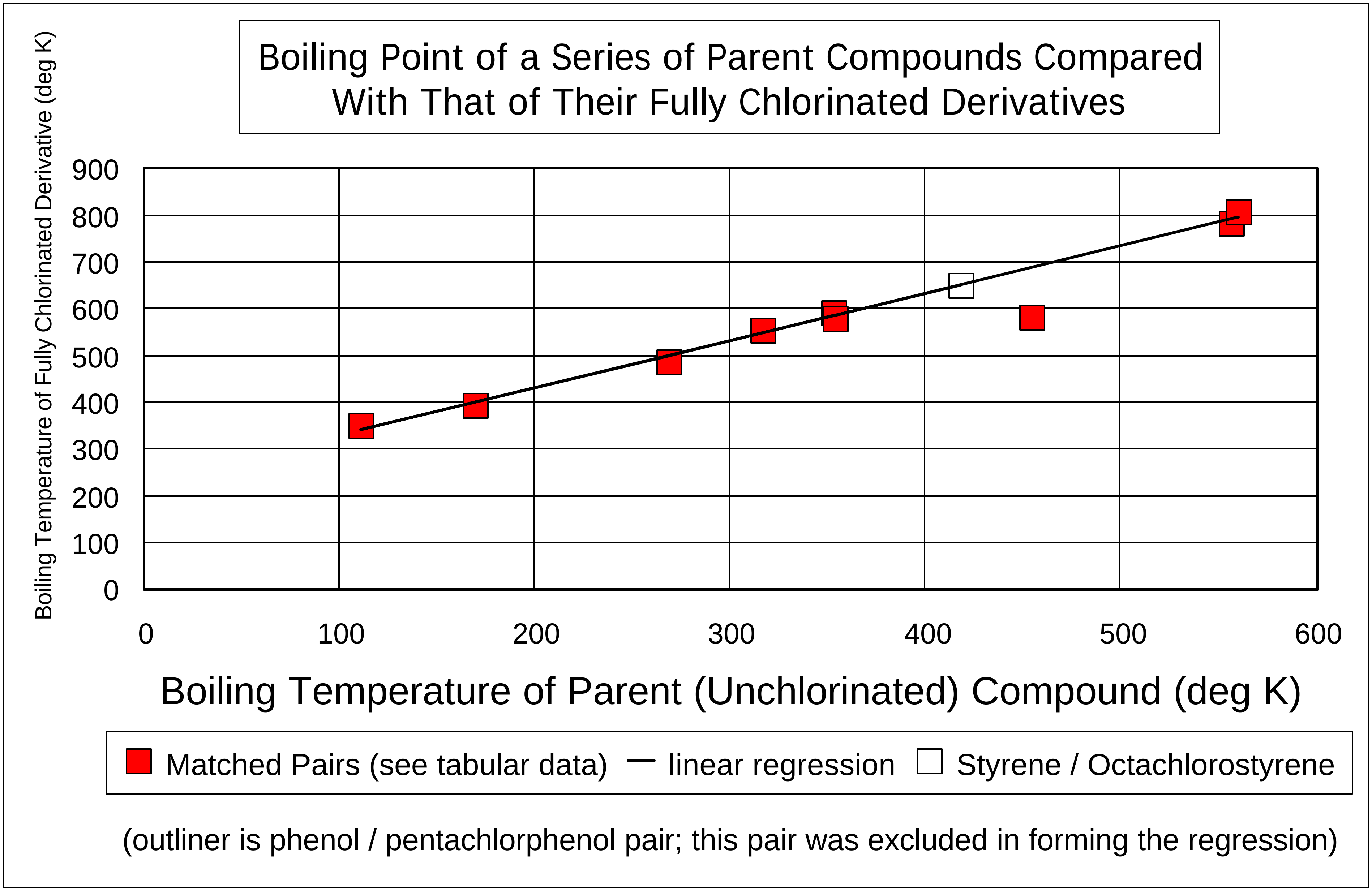
Constant	**226.7086**
Std Err of Y Est	**10.6820**
R Squared	**0.9964**
No. of Observations	**8**
Degrees of Freedom	**6**
X Coefficient(s)	**1.0180**
Std Err of Coef.	**0.0250**

Regression Output for Melting Temperature

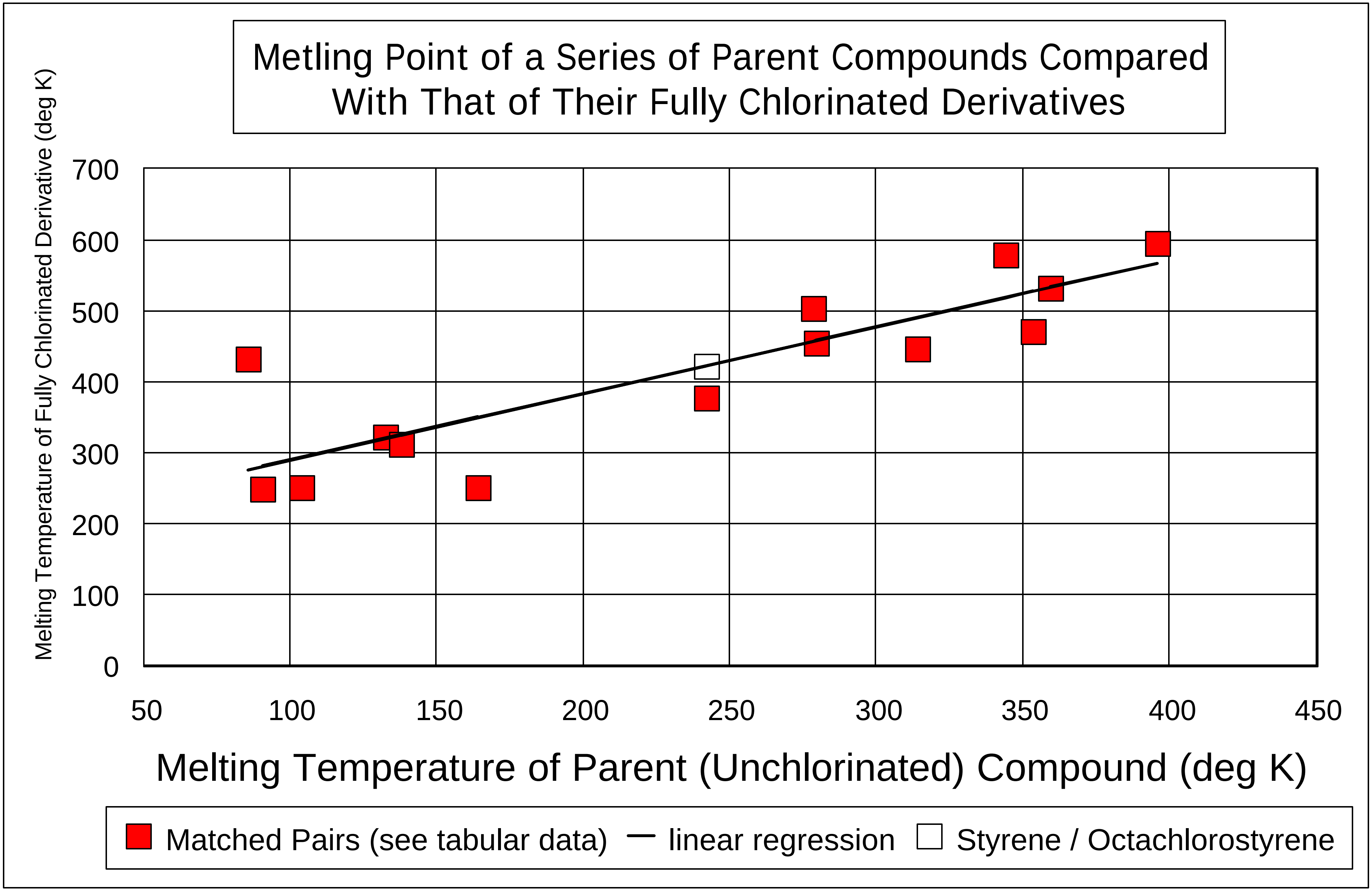
Constant	**195.8783**
Std Err of Y Est	**66.7442**
R Squared	**0.7372**
No. of Observations	**13**
Degrees of Freedom	**11**
X Coefficient(s)	**0.9386**
Std Err of Coef.	**0.1690**

Notes:

Phenol/Pentachlorophenol not included in regression; this pair seemed to be an outlier
Shaded data were included in regression
The purpose of this exercise was to crudely estimate physical properties of octachlorostyrene


Boiling Point of a Series of Parent Compounds Compared With That of Their Fully Chlorinated Derivatives

(outliner is phenol / pentachlorphenol pair; this pair was excluded in forming the regression)


Metling Point of a Series of Parent Compounds Compared
With That of Their Fully Chlorinated Derivatives
Melting Temperature of Fully Chlorinated Derivative (deg K)
0
100
200
300
400
500
600
700
50
100
150
200
250
300
350
400
450
Melting Temperature of Parent (Unchlorinated) Compound (deg K)
🟥 Matched Pairs (see tabular data)
— linear regression
☐ Styrene / Octachlorostyrene

Appendix B.3.

Estimation of Physical Properties for Dinitropyrenes

all references equal 88, unless stated
ref 88 = CRC Properties of Organic Compounds,
Personal Edition CD ROM, 1996

Some Physical Property Data for a Series of Compounds, with Parent Compounds
compared with Nitro- and Dinitro- substituted Derivatives

CHEMICAL IDENTITY DATA				Melt Temp		BOILING TEMPERATURE DATA								
				Melt Temp		Boil Temp @ 1 atm			Boil Temp @ other pressure 1			Boil Temp @ other pressure 2		
TYPE	compound	cas #	molecular weight	deg C	ref	deg C	ref	notes	deg C	pressure mm Hg	ref	deg C	pressure mm Hg	ref
parent	Benzene	71-43-2	78.11	6		80								
+ 1 nitro	Benzene, nitro-	98-95-3	123.11	6		211								
+2 nitro's	Benzene, 1,2-dinitro-	528-29-0	168.11	119		318			194	30				
+2 nitro's	Benzene, 1,3-dinitro-	99-65-0	168.11	90		291			167	14				
+2 nitro's	Benzene, 1,4-dinitro-	100-25-4	168.11	174		297			183	34				
parent	Naphthalene	91-20-3	128.17	80		218								
+ 1 nitro	Naphthalene, 1-nitro-	86-57-7	173.17	61					180	14				
+ 1 nitro	Naphthalene, 2-nitro-	581-89-5	173.17	79		314			165	15				
+2 nitro's	Naphthalene, 1,2-dinitro-	24934-47-2	218.17	163										
+2 nitro's	Naphthalene, 1,3-dinitro-	606-37-1	218.17	148				sublimates						
+2 nitro's	Naphthalene, 1,4-dinitro-	6921-26-2	218.17	133										
+2 nitro's	Naphthalene, 1,5-dinitro-	605-71-0	218.17	219				sublimates						
+2 nitro's	Naphthalene, 1,8-dinitro-	602-38-0	218.17	173		445		decompose						
+2 nitro's	Naphthalene, 2,3-dinitro-	1875-63-4	218.17	174										
+2 nitro's	Naphthalene, 2,7-dinitro-	24824-27-9	218.17	234										

all references equal 88, unless stated
ref 88 = CRC Properties of Organic Compounds,
Personal Edition CD ROM, 1996

Some Physical Property Data for a Series of Compounds, with Parent Compounds
compared with Nitro- and Dinitro- substituted Derivatives

CHEMICAL IDENTITY DATA				Melt Temp		BOILING TEMPERATURE DATA								
				Melt Temp		Boil Temp @ 1 atm			Boil Temp @ other pressure 1			Boil Temp @ other pressure 2		
TYPE	compound	cas #	molecular weight	deg C	ref	deg C	ref	notes	deg C	pressure mm Hg	ref	deg C	pressure mm Hg	ref
parent	1,1'-Biphenyl	92-52-4	154.21	69		256								
+ 1 nitro	1,1'-Biphenyl, 2-nitro-	86-00-0	199.21	37		320								
+ 1 nitro	1,1'-Biphenyl, 3-nitro-	2113-58-8	199.21	62					227	35		143	9	
+ 1 nitro	1,1'-Biphenyl, 4-nitro-	92-93-3	199.21	114		340								
+2 nitro's	1,1'-Biphenyl, 2,2'-dinitro-	2436-96-6	244.21	126		305								
+2 nitro's	1,1'-Biphenyl, 2,3'-dinitro-	7391-72-2	244.21	119										
+2 nitro's	1,1'-Biphenyl, 2,4'-dinitro-	608-81-5	244.21	94										
+2 nitro's	1,1'-Biphenyl, 3,3'-dinitro-	958-96-3	244.21	201										
+2 nitro's	1,1'-Biphenyl, 3,4'-dinitro-	6311-43-9	244.21	189										
+2 nitro's	1,1'-Biphenyl, 4,4'-dinitro-	1528-74-1	244.21	242										
parent	Dibenzofuran	132-64-9	168.19	87		287								
+ 1 nitro	Dibenzofuran, 1-nitro-	87812-99-5	213.19	121										
+ 1 nitro	Dibenzofuran, 3-nitro-	5410-97-9	213.19	182					182.5	3				
+ 1 nitro	Dibenzofuran, 4-nitro-	86607-81-0	213.19	139					197.5	15				
+2 nitro's	Dibenzofuran, 2,7-dinitro-	5408-55-9	258.19	256										
parent	Acenaphthene	83-32-9	154.21	93		279								
+ 1 nitro	Acenaphthene, 3-nitro-	3807-77-0	199.21	151.5										
+ 1 nitro	Acenaphthene, 5-nitro-	602-87-9	199.21	103.5										
+2 nitro's	Acenaphthene, 5,6-dinitro-	4406-87-5	244.21	223										

all references equal 88, unless stated
ref 88 = CRC Properties of Organic Compounds,
Personal Edition CD ROM, 1996

Some Physical Property Data for a Series of Compounds, with Parent Compounds
compared with Nitro- and Dinitro- substituted Derivatives

	CHEMICAL IDENTITY DATA			VAPOR PRESSURE DATA															
				Vp: -25 C		Vp: 0 C		Vp: 25 C		Vp: 50 C		Vp: 75 C		Vp: 100 C		Vp: 125 C		Vp: 150 C	
TYPE	**compound**	**cas #**	**molecular weight**	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref
parent	Benzene	71-43-2	78.11	0.485		3.29		12.7		36.2		86.4		180		338		583	
+ 1 nitro	Benzene, nitro-	98-95-3	123.11					0.03										18.8	
+2 nitro's	Benzene, 1,2-dinitro-	528-29-0	168.11																
+2 nitro's	Benzene, 1,3-dinitro-	99-65-0	168.11																
+2 nitro's	Benzene, 1,4-dinitro-	100-25-4	168.11																
parent	Naphthalene	91-20-3	128.17					0.011				0.768		2.5		6.84		16.2	
+ 1 nitro	Naphthalene, 1-nitro-	86-57-7	173.17																
+ 1 nitro	Naphthalene, 2-nitro-	581-89-5	173.17																
+2 nitro's	Naphthalene, 1,2-dinitro-	24934-47-2	218.17																
+2 nitro's	Naphthalene, 1,3-dinitro-	606-37-1	218.17																
+2 nitro's	Naphthalene, 1,4-dinitro-	6921-26-2	218.17																
+2 nitro's	Naphthalene, 1,5-dinitro-	605-71-0	218.17																
+2 nitro's	Naphthalene, 1,8-dinitro-	602-38-0	218.17																
+2 nitro's	Naphthalene, 2,3-dinitro-	1875-63-4	218.17																
+2 nitro's	Naphthalene, 2,7-dinitro-	24824-27-9	218.17																

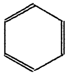
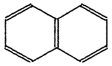
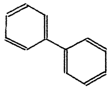
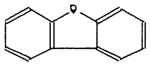
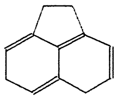
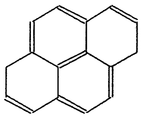
all references equal 88, unless stated
ref 88 = CRC Properties of Organic Compounds,
Personal Edition CD ROM, 1996

Some Physical Property Data for a Series of Compounds, with Parent Compounds
compared with Nitro- and Dinitro- substituted Derivatives

CHEMICAL IDENTITY DATA				VAPOR PRESSURE DATA															
				Vp: -25 C		Vp: 0 C		Vp: 25 C		Vp: 50 C		Vp: 75 C		Vp: 100 C		Vp: 125 C		Vp: 150 C	
TYPE	**compound**	**cas #**	**molecular weight**	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref	Vp kPa	ref
parent	1,1'-Biphenyl	92-52-4	154.21									0.149		0.586		1.87		5.05	
+ 1 nitro	1,1'-Biphenyl, 2-nitro-	86-00-0	199.21																
+ 1 nitro	1,1'-Biphenyl, 3-nitro-	2113-58-8	199.21																
+ 1 nitro	1,1'-Biphenyl, 4-nitro-	92-93-3	199.21																
+2 nitro's	1,1'-Biphenyl, 2,2'-dinitro-	2436-96-6	244.21																
+2 nitro's	1,1'-Biphenyl, 2,3'-dinitro-	7391-72-2	244.21																
+2 nitro's	1,1'-Biphenyl, 2,4'-dinitro-	608-81-5	244.21																
+2 nitro's	1,1'-Biphenyl, 3,3'-dinitro-	958-96-3	244.21																
+2 nitro's	1,1'-Biphenyl, 3,4'-dinitro-	6311-43-9	244.21																
+2 nitro's	1,1'-Biphenyl, 4,4'-dinitro-	1528-74-1	244.21																
parent	Dibenzofuran	132-64-9	168.19																
+ 1 nitro	Dibenzofuran, 1-nitro-	87812-99-5	213.19																
+ 1 nitro	Dibenzofuran, 3-nitro-	5410-97-9	213.19																
+ 1 nitro	Dibenzofuran, 4-nitro-	86607-81-0	213.19																
+2 nitro's	Dibenzofuran, 2,7-dinitro-	5408-55-9	258.19																
parent	Acenaphthene	83-32-9	154.21											0.281		0.949			
+ 1 nitro	Acenaphthene, 3-nitro-	3807-77-0	199.21																
+ 1 nitro	Acenaphthene, 5-nitro-	602-87-9	199.21																
+2 nitro's	\cenaphthene, 5,6-dinitro-	4406-87-5	244.21																

Summary of Data Trends for: Parent Compounds, “+ 1 nitro group ”, “+ 2 nitro groups”

(can we make an educated guess at property value(s) for dinitropyrenes?)

Parent Compound	**Molecular Weight of Parent**	**Structure of Parent**	**Melting Temperature**	**Boiling Temperature**	**Vapor Pressure**
benzene	78		**parent ~ nitro << dinitro** parent: 279 deg K	**parent << nitro << dinitro** parent: 353 deg K	**parent >> nitro** *no data for dinitro*
naphthalene	128		**parent ~ nitro << dinitro** parent: 353 deg K	**parent << nitro << dinitro** *but, not much data...;* *& some dinitro cmpnds sublimate or decompose* parent: 491 deg K	**?** *no data for nitro/dinitro*
biphenyl	154		**parent ~ nitro << dinitro** parent: 342 deg K	**parent < nitro ~ dinitro** *but, not much data...* parent: 529 deg K	**?** *no data for nitro/dinitro*
dibenzofuran	168		**parent << nitro << dinitro** parent: 360 deg K	**?** *no data for nitro/dinitro* parent: 560 deg K	**?** *no data for nitro/dinitro*
acenaphthene	154		**parent < nitro << dinitro** parent = 366 deg K	**?** *no data for nitro/dinitro* parent: 552 deg K	**?** *no data for nitro/dinitro*
pyrene	202		parent = 424 deg K	parent = 677 deg K	

Estimation of Vapor Pressure, Using "Method 2" in:
Lyman, W., 1982, "Vapor Pressure," in Handbook of Chemical Property Estimation Methods
Washington D.C.: American Chemical Society Edition published in 1990

				Pyrene				**Dinitropyrene**			
Parameter		Type	Typical Units	Value	Units	Ref	Notes	Value	Units	Ref	Notes
Tb: Boiling Temp		Data	deg K	677.15	deg K	88		727.15	deg K	88	crude: pyrene+50 C
Kf (from Table 14.4 or 14.5) (?)		Data	dimensionless	1	dimensionless	90	???	1.05	dimensionless	90	???
Temperature		User Specified	deg K	298.15	deg K			298.15	deg K		
Tpb = T/Tb		Calc	dimensionless	0.44	dimensionless			0.41	dimensionless		
Phys State for Estm: "solid" or "liquid"		Specified	text	solid				solid			
m		Data, based on Tpb	dimensionless	1.19	dimensionless	90		1.19	dimensionless	90	
R	= gas constant	Constant	cal/mol K	1.987	cal /mol K			1.987	cal /mol K		
delta Hvb / Tb =		Calc: eqn 14-16	cal /mol K	21.7	cal /mol K			22.9	cal /mol K		
	heat of vaporization at the normal boiling point, divided by the normal boiling point; this equals the entropy of vaporization at the normal boiling point = = Kf (8.75 + R ln Tb)										
delta Zb =		Estimated	dimensionless	0.97	dimensionless	90		0.97	dimensionless	90	
	compressibility factor at normal boiling point										
	factor1 in eqn 14-20	Calc: eqn 14-20	dimensionless	11.3	dimensionless			11.9	dimensionless		
	factor2 in eqn 14-20	Calc: eqn 14-20	dimensionless	1	dimensionless			1	dimensionless		
	factor3 in eqn 14-20	Calc: eqn 14-20	dimensionless	-4.86	dimensionless			-5.39	dimensionless		
	factor4 in eqn 14-20	Calc: eqn 14-20	dimensionless	2.2517903903	dimensionless			2.4604847777	dimensionless		
ln Pvp from equation 14-20		Calc: eqn 14-20	dimensionless	-18.12142957	dimensionless			-22.9672106615	dimensionless		
Pvp	**Vapor Pressure**		**atm**	**1.35E-008**	**atm**			**1.06E-010**	**atm**		
Pvp	**Vapor Pressure**		**mm Hg**	**1.03E-005**	**mm Hg**			**8.06E-008**	**mm Hg**		
Pvp	**Vapor Pressure**		**Pa**	**1.37E-003**	**Pa**			**1.07E-005**	**Pa**		
Pvp	Vapor Pressure -- "Literature Value"		mm Hg	2.45E-006	mm Hg @25C	85	within an order of magnitude				
Pvp	Corrected for Ratio of Literature Value for Parent Compound to Estimated Value for Parent Compound		mm Hg					**1.93E-008**	**mm Hg @25C**		

Some Water Solubility Data for a Series of Compounds, with Parent Compounds
compared with Nitro- and Dinitro- substituted Derivatives

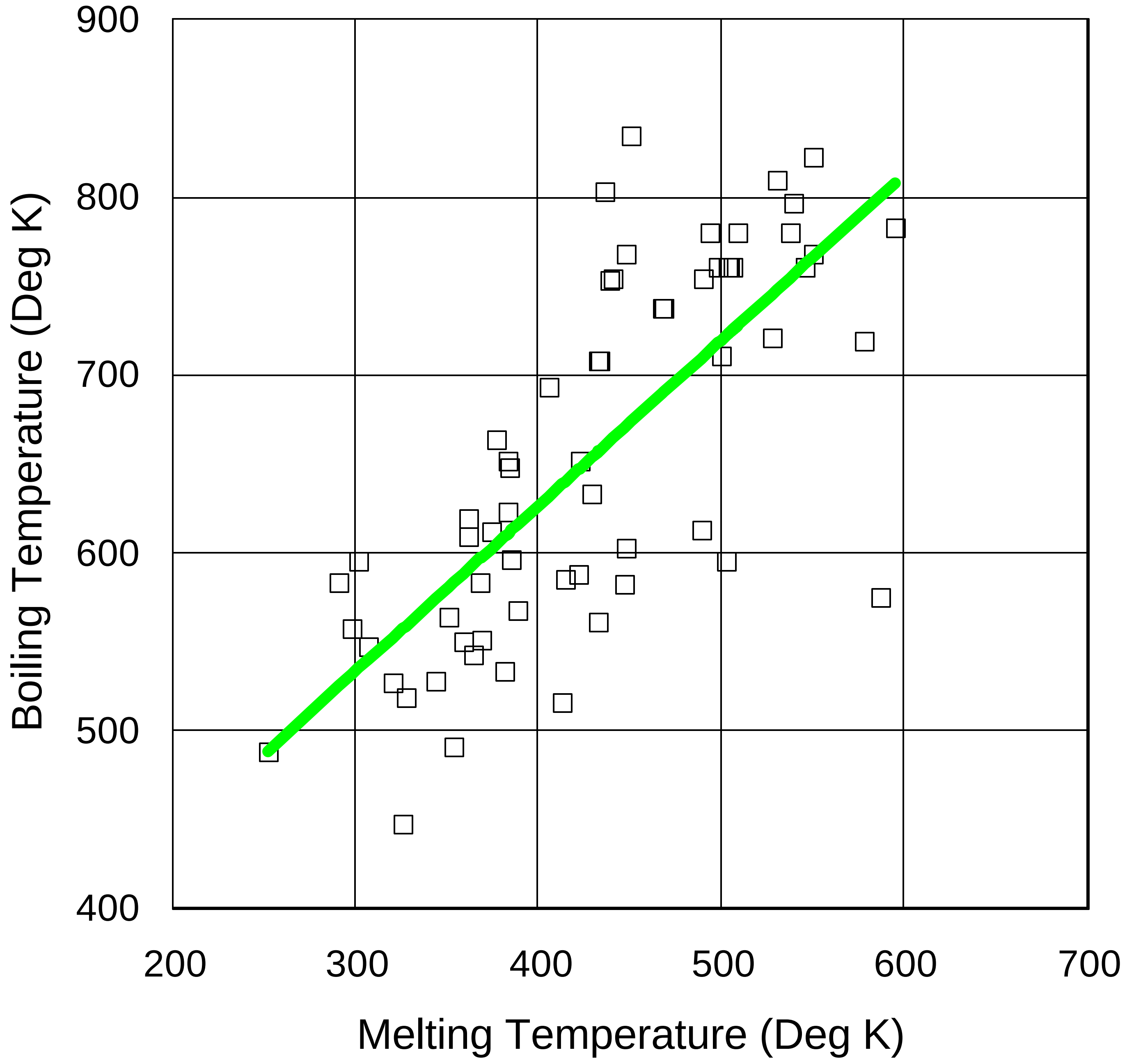
all references equal 97, unless stated

Ref 97 = National Library of Medicine, Hazardous Substances Data Base (HSDB) [various searches: Dec 96, Jan 97]

	CHEMICAL IDENTITY DATA			**Water Solubility**								**ratio of dinitro to parent**	
TYPE	**compound**	**cas #**	**molecular weight**	solubility	units	standard units g/m3	notes on conversion to std units	temp	temp units	ref	notes	ratio of dinitro to parent	avg for chemical group
parent	Benzene	71-43-2	78.11	0.18	g/100 g wat	1800		25	deg C	97			
+ 1 nitro	Benzene, nitro-	98-95-3	123.11	1780	ppm	1780	assume ppm by weight	not given		97			
+2 nitro's	enzene, 1,2-dinitro-	528-29-0	168.11	***************	g/ml	152		"cold water"		97		0.08	0.11
+2 nitro's	enzene, 1,3-dinitro-	99-65-0	168.11	2.2	mol/m3	370		not given		97		0.21	0.11
+2 nitro's	enzene, 1,4-dinitro-	100-25-4	168.11	0.00008	g/ml	80		not given		97		0.04	0.11
parent	Naphthalene	91-20-3	128.17	30	mg/lit	30		not given		97			
+ 1 nitro	aphthalene, 1-nitro-	86-57-7	173.17	18	mg/lit	18		not given		97	estimated		
parent	Cresol	1319-77-3		50	parts water	20000	assume by weight	not given					
+ 1 nitro													
+2 nitro's	Cresol, 4,6-dinitro-o	534-52-1	198.13	130	mg/lit	130		15	deg C	97		0.0065	0.011
+2 nitro's	Cresol, 2,6-dinitro-p	609-93-8	198.13	290	mg/lit	290		15	deg C	97		0.0145	0.011
parent	Phenol	108-95-2		***************	g/ml	66667		not given					
+ 1 nitro													
+2 nitro's	Phenol, 2,3-dinitro		184.1	2200	mg/lit	2200		35.5	deg C	97		0.033	0.011
+2 nitro's	Phenol, 2,4-dinitro		184.1	790	mg/lit	790		35.5	deg C	97		0.012	0.011
+2 nitro's	Phenol, 2,5-dinitro		184.1	680	mg/lit	680		35.5	deg C	97		0.010	0.011
+2 nitro's	Phenol, 2,6-dinitro		184.1	420	mg/lit	420		35.5	deg C	97		0.006	0.011
+2 nitro's	Phenol, 3,4-dinitro		184.1	230	mg/lit	230		35.5	deg C	97		0.003	0.011
+2 nitro's	Phenol, 3,5-dinitro		184.1	160	mg/lit	160		35.5	deg C	97		0.002	0.011
parent	Pyrene	129-00-0		0.135	mg/lit	0.135		25	deg C	97			
+ 1 nitro													
+2 nitro's													

Appendix B.4.

Methodology Used to Estimate Boiling Temperature When No Data Were Available (based on Regression Between Melting Temperature and Boiling Temperature for Other Compounds)



Boiling Temperature vs. Melting Temperature For BVES Compounds with Available Data

Line is Best-Fit Linear Regression

IS THERE A CRUDE RELATIONSHIP
BETWEEN MELTING and BOILING
TEMP?; Following Table has Available
Data for BVES Compounds
sorted in Ascending Melting
Point Order

NAME			**PHYSICAL STATE**	
common chemical name	cas # (1)	calc'd molecular weight	physical state (probably at room temperature)	reference
hexachloro-1,3-butadiene	000087-68-3	260.7	liquid	considering Tm
4-bromophenyl phenyl ether	000101-55-3	249.1	varies; melt temp ~ 18 deg C	considering Tm
3-PCB	002051-61-8	188.7	varies	Tm near room temp
3,3'-PCB	002050-67-1	223.1	varies	Tm near room temp
2-PCB	002051-60-7	188.7	varies	Tm near room temp
1,2,3,4-tetrachlorobenzene	000634-66-2	215.9	solid	considering Tm
1,4-dichlorobenzene	000106-46-7	147.0	solid	considering Tm
1,2,3,5-tetrachlorobenzene	000634-90-2	215.9	solid	considering Tm
biphenyl	000092-54-2	154.2	solid	considering Tm
4-PCB	002051-62-9	188.7	solid	considering Tm
naphthalene	000091-20-3	106.2	solid	considering Tm
pentachlorobenzene	000608-93-5	250.3	solid	considering Tm
methoxychlor	000072-43-5	345.6	solid	considering Tm
p,p'-DDE	000072-55-9	318.0	crystalline solid	60; also consistent with Tm
acenaphthylene	000208-96-8	152.2	solid	considering Tm
heptachlor	000076-44-8	373.3	crystalline solid	53; also consistent with Tm
acenaphthene	000083-32-9	154.2	solid	considering Tm
phenanthrene	000085-01-8	178.2	solid	considering Tm
aldrin	000309-00-2	364.9	crystalline solid	47; also consistent with Tm
p,p'-DDT	000050-29-3	354.5	crystalline solid	59; also consistent with Tm
,4'-methylene bis(2-chloroaniline)	000101-14-4	267.2	solid	considering Tm
p,p'-DDD	000072-54-8	320.0	crystalline solid	60; also consistent with Tm
fluoranthene	000206-44-0	202.3	solid	considering Tm
gamma-hexachlorocyclohexane	000058-89-9	290.8	crystalline solid	33; also consistent with Tm
fluorene	000086-73-7	166.2	solid	considering Tm
3,3'-dichlorobenzidene	000091-94-1	253.1	solid	considering Tm
1,2,4,5-tetrachlorobenzene	000095-94-3	215.9	solid	considering Tm
delta-hexachlorocyclohexane	000319-86-8	290.8	fine plates	29; also consistent with Tm
4,4'-PCB	002050-68-2	223.1	solid	considering Tm
octachlorostyrene	029082-74-4	379.7		
pyrene	000129-00-0	202.3	solid	considering Tm
alpha-hexachlorocyclohexane	000319-84-6	290.8	crystalline solid	32; also consistent with Tm
benz [a] anthracene	000056-55-3	228.3	solid	considering Tm
heptachlor epoxide	001024-57-3	389.3	crystalline solid	**53; ref 52 says that its liqui**
indeno [1,2,3-c,d] pyrene	000193-39-5	276.3	solid	considering Tm
benzo [j] fluoranthene	000205-82-2	252.3	solid	considering Tm
benzo [b] fluoranthene	000205-99-2	252.3	solid	considering Tm
pentachlorophenol	000087-86-5	266.3	flakes or crystalline solid	42; also consistent with Tm
benzo [a] pyrene	000050-32-8	252.3	solid	considering Tm

IS THERE A CRUDE RELATIONSHIP
BETWEEN MELTING and BOILING
TEMP?; Following Table has Available
Data for BVES Compounds
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Point Order

NAME			PHYSICAL STATE	
common chemical name	cas # (1)	calc'd molecular weight	physical state (probably at room temperature)	reference
dieldrin	000060-57-1	380.9	crystalline solid	47; also consistent with Tm
benzo [e] pyrene	000192-97-2	252.3	solid	considering Tm
1,2,3,7,8-PeCDD	040321-76-4	356.4	solid	considering Tm
1,2,3,7,8-PeCDF	057117-41-6	340.4	solid	considering Tm
2,3,4,7,8-PeCDF	057117-31-4	340.4	solid	considering Tm
anthracene	000120-12-7	178.2	solid	considering Tm
benzo [k] fluoranthene	000207-08-9	252.3	solid	considering Tm
1,2,3,4,7,8,9-HpCDF	055673-89-7	409.3	solid	considering Tm
1,2,3,4,7,8-HxCDF	070648-26-9	374.8	solid	considering Tm
2,3,7,8-TCDF	051207-31-9	306.0	solid	considering Tm
hexachlorobenzene	000118-74-1	284.8	solid	considering Tm
1,2,3,6,7,8-HxCDF	057117-44-9	374.8	solid	considering Tm
1,2,3,4,6,7,8-HpCDF	067562-39-4	409.3	solid	considering Tm
2,3,4,6,7,8-HxCDF	060851-34-5	374.8	solid	considering Tm
1,2,3,7,8,9-HxCDF	072918-21-9	374.8	solid	considering Tm
chrysene	000218-01-9	228.3	solid	considering Tm
OCDF	039001-02-0	443.7	solid	considering Tm
1,2,3,4,6,7,8-HpCDD	035822-46-9	425.3	solid	considering Tm
dibenz [a,h] anthracene	000053-70-1	278.4	solid	considering Tm
1,2,3,4,7,8-HxCDD	039227-28-6	390.8	solid	considering Tm
1,2,3,6,7,8-HxCDD	057653-85-7	390.8	solid	considering Tm
1,2,3,7,8,9-HxCDD	019408-74-3	390.8	solid	considering Tm
perylene	000198-55-0	252.3	solid	considering Tm
benzo [g,h,i] perylene	000191-24-2	268.4	solid	considering Tm
2,3,7,8-TCDD	001746-01-6	322.0	solid	considering Tm
beta-hexachlorocyclohexane	000319-85-7	290.8	crystalline solid	33; also consistent with Tm
OCDD	003268-87-9	459.7	solid	considering Tm
mirex				
toxaphene			waxy solid	consistent with Tm
endrin			crystalline solid	consistent with Tm
monomethyl mercury chloride			solid	consistent with Tm
2,7-dinitropyrene	117929-15-4	292.3	probably solid	considering Tm of 1,6 DNP
dinitropyrenes (mixed)	078432-19-6	292.3	probably solid	considering Tm of 1,6 DNP
1,3-dinitropyrene	075321-20-9	292.3	probably solid	considering Tm of 1,6 DNP
1,6-dinitropyrene	042397-64-8	292.3	probably solid	considering Tm of 1,6 DNP
1,8-dinitropyrene	042397-65-9	292.3	probably solid	considering Tm of 1,6 DNP

IS THERE A CRUDE RELATIONSHIP
BETWEEN MELTING and BOILING
TEMP?; Following Table has Available
Data for BVES Compounds
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Point Order

NAME		**MELTING POINT**					
common chemical name	cas # (1)	melting point range	melting point average	melting point units	melting point ref	**for V/P melting point deg K**	data notes
hexachloro-1,3-butadiene	000087-68-3		-21	deg C	7	252	
4-bromophenyl phenyl ether	000101-55-3		18	deg C	7	291	
3-PCB	002051-61-8		25	deg C	5	298	
3,3'-PCB	002050-67-1		29	deg C	5	302	
2-PCB	002051-60-7		34	deg C	5	307	
1,2,3,4-tetrachlorobenzene	000634-66-2		48	deg C	5	321	similar in Aldrich catalog
1,4-dichlorobenzene	000106-46-7		53	deg C	5	326	similar in Aldrich catalog
1,2,3,5-tetrachlorobenzene	000634-90-2		55	deg C	5	328	
biphenyl	000092-54-2		71	deg C	5	344	
4-PCB	002051-62-9		78	deg C	5	351	
naphthalene	000091-20-3		81	deg C	6	354	
pentachlorobenzene	000608-93-5		86	deg C	5	359	similar in Aldrich catalog
methoxychlor	000072-43-5		89	deg C	24; 85	362	
p,p'-DDE	000072-55-9	88-90	89	deg C?	aldrich cata	362	same in ref 61 and SRC data set
acenaphthylene	000208-96-8		92	deg C	6	365	
heptachlor	000076-44-8	95-96	96	deg C	25	369	same in ref 85
acenaphthene	000083-32-9		96	deg C	6	369	
phenanthrene	000085-01-8		101	deg C	6	374	
aldrin	000309-00-2		104	deg C	25	377	
p,p'-DDT	000050-29-3	107-110	109	deg C?	aldrich cata	382	same in ref 61
,4'-methylene bis(2-chloroaniline)	000101-14-4		110	deg C	15	383	
p,p'-DDD	000072-54-8	109-111	110	deg C?	aldrich cata	383	same in ref 61
fluoranthene	000206-44-0		111	deg C	6	384	
gamma-hexachlorocyclohexane	000058-89-9		113	deg C	29, 30	386	
fluorene	000086-73-7		116	deg C	6	389	
3,3'-dichlorobenzidene	000091-94-1	132-133	133	deg C	Howard, Vo	406	same in ref 8
1,2,4,5-tetrachlorobenzene	000095-94-3		140	deg C	5	413	similar in Aldrich catalog
delta-hexachlorocyclohexane	000319-86-8		142	deg C	29	415	
4,4'-PCB	002050-68-2		149	deg C	5	422	
octachlorostyrene	029082-74-4		150	deg C	89	423	estimated using linear regression; not i
pyrene	000129-00-0		156	deg C	6	429	
alpha-hexachlorocyclohexane	000319-84-6		160	deg C	29	433	
benz [a] anthracene	000056-55-3		160	deg C	6	433	
heptachlor epoxide	001024-57-3	160-161.5	161	deg C	25	434	same in ref 85
indeno [1,2,3-c,d] pyrene	000193-39-5		164	deg C	9	437	
benzo [j] fluoranthene	000205-82-2		166	deg C	6	439	
benzo [b] fluoranthene	000205-99-2		168	deg C	6	441	
pentachlorophenol	000087-86-5		174	deg C	8	447	
benzo [a] pyrene	000050-32-8		175	deg C	6	448	

IS THERE A CRUDE RELATIONSHIP
BETWEEN MELTING and BOILING
TEMP?; Following Table has Available
Data for BVES Compounds
sorted in Ascending Melting
Point Order

NAME		MELTING POINT					
						for V/P	
		melting	melting	melting	melting	**melting**	
		point	point	point	point	**point**	data
common chemical name	cas # (1)	range	average	units	ref	**deg K**	notes
dieldrin	000060-57-1	175-176	176	deg C	25	449	
benzo [e] pyrene	000192-97-2		178	deg C	6	451	
1,2,3,7,8-PeCDD	040321-76-4		195	deg C	6	468	using value for 12347 PeCDD
1,2,3,7,8-PeCDF	057117-41-6		196	deg C	6	469	using value for 23478 PeCDF
2,3,4,7,8-PeCDF	057117-31-4		196	deg C	6	469	
anthracene	000120-12-7		216	deg C	6	489	
benzo [k] fluoranthene	000207-08-9		217	deg C	6	490	
1,2,3,4,7,8,9-HpCDF	055673-89-7		221	deg C	6	494	
1,2,3,4,7,8-HxCDF	070648-26-9		226	deg C	6	499	
2,3,7,8-TCDF	051207-31-9		227	deg C	6	500	
hexachlorobenzene	000118-74-1		230	deg C	5	503	similar in Aldrich catalog
1,2,3,6,7,8-HxCDF	057117-44-9		232	deg C	6	505	
1,2,3,4,6,7,8-HpCDF	067562-39-4		236	deg C	6	509	
2,3,4,6,7,8-HxCDF	060851-34-5		231	deg C	6	504	using avg of values for 123478 HxCDF
1,2,3,7,8,9-HxCDF	072918-21-9		234	deg C	6	507	using avg of values for 123478 HxCDF
chrysene	000218-01-9		255	deg C	6	528	
OCDF	039001-02-0		258	deg C	6	531	
1,2,3,4,6,7,8-HpCDD	035822-46-9		265	deg C	6	538	
dibenz [a,h] anthracene	000053-70-1		267	deg C	6	540	
1,2,3,4,7,8-HxCDD	039227-28-6		273	deg C	6	546	
1,2,3,6,7,8-HxCDD	057653-85-7		273	deg C	6	546	using value for 123478 HxCDD
1,2,3,7,8,9-HxCDD	019408-74-3		273	deg C	6	546	using value for 123478 HxCDD
perylene	000198-55-0		277	deg C	6	550	
benzo [g,h,i] perylene	000191-24-2		277	deg C	6	550	
2,3,7,8-TCDD	001746-01-6		305	deg C	6	578	
beta-hexachlorocyclohexane	000319-85-7		315	deg C	29	588	
OCDD	003268-87-9		322	deg C	6	595	
mirex						758	
toxaphene		65-90	77.5	deg C	25	351	using avg of range
endrin		226-230	228.0	deg C	25	501	decomposes at around this temperature
monomethyl mercury chloride			170.0	deg C	95	443	
2,7-dinitropyrene	117929-15-4					479	crude: pyrene+50 C
dinitropyrenes (mixed)	078432-19-6					479	crude: pyrene+50 C
1,3-dinitropyrene	075321-20-9					479	crude: pyrene+50 C
1,6-dinitropyrene	042397-64-8	> 300		deg C	aldrich cata	479	crude: pyrene+50 C
1,8-dinitropyrene	042397-65-9					479	crude: pyrene+50 C

IS THERE A CRUDE RELATIONSHIP
BETWEEN MELTING and BOILING
TEMP?; Following Table has Available
Data for BVES Compounds
sorted in Ascending Melting
Point Order

NAME **BOILING POINT**

common chemical name	cas # (1)	boiling point range	boiling point average	boiling point units	boiling point ref	for V/P **boiling point deg K**	boiling point data notes	T boil estimated using regression deg K	percent error in estimate
hexachloro-1,3-butadiene	000087-68-3		215	deg C	19	488		489	0%
4-bromophenyl phenyl ether	000101-55-3		310	deg C	7	583		525	-10%
3-PCB	002051-61-8		284	deg C	5	557		532	-5%
3,3'-PCB	002050-67-1		322	deg C	5	595		535	-10%
2-PCB	002051-60-7		274	deg C	5	547		540	-1%
1,2,3,4-tetrachlorobenzene	000634-66-2		254	deg C	5	527	similar in Aldrich catalog	552	5%
1,4-dichlorobenzene	000106-46-7		175	deg C	5	448		558	25%
1,2,3,5-tetrachlorobenzene	000634-90-2		246	deg C	5	519		559	8%
biphenyl	000092-54-2		255	deg C	5	528		574	9%
4-PCB	002051-62-9		291	deg C	5	564		581	3%
naphthalene	000091-20-3		218	deg C	6	491		583	19%
pentachlorobenzene	000608-93-5		277	deg C	5	550	similar in Aldrich catalog	588	7%
methoxychlor	000072-43-5		346	deg C	85	619	one ref says that it decomposes when heated, so no data.	591	-5%
p,p'-DDE	000072-55-9		336	deg C	85	609		591	-3%
acenaphthylene	000208-96-8	265-275	270	deg C	6	543		594	9%
heptachlor	000076-44-8		310	deg C	85	583		597	2%
acenaphthene	000083-32-9		278	deg C	6	551		598	9%
phenanthrene	000085-01-8		339	deg C	6	612		602	-2%
aldrin	000309-00-2		664	deg K	87	664	estimated using Clausius Clapyron equation	605	-9%
p,p'-DDT	000050-29-3		260	deg C	60	533	not given in ref 85	609	14%
,4'-methylene bis(2-chloroaniline)	000101-14-4		379	deg C	83	652		611	-6%
p,p'-DDD	000072-54-8		350	deg C	85	623		611	-2%
fluoranthene	000206-44-0		375	deg C	6	648		612	-6%
gamma-hexachlorocyclohexane	000058-89-9		323	deg C	31	597		613	3%
fluorene	000086-73-7		295	deg C	6	568		616	8%
3,3'-dichlorobenzidene	000091-94-1		420	deg C	18	693		632	-9%
1,2,4,5-tetrachlorobenzene	000095-94-3		243	deg C	5	516	similar in Aldrich catalog	639	24%
delta-hexachlorocyclohexane	000319-86-8		312	deg C	29	586	estm based on 60 deg C @ 0.36 mm Hg	640	9%
4,4'-PCB	002050-68-2		315	deg C	5	588		647	10%
octachlorostyrene	029082-74-4		379	deg C	89	652	estimated using linear regression; not in SRC database	648	-1%
pyrene	000129-00-0		360	deg C	6	633		653	3%
alpha-hexachlorocyclohexane	000319-84-6		288	deg C	31	561		657	17%
benz [a] anthracene	000056-55-3		435	deg C	6	708		657	-7%
heptachlor epoxide	001024-57-3		no data			708	**No data available; use value for heptachlor for now**	658	-7%
indeno [1,2,3-c,d] pyrene	000193-39-5		530	deg C	11	803		660	-18%
benzo [j] fluoranthene	000205-82-2		480	deg C	6	753		663	-12%
benzo [b] fluoranthene	000205-99-2		481	deg C	6	754		665	-12%
pentachlorophenol	000087-86-5		310	deg C	25	583	decomposes	670	15%
benzo [a] pyrene	000050-32-8		495	deg C	6	768		671	-13%

IS THERE A CRUDE RELATIONSHIP
BETWEEN MELTING and BOILING
TEMP?; Following Table has Available
Data for BVES Compounds
sorted in Ascending Melting
Point Order

NAME							**BOILING POINT**		
						for V/P		T boil	
							boiling	estimated	percent
		boiling	boiling	boiling	boiling	**boiling**	point	using	error
		point	point	point	point	**point**	data	regression	in
common chemical name	cas # (1)	range	average	units	ref	**deg K**	notes	deg K	estimate
dieldrin	000060-57-1		330	deg C	48	603	estm'd?; same data given in SRC data set	672	11%
benzo [e] pyrene	000192-97-2		561	deg C	79	835	Estimated using calculation; value not given in Ref 6; 310-3	674	-19%
1,2,3,7,8-PeCDD	040321-76-4		465	deg C	6	738	using value for 12347 PeCDD	690	-7%
1,2,3,7,8-PeCDF	057117-41-6		465	deg C	6	738	using value for 23478 PeCDF	691	-6%
2,3,4,7,8-PeCDF	057117-31-4		465	deg C	6	738		691	-6%
anthracene	000120-12-7		340	deg C	6	613		709	16%
benzo [k] fluoranthene	000207-08-9		481	deg C	6	754		710	-6%
1,2,3,4,7,8,9-HpCDF	055673-89-7		507	deg C	6	780		714	-9%
1,2,3,4,7,8-HxCDF	070648-26-9		488	deg C	6	761		718	-6%
2,3,7,8-TCDF	051207-31-9		438	deg C	6	711		720	1%
hexachlorobenzene	000118-74-1		322	deg C	5	595	similar in Aldrich catalog	722	21%
1,2,3,6,7,8-HxCDF	057117-44-9		488	deg C	6	761		724	-5%
1,2,3,4,6,7,8-HpCDF	067562-39-4		507	deg C	6	780		728	-7%
2,3,4,6,7,8-HxCDF	060851-34-5		488	deg C	6	761	using avg of values for 123478 HxCDF and 123678 HxCD	723	-5%
1,2,3,7,8,9-HxCDF	072918-21-9		488	deg C	6	761	using avg of values for 123478 HxCDF and 123678 HxCD	726	-5%
chrysene	000218-01-9		448	deg C	6	721		746	3%
OCDF	039001-02-0		537	deg C	6	810		748	-8%
1,2,3,4,6,7,8-HpCDD	035822-46-9		507	deg C	6	780		755	-3%
dibenz [a,h] anthracene	000053-70-1		524	deg C	6	797		757	-5%
1,2,3,4,7,8-HxCDD	039227-28-6		488	deg C	6	761		762	0%
1,2,3,6,7,8-HxCDD	057653-85-7		488	deg C	6	761	using value for 123478 HxCDD	762	0%
1,2,3,7,8,9-HxCDD	019408-74-3		488	deg C	6	761	using value for 123478 HxCDD	762	0%
perylene	000198-55-0		495	deg C	6	768		766	-0%
benzo [g,h,i] perylene	000191-24-2		550	deg C	11	823		766	-7%
2,3,7,8-TCDD	001746-01-6		447	deg C	6	720		792	10%
beta-hexachlorocyclohexane	000319-85-7		302	deg C	29	575	estm based on 60 deg C @ 0.5 mm Hg	801	39%
OCDD	003268-87-9		510	deg C	6	783		808	3%
mirex								960	
toxaphene								580	
endrin								720	
monomethyl mercury chloride								666	
2,7-dinitropyrene	117929-15-4					683	crude: pyrene + 50 C	700	
dinitropyrenes (mixed)	078432-19-6					683	crude: pyrene + 50 C	700	
1,3-dinitropyrene	075321-20-9					683	crude: pyrene + 50 C	700	
1,6-dinitropyrene	042397-64-8					683	crude: pyrene + 50 C	700	
1,8-dinitropyrene	042397-65-9					683	crude: pyrene + 50 C	700	

IS THERE A CRUDE RELATIONSHIP
BETWEEN MELTING and BOILING
TEMP?; Following Table has Available
Data for BVES Compounds
sorted in Ascending Melting
Point Order

NAME		**BOILING POINT**							
common chemical name	cas # (1)	boiling point range	boiling point average	boiling point units	boiling point ref	**for V/P boiling point deg K**	boiling point data notes	T boil estimated using regression deg K	percent error in estimate
dieldrin	000060-57-1		330	deg C	48	603	estm'd?; same data given in SRC data set	672	11%
benzo [e] pyrene	000192-97-2		561	deg C	79	835	Estimated using calculation; value not given in Ref 6; 310-3	674	-19%
1,2,3,7,8-PeCDD	040321-76-4		465	deg C	6	738	using value for 12347 PeCDD	690	-7%
1,2,3,7,8-PeCDF	057117-41-6		465	deg C	6	738	using value for 23478 PeCDF	691	-6%
2,3,4,7,8-PeCDF	057117-31-4		465	deg C	6	738		691	-6%
anthracene	000120-12-7		340	deg C	6	613		709	16%
benzo [k] fluoranthene	000207-08-9		481	deg C	6	754		710	-6%
1,2,3,4,7,8,9-HpCDF	055673-89-7		507	deg C	6	780		714	-9%
1,2,3,4,7,8-HxCDF	070648-26-9		488	deg C	6	761		718	-6%
2,3,7,8-TCDF	051207-31-9		438	deg C	6	711		720	1%
hexachlorobenzene	000118-74-1		322	deg C	5	595	similar in Aldrich catalog	722	21%
1,2,3,6,7,8-HxCDF	057117-44-9		488	deg C	6	761		724	-5%
1,2,3,4,6,7,8-HpCDF	067562-39-4		507	deg C	6	780		728	-7%
2,3,4,6,7,8-HxCDF	060851-34-5		488	deg C	6	761	using avg of values for 123478 HxCDF and 123678 HxCD	723	-5%
1,2,3,7,8,9-HxCDF	072918-21-9		488	deg C	6	761	using avg of values for 123478 HxCDF and 123678 HxCD	726	-5%
chrysene	000218-01-9		448	deg C	6	721		746	3%
OCDF	039001-02-0		537	deg C	6	810		748	-8%
1,2,3,4,6,7,8-HpCDD	035822-46-9		507	deg C	6	780		755	-3%
dibenz [a,h] anthracene	000053-70-1		524	deg C	6	797		757	-5%
1,2,3,4,7,8-HxCDD	039227-28-6		488	deg C	6	761		762	0%
1,2,3,6,7,8-HxCDD	057653-85-7		488	deg C	6	761	using value for 123478 HxCDD	762	0%
1,2,3,7,8,9-HxCDD	019408-74-3		488	deg C	6	761	using value for 123478 HxCDD	762	0%
perylene	000198-55-0		495	deg C	6	768		766	-0%
benzo [g,h,i] perylene	000191-24-2		550	deg C	11	823		766	-7%
2,3,7,8-TCDD	001746-01-6		447	deg C	6	720		792	10%
beta-hexachlorocyclohexane	000319-85-7		302	deg C	29	575	estm based on 60 deg C @ 0.5 mm Hg	801	39%
OCDD	003268-87-9		510	deg C	6	783		808	3%
mirex								960	
toxaphene								580	
endrin								720	
monomethyl mercury chloride								666	
2,7-dinitropyrene	117929-15-4					683	crude: pyrene + 50 C	700	
dinitropyrenes (mixed)	078432-19-6					683	crude: pyrene + 50 C	700	
1,3-dinitropyrene	075321-20-9					683	crude: pyrene + 50 C	700	
1,6-dinitropyrene	042397-64-8					683	crude: pyrene + 50 C	700	
1,8-dinitropyrene	042397-65-9					683	crude: pyrene + 50 C	700	

Appendix C.

Vapor/Particle Partitioning

C.1. Vapor/Particle Partitioning Theory

C.2. Results of Vapor/Particle Partitioning Estimates

C.3. Comparison of Vapor/Particle Partitioning Estimates with Examples of Vapor/Particle Partitioning Measurements from the Literature

C.4. Vapor-Particle Partitioning of PAH's: Detailed Comparison of Theoretical Estimates with Recent Experimental Data

Appendix C.1.

Vapor/Particle Partitioning Theory

In the atmosphere, pollutants can exist, generally, in the vapor phase or associated with particles, i.e., the aerosol phase. For semivolatile compounds there can be there can be significant fractions associated with either phase. This phenomenon is of crucial importance in determining the fate of semivolatile compounds in the atmosphere, because each of the deposition and destruction mechanisms depend a great deal on the physical form of the pollutant. The vapor/particle partitioning phenomenon was first introduced by Junge (1977), and has been extended and reviewed by many, including the following: Eisenreich et al 1981; Bidleman et al 1986; Bidleman and Foreman, 1987; Foreman and Bidleman, 1987; Bidleman 1988; Pankow 1987, 1988, 1991; Pankow and Bidleman, 1991, 1992; and Johnson et al, 1990. The phenomenon as it relates to atmospheric PCDD/PCDF has been recently measured (Nakano et al, 1990) and summarized (USEPA 1994A).

In essence, the theory of vapor-particle partitioning postulates that for any species in the atmosphere, there is an equilibrium between vapor phase and the particle phase that depends primarily on the physical-chemical properties of the species of interest, the nature of the atmospheric aerosol, and the temperature. As proposed by Junge (1977), the vapor-particle partitioning of exchangeable material can be estimated from the following equation:

$$\Phi = c\,S_t / (p(T) + cS_t)$$

where

Φ = the fraction of the total mass of the species absorbed to the particle phase (dimensionless)

S_t = the total surface area of particles, per unit volume of air (cm^2/cm^3)

$p(T)$ = the saturation vapor pressure of the species of interest (atm), at the ambient temperature (T)

c = an empirical constant, estimated by Junge to be approximately 1.7×10^{-4} atm-cm

The most thermodynamically stable form of many semivolatile species at ambient temperatures is typically a solid, but, Bidleman (1988) has argued that it is the "non-equilibrium" or subcooled liquid phase which controls the dynamic equilibrium partitioning of such compounds between the vapor phase and the atmospheric aerosol. Thus, the subcooled liquid vapor pressure at the ambient temperature should be used in the above equation. This vapor pressure can be approximately estimated from the following equation:

$$\ln (P_l/P_s) = \Delta S_f\,(T_m - T) / RT$$

where

P_l = subcooled liquid vapor pressure (atm) at temp. T
P_s = solid vapor pressure (atm) at temperature T
ΔS_f = entropy of fusion (atm m^3/mole deg K) (approximately equal to 6.79 R)
T_m = melting temperature of the solid compound (deg K)
T = ambient temperature (deg K)
R = the gas constant (atm m^3/mole deg K)

Mackay et al (1986) have suggested that the solid vapor pressure at the temperature of interest can be estimated from the reported solid vapor pressure at a standard temperature with the Clausius-Clapeyron equation using the enthalpy of vaporization, according to the following equation:

$$\ln (P^s_1 / P^s_2) = (\Delta H / R)(1/T_2 - 1/T_1)$$

where

P^s_1 = solid vapor pressure (atm) at temperature T_1

P^s_2 = solid vapor pressure (atm) at temperature T_2

ΔH = enthalpy of vaporization (J/mole)

Note: according to Trouton's Rule, ΔH can be approximately estimated by the following relation: $\Delta H / T_{boil} = 84$ J/(mol degK) (Mackay et al 1986).

R = gas constant (J/mole degK [=] (atm m^3/mole deg K)

T_2 = temperature 1 (deg K)

T_1 = temperature 2 (deg K)

Thus, the vapor particle partitioning for a given compound in the atmosphere can be estimated from the first of the above two equations, with P_l from the second equation used for P(T). From the foregoing, it is seen that the only species-specific physical-chemical property data required to make a vapor/particle partitioning estimate according to the above simplified approach are the species' solid vapor pressure at one temperature, and the species' boiling and melting temperatures.

It is typically assumed that semivolatile compounds in the atmosphere are "fully exchangeable", i.e., that the compound can move freely between the vapor and particle phases, depending on the dictates of thermodynamics. To the extent that a portion of the material was "locked-up" within particles and was not available for exchange, this assumption would be in error.

There is some experimental evidence that suggests that many semivolatile compounds are indeed fully exchangeable in the atmosphere. For example, Eitzer and Hites (1989a and 1989c) measured vapor- and particulate-phase PCDD/F in the atmosphere of Bloomington, IN and found that while there was no temperature-related effect on the <u>total</u> concentration of PCDD/F in the atmosphere, the <u>proportions</u> in the two phases were dependent on the ambient temperature at the time of the measurement. Further, in agreement with V/P theory, it was found that the V/P partitioning of each of the congeners was dependent on each congener’s subcooled liquid vapor pressure (Eitzer and Hites, 1989a).[9]

Some compounds, such as HCB, are predicted and found to exist predominantly in the vapor phase, and the issue of exchangeability is moot.

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[9] Koester and Hites (1992) measured wet and dry deposition of atmospheric PCDD/F, and found that dry deposition was inversely related to ambient temperature. These authors assumed that vapor-phase dry deposition was negligible and that only particle-phase dry deposition was significant. With this assumption, their results are consistent with the hypothesis that the proportion of vapor-phase and particle-phase PCDD/F changes with ambient temperature. On the other hand, if their assumption of vapor-phase deposition being insignificant is not valid, then their finding is not relevant to the vapor/particle exchangeability issue.

Vapor/particle partitioning of PAH's is found to vary with ambient temperature (e.g., Yamasaki et al., 1982) suggesting that most or all of PAH's in the atmosphere are exchangeable. Kamens et al. (1995) have suggested that the equilibration time for atmospheric PAH's may be relatively long (on the order of hours) because of mass transfer resistance within organic layers on atmospheric particles.

Aerosol Characteristics

As described above in the formulation of the vapor/particle partitioning equations, the aerosol surface area plays a role in determining the vapor/particle partitioning behavior of a compound in the atmosphere. Bidleman (1988), citing a study by Whitby (1978), summarizes data on the total aerosol surface area found in measurements. These "typical values" are summarized in the table below. In reality, the characteristics of the atmospheric aerosol vary from point to point in the atmosphere, and at any given point, changes with time.

Table __. Typical Aerosol Surface Areas per Unit Volume
[from Whitby (1978)]

Type of Atmospheric Location	**Typical Aerosol Surface Area** (cm^2 surface area / cm^3 air)
Clean Continental Background	4.2×10^{-7}
Average Background	1.5×10^{-6}
Background + Local Sources	3.5×10^{-6}
Urban	1.1×10^{-5}

Uncertainties

There are many uncertainties associated with vapor/particle partitioning theory and measurements.

For example, the vapor pressure of many compounds is relatively uncertain, with reported values often differing by more than an order of magnitude. Moreover, the estimation of subcooled liquid vapor pressures from solid phase values introduces additional uncertainties. In addition, the surface area of the atmospheric aerosol can vary widely. Thus, even if the above theory "perfectly" described the vapor/particle partitioning phenomenon, there would be large uncertainties related to uncertainties in vapor pressure and aerosol surface area. Possible deviations from the above theory due to the effects of relative humidity, non-exchangeable material and intra-particle mass-transfer phenomena (possibly important for PAH's, for example) also indicate that the estimates made here are somewhat uncertain. Compounds that are predicted in this analysis to exist *overwhelmingly* in either the vapor or particle phase probably exist in the predicted phase, but, it is acknowledged that for *intermediate* compounds, the estimates for the relative proportion of vapor and particle fractions is relatively uncertain.

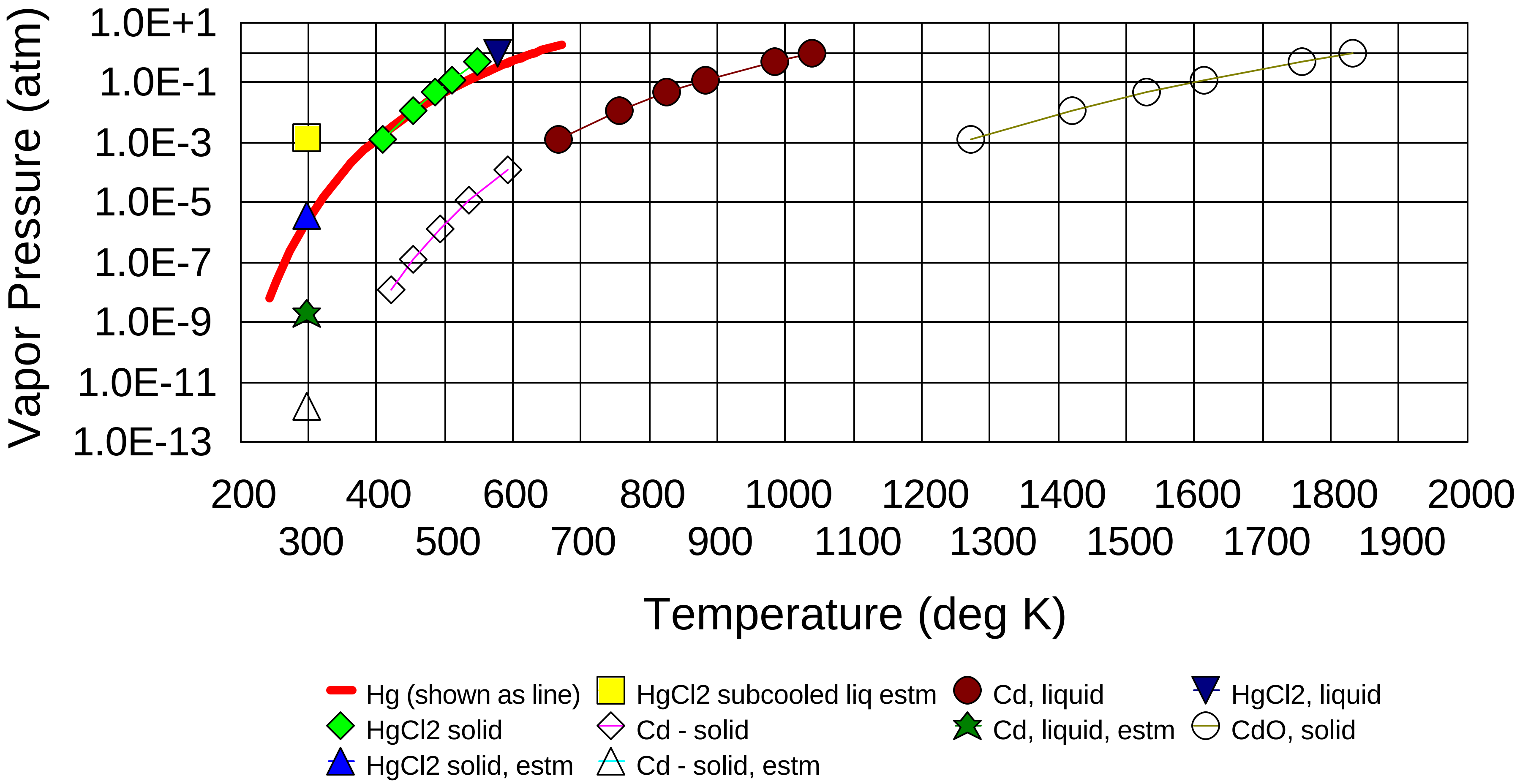
Thibodeaux et al (1991) have extended the theory of vapor/particle partitioning of semivolatile organic compounds (SOC) to include the effect of the competition of water vapor for adsorption sites on an atmospheric particle before deliquesence. The effect of moisture was shown to reduce the fraction of the SOC that is predicted to be adsorbed to atmospheric particles.

Rounds and Pankow (1990) considered the mass transfer aspects of vapor/particle partitioning and concluded that vapor/particle equilibrium would be achieved in several hours or less, depending on the compound.

More recently, Rounds et al. (1993) attempted to measure the vapor/particle partitioning of selected PAH's and other compounds in a laboratory desorption experiment on filter-collected atmospheric particles. They found that 6 of the 9 PAH's measured (acenaphthene, acenaphthylene, benz(a)anthracene, chrysene, fluoranthene, 2-methyl phenanthrene, and pyrene) were more or less fully exchangeable, but, the time scales for vapor/particle exchange (including intraparticle diffusion) in their experiments were much longer than those predicted by Rounds and Pankow (1990). Based on these results, they concluded that for the PAH's considered, vapor/particle equilibrium may not be achieved in the atmosphere, even for PAH's that are fully exchangeable. Three of the PAH's measured had apparently non-exchangeable particle-associated fractions: phenanthrene, fluorene, and 9-fluorenone.

One interesting question that has been raised by this analysis concerns the phase distribution of cadmium in the atmosphere. Cadmium is generally assumed to be associated with particles in the atmosphere, although it can be in the vapor phase in combustion and incineration processes. The simplified vapor/particle partitioning analysis conducted in this study *suggests* that there may be some cadmium in the vapor phase in the atmosphere under certain conditions, but, this is very uncertain. Cadmium melts at about 321 ^{o}C and is a relatively volatile metal. While it is more volatile than many metals, it is not nearly as volatile as mercury. Cadmium has a vapor pressure on the order of 10,000 - 100,000 times lower than mercury at the same temperature; a crude estimate of the saturation vapor pressure of pure cadmium metal at 25 ^{o}C is of the order of 1e-12 atm ($1x10^{-12}$ atm). (Vapor pressure data and estimates are shown in the figure below.) If this is "correct", its vapor pressure at 25 ^{o}C is similar to that of 2,3,7,8-TCDD, a compound that is predicted to exist in both the vapor and particle phases in the atmosphere, depending intimately on the micro-meteorological conditions. Of course, different cadmium compounds have different vapor pressures, and, the form of cadmium in the atmosphere may play an important role. Cadmium oxide and cadmium chloride, for example, have much lower vapor pressures than pure cadmium metal.

Vapor Pressure Data for Some Metals and Metallic Compounds



Data from CRC Handbook of Chemistry and Physics, 56th Edition, 1975-6

Appendix C.2.

Results of Vapor/Particle Partitioning Estimates

In the table below, results are given for vapor/particle partitioning calculations -- using the theory described in Appendix C.1. above -- for the compounds considered in this analysis.

Vapor/Particle Partitioning Estimates

NAME			Vapor/Particle Partitioning Estimates		
common chemical name	IUPAC #	cas # (1)	low end of fraction adsorbed range T = 310K sa=4.2e-7 cm2/cm3 *values from calc*	middle of fraction adsorbed range T = 290K sa=3.5e-6 cm2/cm3 *values from calc*	high end of fraction adsorbed range T = 260K sa=1.1e-5 cm2/cm3 *values from calc*
octachlorostyrene		029082-74-4	1.5E-004	2.8E-003	3.8E-002
4-bromophenyl phenyl ether		000101-55-3	1.7E-005	5.2E-004	1.7E-002
3,3'-dichlorobenzidene		000091-94-1	2.9E-001	9.0E-001	9.9E-001
1,3-dinitropyrene		075321-20-9	2.8E-002	3.5E-001	8.8E-001
1,6-dinitropyrene		042397-64-8	2.8E-002	3.5E-001	8.8E-001
1,8-dinitropyrene		042397-65-9	2.8E-002	3.5E-001	8.8E-001
2,7-dinitropyrene		117929-15-4	2.8E-002	3.5E-001	8.8E-001
dinitropyrenes (mixed)		078432-19-6	2.8E-002	3.5E-001	8.8E-001
hexachloro-1,3-butadiene		000087-68-3	1.9E-007	4.8E-006	1.1E-004
4,4'-methylene bis(2-chloroaniline)		000101-14-4	4.7E-004	9.4E-003	1.3E-001
pentachlorophenol		000087-86-5	4.1E-005	6.4E-004	6.2E-003
aldrin		000309-00-2	4.4E-005	9.2E-004	1.5E-002
dieldrin		000060-57-1	2.0E-004	3.3E-003	3.4E-002
p,p'-DDT		000050-29-3	2.5E-002	2.9E-001	7.9E-001
p,p'-DDD		000072-54-8	5.1E-003	8.8E-002	5.7E-001
p,p'-DDE		000072-55-9	1.3E-003	2.4E-002	2.5E-001
heptachlor		000076-44-8	1.8E-005	3.1E-004	3.8E-003
heptachlor epoxide		001024-57-3	1.2E-004	1.9E-003	1.9E-002
methoxychlor		000072-43-5	5.4E-003	9.5E-002	6.0E-001
mirex		002385-85-5	1.1E-006	2.4E-005	4.7E-004
toxaphene		008001-35-2	3.8E-003	1.1E-001	7.9E-001
endrin		000072-20-8	7.1E-005	1.4E-003	2.0E-002
alpha-hexachlorocyclohexane		000319-84-6	4.0E-005	6.1E-004	5.6E-003
beta-hexachlorocyclohexane		000319-85-7	1.3E-004	1.6E-003	1.0E-002
delta-hexachlorocyclohexane		000319-86-8	7.3E-005	1.2E-003	1.3E-002
gamma-hexachlorocyclohexane		000058-89-9	1.6E-004	2.8E-003	3.3E-002
mixed hexachlorocyclohexanes		000319-84-6			

Vapor/Particle Partitioning Estimates

NAME			**Vapor/Particle Partitioning Estimates**		
common chemical name	IUPAC #	cas # (1)	low end of fraction adsorbed range T = 310K sa=4.2e-7 cm2/cm3 *values from calc*	middle of fraction adsorbed range T = 290K sa=3.5e-6 cm2/cm3 *values from calc*	high end of fraction adsorbed range T = 260K sa=1.1e-5 cm2/cm3 *values from calc*
cadmium		007440-43-9	8.0E-001	1.0E+000	1.0E+000
cadmium carbonate		000513-78-0			
cadmium chloride		010108-64-2	1.0E+000	1.0E+000	1.0E+000
cadmium oxide		001306-19-0			
cadmium sulfate		010124-36-4			
cadmium sulfide		001306-23-6			
elemental mercury		007439-97-6	1.4E-005	4.8E-004	1.8E-002
mercury oxide		021908-53-2			
mercuric chloride		007487-94-7	2.7E-008	3.6E-007	2.6E-006
monomethyl mercury chloride		000115-09-3	1.5E-007	2.8E-006	3.8E-005
dimethyl mercury		000593-74-8			
tetraethyl lead		000078-00-2	7.4E-008	1.8E-006	4.1E-005
tetramethyl lead		000075-74-1	8.6E-010	2.5E-008	7.0E-007
triethyl lead radical (1+ cation)		014570-15-1			
triethyl lead hydride		005224-23-7			
triethyl lead chloride		001067-14-7			
diethyl lead radical (2+ cation)		024952-65-6			
diethyl lead dihydride		081494-11-3			
diethyl lead dichloride		013231-90-8			
trimethyl lead radical (1+ cation)		014570-16-2			
trimethyl lead hydride		007442-13-9			
trimethyl lead chloride		001520-78-1			
dimethyl lead radical (2+ cation)		021774-13-0			
dimethyl lead dihydride		030691-92-0			
dimethyl lead dichloride		001520-77-0			
bis (tributyltin) oxide		000056-35-9	2.4E-002	4.8E-001	9.8E-001
tributyl tin		000688-75-3			
tributyltin fluoride		001983-10-4			
tributyltin chloride		001461-22-9			
tributyltin hydroxide		001067-97-6			
tributyltin naphthenate					
tris(tributylstannyl) phosphate		013435-05-7			

Vapor/Particle Partitioning Estimates

NAME			Vapor/Particle Partitioning Estimates		
			low end of fraction adsorbed range	middle of fraction adsorbed range	high end of fraction adsorbed range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm2/cm3	sa=3.5e-6 cm2/cm3	sa=1.1e-5 cm2/cm3
common chemical name	IUPAC #	cas # (1)	*values from calc*	*values from calc*	*values from calc*
1,4-dichlorobenzene		000106-46-7	3.1E-008	4.4E-007	3.4E-006
1,2,3,4-tetrachlorobenzene		000634-66-2	5.6E-007	9.3E-006	1.0E-004
1,2,4,5-tetrachlorobenzene		000095-94-3	5.4E-007	7.7E-006	6.3E-005
1,2,3,5-tetrachlorobenzene		000634-90-2	2.6E-007	4.2E-006	4.4E-005
pentachlorobenzene		000608-93-5	5.5E-006	9.2E-005	1.0E-003
hexachlorobenzene		000118-74-1	2.1E-005	3.1E-004	2.8E-003
naphthalene		000091-20-3	1.4E-007	2.1E-006	1.8E-005
acenaphthene		000083-32-9	3.2E-006	5.3E-005	5.6E-004
acenaphthylene		000208-96-8	1.2E-006	1.9E-005	2.0E-004
fluorene		000086-73-7	6.8E-006	1.1E-004	1.2E-003
phenanthrene		000085-01-8	4.0E-005	7.5E-004	1.0E-002
anthracene		000120-12-7	6.4E-005	1.0E-003	9.9E-003
pyrene		000129-00-0	3.9E-004	7.0E-003	8.2E-002
fluoranthene		000206-44-0	5.0E-004	9.9E-003	1.3E-001
chrysene		000218-01-9	4.0E-002	4.4E-001	9.2E-001
benz [a] anthracene		000056-55-3	4.6E-002	5.0E-001	9.4E-001
benzo [b] fluoranthene		000205-99-2	2.3E-003	5.1E-002	5.2E-001
benzo [j] fluoranthene		000205-82-3	7.5E-002	6.5E-001	9.7E-001
benzo [k] fluoranthene		000207-08-9	5.0E-001	9.6E-001	1.0E+000
benzo [a] pyrene		000050-32-8	1.6E-001	8.2E-001	9.9E-001
benzo [e] pyrene		000192-97-2	1.3E-001	8.1E-001	9.9E-001
perylene		000198-55-0	5.0E-001	9.5E-001	1.0E+000
benzo [g,h,i] perylene		000191-24-2	4.9E-001	9.6E-001	1.0E+000
dibenz [a,h] anthracene		000053-70-3	9.8E-001	1.0E+000	1.0E+000
indeno [1,2,3-c,d] pyrene		000193-39-5	8.8E-001	9.9E-001	1.0E+000

Vapor/Particle Partitioning Estimates

NAME			**Vapor/Particle Partitioning Estimates**		
			low end	middle	high end
			of fraction	of fraction	of fraction
			adsorbed	adsorbed	adsorbed
			range	range	range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm2/cm3	sa=3.5e-6 cm2/cm3	sa=1.1e-5 cm2/cm3
common chemical name	IUPAC #	cas # (1)	*values from calc*	*values from calc*	*values from calc*
2,3,7,8-TCDD		001746-01-6	7.5E-002	5.9E-001	9.4E-001
1,2,3,7,8-PeCDD		040321-76-4	5.0E-001	9.6E-001	1.0E+000
1,2,3,4,7,8-HxCDD		039227-28-6	7.5E-001	9.8E-001	1.0E+000
1,2,3,6,7,8-HxCDD		057653-85-7	7.5E-001	9.8E-001	1.0E+000
1,2,3,7,8,9-HxCDD		019408-74-3	7.5E-001	9.8E-001	1.0E+000
1,2,3,4,6,7,8-HpCDD		035822-46-9	9.6E-001	1.0E+000	1.0E+000
OCDD		003268-87-9	9.8E-001	1.0E+000	1.0E+000
2,3,7,8-TCDF		051207-31-9	2.2E-002	3.0E-001	8.6E-001
2,3,4,7,8-PeCDF		057117-31-4	2.0E-001	8.4E-001	9.9E-001
1,2,3,7,8-PeCDF		057117-41-6	2.0E-001	8.4E-001	9.9E-001
1,2,3,4,7,8-HxCDF		070648-26-9	5.8E-001	9.7E-001	1.0E+000
1,2,3,6,7,8-HxCDF		057117-44-9	5.2E-001	9.6E-001	1.0E+000
1,2,3,7,8,9-HxCDF		072918-21-9	5.5E-001	9.6E-001	1.0E+000
2,3,4,6,7,8-HxCDF		060851-34-5	5.5E-001	9.6E-001	1.0E+000
1,2,3,4,6,7,8-HpCDF		067562-39-4	8.8E-001	9.9E-001	1.0E+000
1,2,3,4,7,8,9-HpCDF		055673-89-7	8.8E-001	9.9E-001	1.0E+000
OCDF		039001-02-0	9.8E-001	1.0E+000	1.0E+000

Vapor/Particle Partitioning Estimates

NAME			Vapor/Particle Partitioning Estimates		
			low end	middle	high end
			of fraction	of fraction	of fraction
			adsorbed	adsorbed	adsorbed
			range	range	range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm2/cm3	sa=3.5e-6 cm2/cm3	sa=1.1e-5 cm2/cm3
common chemical name	IUPAC #	cas # (1)	*values from calc*	*values from calc*	*values from calc*
biphenyl	0	000092-52-4	1.33E-006	2.16E-005	2.24E-004
2-PCB	1	002051-60-7	1.4E-006	6.6E-005	4.5E-003
3-PCB	2	002051-61-8	2.6E-006	1.3E-004	9.8E-003
4-PCB	3	002051-62-9	2.8E-006	1.4E-004	1.0E-002
count			3	3	3
average			**2.27E-006**	**1.11E-004**	**8.25E-003**
standard deviation			6.14E-007	3.24E-005	2.67E-003
minimum			**1.40E-006**	6.56E-005	4.48E-003
maximum			2.76E-006	1.37E-004	**1.04E-002**
2,2'-PCB	4	013029-08-8	7.5E-006	4.1E-004	3.5E-002
2,3-PCB	5	016605-91-7	1.6E-005	9.3E-004	8.4E-002
2,4-PCB	7	033284-50-3	1.3E-005	7.5E-004	7.4E-002
2,4'-PCB	8	034883-43-7	1.5E-005	8.6E-004	7.9E-002
2,5-PCB	9	034883-39-1	1.3E-005	7.5E-004	7.5E-002
2,6-PCB	10	033146-45-1	7.4E-006	4.0E-004	3.4E-002
3,3'-PCB	11	002050-67-1	2.6E-005	1.6E-003	1.6E-001
3,4-PCB	12	002974-92-7	3.0E-005	1.8E-003	1.7E-001
3,5-PCB	14	034883-41-5	1.8E-005	1.1E-003	1.1E-001
4,4'-PCB	15	002050-68-2	3.1E-005	2.0E-003	1.9E-001
count			10	10	10
average			**1.76E-005**	**1.06E-003**	**1.01E-001**
standard deviation			8.11E-006	5.30E-004	5.17E-002
minimum			**7.38E-006**	3.97E-004	3.39E-002
maximum			3.08E-005	1.96E-003	**1.90E-001**

Vapor/Particle Partitioning Estimates

NAME			Vapor/Particle Partitioning Estimates		
common chemical name	IUPAC #	cas # (1)	low end of fraction adsorbed range T = 310K sa=4.2e-7 cm2/cm3 *values from calc*	middle of fraction adsorbed range T = 290K sa=3.5e-6 cm2/cm3 *values from calc*	high end of fraction adsorbed range T = 260K sa=1.1e-5 cm2/cm3 *values from calc*
2,2',3-PCB	16	038444-78-9	4.2E-005	2.6E-003	2.3E-001
2,2',5-PCB	18	037680-65-2	2.9E-005	1.8E-003	1.7E-001
2,3,3'-PCB	20	038444-84-7	7.7E-005	5.1E-003	4.0E-001
2,3,4-PCB	21	055702-46-0	7.8E-005	5.2E-003	4.1E-001
2,3',5-PCB	26	038444-85-8	5.3E-005	3.6E-003	3.2E-001
2,4,4'-PCB	28	007012-37-5	6.4E-005	4.3E-003	3.6E-001
2,4,5-PCB	29	015862-07-4	5.0E-005	3.2E-003	2.8E-001
2,4,6-PCB	30	035693-92-6	2.4E-005	1.4E-003	1.4E-001
2,4',5,-PCB	31	016606-02-3	7.9E-005	5.3E-003	4.1E-001
2',3,4-PCB	33	038444-86-9	8.2E-005	5.5E-003	4.2E-001
3,3',4-PCB	35	037680-69-6	1.5E-004	1.1E-002	6.3E-001
3,4,4'-PCB	37	038444-90-5	1.6E-004	1.2E-002	6.5E-001
count			12	12	12
average			**7.42E-005**	**5.05E-003**	**3.68E-001**
standard deviation			4.13E-005	3.09E-003	1.50E-001
minimum			**2.37E-005**	1.44E-003	1.38E-001
maximum			1.63E-004	1.18E-002	**6.47E-001**
2,2',3,3'-PCB	40	038444-93-8	2.1E-004	1.5E-002	7.1E-001
2,2',3,5'-PCB	44	041464-39-5	1.6E-004	1.2E-002	6.4E-001
2,2',4,4'-PCB	47	002437-79-8	1.4E-004	9.7E-003	6.0E-001
2,2',4,5'-PCB	49	041464-40-8	1.2E-004	8.9E-003	5.8E-001
2,2',4,6-PCB	50	062796-65-0	2.5E-003	4.2E-002	3.5E-001
2,2',4,6'-PCB	51	068194-04-7	8.7E-005	5.9E-003	4.5E-001
2,2,5,5'-PCB	52	035693-99-3	1.3E-004	9.3E-003	5.8E-001
2,2,5,6'-PCB	53	041464-41-9	7.8E-005	5.3E-003	4.2E-001
2,2,6,6'-PCB	54	015968-05-5	6.2E-005	3.5E-003	2.6E-001
2,3,4,4'-PCB	60	033025-41-1	3.8E-004	2.9E-002	8.4E-001
2,3,4,5-PCB	61	033284-53-6	1.6E-004	1.3E-002	6.9E-001
2,3,5,6-PCB	65	033284-54-7	1.5E-004	1.1E-002	6.2E-001
2,3,4,4'-PCB	66	032598-10-0	3.2E-004	2.4E-002	8.1E-001
2,3',4',5-PCB	70	032598-11-1	3.6E-004	2.8E-002	8.4E-001
2,4,4',6-PCB	75	032598-12-2	1.2E-004	8.3E-003	5.6E-001
3,3',4,4'-PCB	77	032598-13-3	8.6E-004	6.9E-002	9.4E-001
3,3',5,5'-PCB	80	033284-52-5	3.4E-004	2.9E-002	8.6E-001
3,4,4',5-PCB	81	070362-50-4	6.5E-004	5.4E-002	9.2E-001
count			18	18	18
average			**3.77E-004**	**2.09E-002**	**6.48E-001**
standard deviation			5.49E-004	1.77E-002	1.92E-001
minimum			**6.16E-005**	3.49E-003	2.55E-001
maximum			2.48E-003	6.85E-002	**9.37E-001**

Vapor/Particle Partitioning Estimates

NAME			**Vapor/Particle Partitioning Estimates**		
			low end of fraction adsorbed range	middle of fraction adsorbed range	high end of fraction adsorbed range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm2/cm3	sa=3.5e-6 cm2/cm3	sa=1.1e-5 cm2/cm3
common chemical name	IUPAC #	cas # (1)	*values from calc*	*values from calc*	*values from calc*
2,2',3,3',5-PCB	83	060145-20-2	7.0E-004	5.6E-002	9.2E-001
2,2',3,4,5-PCB	86	065510-45-4	6.9E-004	5.5E-002	9.2E-001
2,2',3,4,5'-PCB	87	038380-02-8	8.2E-004	6.6E-002	9.4E-001
2,2',3,4,6-PCB	88	055215-17-3	3.3E-004	2.6E-002	8.2E-001
2,2',3,5,6-PCB	95	038379-99-6	3.7E-004	2.9E-002	8.4E-001
2,2',4,4',5-PCB	99	038380-01-7	6.3E-004	5.1E-002	9.2E-001
2,2',4,4',6-PCB	100	039485-83-1	1.2E-002	2.5E-001	8.9E-001
2,2',4,5,5'-PCB	101	037680-73-2	5.6E-004	4.5E-002	9.0E-001
2,2',4,6,6'-PCB	104	056558-16-8	7.0E-004	5.6E-002	9.2E-001
2,3,3',4,4'-PCB	105	032598-14-4	2.0E-003	1.6E-001	9.8E-001
2,3,3',4',6-PCB	110	038380-03-9	1.0E-003	8.1E-002	9.5E-001
2,3,4,4',5-PCB	114	074472-37-0	1.4E-003	1.2E-001	9.7E-001
2,3,4,5,6-PCB	116	018259-05-7	8.2E-004	6.5E-002	9.3E-001
2,3',4,4',5-PCB	118	031508-00-6	1.5E-003	1.2E-001	9.7E-001
2',3,4,5,5'-PCB	124	070424-70-3	2.3E-003	1.7E-001	9.8E-001
3,3',4,4',5-PCB	126	057465-28-8	3.4E-003	2.7E-001	9.9E-001
count			16	16	16
average			**1.87E-003**	**1.01E-001**	**9.27E-001**
standard deviation			2.86E-003	7.27E-002	4.64E-002
minimum			**3.31E-004**	2.56E-002	8.23E-001
maximum			1.25E-002	2.66E-001	**9.91E-001**
2,2',3,3',4,4'-PCB	128	038380-07-3	4.9E-003	3.3E-001	9.9E-001
2,2',3,3',4,5-PCB	129	055215-18-4	3.9E-003	2.8E-001	9.9E-001
2,2',3,3',5,6-PCB	134	052704-70-8	1.5E-003	1.2E-001	9.7E-001
2,2',3,3',6,6'-PCB	136	038411-22-2	1.3E-003	8.9E-002	9.4E-001
2,2',3,4,4',5'-PCB	138	035065-28-2	3.4E-003	2.5E-001	9.9E-001
2,2',3,4',5',6-PCB	149	038380-04-0	1.6E-003	1.3E-001	9.7E-001
2,2',4,4',5,5'-PCB	153	035065-27-1	2.6E-003	2.0E-001	9.8E-001
2,2',4,4',6,6'-PCB	155	033979-03-2	5.2E-004	3.8E-002	8.7E-001
2,3,3',4,4',5-PCB	156	038380-08-4	7.6E-003	4.5E-001	1.0E+000
2,3,3',4,4',5'-PCB	157	069782-90-7	8.2E-003	4.7E-001	1.0E+000
2,3',4,4',5,5'-PCB	167	052663-72-6	5.8E-003	3.9E-001	9.9E-001
3,3',4,4',5,5'-PCB	169	032774-16-6	2.2E-002	7.4E-001	1.0E+000
count			12	12	12
average			**5.31E-003**	**2.90E-001**	**9.74E-001**
standard deviation			5.65E-003	1.92E-001	3.65E-002
minimum			**5.25E-004**	3.81E-002	8.65E-001
maximum			2.23E-002	7.43E-001	**9.99E-001**

Vapor/Particle Partitioning Estimates

NAME			**Vapor/Particle Partitioning Estimates**		
			low end of fraction adsorbed range	middle of fraction adsorbed range	high end of fraction adsorbed range
			T = 310K	T = 290K	T = 260K
			sa=4.2e-7 cm2/cm3	sa=3.5e-6 cm2/cm3	sa=1.1e-5 cm2/cm3
common chemical name	IUPAC #	cas # (1)	*values from calc*	*values from calc*	*values from calc*
2,2',3,3',4,4',5-PCB	170	035065-30-6	1.8E-002	6.8E-001	1.0E+000
2,2',3,3',4,4',6-PCB	171	052663-71-5	8.7E-003	4.9E-001	1.0E+000
2,2',3,4,4',5,5'-PCB	180	035065-29-3	1.2E-002	5.8E-001	1.0E+000
2,2',3,4,5,5',6-PCB	185	052712-05-7	5.2E-003	3.5E-001	9.9E-001
2,2',3,4',5,5',6-PCB	187	052663-68-0	5.5E-003	3.6E-001	9.9E-001
2,3,3',4,4',5,5'-PCB	189	039635-31-9	3.0E-002	8.0E-001	1.0E+000
count			6	6	6
average			**1.34E-002**	**5.44E-001**	**9.97E-001**
standard deviation			8.80E-003	1.61E-001	2.17E-003
minimum			**5.17E-003**	3.55E-001	9.94E-001
maximum			3.04E-002	7.98E-001	**9.99E-001**
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	6.7E-002	9.0E-001	1.0E+000
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	3.3E-003	2.5E-001	9.9E-001
count			2	2	2
average			**3.51E-002**	**5.76E-001**	**9.94E-001**
standard deviation			3.18E-002	3.28E-001	5.49E-003
minimum			**3.28E-003**	2.48E-001	9.89E-001
maximum			6.69E-002	9.05E-001	**1.00E+000**
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	1.2E-001	9.5E-001	1.0E+000
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	4.8E-002	8.5E-001	1.0E+000
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	5.0E-002	8.6E-001	1.0E+000
count			3	3	3
average			**7.08E-002**	**8.86E-001**	**1.00E+000**
standard deviation			3.15E-002	4.43E-002	1.81E-004
minimum			**4.75E-002**	8.52E-001	9.99E-001
maximum			1.15E-001	9.49E-001	**1.00E+000**
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	9.38E-002	9.32E-001	1.00E+000

Appendix C.3.

Comparison of Vapor/Particle Partitioning Estimates with Examples of Vapor/Particle Partitioning Measurements from the Literature

As described in Appendix C.1. and presented in Appendix C.2., above, estimates were made using the adsorption-based theory of Junge (1977), with the subcooled liquid-phase vapor pressure substituted for the solid phase vapor pressure, as recommended by Bidleman (1988).

The central estimates of this analysis — shown in the table below in bold face — were carried out using a temperature of 290 ^oK (~17 ^oC; ~62 ^oF). An aerosol surface area of $3.5x10^{-6}$ cm^2 aerosol surface area per cm^3 of air (cm^2/cm^3) was selected, corresponding to the "background + local sources" aerosol surface area category (Whitby, 1978; Bidleman, 1988). In addition to the physical-chemical properties of the pollutant in question, vapor/particle partitioning depends intimately on local meteorological conditions and on the local nature of the atmospheric aerosol.

In order to gain some perspective on the range of vapor/particle partitioning that might be encountered, estimates were also made for a scenarios in which adsorption to particles was at the low and high ends of the expected environmental range.

For the estimated low end of the expected particle-adsorbed range, a relatively high temperature was selected, and a relatively low aerosol surface area was assumed. The conditions chosen were a temperature of 310 ^oK (~37 ^oC; ~98 ^oF) and an aerosol surface area of $4.2x10^{-7}$ cm^2/cm^3. This surface area corresponds to the "clean continental background" aerosol surface area category (Whitby, 1978; Bidleman, 1988).

For the estimated high end of the expected particle-adsorbed range, a relatively low temperature was selected, and a relatively high aerosol surface area was assumed. The conditions chosen were a temperature of 260 ^oK (~ -13 ^oC; ~8 ^oF) and an aerosol surface area of $1.1x10^{-5}$ cm^2/cm^3. This surface area corresponds to the "urban" aerosol surface area category (Whitby, 1978; Bidleman, 1988). [Note: the global mean temperature at a height of 4000 meters is estimated to be on the order of 262 ^oK (Ballschmiter and Wittlinger, 1991)].

In Table C.3.-(1) below, the results of these estimates are presented, along with examples of information from the literature regarding vapor/particle partitioning of the selected compounds in the atmosphere.

The range of the above conditions is rather large, but, for many of the compounds considered in this analysis, their physical chemical properties suggest that they will reside predominantly in the vapor phase (e.g., hexachlorobenzene) or the particle phase (e.g., OCDD) under most ambient conditions. Some of the compounds, however, are predicted to vary quite significantly over the above range of conditions. For example, in the "central" partitioning scenario, approximately 60% of atmospheric 2,3,7,8-TCDD is estimated to associated with the particle phase; for the high and low scenarios considered, the estimated fraction-adsorbed ranges from 8% to 90%.

Table C.3.-(1). Vapor Particle Partitioning Summary for Compounds Considered in this Study

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate (**bold**) T = 290°K; Aerosol surface area = 3.5e-6 cm^2/cm ^{3}] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm^2/cm ^{3}]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
METALS / ORGANOMETALLICS					
Alkylated Lead TEL = Tetraethyl Lead TML = Tetramethyl Lead	I	**0.000002** (TEL) (0.00000007 - 0.00004)	**< 0.00003**		13
		0.00000003 (TML) (1e-9 - 0.00004)	**< 0.00001**		13
Mercury	I	**0.0005** (Hg) (0.00001 - 0.02)	"... it is now known that only a few percent of the total airborne Hg is in the particulate phase. The major chemical form(s) of Hg associated with atmospheric aerosols have so far not been identified ." (11) "Currently it is felt that Hg(p) contributes a small (<5%) fraction of the total amount of Hg found in the ambient air." Several studies at sites in the Great Lakes region are cited showing a range of particulate fraction of total Hg to be (12): 0.006 - 0.023 (over Lake Michigan); 0.001 - 0.073 (Chicago, IL); 0.007 - 0.117 (South Haven, MI); 0.003 - 0.126 (Chicago, IL); 0.020 - 0.162 (South Haven, MI); 0.003 - 0.200 (Ann Arbor, MI); 0.001 - 0.410 (Detroit, MI)		
		0.0000004 ($HgCl_2$) (0.00000003 - 0.000003)			
		0.000003 ($HgCH_3Cl$ (0.0000002 - 0.00004)			
Cadmium	II	**1** (Cd) (0.8 - 1)	Cadmium is generally assumed to be associated with particles in the atmosphere, although it can be in the vapor phase in combustion and incineration processes. The simplified vapor/particle partitioning analysis conducted in this study *suggests* that there may be a small amount of cadmium in the vapor phase in the atmosphere under certain conditions, but, this is very uncertain. Additional details are given in Appendix C, in the discussion of vapor/particle partitioning.		
		1 ($CdCl_2$)			
Tributyltin TBTO = Tributyltin Oxide	II	**0.5** (TBTO) (0.02 -0.98)	If released to the atmosphere, TBTO can be expected to exist in both the particle phase and the vapor phase in the ambient atmosphere (14) The ATSDR Toxicological Profile for Tin (1992) reports that no information on tributyltin compounds in the ambient atmosphere is available. In general, no information on tributyltin compounds in the atmosphere could be found. Measurements of tin in the atmosphere generally measure only the total tin content, and do not attempt to speciate the tin compounds.		

Table C.3.-(1). Vapor Particle Partitioning Summary for Compounds Considered in this Study

Chemical or Group	Level	**Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C** [Central Estimate (**bold**) T = 290°K; Aerosol surface area = 3.5e-6 cm^2/cm^3] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm^2/cm^3]	**Examples from the Literature of Information Regarding Vapor/Particle Partitioning**		
			fraction adsorbed to atmospheric particles	**Temperature (°C)**	**Reference (see end of Table)**
ORGANOCHLORINE BIOCIDES					
Aldrin / Dieldrin	I	**0.0009** (Aldrin) (0.00004 - 0.02)			
		0.003 (Dieldrin) (0.0002 - 0.03)			
DDT / DDD / DDE	I	**0.3** (DDT) (0.03 - 0.8)	**0.73 - 0.88** **0.089 - 0.74**	-5.9 to 1.8 0 - 20	1 4
		0.09 (DDD) (0.005 - 0.6)			
		0.02 (DDE) (0.001 - 0.3)	**0.18 - 0.41** ≤ **0.03** **0.05** (avg) **0.02 - 0.24**	-5.9 to 1.8 8 - 26 20 - 28 0 - 20	1 2 3 4
Mirex	I	**0.00002** (0.000001 - 0.0005)			
Toxaphene	I	**0.1** (0.004 - 0.8)			
Endrin	II	**0.001** (0.00007 - 0.02)			
Heptachlor / Heptachlor Epoxide	II	**0.0003** Hept. (0.00002 - 0.004)			
		0.002 Hept. Epox. (0.0001 - 0.02)			
Hexachloro-cyclohexane	II	**0.0006** (α) (0.00004 - 0.006)	**0.0008 - 0.004**	0 - 20	4
		0.002 (β) (0.0001 - 0.01)			
		0.001 (δ) (0.00007 - 0.01)			
		0.003 (γ) (0.0002 - 0.03)			
Methoxychlor	II	**0.1** (0.005 - 0.6)			

Table C.3.-(1). Vapor Particle Partitioning Summary for Compounds Considered in this Study

Chemical or Group	Level	**Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C** [Central Estimate (**bold**) T = 290°K; Aerosol surface area = 3.5e-6 cm^2/cm^3] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm^2/cm^3]	**Examples from the Literature of Information Regarding Vapor/Particle Partitioning**		
			fraction adsorbed to atmospheric particles	**Temperature (°C)**	**Reference (see end of Table)**
Pentachlorophenol	II	**0.0006** (0.00004 - 0.006)			
INDUSTRIAL / MISCELLANEOUS					
Octachlorostyrene	I	**0.003** (0.0001 - 0.04)			
3,3'-Dichloro-benzidene	II	**0.9** (0.3 - 0.99)			
4,4'-Methylene bis (2-Chloroaniline) “MBOCA”	II	**0.009** (0.0005 - 0.1)			
4-Bromophenyl Phenyl Ether “4BPE”	II	**0.0005** (0.00002 - 0.02)			
Hexachloro-1,3-Butadiene “HCBD”	II	**0.000005** (0.0000002 - 0.0001)	“Hexachlorobutadiene can exist in the atmosphere as a vapor or adsorbed to airborne particulate matter... A high partition coefficient (Log Koc) value of 3.67 ... indicates that adsorption to soils with high organic content can occur. Wind erosion of contaminated surface soils can then lead to airborne hexachlorobutadiene-containing particulate matter. Levels of hexachlorobutadiene have been detected in flyash from the incineration of hexachlorobutadiene-containing hazardous waste (Junk and Ford 1980). The transport of particulate matter is a function of particle size and wind speed, however no data were located regarding the transport of hexachlorobutadiene particles in air.” (ATSDR-Hexachlorobutadiene, 1994)		

Table C.3.-(1). Vapor Particle Partitioning Summary for Compounds Considered in this Study

Chemical or Group	Level	**Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C** [Central Estimate (**bold**) T = 290^{o}K; Aerosol surface area = 3.5e-6 cm^2/cm ^{3}] [RANGE (in parentheses): 310 to 260 ^{o}K; 4.2e-7 to 1.1e-5 cm^2/cm ^{3}]	**Examples from the Literature of Information Regarding Vapor/Particle Partitioning**		
			fraction adsorbed to atmospheric particles	**Temperature (°C)**	**Reference (see end of Table)**
CHLOROBENZENES					
1,4-dichlorobenzene “pDCB”	II	**0.0000004** (0.00000003 - 0.000003)			
Tetrachlorobenzenes 1234 Tetrachlorbenzene 1245 Tetrachlorobenzene 1235 Tetrachlorobenzene “1234TCB” “1245TCB” “1235TCB”	II	**0.000009** (1234TCB) (0.0000006 - 0.0001)			
		0.000008 (1245TCB) (0.0000005 - 0.00006)			
		0.000004 (1235TCB) (0.0000003 - 0.00004)			
Pentachlorobenzene “PeCB”	II	**0.00009** (0.000006 - 0.001)			
Hexachlorobenzene “HCB”	I	**0.0003** (0.00002 - 0.003)	**0.001 - 0.007**	0 - 20	4

Table C.3.-(1). Vapor Particle Partitioning Summary for Compounds Considered in this Study

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate (**bold**) T = 290°K; Aerosol surface area = 3.5e-6 cm^2/cm^3] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm^2/cm^3]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
POLYCHLORINATED DIBENZO-P-DIOXINS AND DIBENZOFURANS (PCDD/F'S)					
2,3,7,8-TCDD	I	**0.6** (0.08 - 0.9)	**0.13** avg for all samples: total TCDD	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
2,3,7,8-TCDF	I	**0.3** (0.02 - 0.9)	**0.09** avg for all samples: total TCDF	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
PeCDD/F's (pentachloro-)	I	**0.9** (0.2 - 0.99)	**0.36** avg for all samples: PeCDD/F's	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
HxCDD/F's (hexachloro-)	I	**0.97** (0.6 - 1)	**0.76** avg for all samples: total HxCDD/F's	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
HpCDD/F's (heptachloro-)	I	**0.99** (0.9 - 1)	**0.97** avg for all samples: total HpCDD/F's	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
OCDD/F's (octachloro-)	I	**1** (0.98 - 1)	**0.99** avg for all samples: total OCDD/F	38 samples over 3 yrs; <3 °C: 11 samples 16-20 °C: 15 samples >28 °C: 12 samples	15
PCDD/F's (as a group)	I		~ **0.87** (avg)	20 - 28	3
			0.54 - 0.74 **0.91 - 0.94**	25 - 28 8 -12	5 5
			0.31 - 0.56 **0.87 - 0.96**	25 - 28 8 - 12	5 (TEQ) 5 (TEQ)
			0.74 (avg)	38 samples over 3 yrs; <3 °C:11 samples 16-20 °C:15 samples >28 °C: 12 samples	15

Table C.3.-(1). Vapor Particle Partitioning Summary for Compounds Considered in this Study

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate (**bold**) T = 290°K; Aerosol surface area = 3.5e-6 cm^2/cm^3] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm^2/cm^3]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	**Temperature (°C)**	**Reference (see end of Table)**
POLYCHLORINATED BIPHENYLS (PCB'S)					
Cl_1-PCB		**0.00007 - 0.00014** (0.000001 - 0.01)			
Cl_2-PCB		**0.0004 - 0.0020** (0.000007 - 0.2)	**< 0.01** (avg)	20 - 28	3
Cl_3-PCB		**0.001 - 0.012** (0.00002 - 0.6)	**< 0.001** (avg)	20 - 28	3
Cl_4-PCB		**0.003 - 0.069** (0.00006 - 0.94)	**~ 0.024** (avg) **0.016 - 0.069** **0.11 - 0.22**	20 - 28 25 - 28 8 - 12	3 5 (coplanar) 5 (coplanar)
Cl_5-PCB		**0.03 - 0.27** (0.0003 - 0.99)	**n.d - 0.13** **~ 0.04** (avg) **0.03 - 0.04** **0.39 - 0.55**	-5.9 to 1.8 20 - 28 25 - 28 8 - 12	1 (PCB-101) 3 5 (coplanar) 5 (coplanar)
Cl_6-PCB		**0.04 - 0.74** (0.0005 - 0.999)	**n.d - 0.47** **~ 0.067** (avg) **0.02 - 0.41** **0.56 - 0.98**	-5.9 to 1.8 20 - 28 25 - 28 8 - 12	1 (PCB-153) 3 5 (coplanar) 5 (coplanar)
Cl_7-PCB		**0.36 - 0.80** (0.005 - 0.999)	**~ 0.2**	20 - 28	3
Cl_8-PCB		**0.25 - 0.91** (0.003 - 1.000)	**~ 0.6**	20 - 28	3
Cl_9-PCB		**0.85 - 0.95** (0.05 - 1.000)			
Cl_{10}-PCB		**0.93** (0.09 - 1.00)			
PCB's as a group	I		**~ 0.04** **0.02 - 0.25**	20 - 28 0 - 20	3 4 (Arochlor 1254)

Table C.3.-(1). Vapor Particle Partitioning Summary for Compounds Considered in this Study

Chemical or Group	Level	**Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C** [Central Estimate (**bold**) T = 290°K; Aerosol surface area = 3.5e-6 cm^2/cm^3] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm^2/cm^3]	**Examples from the Literature of Information Regarding Vapor/Particle Partitioning**		
			fraction adsorbed to atmospheric particles	**Temperature (°C)**	**Reference (see end of Table)**
POLYCYCLIC AROMATIC HYDROCARBONS					
Naphthalene “Naph”		**0.000002** (0.0000001 - 0.00002)	**< 0.02**	16	10-a
Acenaphthene “Acn”		**0.00005** (0.000003 - 0.0006)	**< 0.02**	16	10-a (Acn + Acl)
Acenaphthylene “Acl”		**0.00002** (0.000001 - 0.0002)	**< 0.02**	16	10-a (Acn + Acl)
Fluorene “Flr”		**0.0001** (0.000007 - 0.001)	**~ 0 - 0.004**	10 - 24	7
			< 0.02	16	10-a
			0.0004 - 0.0166	0 - 30	16(range)
			0.0039	0 - 30	16(median)
Phenanthrene “Phen”	II	**0.0008** (0.00004 - 0.01)	**0.003 - 0.007**	10 - 24	7
			0.01	12	9
			< 0.11	16	10-a
			0.08 +/- 0.02	21	10-b
			0.03 +/- 0.01	21	10-c
			0.0004 - 0.1025	0 - 30	16(range)
			0.0103	0 - 30	16(median)
Anthracene “Anth”	II	**0.001** (0.00006 - 0.01)	**< 0.03**	16	10-a
			0.0006 - 0.97	0 - 30	16(range)
			0.04	0 - 30	16(median)
Pyrene “Pyr”		**0.007** (0.0004 - 0.08)	**0.017 - 0.095**	10 - 24	7
			0.01 - 0.29	5 - 29	8
			0.28	12	9
			0.15 +/- 0.07	21	10-b
			0.06 +/- 0.03	21	10-c
			0.005 - .520	0 - 30	16(range)
			0.08	0 - 30	16(median)
Fluoranthene “Fln”		**0.01** (0.0005 - 0.1)	**0.012 - 0.082**	10 - 24	7
			0.009 - 0.234	5 - 29	8
			0.28	12	9
			0.0014 - .4422	0 - 30	16(range)
			0.064	0 - 30	16(median)
Chrysene “Chr”		**0.4** (0.04 - 0.9)	**0.97**	12	9
			0.21 +/- 0.04	21	10-b
			0.15 +/- 0.03	21	10-c
			0.16 - 0.48	10 - 24	7 (combined with triphenylene)
			0.01 - ~ 1	0 - 30	16(range)
			0.5	0 - 30	16(median)

Table C.3.-(1). Vapor Particle Partitioning Summary for Compounds Considered in this Study

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate (**bold**) T = 290^{o}K; Aerosol surface area = 3.5e-6 cm^{2}/cm ^{3}] [RANGE (in parentheses): 310 to 260 ^{o}K; 4.2e-7 to 1.1e-5 cm^{2}/cm ^{3}]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)
Benz (a) Anthracene “BaA”	II	**0.5** (0.05 - 0.95)	**~ 0.6** **0.023 - 0.67** **0.016 - ~1** **0.87**	4 - 13 10 - 24 0 - 30 0 - 30	6 7 16(range) 16(median)
Benzo (b) Fluoranthene “BbF”		**0.05** (0.002 - 0.5)	**035 - 0.57** **0.21 - ~1** **0.93**	10 - 24 0 - 20 0 - 30	7 16(range) 16(median)
Benzo (j) Fluoranthene “BjF”		**0.7** (0.08 - 0.97)			
Benzo (k) Fluoranthene “BkF”		**0.96** (0.5 - 1)	**034 - 0.52** .50 - ~1 ~ 1	10 - 24 0 - 30 0 - 30	7 16(range) 16(median)
Benzo (a) Pyrene “BaP”	I	**0.8** (0.2 - 0.99)	**~1** **0.72 - 1.00** **0.8 - 1.0** **0.09 - ~1** **~1**	-5.9 to 1.8 10 - 24 5 - 29 0 - 30 0 - 30	1 7 8 (BaP + BeP) 16(range) 16(median)
Benzo (e) Pyrene “BeP”		**0.8** (0.1 - 0.99)	**0.8 - 1.0** **0.17 - ~1** **0.93**	5 - 29 0 - 30 0 - 30	8 (BaP + BeP) 16(range) 16(median)
Perylene “Per”	II	**0.95** (0.5 - 1)			
Benzo (g,h,i) Perylene “BgP”	II	**0.96** (0.5 - 1)	**~1** **0.32 - 1.00** **0.17 - ~1** **0.98**	-5.9 - 1.8 10 - 24 0 - 30 0 - 30	1 7 16(range) 16(median)
Dibenz (a,h) Anthracene “dBA”		**1** (0.98 - 1)	**0.29 - ~1** **> 0.95**	0 - 30 0 - 30	16(range) 16(median)
Indeno (1,2,3-c,d) Pyrene “IPyr”		**0.99** (0.9 -1)	**0.77 - 1.00** **0.46 - ~1** **> 0.989**	10 - 24 0 - 30 0 - 30	7 16(range) 16(median)
Dinitropyrenes “DNPs”	II	**0.4** (0.03 - 0.9)			
PAH’s (as a group)	II				

Table C.3.-(1). Vapor Particle Partitioning Summary for Compounds Considered in this Study

Chemical or Group	Level	Estimated Fraction Adsorbed to Particle Phase in Atmosphere Based on Calculations in Appendix C [Central Estimate (**bold**) T = 290°K; Aerosol surface area = 3.5e-6 cm^2/cm^3] [RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm^2/cm^3]	Examples from the Literature of Information Regarding Vapor/Particle Partitioning		
			fraction adsorbed to atmospheric particles	Temperature (°C)	Reference (see end of Table)

References for above Table

(1) Kaupp and Umlauf, 1990 (Northern Bavaria, Germany: urban area)
(2) Hawthorne et al., 1996 (South Dakota, U.S.: agricultural area)
(3) Nakano et al., 1990a (Japan, urban area) (Note: The average particle-associated fraction was not explicitly reported; for the estimates of average particle-associated fraction reported in this table, the reported average particle-phase concentration was divided by reported average total particle- + vapor-phase concentration.)
(4) Bidleman, Billings, and Foreman, 1986 (Columbia, South Carolina, U.S.; New Bedford, Mass., U.S.; Denver, Colorado, U.S.; Stockholm, Sweden: all urban areas). (Note: averages given here, as reported in paper, based on correlations of field data)
(5) Kurokawa et al., 1996 (Japan: 2 urban sites, 1 rural site)
(6) Nakano et al., 1990b (Kobe, Japan: urban area)
(7) Baker and Eisenreich, 1990 (over Lake Superior)
(8) Yamasaki et al., 1982 (Osaka City, Japan: urban area)
(9) Albaiges et al., 1991 (Barcelona, Spain: urban area)
(10) Gundel et al., 1995 (a: partitioning to simulated environmental tobacco smoke was studied; a relatively high aerosol concentration was employed; b: partitioning in laboratory air - denuder method; c: laboratory air - filter-sorbent (conventional) method)
(11) Schroeder et al., 1991
(12) Lamborg et al., 1994
(13) Harrison and Laxen, 1978 (as cited in Grandjean and Nielsen, 1979)
(14) information downloaded from U.S. National Institutes of Health Hazardous Substances Database (HSDB), Nov.- Dec., 1996
(15) Eitzer and Hites, 1989a (Bloomington, Indiana, urban area)
(16) Gustafson & Dickhut, 1997 (Southern Chesapeake Bay region; 4 sites: rural, semi-urban, urban, industrial)

Appendix C.4.
Vapor-Particle Partitioning of PAH's: Detailed Comparison of Theoretical Estimates with Recent Experimental Data

In a recent paper, a detailed set of vapor/particle partitioning data for PAH's is described (Gustafson and Dickhut, 1997). The supplementary data (i.e., the detailed data set) was obtained and a comparison was made between the measurements and the "simplified" theoretical estimates used in this analysis.

The measurements were made at four sites in the southern Chesapeake Bay region, including one rural site, one semi-urban site, one urban site, and one industrial site (as characterized by the authors). Various measurements of the gas and particle phase concentrations of PAH's were made at the four sites, over the period from October 1993 through May 1995 (the period of measurements at the four sites varied). In all, a total of 44 paired sets of vapor and particle measurements were made, with 24 of these being made at the Haven Beach (rural) site. A set of 14 PAH's were measured, as listed in Table C.4.-(1), below.

Table C.4.-(1). List of PAH Compounds

Chemical	Measured by Gustafson and Dickhut (1997)	Specifically Identified on IJC Target Compound List	ATSDR List of 17 PAH's	USEPA List of 16 PAH's	USEPA List of 7 PAH's
naphthalene	0	0	0	1	0
acenaphthene	0	0	1	1	0
acenaphthylene	0	0	1	1	0
fluorene	**1**	0	1	1	0
phenanthrene	**1**	1	1	1	0
anthracene	**1**	1	1	1	0
pyrene	**1**	0	1	1	0
fluoranthene	**1**	0	1	1	0
chrysene	**1**	0	1	1	1
benz [a] anthracene	**1**	1	1	1	1
benzo [b] fluoranthene	**1**	0	1	1	1
benzo [j] fluoranthene	0	0	1	0	0
benzo [k] fluoranthene	**1**	0	1	1	1
benzo [a] pyrene	**1**	1	1	1	1
benzo [e] pyrene	**1**	0	1	0	0
perylene	0	1	0	0	0
benzo [g,h,i] perylene	**1**	1	1	1	0
dibenz [a,h] anthracene	**1**	0	1	1	1
indeno [1,2,3-c,d] pyrene	**1**	0	1	1	1
total # in list -->	**14**	**6**	**17**	**16**	**7**

The complete data set is summarized in Table C.4.-(2) (page C-29) and given in Table C.4.-(3) (pages C-46 through C-54), below. In Table C.4.-(3), an "n.d." means "not detected"; "n.q." means "not quantified". These were assumed to be the meaning of the abbreviations used by the authors. An average detection limit of 0.30 pg/m3 was reported, and, this value was used in the calculations shown. In these Tables, the "fraction associated with particles" is calculated from the available data.

When either the vapor or particle phase measurement was reported as "n.q.", or, if both the vapor and particle phase measurements were reported as "n.d.", then it was assumed that no estimate of the vapor/particle partitioning could be made from the data. In these cases, the term "n.a." (for "not available") was used in Table C.4.-(3). In general, out of the 44 measurements, about 40 estimates could be made for each of the PAH's measured.

A summary of the theoretical predictions for PAH's — as described in earlier portions of this Appendix — is shown in Figure C.4.-(1). In this Figure, the mid-range estimates are shown as "data points" and the low- and high-range of the estimates are shown as "error bars".

A comparison of the measurements of Dickhut and Gustafson (1997) with the simple theory used in this analysis is summarized in Table C.4.-(2). A plot of the median experimental measurements vs. the mid-range theoretical estimates is shown in Figure C.4.-(2). A detailed set of plots showing the experimental measurements and the theoretical predictions for each of the 14 PAH's measured are given as Figures C.4.-(3) through C.4.-(16).

It can be seen from the overall summary plot [Figure C.4.-(2)] that for most of the PAH's considered, the simple theory has done a relatively adequate job of predicting the overall tendency of the compounds. That is, compounds measured largely in the vapor phase were more or less predicted to exist largely in the vapor phase, etc.

For one (and maybe two) compounds, the predictions seem to be qualitatively wrong. Benzo(b)Fluoranthene is predicted by the theory to exist largely in the vapor phase. The particle-associated fractions are theoretically estimated to be:

low estimate = 0.002
mid-range estimate = 0.050
high-range estimate = 0.520

There were 44 available measurements for benzo(b)fluoranthene; a statistical summary of the <u>particle-associated fractions</u> of these measurements is as follows:

minimum = 0.21
maximum = ~ 1
median = 0.93

The reason for this discrepancy can not be unambiguously determined at this time, but, likely explanations are the following:

- The physical-chemical properties used for this compound were in error (i.e., the vapor-pressure may be have been incorrect);

- Factors leading towards increased particle associated fractions (as discussed below) played a more dramatic role for this compound.

A similar but less dramatic discrepancy is seen for Benzo(a)Anthracene. In fact, the discrepancy was even larger than displayed, prompting a reconsideration of physical-chemical property data for this compound. A revised value for the vapor/pressure was adopted (as cited in Howard and Meylan, 1997), and the earlier used value (taken from MacKay et al, 1992) was discarded.

Even with this "correction" the theoretical predictions for Benzo(a)Anthracene indicate a lower particle associated fraction than observed. However, as shown in Figure C.4.-(8), there is somewhat of an overlap between the measured and theoretical ranges.

Throughout the many comparisons shown in this Appendix, there is a general pattern of the measured particle-associated fractions being somewhat higher than the predicted values. There are many possible reasons for this systematic trend, including the following:

- The parameters used in the simplified absorption theory were not exactly appropriate for the PAH's and atmospheric conditions measured (i.e., there are potential "errors" in Junge's constant or the aerosol surface area, etc.);
- The physical-chemical properties for the PAH's are not exactly specified (i.e., there could have been errors in the "underlying data" used, or, possibly more likely, a systematic bias in the simplified extrapolation procedures used in this analysis could exist);
- An absorption theory or combined absorption/adsorption theory should have been used;
- A fraction of the PAH's are non-exchangeable;
- The measured particle-associated fractions are artificially high due to adsorption/absorption of gas-phase material onto particles already collected by the filter (a potential bias common to these types of measurements and acknowledged by the authors).

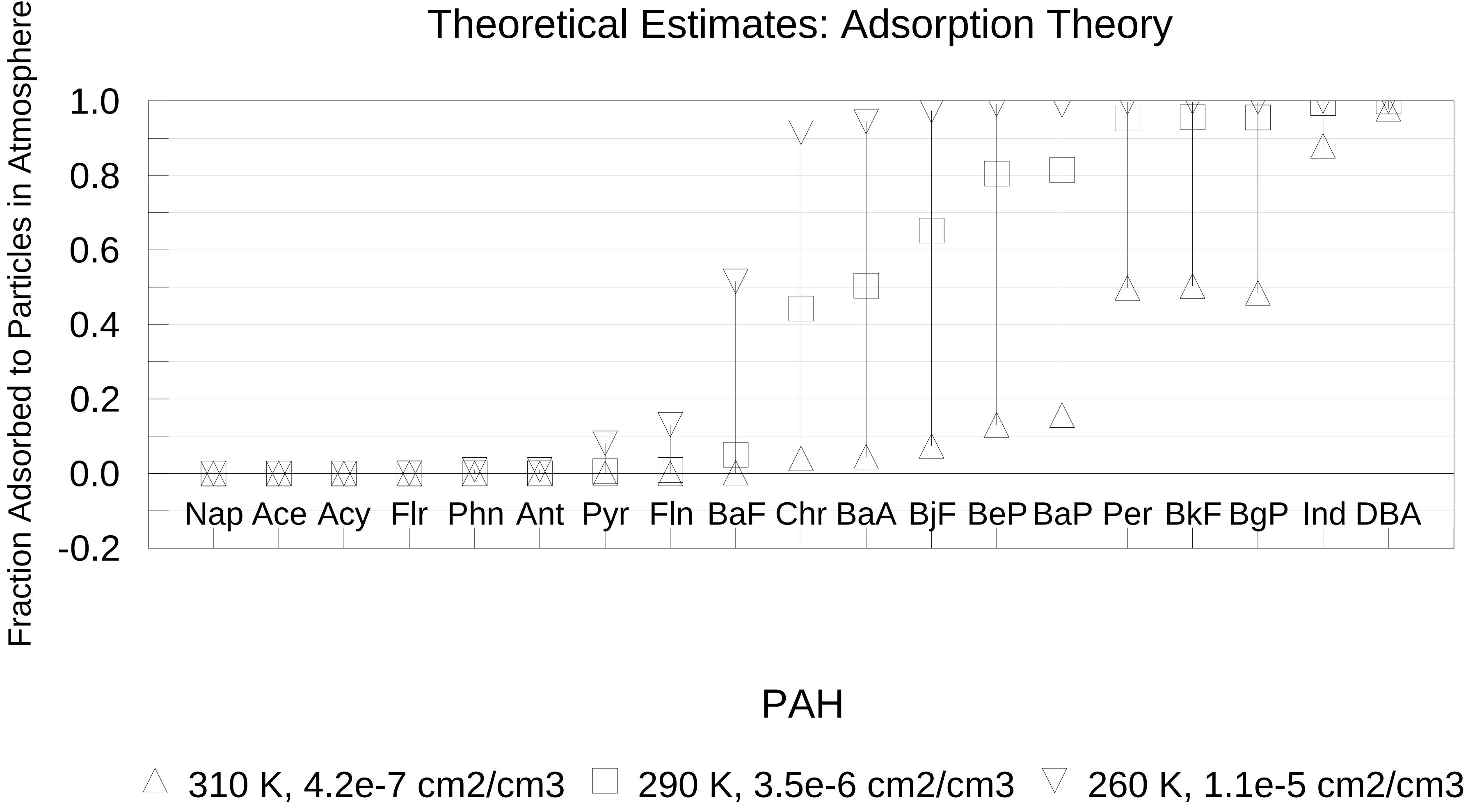
In reality, probably all of the above potential sources of error play a role in the differences observed between the measurements and the theoretical predictions.

Table C.4.-(2)

SUMMARY DATA from Gustafson and Dickhut, 1997: ES&T 31:140-147 (supplementary information)

	TOTAL	TOTAL	TOTAL		TOTAL		TOTAL		TOTAL		TOTAL	TOTAL	THEORY	THEORY	THEORY
		# of	# of										Junge	Junge	Junge
		"Greater	"Less										theory	theory	theory
	Count	Thans"	Thans"		Min		Max		Median		Avg	Std	low-range	mid-range	high-range
					fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase	fraction in particle phase	fraction in particle phase	fraction in particle phase	fraction in particle phase
fluorene	39	0	0		0.0004		0.0166		0.0039		0.0046	0.0035	0.0000	0.0001	0.0012
phenanthrene	42	0	0		0.0004		0.1025		0.0103		0.0206	0.0249	0.0000	0.0008	0.0100
anthracene	39	15	0		0.0006	>	0.9680		0.0400	>	0.3685	0.4407	0.0001	0.0010	0.0099
fluoranthene	43	0	0		0.0014		0.4422		0.0636		0.1079	0.1126	0.0005	0.0099	0.1312
pyrene	43	0	0		0.0050		0.5172		0.0795		0.1203	0.1336	0.0004	0.0070	0.0815
benzo(a)anthracene	42	20	3		0.0161	>	0.9972		0.8753	>	0.7213	0.3258	0.0457	0.5048	0.9448
chrysene	44	1	0		0.0118	>	0.9978		0.5058	>	0.5110	0.2903	0.0403	0.4432	0.9160
benzo(b)flouranthene	44	3	0		0.2082	>	0.9990		0.9299	>	0.8304	0.1943	0.0023	0.0511	0.5159
benzo(k)flouranthene	43	24	0		0.5030	>	0.9989	>	0.9769	>	0.9316	0.1116	0.5032	0.9564	0.9974
benzo(e)pyrene	44	6	0		0.1749	>	0.9987		0.9313	>	0.8154	0.2347	0.1309	0.8056	0.9910
benzo(a)pyrene	43	25	0		0.0890	>	0.9983	>	0.9718	>	0.8663	0.2079	0.1564	0.8152	0.9891
indeno(123cd)pyrene	42	36	0		0.4637	>	0.9995	>	0.9881	>	0.9470	0.1149	0.8793	0.9948	0.9998
dibenzo(ah)anthracene	39	34	0		0.2940	>	0.9932	>	0.9544	>	0.8973	0.1333	0.9783	0.9990	0.9999
benzo(ghi)perylene	43	19	0		0.1709	>	0.9989		0.9796	>	0.8691	0.2073	0.4852	0.9561	0.9976

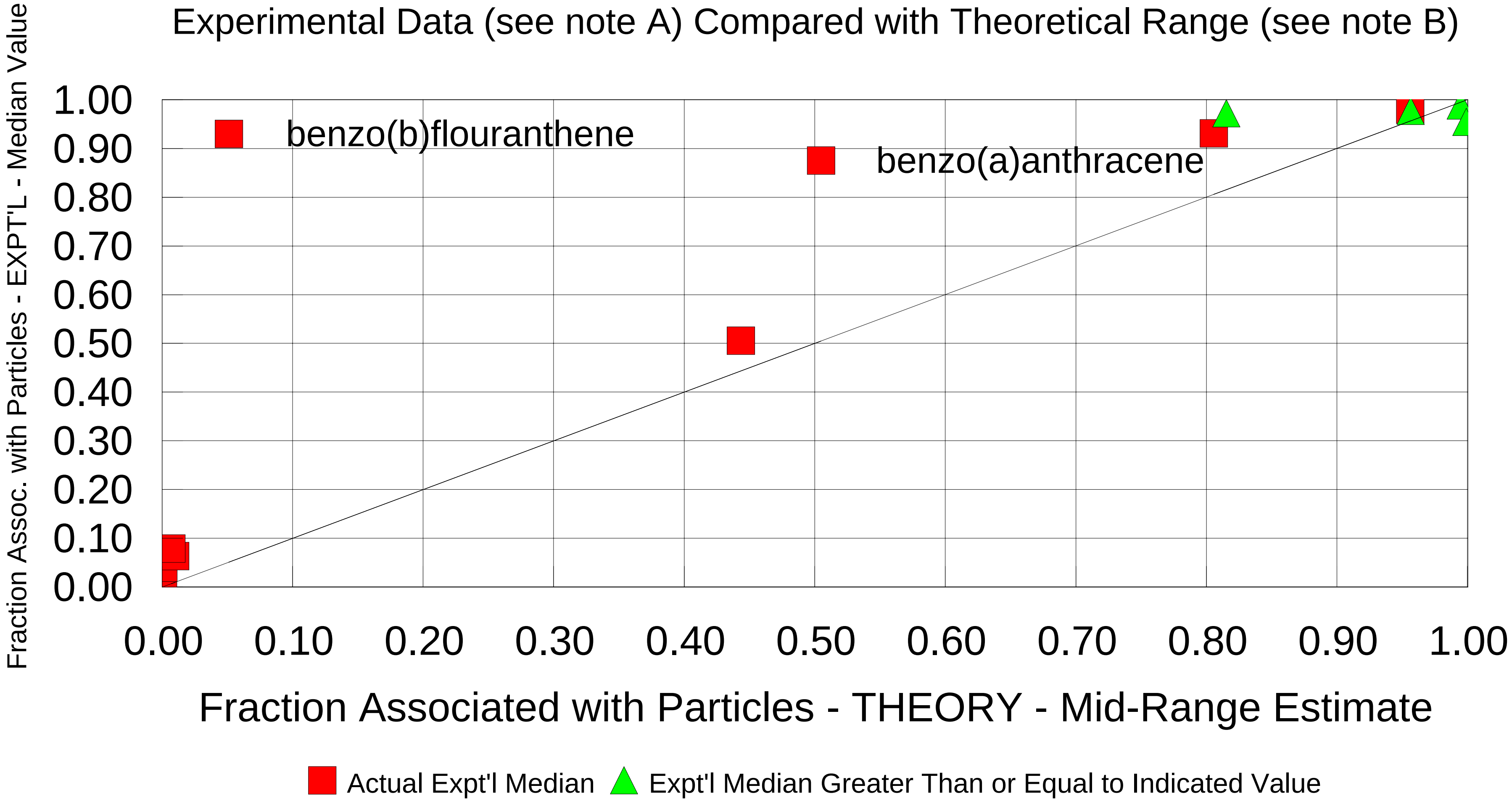
Figure C.4.-(1). Vapor/Particle Partitioning of PAH's in the Atmosphere
Theoretical Estimates: Adsorption Theory



Estimates are based on Junge's Adsorption Theory, using subcooled liquid vapor pressure

Figure C.4.-(2). Vapor/Particle Partitioning for PAH's (SUMMARY)

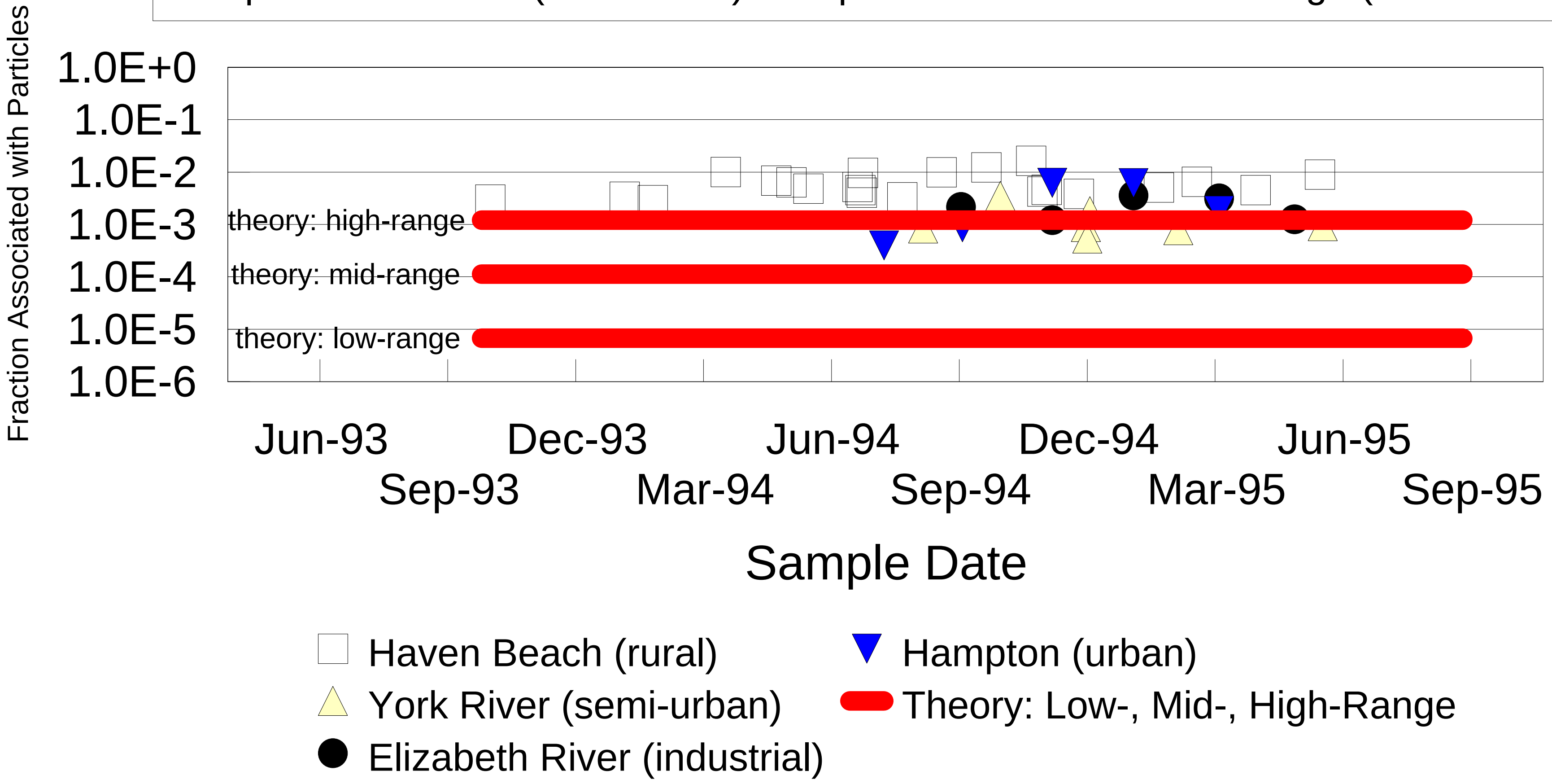
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A. Gustafson & Dickhut, ES&T 31:140-147, 1997. Atmos. meas. in the southern Ches. Bay region (~40 meas., 1993-1995)
B. Junge's Adsorption Theory, using subcooled liquid vapor pressure; Temp. = 290 K; Aerosol Surface Area = 3.5e-6 cm2/cm3

Figure C.4.-(3). Vapor/Particle Partitioning for PAH's: FLOURENE

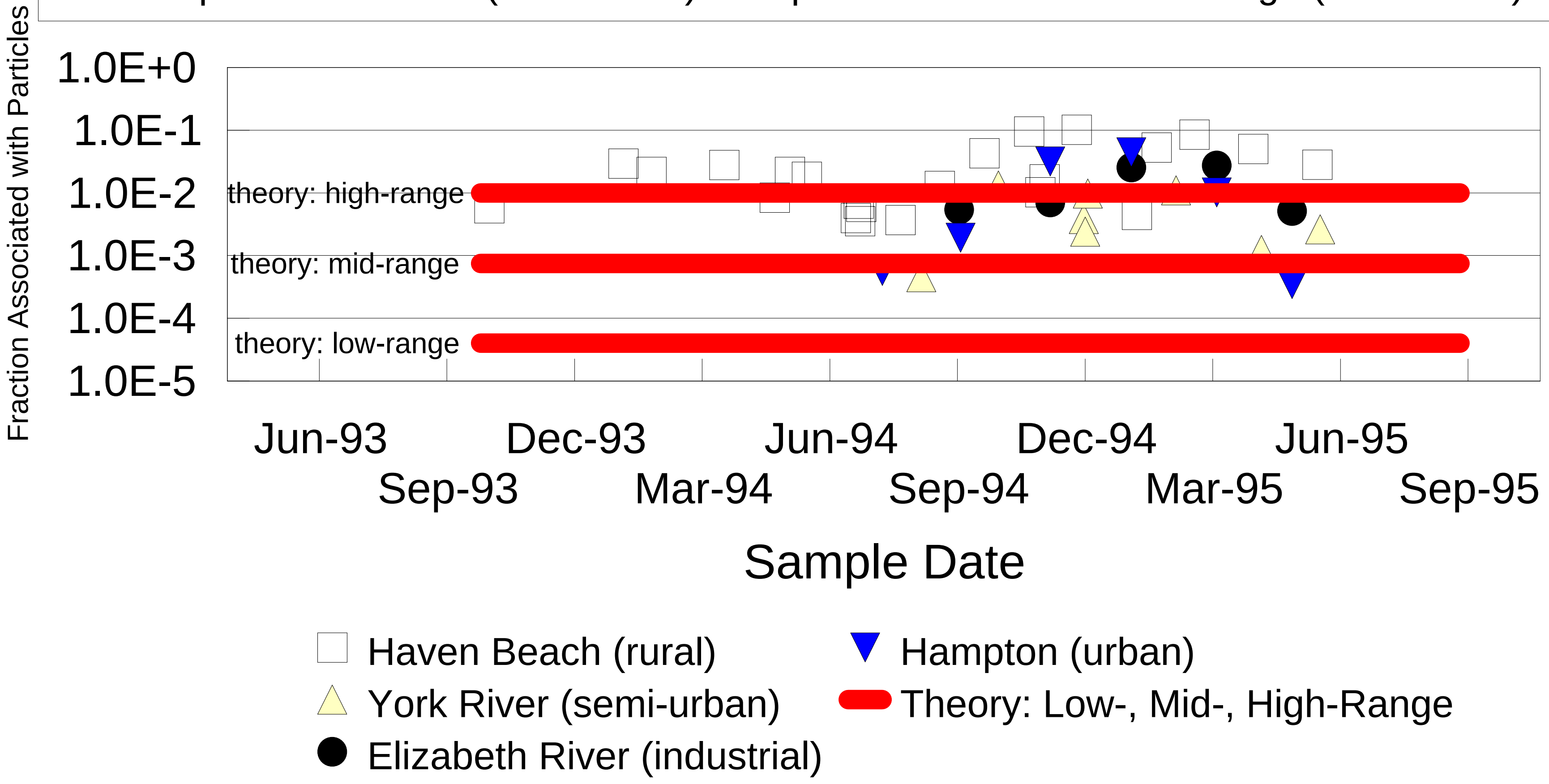
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(4). Vapor/Particle Partitioning for PAH's: PHENANTHRENE

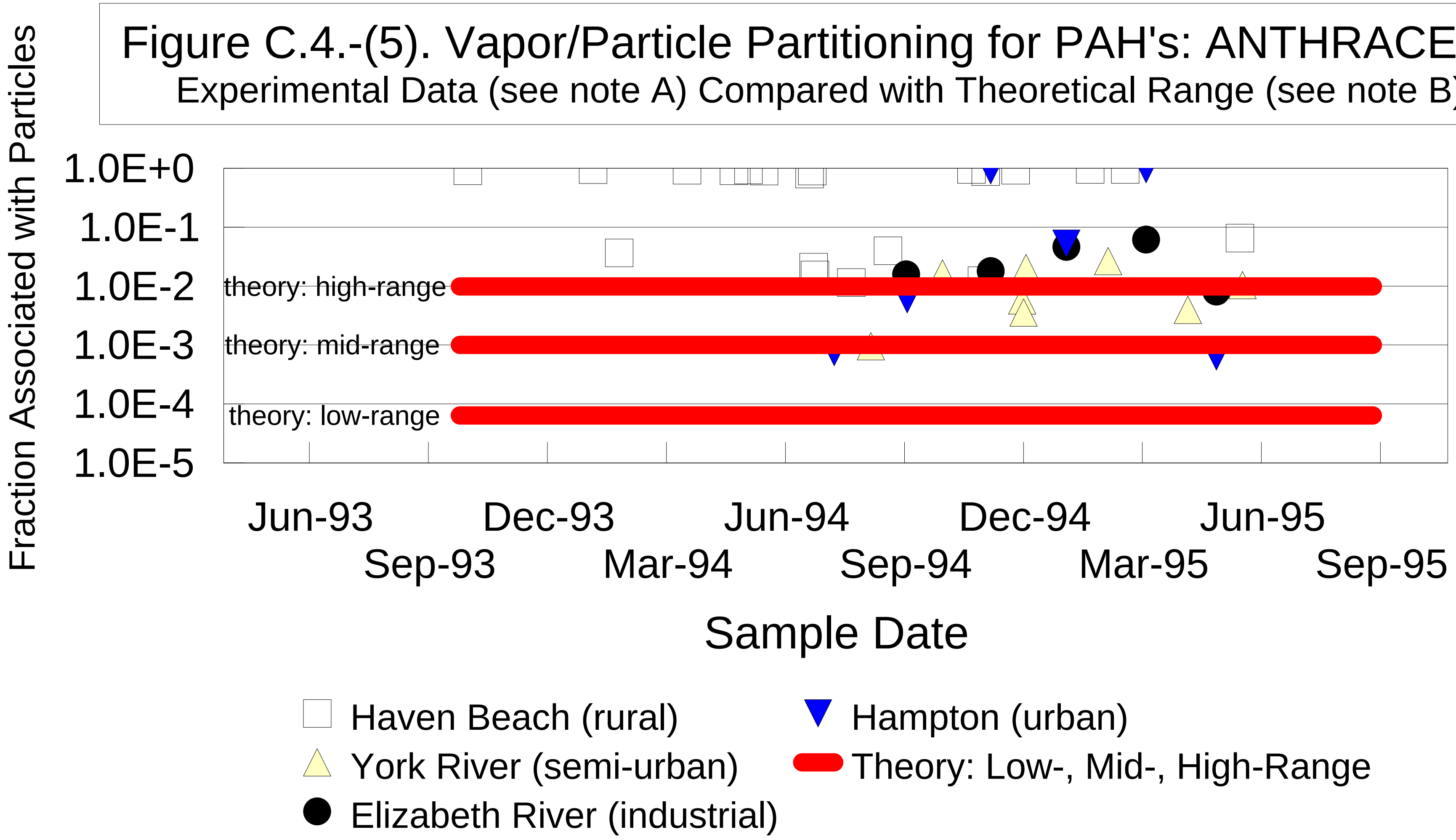
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(5). Vapor/Particle Partitioning for PAH's: ANTHRACENE

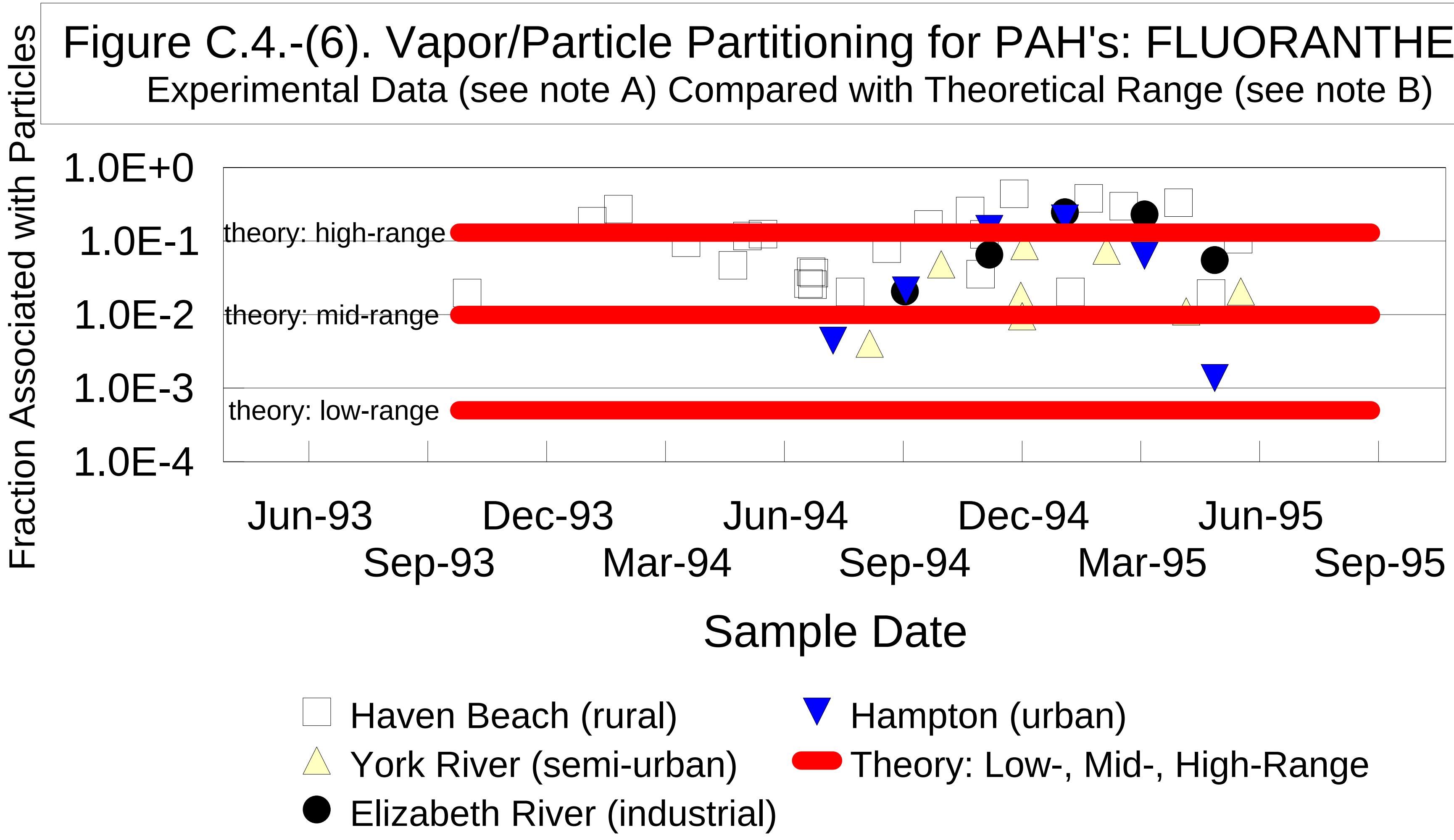
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(6). Vapor/Particle Partitioning for PAH's: FLUORANTHENE

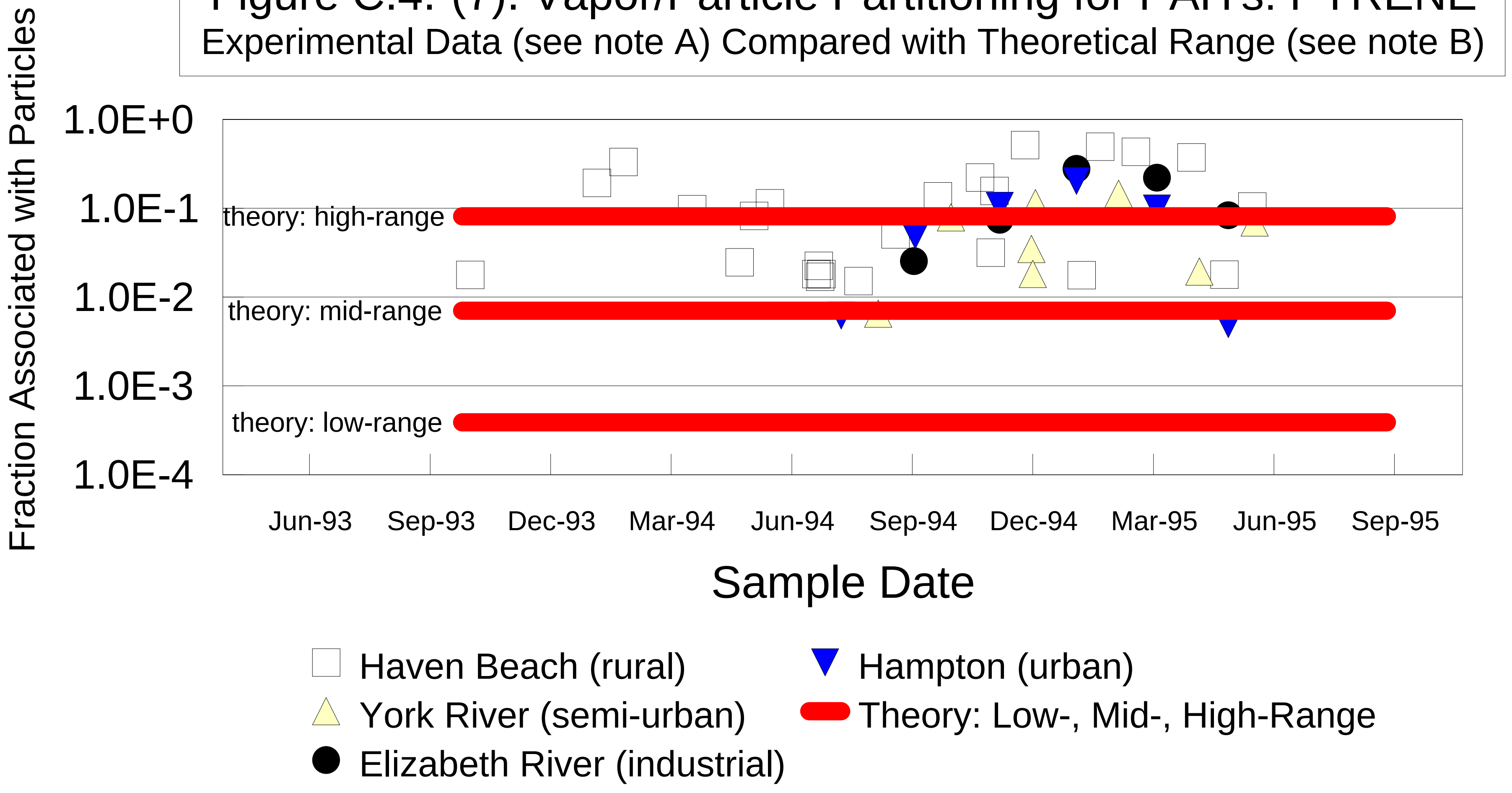
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

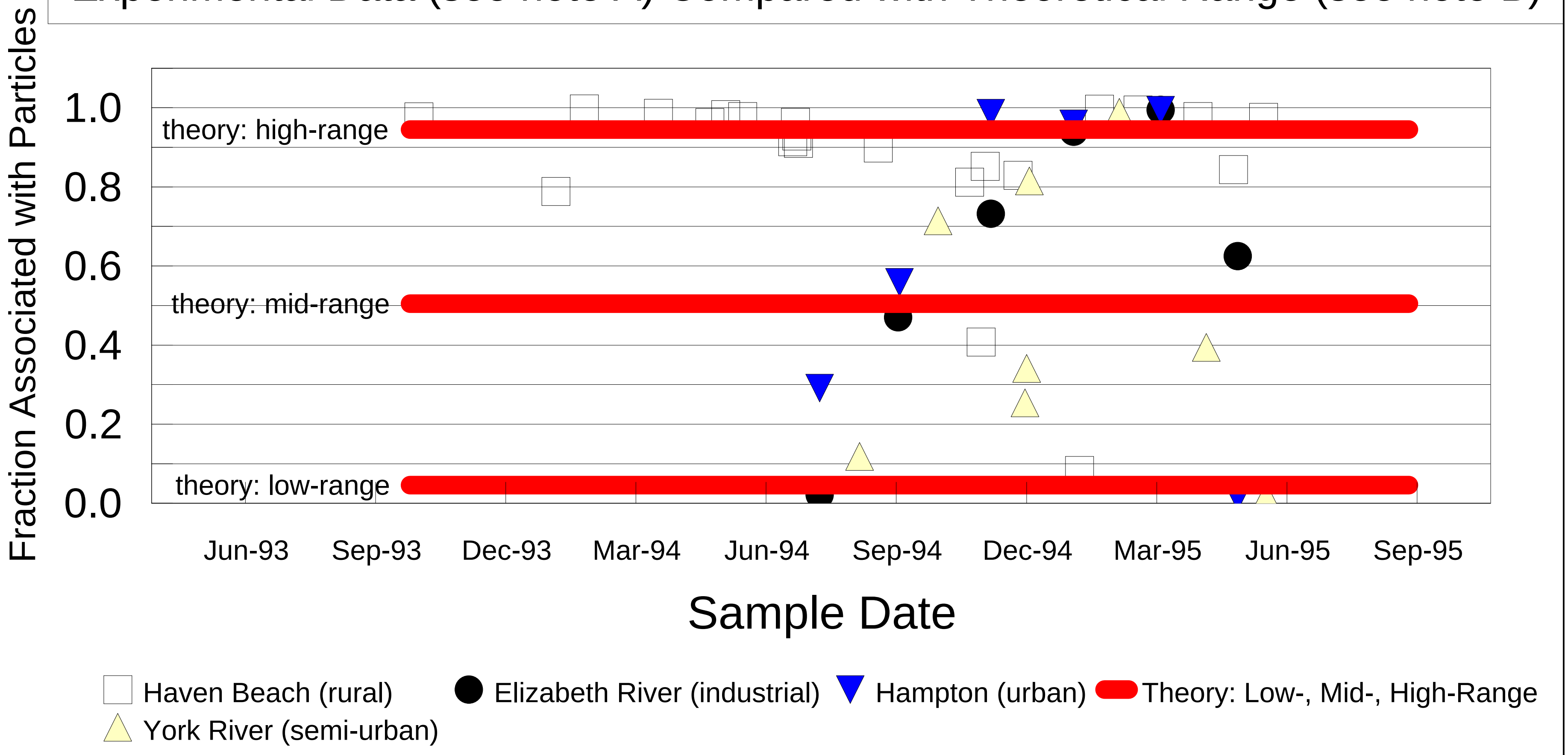
Figure C.4.-(7). Vapor/Particle Partitioning for PAH's: PYRENE

Experimental Data (see note A) Compared with Theoretical Range (see note B)



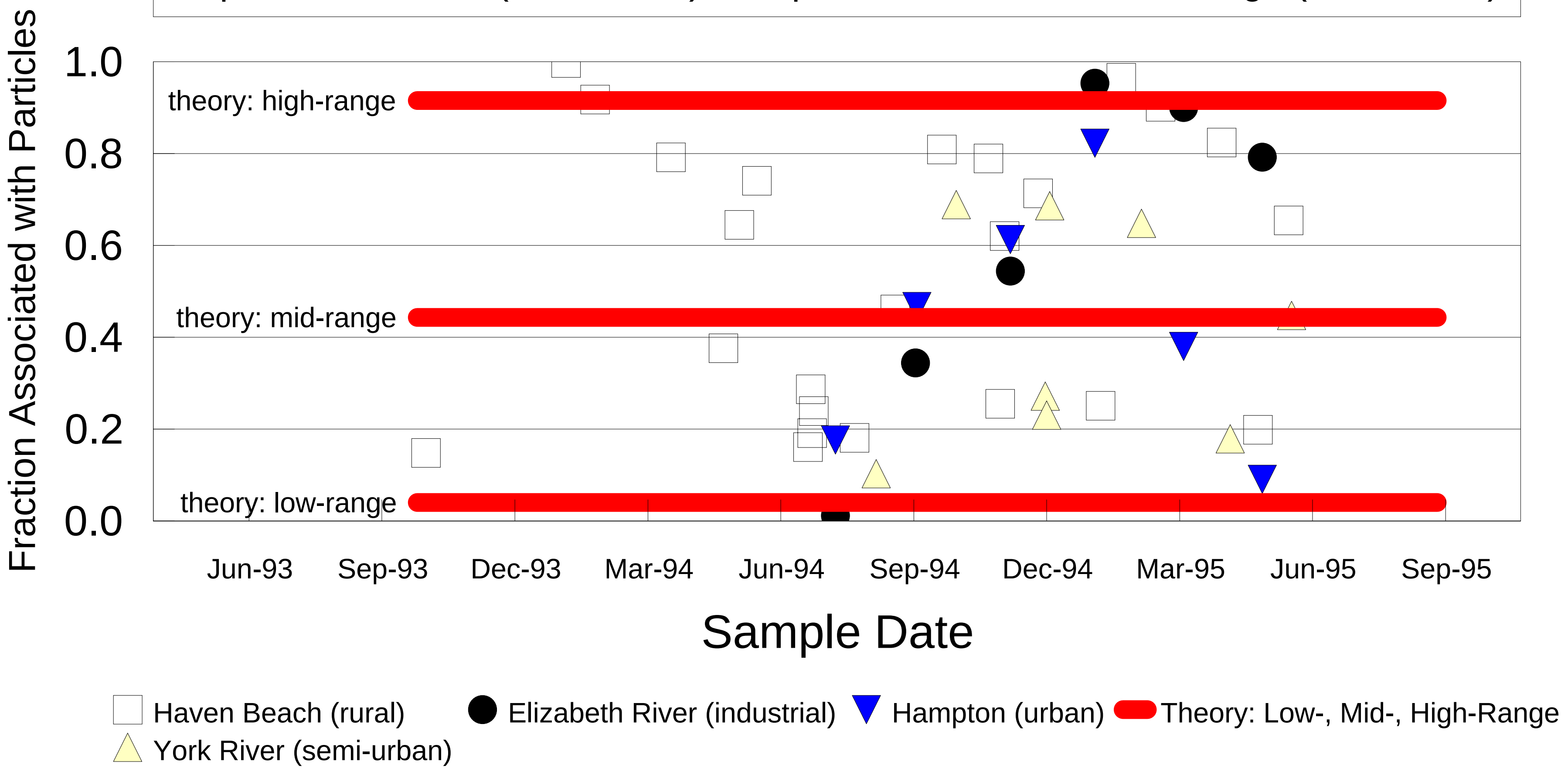
A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(8). Vapor/Particle Partitioning for PAH's: BENZO(a)ANTHRACENE
Experimental Data (see note A) Compared with Theoretical Range (see note B)



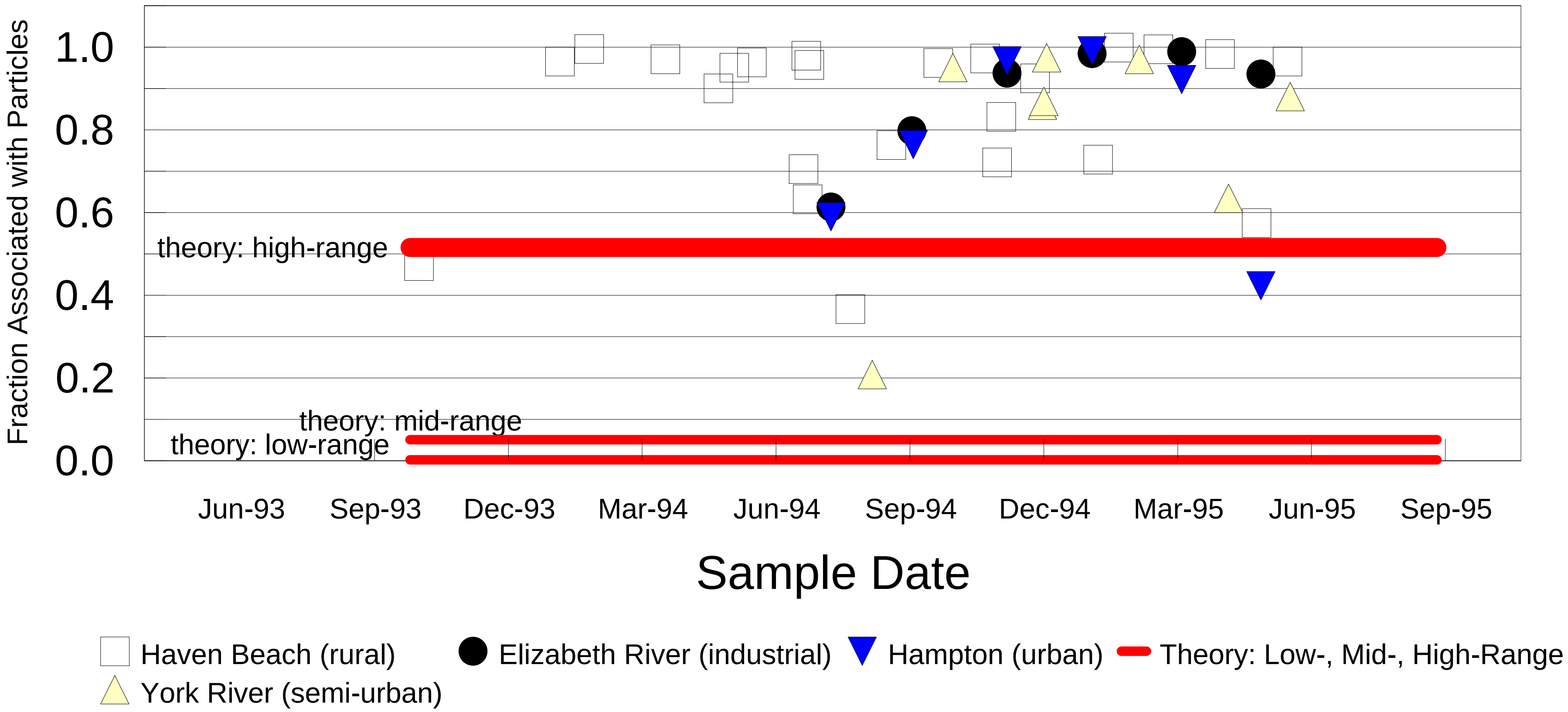
A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(9). Vapor/Particle Partitioning for PAH's: CHRYSENE
Experimental Data (see note A) Compared with Theoretical Range (see note B)



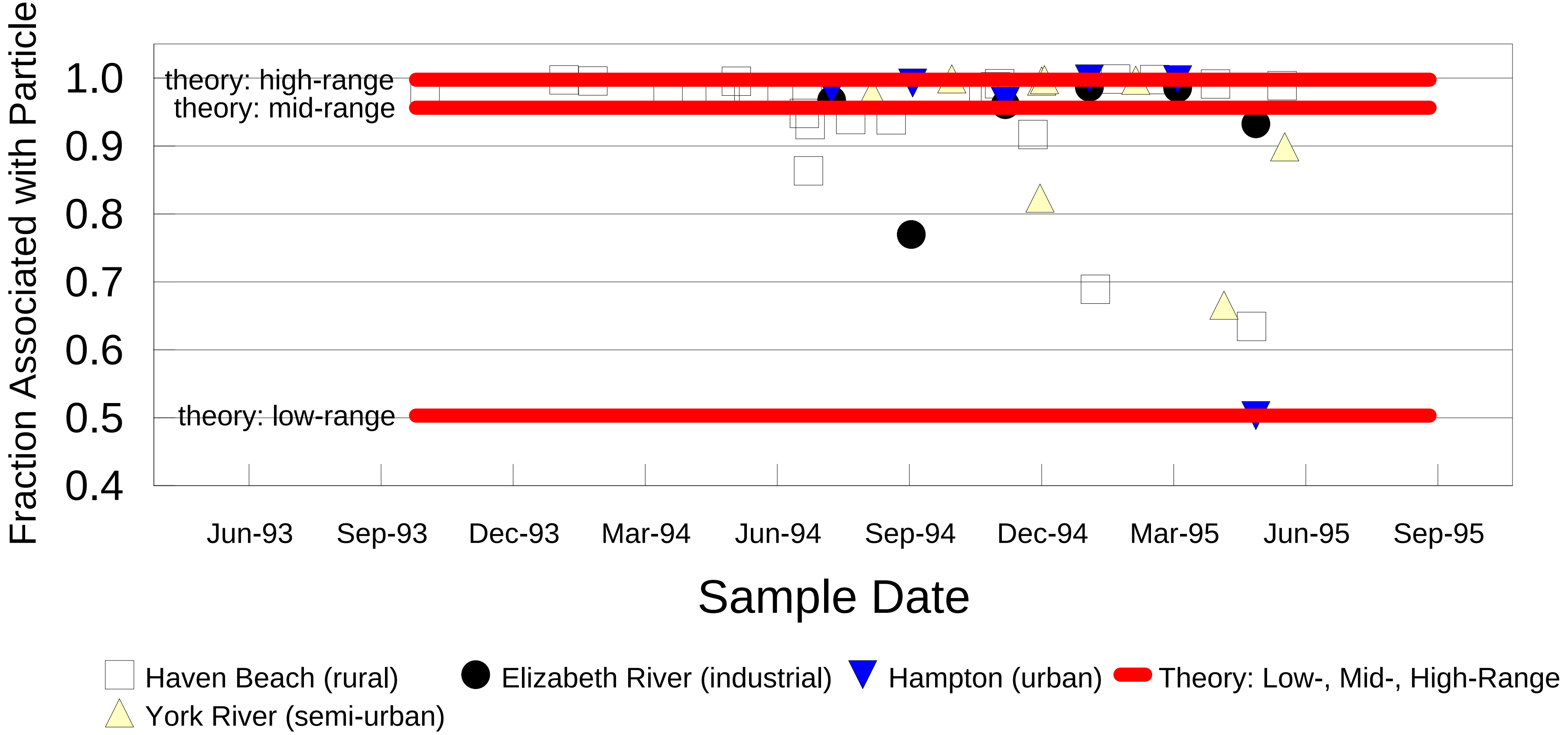
A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(10). Vapor/Particle Partitioning for PAH's: BENZO(b)FLUORANTHENE
Experimental Data (see note A) Compared with Theoretical Range (see note B)



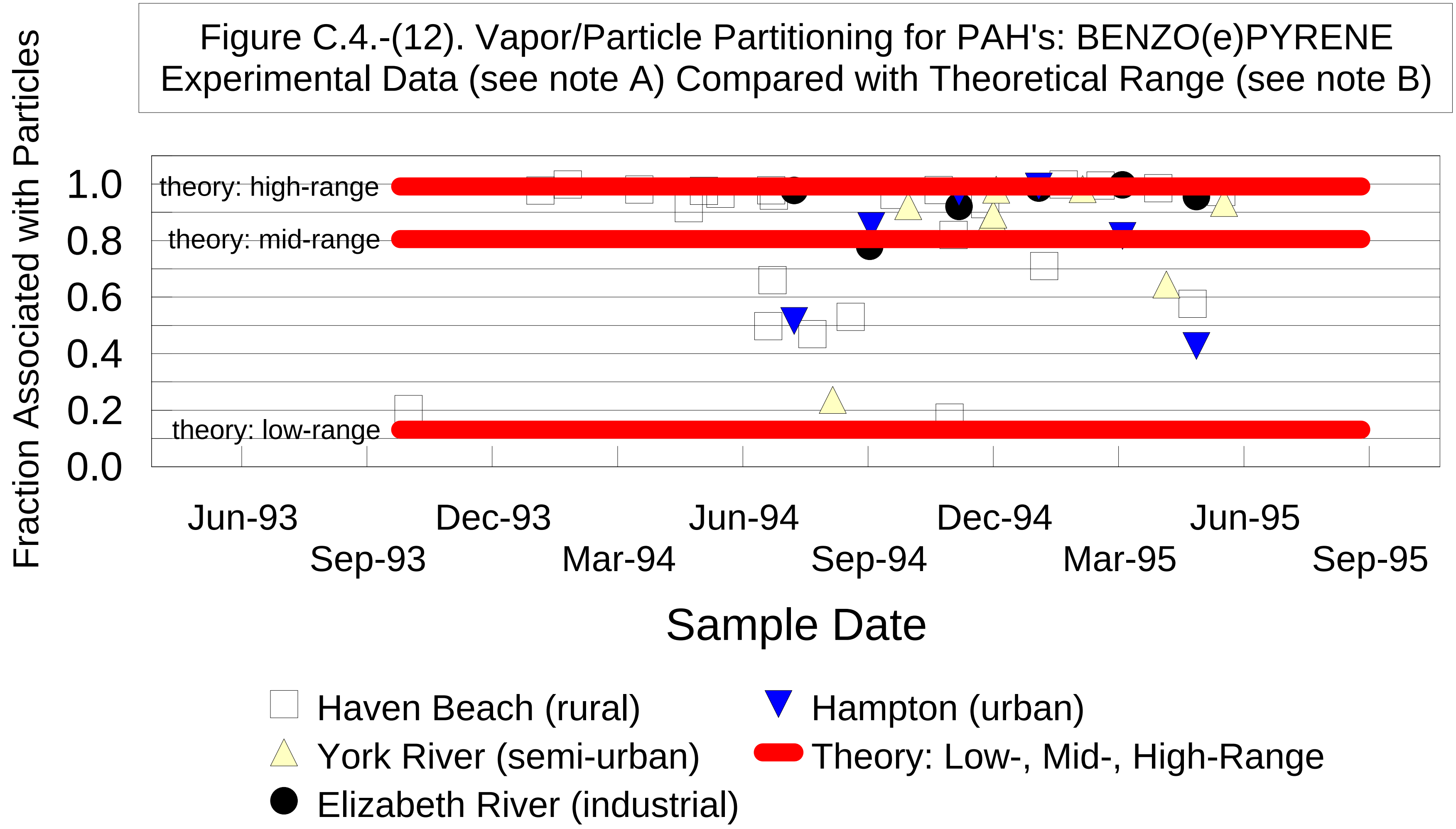
A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(11). Vapor/Particle Partitioning for PAH's: BENZO(k)FLUORANTHENE
Experimental Data (see note A) Compared with Theoretical Range (see note B)



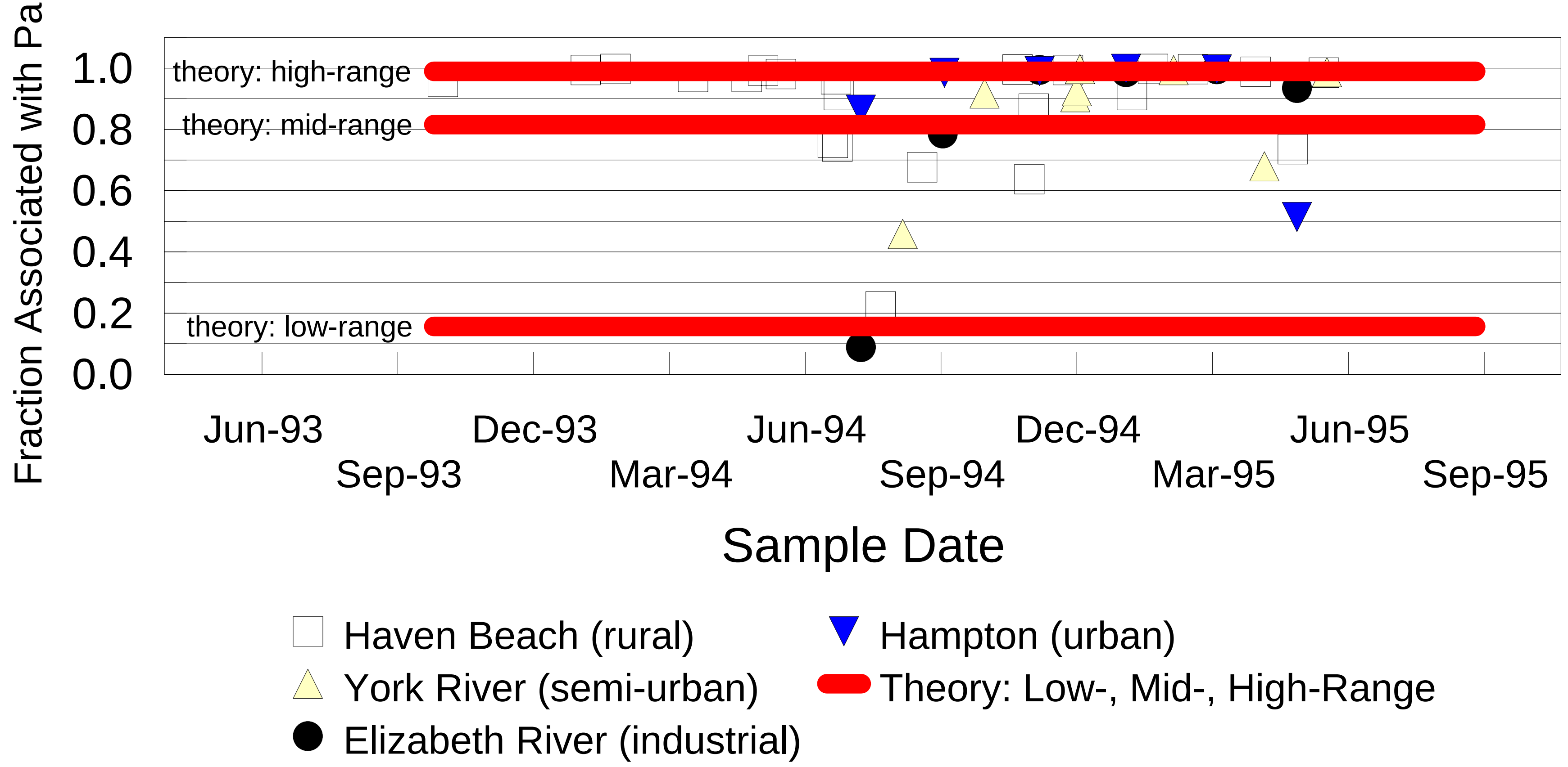
A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(12). Vapor/Particle Partitioning for PAH's: BENZO(e)PYRENE
Experimental Data (see note A) Compared with Theoretical Range (see note B)



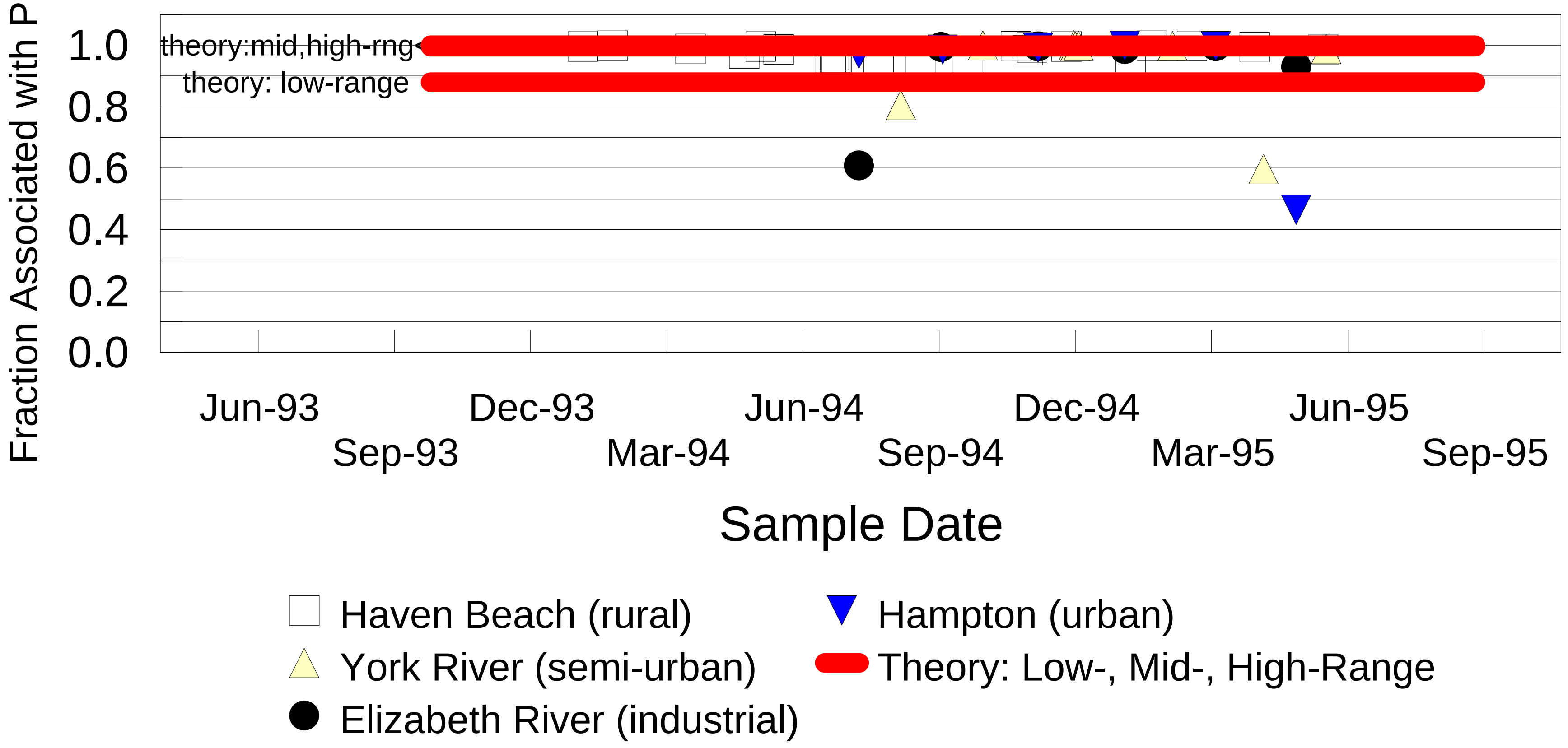
A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(13). Vapor/Particle Partitioning for PAH's: BENZO(a)PYRENE
Experimental Data (see note A) Compared with Theoretical Range (see note B)



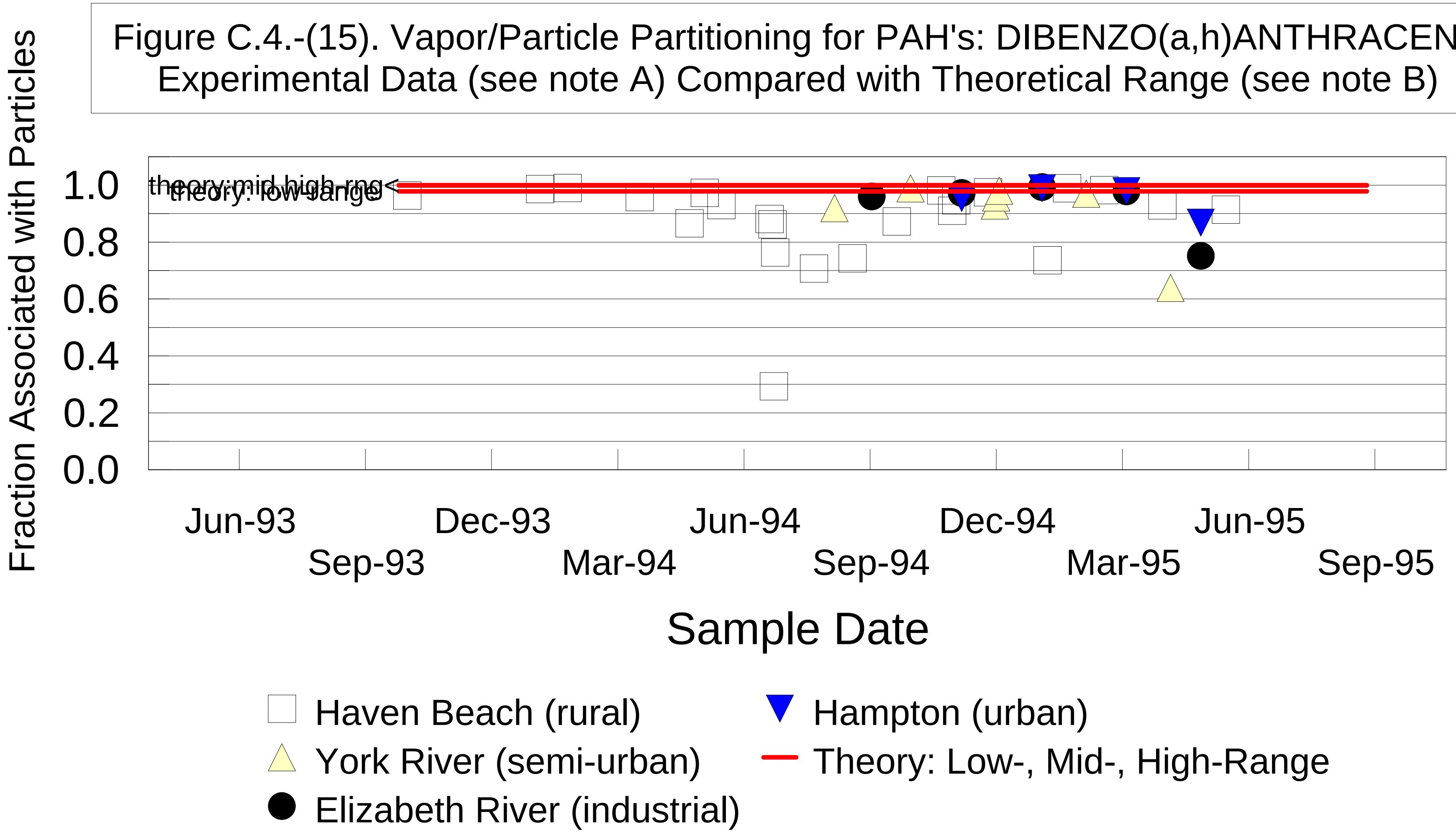
A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(14). Vapor/Particle Partitioning for PAH's: INDENO(1,2,3-cd)PYRENE
Experimental Data (see note A) Compared with Theoretical Range (see note B)



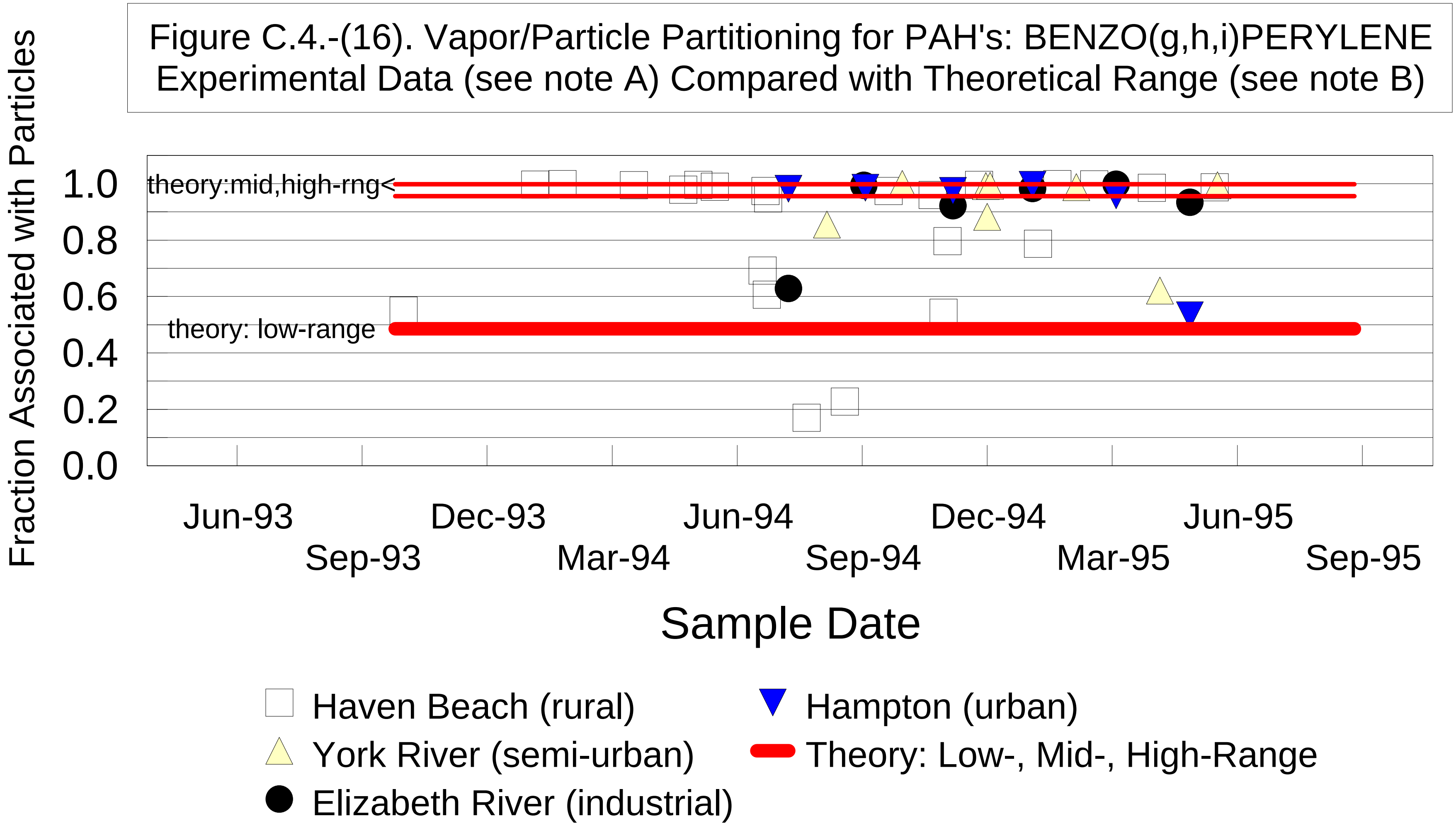
A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(15). Vapor/Particle Partitioning for PAH's: DIBENZO(a,h)ANTHRACENE
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Figure C.4.-(16). Vapor/Particle Partitioning for PAH's: BENZO(g,h,i)PERYLENE
Experimental Data (see note A) Compared with Theoretical Range (see note B)



A: Gustafson & Dickhut, ES&T 31:140-147, 1997 (sample durations 4 - 10 hours)
B: Junge ads. (subcooled liq.Vp); Low:T=310K; Surface Area=4.2e-7cm2/cm3;
Mid:290K, Surface Area=3.5e-6cm2/cm3; High:260K, Surface Area=1.1e-5cm2/cm3

Data from Gustafson and Dickhut (1997)

value to use for ND =		HAVEN		HAVEN		HAVEN		HAVEN		HAVEN
0.3		BEACH		BEACH		BEACH		BEACH		BEACH
pg/m3 (avg value per article)		07-Oct-93		11-Jan-94		31-Jan-94		24-Mar-94		29-Apr-94
	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase
fluorene	1	2398.91	1	2446.07	1	3052.15	1	663.91	1	482.43
phenanthrene	1	5617.75	1	3579.03	1	6900.56	1	1729.54	1	3395.83
anthracene	0	**0.30**	0	**0.30**	1	292.84	0	**0.30**	0	**0.30**
fluoranthene	1	651.16	1	588.62	1	599.5	1	354.95	1	535.75
pyrene	1	942.49	1	449.17	1	396.3	1	339.36	1	967.82
benzo(a)anthracene	0	**0.30**	1	10.64	0	**0.30**	0	**0.30**	0	**0.30**
chrysene	1	74.04	0	**0.30**	1	22.9	1	22.77	1	32.85
benzo(b)flouranthene	1	17.18	1	4.24	1	1.2	1	2.2	1	2.13
benzo(k)flouranthene	0	**0.30**	0	**0.30**	1	1	1	1.16	0	**0.30**
benzo(e)pyrene	1	40.57	1	2.46	0	**0.30**	1	1.34	1	1.53
benzo(a)pyrene	0	**0.30**	0	**0.30**	0	**0.30**	1	0.61	0	**0.30**
indeno(123cd)pyrene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
dibenzo(ah)anthracene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
benzo(ghi)perylene	1	10.20	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase
fluorene	1	7.279	1	8.361	1	8.990	1	6.807	1	3.358
phenanthrene	1	32.437	1	108.962	1	154.465	1	50.010	1	28.969
anthracene	1	3.089	1	6.593	1	11.264	1	4.416	1	3.121
fluoranthene	1	13.244	1	136.943	1	227.957	1	37.798	1	26.550
pyrene	1	17.210	1	108.713	1	199.634	1	37.086	1	24.577
benzo(a)anthracene	1	12.815	1	39.680	1	108.298	1	21.455	1	7.818
chrysene	1	12.946	1	138.436	1	258.172	1	86.925	1	19.842
benzo(b)flouranthene	1	15.293	1	118.607	1	282.670	1	72.587	1	19.305
benzo(k)flouranthene	1	10.571	1	122.957	1	252.678	1	45.599	1	13.927
benzo(e)pyrene	1	10.413	1	106.646	1	229.789	1	69.987	1	16.523
benzo(a)pyrene	1	6.477	1	48.973	1	170.597	1	21.270	1	10.353
indeno(123cd)pyrene	0	**0.300**	1	85.299	1	205.855	1	25.445	1	11.243
dibenzo(ah)anthracene	1	8.099	1	21.744	1	31.646	1	6.850	1	1.942
benzo(ghi)perylene	1	12.488	1	97.422	1	223.031	1	65.399	1	14.442
		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase
fluorene	**=**	0.00303	**=**	0.00341	**=**	0.00294	**=**	0.01015	**=**	0.00691
phenanthrene	**=**	0.00574	**=**	0.02955	**=**	0.02189	**=**	0.02810	**=**	0.00846
anthracene	**>**	0.91148	**>**	0.95648	**=**	0.03704	**>**	0.93639	**>**	0.91231
fluoranthene	**=**	0.01993	**=**	0.18874	**=**	0.27549	**=**	0.09624	**=**	0.04722
pyrene	**=**	0.01793	**=**	0.19487	**=**	0.33499	**=**	0.09852	**=**	0.02477
benzo(a)anthracene	**>**	0.97713	**=**	0.78855	**>**	0.99724	**>**	0.98621	**>**	0.96305
chrysene	**=**	0.14883	**>**	0.99784	**=**	0.91853	**=**	0.79242	**=**	0.37657
benzo(b)flouranthene	**=**	0.47095	**=**	0.96549	**=**	0.99577	**=**	0.97058	**=**	0.90063
benzo(k)flouranthene	**>**	0.97240	**>**	0.99757	**=**	0.99606	**=**	0.97519	**>**	0.97891
benzo(e)pyrene	**=**	0.20424	**=**	0.97745	**>**	0.99870	**=**	0.98121	**=**	0.91525
benzo(a)pyrene	**>**	0.95573	**>**	0.99391	**>**	0.99824	**=**	0.97212	**>**	0.97184
indeno(123cd)pyrene	**na**		**>**	0.99650	**>**	0.99854	**>**	0.98835	**>**	0.97401
dibenzo(ah)anthracene	**>**	0.96428	**>**	0.98639	**>**	0.99061	**>**	0.95804	**>**	0.86619
benzo(ghi)perylene	**=**	0.55042	**>**	0.99693	**>**	0.99866	**>**	0.99543	**>**	0.97965

Table C.4.(3)

Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =		HAVEN		HAVEN		HAVEN		HAVEN		HAVEN
0.3		BEACH		BEACH		BEACH		BEACH		BEACH
pg/m3 (avg value per article)		30-Jun-94		28-Jul-94		25-Aug-94		26-Sep-94		28-Oct-94
	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase
fluorene	1	255.82	1	729.39	1	224.33	1	782.74	1	942.47
phenanthrene	1	2748.83	1	4784.67	1	1291.99	1	1076.28	1	1936.58
anthracene	1	69.31	1	83.91	1	21.54	nq		0	**0.30**
fluoranthene	1	430.2	1	577.14	1	167.59	1	97.98	1	433.65
pyrene	1	650.56	1	902.11	1	308.32	1	160.98	1	519.49
benzo(a)anthracene	0	**0.30**	0	**0.30**	0	**0.30**	nq		1	13.2
chrysene	1	27.9	1	33.76	1	13.27	1	7.87	1	110.02
benzo(b)flouranthene	0	**0.30**	1	13.64	1	3.23	1	2.49	1	9.05
benzo(k)flouranthene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	1	4.62
benzo(e)pyrene	0	**0.30**	1	9.97	1	7.37	1	1.41	1	5.37
benzo(a)pyrene	0	**0.30**	1	6.36	1	1.38	nq		0	**0.30**
indeno(123cd)pyrene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
dibenzo(ah)anthracene	0	**0.30**	0	**0.30**	1	0.6	0	**0.30**	0	**0.30**
benzo(ghi)perylene	0	**0.30**	1	32.31	1	19.8	0	**0.30**	1	5.62
	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase
fluorene	1	2.520	1	2.436	1	2.281	1	9.816	1	15.901
phenanthrene	1	16.787	1	17.870	1	17.097	1	48.746	1	205.168
anthracene	1	1.101	1	0.990	1	0.897	0	**0.300**	1	7.473
fluoranthene	1	16.545	1	12.081	1	14.457	1	20.149	1	152.213
pyrene	1	12.086	1	14.003	1	16.662	1	25.512	1	149.591
benzo(a)anthracene	1	3.055	0	**0.300**	1	2.653	0	**0.300**	1	56.979
chrysene	1	8.801	1	7.491	1	11.349	1	33.383	1	413.691
benzo(b)flouranthene	1	6.748	1	7.901	1	10.434	1	63.298	1	322.224
benzo(k)flouranthene	1	4.109	1	4.636	1	4.598	0	**0.300**	1	222.406
benzo(e)pyrene	1	7.023	1	8.826	1	8.345	1	35.634	1	254.591
benzo(a)pyrene	1	3.117	1	1.822	1	2.883	1	4.693	1	81.514
indeno(123cd)pyrene	1	4.319	1	3.398	1	5.657	1	7.004	1	116.552
dibenzo(ah)anthracene	1	0.973	1	0.726	1	1.739	1	2.057	1	16.395
benzo(ghi)perylene	1	5.510	1	6.661	1	5.848	1	11.527	1	135.948
		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase
fluorene	**=**	0.00975	**=**	0.00333	**=**	0.01007	**=**	0.01239	**=**	0.01659
phenanthrene	**=**	0.00607	**=**	0.00372	**=**	0.01306	**=**	0.04333	**=**	0.09579
anthracene	**=**	0.01564	**=**	0.01166	**=**	0.03998	**na**		**>**	0.96140
fluoranthene	**=**	0.03703	**=**	0.02050	**=**	0.07941	**=**	0.17057	**=**	0.25981
pyrene	**=**	0.01824	**=**	0.01529	**=**	0.05127	**=**	0.13680	**=**	0.22358
benzo(a)anthracene	**>**	0.91058	**na**		**>**	0.89841	**na**		**=**	0.81191
chrysene	**=**	0.23980	**=**	0.18160	**=**	0.46099	**=**	0.80923	**=**	0.78992
benzo(b)flouranthene	**>**	0.95743	**=**	0.36679	**=**	0.76361	**=**	0.96215	**=**	0.97268
benzo(k)flouranthene	**>**	0.93196	**>**	0.93922	**>**	0.93875	**na**		**=**	0.97965
benzo(e)pyrene	**>**	0.95903	**=**	0.46957	**=**	0.53102	**=**	0.96194	**=**	0.97934
benzo(a)pyrene	**>**	0.91220	**=**	0.22268	**=**	0.67628	**NQ**		**>**	0.99633
indeno(123cd)pyrene	**>**	0.93505	**>**	0.91888	**>**	0.94964	**>**	0.95893	**>**	0.99743
dibenzo(ah)anthracene	**>**	0.76434	**>**	0.70760	**=**	0.74348	**>**	0.87272	**>**	0.98203
benzo(ghi)perylene	**>**	0.94836	**=**	0.17092	**=**	0.22801	**>**	0.97463	**=**	0.96030

Table C.4.(3)

Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =		HAVEN		HAVEN		HAVEN		HAVEN		HAVEN
0.3		BEACH		BEACH		BEACH		BEACH		BEACH
pg/m3 (avg value per article)		01-Dec-94		13-Jan-95		27-Jan-95		23-Feb-95		06-Apr-95
	detect?	pg/m3 gas phase	detect?	pg/m3 gas phase	detect?	pg/m3 gas phase	detect?	pg/m3 gas phase	detect?	pg/m3 gas phase
fluorene	1	961.19	1	1277.53	1	1919.33	1	1813.15	1	1038.75
phenanthrene	1	523.98	1	2329.37	1	2199.9	1	1843.46	1	901.1
anthracene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
fluoranthene	1	114.18	1	359.29	1	323.17	1	507.26	1	190.4
pyrene	1	62.88	1	417.78	1	169.11	1	198.26	1	100.65
benzo(a)anthracene	1	6.56	1	3.3	0	**0.30**	0	**0.30**	0	**0.30**
chrysene	1	28.86	1	34.48	1	7.15	1	16.89	1	16.44
benzo(b)flouranthene	1	9.47	1	3.36	0	**0.30**	1	0.93	1	1.7
benzo(k)flouranthene	1	7.91	1	2.81	0	**0.30**	0	**0.30**	1	0.62
benzo(e)pyrene	1	6.18	1	2.58	0	**0.30**	1	0.58	1	1.02
benzo(a)pyrene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
indeno(123cd)pyrene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
dibenzo(ah)anthracene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
benzo(ghi)perylene	0	**0.30**	1	1.84	0	**0.30**	0	**0.30**	1	0.8
	detect?	pg/m3 particle phase	detect?	pg/m3 particle phase	detect?	pg/m3 particle phase	detect?	pg/m3 particle phase	detect?	pg/m3 particle phase
fluorene	1	3.750	nq		1	9.890	1	12.044	1	4.768
phenanthrene	1	59.855	1	10.499	1	124.374	1	173.210	1	48.086
anthracene	1	4.305	0	**0.300**	1	7.309	1	8.167	0	**0.300**
fluoranthene	1	90.511	1	7.555	1	202.873	1	218.824	1	96.263
pyrene	1	67.363	1	7.530	1	166.673	1	153.065	1	60.623
benzo(a)anthracene	1	31.850	0	**0.300**	1	84.251	1	53.118	1	13.286
chrysene	1	72.050	1	11.572	1	201.870	1	156.003	1	77.419
benzo(b)flouranthene	1	116.755	1	8.993	1	306.389	1	190.353	1	102.188
benzo(k)flouranthene	1	87.332	1	6.237	1	265.667	1	151.233	1	72.411
benzo(e)pyrene	1	81.282	1	6.313	1	213.795	1	128.535	1	71.228
benzo(a)pyrene	1	55.222	1	3.113	1	174.100	1	100.862	1	26.738
indeno(123cd)pyrene	1	83.171	1	5.766	1	229.410	1	127.890	1	48.807
dibenzo(ah)anthracene	1	11.719	1	0.838	1	28.642	1	16.986	1	3.975
benzo(ghi)perylene	1	79.027	1	6.818	1	220.831	1	131.981	1	56.387
		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase
fluorene	**=**	0.00389	**NQ**		**=**	0.00513	**=**	0.00660	**=**	0.00457
phenanthrene	**=**	0.10252	**=**	0.00449	**=**	0.05351	**=**	0.08589	**=**	0.05066
anthracene	**>**	0.93485	**na**		**>**	0.96057	**>**	0.96457	**na**	
fluoranthene	**=**	0.44218	**=**	0.02059	**=**	0.38566	**=**	0.30138	**=**	0.33581
pyrene	**=**	0.51721	**=**	0.01770	**=**	0.49637	**=**	0.43568	**=**	0.37590
benzo(a)anthracene	**=**	0.82921	**<**	0.08333	**>**	0.99645	**>**	0.99438	**>**	0.97792
chrysene	**=**	0.71400	**=**	0.25128	**=**	0.96579	**=**	0.90231	**=**	0.82484
benzo(b)flouranthene	**=**	0.92498	**=**	0.72800	**>**	0.99902	**=**	0.99514	**=**	0.98364
benzo(k)flouranthene	**=**	0.91695	**=**	0.68940	**>**	0.99887	**>**	0.99802	**=**	0.99151
benzo(e)pyrene	**=**	0.92934	**=**	0.70988	**>**	0.99860	**=**	0.99551	**=**	0.98588
benzo(a)pyrene	**>**	0.99460	**>**	0.91210	**>**	0.99828	**>**	0.99703	**>**	0.98890
indeno(123cd)pyrene	**>**	0.99641	**>**	0.95054	**>**	0.99869	**>**	0.99766	**>**	0.99389
dibenzo(ah)anthracene	**>**	0.97504	**>**	0.73638	**>**	0.98963	**>**	0.98264	**>**	0.92982
benzo(ghi)perylene	**>**	0.99622	**=**	0.78748	**>**	0.99864	**>**	0.99773	**=**	0.98601

Table C.4.(3)

Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =		HAVEN		HAVEN		YORK		YORK		YORK
0.3		BEACH		BEACH		RIVER		RIVER		RIVER
pg/m3 (avg value per article)		01-May-95		22-May-95		12-Aug-94		06-Oct-94		06-Dec-94
	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase
fluorene	1	487.27	1	390.6	1	4764.90	1	9638.81	1	15377.24
phenanthrene	1	516.14	1	1083.27	1	65243.00	1	21219.87	1	28183.18
anthracene	0	**0.30**	1	36.96	1	3234.85	1	1153.42	1	2424.90
fluoranthene	1	116.97	1	412.89	1	8056.13	1	3992.61	1	5338.88
pyrene	1	82.25	1	307.88	1	3067.21	1	1826.02	1	2631.84
benzo(a)anthracene	0	**0.30**	0	**0.30**	1	48.36	1	30.14	1	182.93
chrysene	1	8.91	1	19.96	1	157.35	1	75.03	1	364.72
benzo(b)flouranthene	1	1.45	1	1.4	1	67.52	1	15.15	1	63.36
benzo(k)flouranthene	1	0.8	0	**0.30**	0	**0.30**	0	**0.30**	1	71.35
benzo(e)pyrene	1	0.93	1	0.75	1	25.21	1	19.83	1	47.96
benzo(a)pyrene	0	**0.30**	0	**0.30**	1	8.68	1	11.30	1	14.57
indeno(123cd)pyrene	0	**0.30**	0	**0.30**	1	4.94	0	**0.30**	0	**0.30**
dibenzo(ah)anthracene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	1	2.81
benzo(ghi)perylene	0	**0.30**	0	**0.30**	1	5.00	0	**0.30**	1	6.44

	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase
fluorene	nq		1	3.558	1	4.001	1	33.787	1	13.905
phenanthrene	nq		1	31.549	1	29.484	1	282.348	1	108.587
anthracene	0	**0.300**	1	2.604	1	3.115	1	19.191	1	13.905
fluoranthene	1	2.335	1	49.257	1	32.765	1	203.452	1	98.235
pyrene	1	1.512	1	36.161	1	20.058	1	157.649	1	94.720
benzo(a)anthracene	1	1.627	1	12.328	1	6.518	1	75.405	1	62.300
chrysene	1	2.211	1	37.856	1	18.034	1	166.363	1	136.365
benzo(b)flouranthene	1	1.962	1	38.805	1	17.752	1	292.194	1	386.033
benzo(k)flouranthene	1	1.390	1	27.149	1	12.714	1	221.273	1	332.469
benzo(e)pyrene	1	1.266	1	26.320	1	7.795	1	234.671	1	358.517
benzo(a)pyrene	1	0.833	1	20.766	1	7.353	1	125.562	1	138.628
indeno(123cd)pyrene	0	**0.300**	1	21.473	1	20.425	1	196.521	1	584.253
dibenzo(ah)anthracene	0	**0.300**	1	3.197	1	3.407	1	25.043	1	36.655
benzo(ghi)perylene	0	**0.300**	1	24.121	1	29.530	1	261.975	1	746.305

		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase
fluorene	**NQ**		**=**	0.00903	**=**	0.00084	**=**	0.00349	**=**	0.00090
phenanthrene	**NQ**		**=**	0.02830	**=**	0.00045	**=**	0.01313	**=**	0.00384
anthracene	**na**		**=**	0.06582	**=**	0.00096	**=**	0.01637	**=**	0.00570
fluoranthene	**=**	0.01957	**=**	0.10658	**=**	0.00405	**=**	0.04849	**=**	0.01807
pyrene	**=**	0.01805	**=**	0.10511	**=**	0.00650	**=**	0.07947	**=**	0.03474
benzo(a)anthracene	**>**	0.84432	**>**	0.97624	**=**	0.11877	**=**	0.71443	**=**	0.25405
chrysene	**=**	0.19881	**=**	0.65477	**=**	0.10283	**=**	0.68918	**=**	0.27214
benzo(b)flouranthene	**=**	0.57503	**=**	0.96518	**=**	0.20818	**=**	0.95071	**=**	0.85901
benzo(k)flouranthene	**=**	0.63470	**>**	0.98907	**>**	0.97695	**>**	0.99865	**=**	0.82331
benzo(e)pyrene	**=**	0.57650	**=**	0.97229	**=**	0.23618	**=**	0.92208	**=**	0.88201
benzo(a)pyrene	**>**	0.73522	**>**	0.98576	**=**	0.45862	**=**	0.91744	**=**	0.90489
indeno(123cd)pyrene	**na**		**>**	0.98622	**=**	0.80524	**>**	0.99848	**>**	0.99949
dibenzo(ah)anthracene	**na**		**>**	0.91421	**>**	0.91907	**>**	0.98816	**=**	0.92880
benzo(ghi)perylene	**na**		**>**	0.98772	**=**	0.85520	**>**	0.99886	**=**	0.99144

Data from Gustafson and Dickhut (1997)

value to use for ND =		YORK		YORK		YORK		YORK		YORK
0.3		RIVER		RIVER		RIVER		RIVER		RIVER
pg/m3 (avg value per article)		07-Dec-94		09-Dec-94		10-Feb-95		12-Apr-95		24-May-95
	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase
fluorene	1	9000.11	1	3885.72	1	5714.64	1	6557.20	1	16420.99
phenanthrene	1	21384.75	1	8782.73	1	5925.09	1	16133.94	1	31113.35
anthracene	1	932.55	1	317.48	1	151.80	1	267.26	1	595.91
fluoranthene	1	5795.52	1	1438.16	1	1488.32	1	2189.64	1	5019.09
pyrene	1	2350.18	1	978.73	1	506.78	1	785.96	1	1467.32
benzo(a)anthracene	1	38.96	1	12.89	0	**0.30**	1	8.00	1	18.34
chrysene	1	177.40	1	71.57	1	47.42	1	64.50	1	97.85
benzo(b)flouranthene	1	12.07	1	4.42	1	3.63	1	7.76	1	6.97
benzo(k)flouranthene	0	**0.30**	0	**0.30**	0	**0.30**	1	4.86	1	3.29
benzo(e)pyrene	1	7.89	1	2.74	1	1.41	1	5.06	1	4.34
benzo(a)pyrene	1	3.04	0	**0.30**	0	**0.30**	1	2.88	0	**0.30**
indeno(123cd)pyrene	0	**0.30**	0	**0.30**	0	**0.30**	1	4.85	0	**0.30**
dibenzo(ah)anthracene	0	**0.30**	0	**0.30**	0	**0.30**	1	0.95	0	**0.30**
benzo(ghi)perylene	1	12.11	1	1.39	1	1.10	1	5.27	0	**0.30**
	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase
fluorene	1	4.910	1	7.030	1	4.495	nq		1	15.278
phenanthrene	1	51.958	1	86.516	1	65.786	1	19.892	1	82.177
anthracene	1	3.334	1	6.543	1	4.162	1	1.063	1	6.277
fluoranthene	1	55.919	1	135.613	1	119.632	1	24.635	1	105.852
pyrene	1	43.647	1	126.910	1	86.654	1	15.626	1	109.704
benzo(a)anthracene	1	20.143	1	56.771	1	26.381	1	5.199	0	**0.30**
chrysene	1	53.127	1	156.929	1	87.392	1	14.094	1	79.359
benzo(b)flouranthene	1	80.040	1	165.008	1	116.123	1	13.453	1	51.104
benzo(k)flouranthene	1	66.081	1	131.444	1	85.991	1	9.678	1	29.249
benzo(e)pyrene	1	64.860	1	133.200	1	77.324	1	9.171	1	60.762
benzo(a)pyrene	1	37.374	1	89.722	1	41.656	1	6.098	1	22.264
indeno(123cd)pyrene	1	75.998	1	139.859	1	88.177	1	7.172	1	24.444
dibenzo(ah)anthracene	1	6.635	1	14.765	1	9.574	1	1.682	0	**0.30**
benzo(ghi)perylene	1	90.836	1	186.523	1	88.744	1	8.638	1	48.817
		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase
fluorene	**=**	0.00055	**=**	0.00181	**=**	0.00079	**NQ**		**=**	0.00093
phenanthrene	**=**	0.00242	**=**	0.00975	**=**	0.01098	**=**	0.00123	**=**	0.00263
anthracene	**=**	0.00356	**=**	0.02019	**=**	0.02669	**=**	0.00396	**=**	0.01042
fluoranthene	**=**	0.00956	**=**	0.08617	**=**	0.07440	**=**	0.01113	**=**	0.02065
pyrene	**=**	0.01823	**=**	0.11478	**=**	0.14602	**=**	0.01949	**=**	0.06956
benzo(a)anthracene	**=**	0.34081	**=**	0.81496	**>**	0.98876	**=**	0.39389	**<**	0.01609
chrysene	**=**	0.23046	**=**	0.68678	**=**	0.64825	**=**	0.17933	**=**	0.44783
benzo(b)flouranthene	**=**	0.86896	**=**	0.97391	**=**	0.96969	**=**	0.63419	**=**	0.87998
benzo(k)flouranthene	**>**	0.99548	**>**	0.99772	**>**	0.99652	**=**	0.66570	**=**	0.89889
benzo(e)pyrene	**=**	0.89155	**=**	0.97984	**=**	0.98209	**=**	0.64444	**=**	0.93334
benzo(a)pyrene	**=**	0.92478	**>**	0.99667	**>**	0.99285	**=**	0.67922	**>**	0.98670
indeno(123cd)pyrene	**>**	0.99607	**>**	0.99786	**>**	0.99661	**=**	0.59657	**>**	0.98788
dibenzo(ah)anthracene	**>**	0.95674	**>**	0.98009	**>**	0.96962	**=**	0.63906	**na**	
benzo(ghi)perylene	**=**	0.88237	**=**	0.99260	**=**	0.98776	**=**	0.62108	**>**	0.99389

Table C.4.(3)

Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =		HAVEN		HAVEN		HAVEN		HAVEN		HAVEN
0.3		BEACH		BEACH		BEACH		BEACH		BEACH
pg/m3 (avg value per article)		10-May-94		22-May-94		26-Jun-94		28-Jun-94		29-Jun-94
	det-	pg/m3	det-	pg/m3	det-	pg/m3	det-	pg/m3	det-	pg/m3
	ect?	gas phase	ect?	gas phase	ect?	gas phase	ect?	gas phase	ect?	gas phase
fluorene	1	731.33	1	671.62	1	439.96	1	725.87	1	376.65
phenanthrene	1	1914.11	1	1718.83	1	3711.71	1	4227.41	1	3688.97
anthracene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	1	54.50
fluoranthene	1	353.22	1	305.98	1	416.55	1	630.83	1	492.20
pyrene	1	451.54	1	277.54	1	512.98	1	984.84	1	556.21
benzo(a)anthracene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
chrysene	1	25.69	1	12.80	1	42.71	1	41.60	1	39.90
benzo(b)flouranthene	1	4.36	1	1.34	1	3.32	0	**0.30**	1	5.30
benzo(k)flouranthene	0	**0.30**	1	0.62	0	**0.30**	0	**0.30**	1	1.47
benzo(e)pyrene	1	1.89	1	1.01	1	7.76	0	**0.30**	1	4.56
benzo(a)pyrene	0	**0.30**	0	**0.30**	1	1.16	0	**0.30**	1	1.53
indeno(123cd)pyrene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
dibenzo(ah)anthracene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	1	3.40
benzo(ghi)perylene	0	**0.30**	0	**0.30**	1	3.02	0	**0.30**	1	5.58
	det-	pg/m3	det-	pg/m3	det-	pg/m3	det-	pg/m3	det-	pg/m3
	ect?	particle phase	ect?	particle phase	ect?	particle phase	ect?	particle phase	ect?	particle phase
fluorene	1	4.757	1	3.302	1	2.340	1	3.339	1	1.548
phenanthrene	1	42.833	1	32.010	1	14.953	1	28.781	1	13.196
anthracene	1	4.703	1	2.802	1	1.237	1	2.821	1	1.173
fluoranthene	1	47.474	1	43.728	1	11.406	1	25.359	1	13.055
pyrene	1	40.760	1	35.818	1	9.524	1	22.778	1	9.644
benzo(a)anthracene	1	17.539	1	13.286	1	3.207	1	7.948	1	3.939
chrysene	1	46.751	1	36.720	1	8.227	1	16.748	1	9.475
benzo(b)flouranthene	1	83.156	1	35.105	1	7.937	1	14.150	1	9.124
benzo(k)flouranthene	1	69.140	1	24.431	1	5.506	1	10.290	1	9.324
benzo(e)pyrene	1	77.831	1	28.713	1	7.703	1	13.321	1	8.852
benzo(a)pyrene	1	39.360	1	15.296	1	3.595	1	8.134	1	4.451
indeno(123cd)pyrene	1	74.710	1	22.485	1	5.415	1	9.151	1	7.155
dibenzo(ah)anthracene	1	10.876	1	3.980	1	2.228	1	1.881	1	1.416
benzo(ghi)perylene	1	81.975	1	28.505	1	6.813	1	11.433	1	8.606
		fraction in		fraction in		fraction in		fraction in		fraction in
		particle phase		particle phase		particle phase		particle phase		particle phase
fluorene	**=**	0.00646	**=**	0.00489	**=**	0.00529	**=**	0.00458	**=**	0.00409
phenanthrene	**=**	0.02189	**=**	0.01828	**=**	0.00401	**=**	0.00676	**=**	0.00356
anthracene	**>**	0.94004	**>**	0.90329	**>**	0.80481	**>**	0.90388	**=**	0.02107
fluoranthene	**=**	0.11848	**=**	0.12504	**=**	0.02665	**=**	0.03865	**=**	0.02584
pyrene	**=**	0.08280	**=**	0.11430	**=**	0.01823	**=**	0.02261	**=**	0.01704
benzo(a)anthracene	**>**	0.98318	**>**	0.97792	**>**	0.91446	**>**	0.96363	**>**	0.92923
chrysene	**=**	0.64537	**=**	0.74152	**=**	0.16151	**=**	0.28704	**=**	0.19190
benzo(b)flouranthene	**=**	0.95018	**=**	0.96323	**=**	0.70507	**>**	0.97924	**=**	0.63256
benzo(k)flouranthene	**>**	0.99568	**=**	0.97525	**>**	0.94833	**>**	0.97167	**=**	0.86381
benzo(e)pyrene	**=**	0.97629	**=**	0.96602	**=**	0.49816	**>**	0.97798	**=**	0.66001
benzo(a)pyrene	**>**	0.99244	**>**	0.98076	**=**	0.75605	**>**	0.96443	**=**	0.74419
indeno(123cd)pyrene	**>**	0.99600	**>**	0.98683	**>**	0.94751	**>**	0.96826	**>**	0.95976
dibenzo(ah)anthracene	**>**	0.97316	**>**	0.92991	**>**	0.88133	**>**	0.86245	**=**	0.29402
benzo(ghi)perylene	**>**	0.99635	**>**	0.98959	**=**	0.69287	**>**	0.97443	**=**	0.60665

Data from Gustafson and Dickhut (1997)

value to use for ND =		HAVEN		HAVEN		ELIZABETH		ELIZABETH		ELIZABETH
0.3		BEACH		BEACH		RIVER		RIVER		RIVER
pg/m3 (avg value per article)		05-Nov-94		08-Nov-94		15-Jul-94		08-Sep-94		12-Nov-94
	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase
fluorene	1	799.66	1	1007.10	nq		1	5056.24	1	8333.31
phenanthrene	1	2300.57	1	2518.09	nq		1	17823.32	1	12894.94
anthracene	1	123.35	0	**0.30**	nq		1	869.63	1	281.96
fluoranthene	1	432.38	1	363.83	nq		1	4576.92	1	1794.26
pyrene	1	419.17	1	411.92	nq		1	2524.15	1	1209.90
benzo(a)anthracene	1	9.69	1	9.07	1	284.27	1	29.25	1	10.96
chrysene	1	56.78	1	74.57	1	1812.49	1	141.08	1	68.78
benzo(b)flouranthene	1	11.95	1	13.01	1	10.79	1	19.43	1	5.90
benzo(k)flouranthene	0	**0.30**	0	**0.30**	0	**0.30**	1	17.81	1	2.90
benzo(e)pyrene	1	106.62	1	13.53	0	**0.30**	1	15.73	1	5.63
benzo(a)pyrene	1	4.66	1	3.64	1	66.95	1	9.05	0	**0.30**
indeno(123cd)pyrene	0	**0.30**	0	**0.30**	1	6.84	0	**0.30**	0	**0.30**
dibenzo(ah)anthracene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
benzo(ghi)perylene	1	15.00	1	14.17	1	10.77	0	**0.30**	1	7.57
	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase
fluorene	1	3.446	1	4.684	1	7.020	1	11.013	1	10.203
phenanthrene	1	24.101	1	42.327	1	43.053	1	96.969	1	91.788
anthracene	1	1.559	1	2.432	1	3.340	1	14.045	1	5.202
fluoranthene	1	16.101	1	51.709	1	20.530	1	96.673	1	125.574
pyrene	1	13.809	1	76.827	1	16.898	1	66.061	1	96.971
benzo(a)anthracene	1	6.672	1	52.259	1	6.263	1	25.930	1	29.994
chrysene	1	19.495	1	122.188	1	21.719	1	74.070	1	82.156
benzo(b)flouranthene	1	30.932	1	64.173	1	17.122	1	76.709	1	87.384
benzo(k)flouranthene	1	23.166	1	36.751	1	8.885	1	59.517	1	71.376
benzo(e)pyrene	1	22.596	1	61.696	1	13.190	1	55.687	1	65.189
benzo(a)pyrene	1	8.216	1	23.995	1	6.539	1	33.368	1	48.235
indeno(123cd)pyrene	1	18.009	1	43.548	1	10.645	1	48.811	1	68.601
dibenzo(ah)anthracene	1	3.060	1	5.406	0	**0.30**	1	7.321	1	10.669
benzo(ghi)perylene	1	17.821	1	55.657	1	18.206	1	54.589	1	89.452
		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase
fluorene	**=**	0.00429	**=**	0.00463	**NQ**		**=**	0.00217	**=**	0.00122
phenanthrene	**=**	0.01037	**=**	0.01653	**NQ**		**=**	0.00541	**=**	0.00707
anthracene	**=**	0.01248	**>**	0.89019	**NQ**		**=**	0.01589	**=**	0.01812
fluoranthene	**=**	0.03590	**=**	0.12444	**NQ**		**=**	0.02068	**=**	0.06541
pyrene	**=**	0.03189	**=**	0.15719	**NQ**		**=**	0.02550	**=**	0.07420
benzo(a)anthracene	**=**	0.40777	**=**	0.85211	**=**	0.02156	**=**	0.46992	**=**	0.73238
chrysene	**=**	0.25559	**=**	0.62101	**=**	0.01184	**=**	0.34427	**=**	0.54431
benzo(b)flouranthene	**=**	0.72133	**=**	0.83144	**=**	0.61343	**=**	0.79790	**=**	0.93675
benzo(k)flouranthene	**>**	0.98722	**>**	0.99190	**>**	0.96734	**=**	0.76968	**=**	0.96096
benzo(e)pyrene	**=**	0.17487	**=**	0.82014	**>**	0.97776	**=**	0.77974	**=**	0.92050
benzo(a)pyrene	**=**	0.63809	**=**	0.86828	**=**	0.08898	**=**	0.78665	**>**	0.99382
indeno(123cd)pyrene	**>**	0.98361	**>**	0.99316	**=**	0.60881	**>**	0.99389	**>**	0.99565
dibenzo(ah)anthracene	**>**	0.91071	**>**	0.94742	**na**		**>**	0.96064	**>**	0.97265
benzo(ghi)perylene	**=**	0.54298	**=**	0.79707	**=**	0.62831	**>**	0.99453	**=**	0.92198

Table C.4.(3)

Data from Gustafson and Dickhut (1997)

(supplementary information)

value to use for ND =		ELIZABETH		ELIZABETH		ELIZABETH		HAMPTON		HAMPTON
0.3		RIVER		RIVER		RIVER				
pg/m3 (avg value per article)		09-Jan-95		11-Mar-95		04-May-95		15-Jul-94		09-Sep-94
	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase
fluorene	1	5741.74	1	2788.34	1	11204.46	1	29218.03	1	24670.86
phenanthrene	1	11515.13	1	6013.35	1	25225.86	1	124573.46	1	80242.93
anthracene	1	750.63	1	124.01	1	1042.99	1	6939.02	1	2526.69
fluoranthene	1	1607.14	1	677.71	1	3901.73	1	12854.70	1	4080.84
pyrene	1	1629.53	1	500.74	1	2018.29	1	5559.62	1	1678.95
benzo(a)anthracene	1	12.94	0	**0.30**	1	35.48	1	24.99	1	10.37
chrysene	1	42.42	1	15.07	1	91.78	1	144.95	1	49.05
benzo(b)flouranthene	1	6.92	1	1.77	1	10.47	1	16.31	1	16.60
benzo(k)flouranthene	1	4.53	1	1.74	1	6.60	0	**0.30**	0	**0.30**
benzo(e)pyrene	1	5.76	0	**0.30**	1	5.67	1	15.56	1	6.76
benzo(a)pyrene	1	3.71	0	**0.30**	1	4.17	1	1.55	0	**0.30**
indeno(123cd)pyrene	1	4.72	0	**0.30**	1	6.62	0	**0.30**	0	**0.30**
dibenzo(ah)anthracene	0	**0.30**	0	**0.30**	1	9.77	0	**0.30**	0	**0.30**
benzo(ghi)perylene	1	8.93	0	**0.30**	1	10.07	0	**0.30**	0	**0.30**
	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase
fluorene	1	20.671	1	8.870	1	14.098	1	11.708	1	21.773
phenanthrene	1	302.056	1	169.838	1	130.250	1	70.994	1	155.231
anthracene	1	36.721	1	8.170	1	8.561	1	5.270	1	15.271
fluoranthene	1	533.524	1	205.687	1	229.606	1	57.130	1	89.400
pyrene	1	631.710	1	142.532	1	184.695	1	34.809	1	87.818
benzo(a)anthracene	1	200.210	1	52.584	1	59.183	1	10.268	1	13.121
chrysene	1	864.645	1	136.250	1	350.255	1	31.083	1	43.043
benzo(b)flouranthene	1	433.885	1	155.686	1	150.210	1	23.428	1	53.833
benzo(k)flouranthene	1	332.971	1	117.906	1	91.493	1	16.209	1	41.084
benzo(e)pyrene	1	387.036	1	107.813	1	122.232	1	16.592	1	38.778
benzo(a)pyrene	1	271.294	1	81.861	1	60.028	1	9.910	1	19.241
indeno(123cd)pyrene	1	365.048	1	116.611	1	88.778	1	10.125	1	20.923
dibenzo(ah)anthracene	1	43.623	1	13.676	1	29.596	0	**0.30**	0	**0.30**
benzo(ghi)perylene	1	513.626	1	140.102	1	143.076	1	16.677	1	20.750
		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase
fluorene	**=**	0.00359	**=**	0.00317	**=**	0.00126	**=**	0.00040	**=**	0.00088
phenanthrene	**=**	0.02556	**=**	0.02747	**=**	0.00514	**=**	0.00057	**=**	0.00193
anthracene	**=**	0.04664	**=**	0.06181	**=**	0.00814	**=**	0.00076	**=**	0.00601
fluoranthene	**=**	0.24923	**=**	0.23284	**=**	0.05558	**=**	0.00442	**=**	0.02144
pyrene	**=**	0.27936	**=**	0.22157	**=**	0.08384	**=**	0.00622	**=**	0.04971
benzo(a)anthracene	**=**	0.93929	**>**	0.99433	**=**	0.62520	**=**	0.29122	**=**	0.55855
chrysene	**=**	0.95323	**=**	0.90041	**=**	0.79237	**=**	0.17657	**=**	0.46739
benzo(b)flouranthene	**=**	0.98430	**=**	0.98876	**=**	0.93484	**=**	0.58956	**=**	0.76432
benzo(k)flouranthene	**=**	0.98658	**=**	0.98546	**=**	0.93272	**>**	0.98183	**>**	0.99275
benzo(e)pyrene	**=**	0.98534	**>**	0.99723	**=**	0.95567	**=**	0.51605	**=**	0.85155
benzo(a)pyrene	**=**	0.98651	**>**	0.99635	**=**	0.93504	**=**	0.86475	**>**	0.98465
indeno(123cd)pyrene	**=**	0.98724	**>**	0.99743	**=**	0.93061	**>**	0.97122	**>**	0.98586
dibenzo(ah)anthracene	**>**	0.99317	**>**	0.97853	**=**	0.75182	**na**		**na**	
benzo(ghi)perylene	**=**	0.98291	**>**	0.99786	**=**	0.93425	**>**	0.98233	**>**	0.98575

Data from Gustafson and Dickhut (1997)

value to use for ND =		HAMPTON		HAMPTON		HAMPTON		HAMPTON
0.3								
pg/m3 (avg value per article)		12-Nov-94		09-Jan-95		11-Mar-95		04-May-95
	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase	det-ect?	pg/m3 gas phase
fluorene	1	1738.09	1	2417.97	1	4256.63	1	40581.78
phenanthrene	1	2456.33	1	3598.42	1	10770.95	1	47281.54
anthracene	0	**0.30**	1	197.56	0	**0.30**	1	1289.49
fluoranthene	1	800.69	1	834.53	1	2301.69	1	8750.36
pyrene	1	1131.33	1	567.93	1	952.30	1	2078.87
benzo(a)anthracene	0	**0.30**	1	7.48	0	**0.30**	1	17.37
chrysene	1	49.90	1	41.53	1	198.41	1	110.93
benzo(b)flouranthene	1	2.50	1	2.33	1	14.39	1	14.90
benzo(k)flouranthene	1	1.58	0	**0.30**	0	**0.30**	1	7.77
benzo(e)pyrene	1	1.65	1	1.45	1	24.06	1	10.49
benzo(a)pyrene	0	**0.30**	0	**0.30**	0	**0.30**	1	4.69
indeno(123cd)pyrene	0	**0.30**	0	**0.30**	0	**0.30**	1	8.55
dibenzo(ah)anthracene	0	**0.30**	0	**0.30**	0	**0.30**	0	**0.30**
benzo(ghi)perylene	1	1.23	1	0.72	1	4.96	1	9.16

	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase	det-ect?	pg/m3 particle phase
fluorene	1	11.029	1	15.120	1	7.845	nq	
phenanthrene	1	81.170	1	167.214	1	111.240	1	16.709
anthracene	1	3.569	1	11.042	1	9.082	1	0.826
fluoranthene	1	138.903	1	214.940	1	156.416	1	12.088
pyrene	1	135.126	1	146.144	1	105.690	1	10.363
benzo(a)anthracene	1	21.559	1	178.023	1	47.569	0	**0.30**
chrysene	1	79.058	1	192.490	1	121.683	1	11.097
benzo(b)flouranthene	1	72.988	1	259.754	1	169.004	1	10.918
benzo(k)flouranthene	1	44.208	1	208.361	1	119.757	1	7.865
benzo(e)pyrene	1	52.897	1	171.040	1	106.809	1	7.827
benzo(a)pyrene	1	32.684	1	131.059	1	77.120	1	4.953
indeno(123cd)pyrene	1	34.230	1	193.042	1	101.563	1	7.393
dibenzo(ah)anthracene	1	6.285	1	29.495	1	14.160	1	1.985
benzo(ghi)perylene	1	46.531	1	183.864	1	113.417	1	10.486

		fraction in particle phase		fraction in particle phase		fraction in particle phase		fraction in particle phase
fluorene	**=**	0.00631	**=**	0.00621	**=**	0.00184	**NQ**	
phenanthrene	**=**	0.03199	**=**	0.04441	**=**	0.01022	**=**	0.00035
anthracene	**>**	0.92246	**=**	0.05293	**>**	0.96802	**=**	0.00064
fluoranthene	**=**	0.14783	**=**	0.20481	**=**	0.06363	**=**	0.00138
pyrene	**=**	0.10670	**=**	0.20466	**=**	0.09990	**=**	0.00496
benzo(a)anthracene	**>**	0.98628	**=**	0.95968	**>**	0.99373	**<**	0.01698
chrysene	**=**	0.61305	**=**	0.82254	**=**	0.38015	**=**	0.09094
benzo(b)flouranthene	**=**	0.96688	**=**	0.99111	**=**	0.92154	**=**	0.42288
benzo(k)flouranthene	**=**	0.96549	**>**	0.99856	**>**	0.99750	**=**	0.50304
benzo(e)pyrene	**=**	0.96975	**=**	0.99159	**=**	0.81615	**=**	0.42731
benzo(a)pyrene	**>**	0.99090	**>**	0.99772	**>**	0.99613	**=**	0.51364
indeno(123cd)pyrene	**>**	0.99131	**>**	0.99845	**>**	0.99705	**=**	0.46371
dibenzo(ah)anthracene	**>**	0.95444	**>**	0.98993	**>**	0.97925	**>**	0.86871
benzo(ghi)perylene	**=**	0.97425	**=**	0.99610	**=**	0.95810	**=**	0.53375

Appendix D.

Atmospheric Fate Mechanisms and Atmospheric Lifetimes

Appendix D.1.
Characteristic Time for Gas-Phase Washout by Wet Deposition from the Atmosphere

As discussed in Appendix C, compounds can exist in the vapor phase and/or the particle phase in the atmosphere. This analysis has used a simple form of vapor/particle partitioning theory to make qualitative estimates of this phenomenon. The extent to which a chemical exists in either phase at any given location in the atmosphere depends (at least) on the particular physical-chemical properties of the substance as well as the ambient temperature and the nature of the atmospheric aerosol.

One depletion mechanism for atmospheric pollutants is the removal of gas-phase pollutants by rainfall. For pollutants that have very limited water solubility, this mechanism will not be very significant.

A simplified approach was taken to make a qualitative estimate of the time scale for gas-phase washout of pollutants by wet deposition. This approach is described as follows.

The rate of deposition, **W** (g/m^2-day), of a given compound is given by the product of the rainfall rate, **J** (m3/m^2-day [=] m/day), the molar concentration of the pollutant in the rain $\mathbf{C_{aq}}$ (mol/m^3), and the molecular weight of the substance $\mathbf{m_w}$ (g/mol):

(1) $W = J\ C_{aq}\ m_w$

The total amount of a given compound in the atmosphere (per square meter of earth surface), **M** (g/m2), is given by product of the assumed height of the chemical layer in the atmosphere, **L** (m), and the concentration of pollutant in the atmosphere, $\mathbf{C_g}$ (atm):

(2) $M = L\ C_g\ (m_w / R\ T)$

where the term in parentheses (m_w / RT = molecular weight / gas constant * temperature) has been included for dimensional consistency.

A characteristic time for removal of a given pollutant by deposition can be defined as the mass of pollutant in the atmosphere divided by the rate of removal. In the case of <u>w</u>et deposition of <u>g</u>as-phase pollutants, this characteristic time — $\tau_{w,g}$ — can be defined in terms of the above variables as:

(3) $\tau_{w,g} = M / W = L\ C_g\ (m_w / RT) / J\ C_{aq}\ m_w$

Canceling m_w and rearranging, one obtains:

(4) $\tau_{w,g} = (L / J\ R\ T)\ (C_g / C_{aq})$

Assuming equilibrium between the gas phase and aqueous phase and assuming that the atmospheric layer is well mixed, the gas- and aqueous-phase concentrations can be related using Henry's Law:

(5) $C_g(\text{atm}) = C_{aq}\ (\text{mol/m}^3)\ H\ (\text{atm-m}^3/\text{mol})$

where $\mathbf{C_g}$ is the gas phase concentration, $\mathbf{C_{aq}}$ is the aqueous phase concentration, and **H** is the Henry's Law Constant for the particular substance at the temperature of interest.

Substituting equation (5) into (4), one obtains the following expression for the characteristic time for removal of a given pollutant from the atmosphere by wet deposition of gas phase material:

(6) $\tau_{w,g} = H\ L / J\ R\ T$

An example of a consistent set of units for using this equation, giving the characteristic time in days, is the following:

H [=] atm-m3/mol
L [=] m
J [=] m/day
R [=] 8.20575×10^{-5} m^3 atm (deg K)$^{-1}$ mol^{-1}
T [=] deg K

Calculations with equation (6) are shown in the figure below. For this figure, a temperature of 290 K was used, a rainfall rate of 30 inches per year (0.0021 m/day) was assumed, and the chemical layer height, L, ranged from 500 m to 10,000 m. It can be seen that compounds with Henry's Law Constants $\lesssim$ 1×10^{-8} atm-m^3/mol can be fairly effectively removed from the atmosphere (e.g., with characteristic times of less than 1 day) to the extent that they exist in the gas phase. Compounds with Henry's Law Constants $\gtrsim$ 1×10^{-5} atm-m^3/mol will not be removed efficiently from the atmosphere by wet deposition of gas phase material. For compounds with Henry's Law Constants between 1×10^{-8} and 1×10^{-5}, wet deposition of gas phase material — to the extent that the compound exists in the gas phase at all -- may or may not be important.

An approximate way to combine the effects of vapor/particle partitioning into this estimation is to simply divide the estimated characteristic time by the typical fraction that exists in the vapor phase (estimated by the vapor/particle partitioning theory). That is, for example, if 100% of the compound exists in the vapor phase, then the V/P-adjusted characteristic time for gas-phase wet removal is $\tau_{w,g}$ / 100% = $\tau_{w,g}$; if 1% of the compound exists in the vapor phase, then the V/P-adjusted characteristic time for gas-phase wet removal is $\tau_{w,g}$ / 1% = 100 $\tau_{w,g}$. This V/P-adjusted characteristic time will be denoted by $\tau_{w,g}^{(V/P)}$.

It is important to note that $\tau_{w,g}^{(V/P)}$ is *not* an estimate of the atmospheric lifetime of a given compound relative to precipitation. It is simply a qualitative measure of the significance of this deposition pathway.

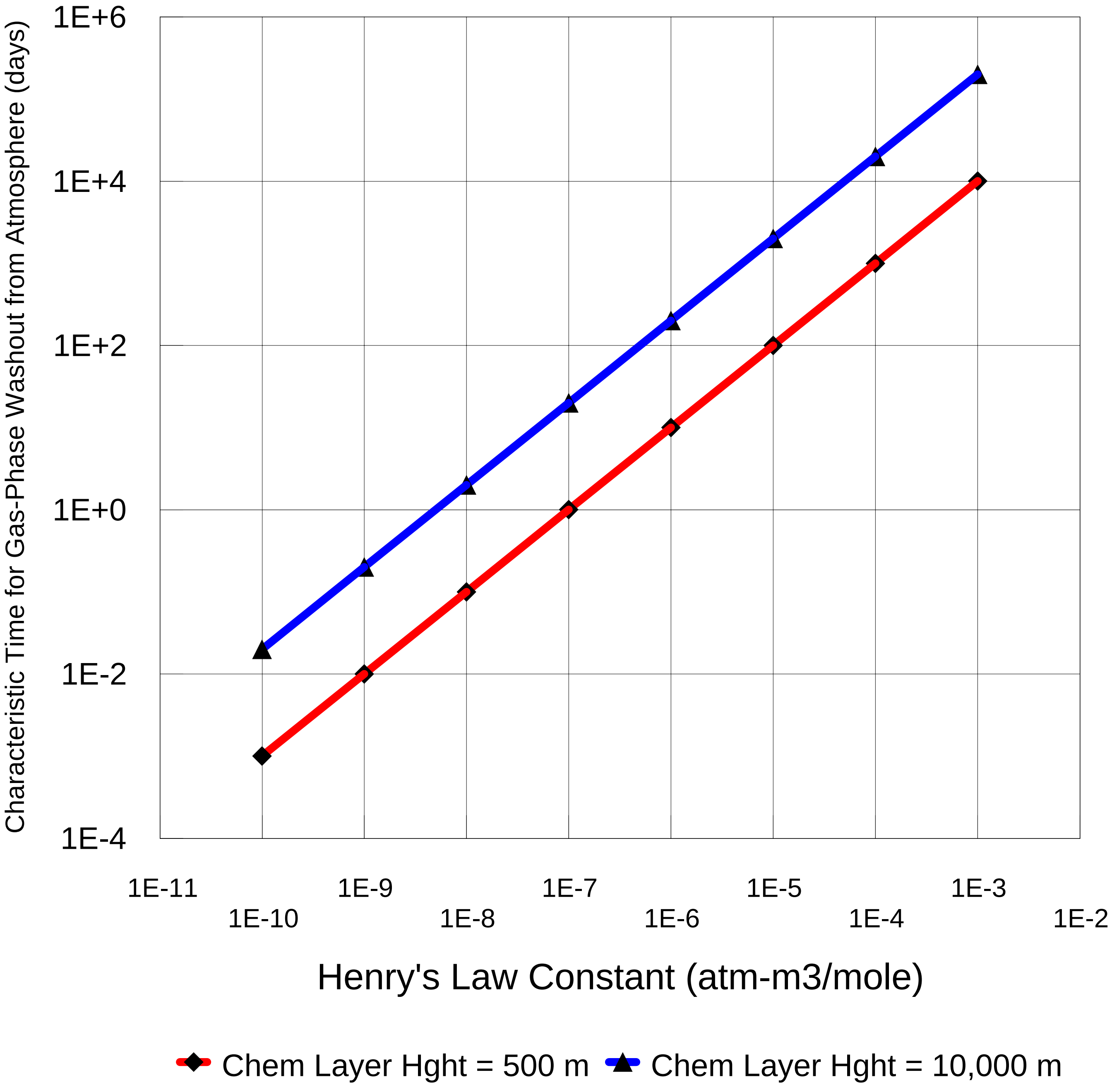
Estimates of $\tau_{w,g}^{(V/P)}$ were made as many of the compounds considered in this analysis for which Henry's Law Constants and basic V/P partitioning estimates could be obtained. These estimates are presented in the table below.

For most of the compounds considered in this analysis, $\tau_{w,g}^{(V/P)}$ is very large — on the order of 100-10,000 days. For one of the compounds -- 4,4'-methylene bis(2-chloroaniline, "MBOCA") — $\tau_{w,g}^{(V/P)} \approx 4.1 \times 10^{-3}$ days $\approx$ 6 minutes, suggesting that this compound will be very effectively removed from the atmosphere by rainfall. Another compound with a relatively low $\tau_{w,g}^{(V/P)}$ was mercuric chloride (HgCl2), with an estimated value of ~1.4 days. Interestingly, mercury in precipitation has been found to be correlated with concentrations of chloride ion, suggesting that an important form of mercury in precipitation is $HgCl_2$ (Keeler, Glinsorn, and Pirrono, 1995).

Of course, rainfall is a sporadic event, and a given "air parcel" may not encounter a rain event for days or weeks. Thus, this very short characteristic time for rain removal does not guarantee that MBOCA will not be transported for long distances in the atmosphere. Rather, it suggests that wet deposition of gas phase material will be a very effective removal process, and the "average" atmospheric lifetime will depend on the frequency with which emitted material encounters a rain event.

Hamrud and Rodhe (1986) have estimated lagrangian time scales related to clouds and precipitation using a trajectory air transport model. They estimate that the average time a lagrangian air parcel exists in the atmosphere after being emitted before encountering its first cloud is on the order of a week, with variations around the world and in different seasons (the range is approximately from 0.5 - 2.5 weeks). Not all clouds produce rain, however, and so the average time to a rain event will be somewhat longer. Thus, the minimum average atmospheric lifetime for compounds relative to wet deposition -- even if they are very effectively removed by rain -- will be on the order of a week.

Figure D.1.-(1). Qualitative Assessment of the Time Scale for Gas Phase Washout by Wet Deposition from the Atmosphere



"Chem Layer Hght" = Height of Atmospheric Layer Within Which Chemical Assumed to be Evenly Mixed
Rainfall Rate assumed to be 30 inches per year (0.0021 m/day)

NAME

Char. Time for Gas Phase Wet Dep. Removal from Atm.

assume precipitation rate of 30"/yr
assume chemcal mixing layer depth of 5000 meters
assume temperature = 290 degrees K
assume mid-range value of average fraction in gas phase

common chemical name	IUPAC #	cas # (1)	characteristic time for gas phase wet deposition of compound [=] days	char. time for gas-phase wet dep divided by avg frac in gas phase [=] days	notes
octachlorostyrene		029082-74-4	1.3E+004	1.3E+004	
4-bromophenyl phenyl ether		000101-55-3	1.0E+004	1.0E+004	
3,3'-dichlorobenzidene		000091-94-1	5.0E+000	4.8E+001	
1,3-dinitropyrene		075321-20-9	5.7E+001	8.7E+001	crude estm of H; uncertainty in this characteristic time at least +/- a factor of 10
1,6-dinitropyrene		042397-64-8	5.7E+001	8.7E+001	crude estm of H; uncertainty in this characteristic time at least +/- a factor of 10
1,8-dinitropyrene		042397-65-9	5.7E+001	8.7E+001	crude estm of H; uncertainty in this characteristic time at least +/- a factor of 10
2,7-dinitropyrene		117929-15-4	5.7E+001	8.7E+001	crude estm of H; uncertainty in this characteristic time at least +/- a factor of 10
dinitropyrenes (mixed)		078432-19-6			
hexachloro-1,3-butadiene		000087-68-3	1.5E+006	1.5E+006	
4,4'-methylene bis(2-chloroaniline)		000101-14-4	4.0E-003	4.1E-003	
pentachlorophenol		000087-86-5	7.8E+001	7.9E+001	will depend on pH of rain; will be less soluble in more acidic rain.
aldrin		000309-00-2	5.0E+004	5.0E+004	
dieldrin		000060-57-1	5.8E+003	5.9E+003	
p,p'-DDT		000050-29-3	5.2E+004	7.2E+004	
p,p'-DDD		000072-54-8	2.2E+003	2.4E+003	
p,p'-DDE		000072-55-9	6.8E+003	7.0E+003	
heptachlor		000076-44-8	1.5E+005	1.5E+005	
heptachlor epoxide		001024-57-3	3.2E+003	3.2E+003	
methoxychlor		000072-43-5	1.6E+003	1.8E+003	
mirex		002385-85-5	8.3E+005	8.3E+005	
toxaphene		008001-35-2	6.0E+002	6.7E+002	
endrin		000072-20-8	7.6E+002	7.6E+002	
alpha-hexachlorocyclohexane		000319-84-6	5.4E+002	5.4E+002	
beta-hexachlorocyclohexane		000319-85-7	4.5E+001	4.5E+001	
delta-hexachlorocyclohexane		000319-86-8	2.1E+001	2.1E+001	
gamma-hexachlorocyclohexane		000058-89-9	5.5E+002	5.6E+002	
mixed hexachlorocyclohexanes		000319-84-6			

NAME			Char. Time for Gas Phase Wet Dep. Removal from Atm.		
common chemical name	IUPAC #	cas # (1)	characteristic time for gas phase wet deposition of compound [=] days	char. time for gas-phase wet dep divided by avg frac in gas phase [=] days	assume precipitation rate of 30"/yr assume chemcal mixing layer depth of 5000 meters assume temperature = 290 degrees K assume mid-range value of average fraction in gas phase notes
cadmium		007440-43-9			
cadmium carbonate		000513-78-0			
cadmium chloride		010108-64-2			
cadmium oxide		001306-19-0			
cadmium sulfate		010124-36-4			
cadmium sulfide		001306-23-6			
elemental mercury		007439-97-6	5.7E+005	5.7E+005	
mercury oxide		021908-53-2			
mercuric chloride		007487-94-7	1.4E+000	1.4E+000	
monomethyl mercury chloride		000115-09-3			
dimethyl mercury		000593-74-8			
tetraethyl lead		000078-00-2	5.7E+007	5.7E+007	
tetramethyl lead		000075-74-1	8.8E+007	8.8E+007	
triethyl lead radical (1+ cation)		014570-15-1			
triethyl lead hydride		005224-23-7			
triethyl lead chloride		001067-14-7			
diethyl lead radical (2+ cation)		024952-65-6			
diethyl lead dihydride		081494-11-3			
diethyl lead dichloride		013231-90-8			
trimethyl lead radical (1+ cation)		014570-16-2			
trimethyl lead hydride		007442-13-9			
trimethyl lead chloride		001520-78-1			
dimethyl lead radical (2+ cation)		021774-13-0			
dimethyl lead dihydride		030691-92-0			
dimethyl lead dichloride		001520-77-0			
bis (tributyltin) oxide		000056-35-9	1.3E+001	2.4E+001	
tributyl tin		000688-75-3			
tributyltin fluoride		001983-10-4			
tributyltin chloride		001461-22-9			
tributyltin hydroxide		001067-97-6			
tributyltin naphthenate					
tris(tributylstannyl) phosphate		013435-05-7			

NAME				Char. Time for Gas Phase Wet Dep. Removal from Atm.	
				char. time	assume precipitation rate of 30"/yr
			characteristic	for gas-phase	assume chemcal mixing layer depth of 5000 meters
			time for	wet dep	assume temperature = 290 degrees K
			gas phase	divided	assume mid-range value of average fraction in gas phase
			wet deposition	by avg frac	
			of compound	in gas phase	
common chemical name	IUPAC #	cas # (1)	[=] days	[=] days	notes
1,4-dichlorobenzene		000106-46-7	1.6E+005	1.6E+005	
1,2,3,4-tetrachlorobenzene		000634-66-2	1.4E+005	1.4E+005	
1,2,4,5-tetrachlorobenzene		000095-94-3	1.2E+005	1.2E+005	
1,2,3,5-tetrachlorobenzene		000634-90-2	5.8E+005	5.8E+005	
pentachlorobenzene		000608-93-5	8.4E+004	8.4E+004	
hexachlorobenzene		000118-74-1	1.3E+005	1.3E+005	
naphthalene		000091-20-3	4.3E+004	4.3E+004	
acenaphthene		000083-32-9	1.2E+004	1.2E+004	
acenaphthylene		000208-96-8	8.3E+003	8.3E+003	
fluorene		000086-73-7	7.8E+003	7.8E+003	
phenanthrene		000085-01-8	3.2E+003	3.2E+003	
anthracene		000120-12-7	3.9E+003	3.9E+003	
pyrene		000129-00-0	9.1E+002	9.2E+002	
fluoranthene		000206-44-0	1.0E+003	1.0E+003	
chrysene		000218-01-9	1.1E+002	1.9E+002	
benz [a] anthracene		000056-55-3	5.8E+002	1.2E+003	
benzo [b] fluoranthene		000205-99-2	1.2E+003	1.3E+003	
benzo [j] fluoranthene		000205-82-3	1.0E+002	2.9E+002	
benzo [k] fluoranthene		000207-08-9	1.6E+001	3.6E+002	
benzo [a] pyrene		000050-32-8	4.6E+001	2.5E+002	
benzo [e] pyrene		000192-97-2	2.0E+001	1.0E+002	
perylene		000198-55-0	3.0E+000	6.3E+001	
benzo [g,h,i] perylene		000191-24-2	7.4E+001	1.7E+003	
dibenz [a,h] anthracene		000053-70-3	7.3E+000	7.3E+003	
indeno [1,2,3-c,d] pyrene		000193-39-5	7.0E+000	1.3E+003	

NAME

Char. Time for Gas Phase Wet Dep. Removal from Atm.

assume precipitation rate of 30"/yr
assume chemcal mixing layer depth of 5000 meters
assume temperature = 290 degrees K
assume mid-range value of average fraction in gas phase

common chemical name	IUPAC #	cas # (1)	characteristic time for gas phase wet deposition of compound [=] days	char. time for gas-phase wet dep divided by avg frac in gas phase [=] days	notes
2,3,7,8-TCDD		001746-01-6	3.3E+003	8.0E+003	
1,2,3,7,8-PeCDD		040321-76-4	2.6E+002	5.9E+003	
1,2,3,4,7,8-HxCDD		039227-28-6	1.1E+003	6.6E+004	
1,2,3,6,7,8-HxCDD		057653-85-7	1.1E+003	6.6E+004	
1,2,3,7,8,9-HxCDD		019408-74-3	1.1E+003	6.6E+004	
1,2,3,4,6,7,8-HpCDD		035822-46-9	1.3E+003	6.4E+005	
OCDD		003268-87-9	6.8E+002	6.2E+005	
2,3,7,8-TCDF		051207-31-9	1.5E+003	2.1E+003	
2,3,4,7,8-PeCDF		057117-31-4	5.0E+002	3.1E+003	
1,2,3,7,8-PeCDF		057117-41-6	5.0E+002	3.1E+003	
1,2,3,4,7,8-HxCDF		070648-26-9	1.4E+003	4.4E+004	
1,2,3,6,7,8-HxCDF		057117-44-9	7.4E+002	1.8E+004	
1,2,3,7,8,9-HxCDF		072918-21-9	1.1E+003	2.9E+004	
2,3,4,6,7,8-HxCDF		060851-34-5	1.1E+003	2.9E+004	
1,2,3,4,6,7,8-HpCDF		067562-39-4	1.4E+003	2.3E+005	
1,2,3,4,7,8,9-HpCDF		055673-89-7	1.4E+003	2.4E+005	
OCDF		039001-02-0	1.9E+002	1.7E+005	

NAME				Char. Time for Gas Phase Wet Dep. Removal from Atm.	
common chemical name	IUPAC #	cas # (1)	characteristic time for gas phase wet deposition of compound [=] days	char. time for gas-phase wet dep divided by avg frac in gas phase [=] days	assume precipitation rate of 30"/yr assume chemcal mixing layer depth of 5000 meters assume temperature = 290 degrees K assume mid-range value of average fraction in gas phase notes
biphenyl	0	000092-52-4	5.3E+004	5.3E+004	
2-PCB	1	002051-60-7	7.0E+004	7.0E+004	
3-PCB	2	002051-61-8	7.5E+004	7.5E+004	
4-PCB	3	002051-62-9	4.2E+004	4.2E+004	
count					
average					
standard deviation					
minimum					
maximum					
2,2'-PCB	4	013029-08-8	5.9E+004	5.9E+004	
2,3-PCB	5	016605-91-7			
2,4-PCB	7	033284-50-3	4.5E+004	4.5E+004	
2,4'-PCB	8	034883-43-7			
2,5-PCB	9	034883-39-1	2.0E+004	2.0E+004	
2,6-PCB	10	033146-45-1			
3,3'-PCB	11	002050-67-1	1.7E+004	1.7E+004	
3,4-PCB	12	002974-92-7			
3,5-PCB	14	034883-41-5			
4,4'-PCB	15	002050-68-2	1.7E+004	1.7E+004	
count					
average					
standard deviation					
minimum					
maximum					

NAME				**Char. Time for Gas Phase Wet Dep. Removal from Atm.**	
				char. time	assume precipitation rate of 30"/yr
			characteristic	for gas-phase	assume chemcal mixing layer depth of 5000 meters
			time for	wet dep	assume temperature = 290 degrees K
			gas phase	divided	assume mid-range value of average fraction in gas phase
			wet deposition	by avg frac	
			of compound	in gas phase	
common chemical name	IUPAC #	cas # (1)	[=] days	[=] days	notes
2,2',3-PCB	16	038444-78-9			
2,2',5-PCB	18	037680-65-2	9.2E+004	9.2E+004	
2,3,3'-PCB	20	038444-84-7			
2,3,4-PCB	21	055702-46-0			
2,3',5-PCB	26	038444-85-8			
2,4,4'-PCB	28	007012-37-5			
2,4,5-PCB	29	015862-07-4	2.4E+004	2.4E+004	
2,4,6-PCB	30	035693-92-6	4.9E+004	4.9E+004	
2,4',5,-PCB	31	016606-02-3			
2',3,4-PCB	33	038444-86-9	4.3E+004	4.4E+004	
3,3',4-PCB	35	037680-69-6			
3,4,4'-PCB	37	038444-90-5			
count					
average					
standard deviation					
minimum					
maximum					
2,2',3,3'-PCB	40	038444-93-8	2.2E+004	2.2E+004	
2,2',3,5'-PCB	44	041464-39-5			
2,2',4,4'-PCB	47	002437-79-8	1.7E+004	1.7E+004	
2,2',4,5'-PCB	49	041464-40-8			
2,2',4,6-PCB	50	062796-65-0			
2,2',4,6'-PCB	51	068194-04-7			
2,2,5,5'-PCB	52	035693-99-3	4.7E+004	4.8E+004	
2,2,5,6'-PCB	53	041464-41-9			
2,2,6,6'-PCB	54	015968-05-5			
2,3,4,4'-PCB	60	033025-41-1			
2,3,4,5-PCB	61	033284-53-6			
2,3,5,6-PCB	65	033284-54-7			
2,3,4,4'-PCB	66	032598-10-0			
2,3',4',5-PCB	70	032598-11-1			
2,4,4',6-PCB	75	032598-12-2			
3,3',4,4'-PCB	77	032598-13-3	1.7E+003	1.8E+003	
3,3',5,5'-PCB	80	033284-52-5			
3,4,4',5-PCB	81	070362-50-4			
count					
average					
standard deviation					
minimum					
maximum					

NAME

Char. Time for Gas Phase Wet Dep. Removal from Atm.

common chemical name	IUPAC #	cas # (1)	characteristic time for gas phase wet deposition of compound [=] days	char. time for gas-phase wet dep divided by avg frac in gas phase [=] days	notes
					assume precipitation rate of 30"/yr assume chemcal mixing layer depth of 5000 meters assume temperature = 290 degrees K assume mid-range value of average fraction in gas phase
2,2',3,3',5-PCB	83	060145-20-2			
2,2',3,4,5-PCB	86	065510-45-4	1.5E+005	1.6E+005	
2,2',3,4,5'-PCB	87	038380-02-8	2.5E+004	2.6E+004	
2,2',3,4,6-PCB	88	055215-17-3			
2,2',3,5,6-PCB	95	038379-99-6			
2,2',4,4',5-PCB	99	038380-01-7			
2,2',4,4',6-PCB	100	039485-83-1			
2,2',4,5,5'-PCB	101	037680-73-2	3.5E+004	3.7E+004	
2,2',4,6,6'-PCB	104	056558-16-8	1.4E+004	1.5E+004	
2,3,3',4,4'-PCB	105	032598-14-4			
2,3,3',4',6-PCB	110	038380-03-9			
2,3,4,4',5-PCB	114	074472-37-0			
2,3,4,5,6-PCB	116	018259-05-7			
2,3',4,4',5-PCB	118	031508-00-6			
2',3,4,5,5'-PCB	124	070424-70-3			
3,3',4,4',5-PCB	126	057465-28-8			
count					
average					
standard deviation					
minimum					
maximum					
2,2',3,3',4,4'-PCB	128	038380-07-3	1.2E+004	1.8E+004	
2,2',3,3',4,5-PCB	129	055215-18-4			
2,2',3,3',5,6-PCB	134	052704-70-8			
2,2',3,3',6,6'-PCB	136	038411-22-2			
2,2',3,4,4',5'-PCB	138	035065-28-2			
2,2',3,4',5',6-PCB	149	038380-04-0			
2,2',4,4',5,5'-PCB	153	035065-27-1	4.3E+004	5.3E+004	
2,2',4,4',6,6'-PCB	155	033979-03-2	8.6E+004	8.9E+004	
2,3,3',4,4',5-PCB	156	038380-08-4			
2,3,3',4,4',5'-PCB	157	069782-90-7			
2,3',4,4',5,5'-PCB	167	052663-72-6			
3,3',4,4',5,5'-PCB	169	032774-16-6			
count					
average					
standard deviation					
minimum					
maximum					

NAME

Char. Time for Gas Phase Wet Dep. Removal from Atm.

common chemical name	IUPAC #	cas # (1)	characteristic time for gas phase wet deposition of compound [=] days	char. time for gas-phase wet dep divided by avg frac in gas phase [=] days	assume precipitation rate of 30"/yr assume chemcal mixing layer depth of 5000 meters assume temperature = 290 degrees K assume mid-range value of average fraction in gas phase notes
2,2',3,3',4,4',5-PCB	170	035065-30-6			
2,2',3,3',4,4',6-PCB	171	052663-71-5	5.4E+003	1.0E+004	
2,2',3,4,4',5,5'-PCB	180	035065-29-3			
2,2',3,4,5,5',6-PCB	185	052712-05-7			
2,2',3,4',5,5',6-PCB	187	052663-68-0			
2,3,3',4,4',5,5'-PCB	189	039635-31-9			
count					
average					
standard deviation					
minimum					
maximum					
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7			
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	3.8E+004	5.0E+004	
count					
average					
standard deviation					
minimum					
maximum					
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	8.2E+004	1.6E+006	
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3			
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1			
count					
average					
standard deviation					
minimum					
maximum					
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	2.1E+004	3.1E+005	

Appendix D.2.

Basic Results for Gas Phase Reaction Rate with Hydroxyl Radical (limited data on reactions with O_3 and NO_3 also summarized)

MDC	MDC	**ESTM RXN RATE with HYDROXYL RADICAL**			**Atm Half Life**			**EXPT'L: RXN RATE with OH**		
		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN
		AOPWIN output text indicating that it tried to estm OH rxn	AOPWIN estimated an OH rxn rate of 0.0e-12 for this	Reaction Rate Estimate with Hydroxyl cm3/	estimated half-life (days) assuming 12 hours/day and [OH]= 1.5E+006	AOPWIN output text indicating that it tried to find expt'l OH		**EXPT'L: RXN RATE with OH cm3/(molecule-sec)** AVG Expt'l OH	LOW Expt'l OH	HIGH Expt'l OH
octachlorostyrene		(OH est)		1.07311E-012	9.968	----(exp OH)	0			
4-bromophenyl phenyl ether		(OH est)		6.33066E-012	1.690	----(exp OH)	0			
3,3'-dichlorobenzidene		(OH est)		3.95704E-011	0.270	----(exp OH)	0			
1,3-dinitropyrene		(OH est)		5.46000E-013	19.591	----(exp OH)	0			
1,6-dinitropyrene		(OH est)		5.46000E-013	19.591	----(exp OH)	0			
1,8-dinitropyrene		(OH est)		5.46000E-013	19.591	----(exp OH)	0			
2,7-dinitropyrene		(OH est)		5.46000E-013	19.591	----(exp OH)	0			
dinitropyrenes (mixed)							0			
hexachloro-1,3-butadiene		(OH est)		3.00200E-014	356.320	----(exp OH)	0			
4,4'-methylene bis(2-chloroaniline)		(OH est)		7.75166E-011	0.138	----(exp OH)	0			
pentachlorophenol		(OH est)		5.50490E-013	19.431	----(exp OH)	0			
aldrin		(OH est)		6.45895E-011	0.166	----(exp OH)	0			
dieldrin		(OH est)		8.83921E-012	1.210	----(exp OH)	0			
p,p'-DDT		(OH est)		3.43505E-012	3.114	----(exp OH)	0			
p,p'-DDD		(OH est)		4.34415E-012	2.462	----(exp OH)	0			
p,p'-DDE		(OH est)		7.43011E-012	1.440	----(exp OH)	0			
heptachlor		(OH est)		6.13278E-011	0.174	----(exp OH)	0			
heptachlor epoxide		(OH est)		3.84870E-012	2.779	----(exp OH)	0			
methoxychlor		(OH est)		5.35478E-011	0.200	----(exp OH)	0			
mirex		(OH est)	0.00E+000			----(exp OH)	0			
toxaphene		(OH est)		2.49555E-012	4.286	----(exp OH)	0			
endrin		(OH est)		8.83921E-012	1.210	----(exp OH)	0			
alpha-hexachlorocyclohexane		(OH est)		5.73250E-013	18.660	----(exp OH)	0			
beta-hexachlorocyclohexane		(OH est)		5.73250E-013	18.660	----(exp OH)	0			
delta-hexachlorocyclohexane		(OH est)		5.73250E-013	18.660	----(exp OH)	0			
gamma-hexachlorocyclohexane		(OH est)		5.73250E-013	18.660	----(exp OH)	0			
mixed hexachlorocyclohexanes		(OH est)		5.73250E-013	18.660	----(exp OH)	0			
cadmium							0			
cadmium carbonate							0			
cadmium chloride		(OH est)	0.00E+000			----(exp OH)	0			
cadmium oxide		(OH est)	0.00E+000			----(exp OH)	0			
cadmium sulfate							0			
cadmium sulfide		(OH est)	0.00E+000			----(exp OH)	0			
elemental mercury							0			
mercury oxide		(OH est)	0.00E+000			----(exp OH)	0			
mercuric chloride		(OH est)	0.00E+000			----(exp OH)	0			
monomethyl mercury chloride		(OH est)		8.16000E-012	1.311	----(exp OH)	0			
dimethyl mercury		(OH est)		1.63200E-011	0.655	----(exp OH)	1	1.90E-011		

MDC	MDC	ESTM RXN RATE with HYDROXYL RADICAL			Atm Half Life			EXPT'L: RXN RATE with OH		
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		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN
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		AOPWIN	AOPWIN		estimated	AOPWIN		EXPT'L: RXN RATE with OH		
		output	estimated	Reaction	half-life (days)	output		cm3/(molecule-sec)		
		text	an OH	Rate	assuming	text	-----------------	--------------------	--------------------	--------------------
		indicating	rxn rate	Estimate	12	indicating				
		that it tried	of	with Hydroxyl	hours/day	that it tried		AVG	LOW	HIGH
		to estm	0.0e-12		and [OH]=	to find		Expt'l	Expt'l	Expt'l
		OH rxn	for this	cm3/	1.5E+006	expt'l OH		OH	OH	OH
tetraethyl lead		(OH est)		4.92371E-011	0.217	----(exp OH)	1	6.00E-011		
tetramethyl lead		(OH est)		7.07200E-012	1.513	----(exp OH)	1	6.00E-012		
triethyl lead radical (1+ cation)		(OH est)		3.69278E-011	0.290	----(exp OH)	0			
triethyl lead hydride		(OH est)		3.69278E-011	0.290	----(exp OH)	0			
triethyl lead chloride		(OH est)		3.69278E-011	0.290	----(exp OH)	0			
diethyl lead radical (2+ cation)		(OH est)		2.46186E-011	0.434	----(exp OH)	0			
diethyl lead dihydride		(OH est)		2.46186E-011	0.434	----(exp OH)	0			
diethyl lead dichloride		(OH est)		2.46186E-011	0.434	----(exp OH)	0			
trimethyl lead radical (1+ cation)		(OH est)		5.30400E-012	2.017	----(exp OH)	0			
trimethyl lead hydride		(OH est)		5.30400E-012	2.017	----(exp OH)	0			
trimethyl lead chloride		(OH est)		5.30400E-012	2.017	----(exp OH)	0			
dimethyl lead radical (2+ cation)		(OH est)		3.53600E-012	3.025	----(exp OH)	0			
dimethyl lead dihydride							0			
dimethyl lead dichloride		(OH est)		3.53600E-012	3.025	----(exp OH)	0			
bis (tributyltin) oxide		(OH est)		8.53041E-011	0.125	----(exp OH)	0			
tributyl tin							0			
tributyltin fluoride		(OH est)		4.26520E-011	0.251	----(exp OH)	0			
tributyltin chloride		(OH est)		4.26520E-011	0.251	----(exp OH)	0			
tributyltin hydroxide		(OH est)		4.27920E-011	0.250	----(exp OH)	0			
tributyltin naphthenate							0			
tris(tributylstannyl) phosphate							0			
1,4-dichlorobenzene		(OH est)		4.00480E-013	26.710	----(exp OH)	1	3.20E-013		
1,2,3,4-tetrachlorobenzene		(OH est)		8.22500E-014	130.051	----(exp OH)	0			
1,2,4,5-tetrachlorobenzene		(OH est)		8.22500E-014	130.051	----(exp OH)	0			
1,2,3,5-tetrachlorobenzene		(OH est)		1.98180E-013	53.975	----(exp OH)	0			
pentachlorobenzene		(OH est)		5.78600E-014	184.872	----(exp OH)	0			
hexachlorobenzene		(OH est)		1.68900E-014	633.317	----(exp OH)	0			
naphthalene		(OH est)		2.16000E-011	0.495	----(exp OH)	1	2.16E-011		
acenaphthene		(OH est)		6.72285E-011	0.159	----(exp OH)	1	7.85E-011	5.40E-011	1.03E-010
acenaphthylene		(OH est)		7.54921E-011	0.142	----(exp OH)	1	1.10E-010		
fluorene		(OH est)		9.00093E-012	1.188	----(exp OH)	1	1.20E-011		
phenanthrene		(OH est)		1.30000E-011	0.823	----(exp OH)	1	1.30E-011		
anthracene		(OH est)		4.00000E-011	0.267	----(exp OH)	1	4.00E-011		
pyrene		(OH est)		5.00000E-011	0.214	----(exp OH)	1	5.00E-011		
fluoranthene		(OH est)		2.92273E-011	0.366	----(exp OH)	1	5.00E-011		
chrysene		(OH est)		5.00000E-011	0.214	----(exp OH)	0			
benz [a] anthracene		(OH est)		5.00000E-011	0.214	----(exp OH)	0			
benzo [b] fluoranthene		(OH est)		1.85540E-011	0.577	----(exp OH)	0			

MDC	MDC	**ESTM RXN RATE with HYDROXYL RADICAL**			**Atm Half Life**			**EXPT'L: RXN RATE with OH**		
		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN
		AOPWIN output text indicating that it tried to estm OH rxn	AOPWIN estimated an OH rxn rate of 0.0e-12 for this	Reaction Rate Estimate with Hydroxyl cm3/	estimated half-life (days) assuming 12 hours/day and [OH]= 1.5E+006	AOPWIN output text indicating that it tried to find expt'l OH		**EXPT'L: RXN RATE with OH cm3/(molecule-sec)**		
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								AVG Expt'l OH	LOW Expt'l OH	HIGH Expt'l OH
benzo [j] fluoranthene		(OH est)		5.36147E-011	0.200	----(exp OH)	0			
benzo [k] fluoranthene		(OH est)		5.36147E-011	0.200	----(exp OH)	0			
benzo [a] pyrene		(OH est)		5.00000E-011	0.214	----(exp OH)	0			
benzo [e] pyrene		(OH est)		5.00000E-011	0.214	----(exp OH)	0			
perylene		(OH est)		5.00000E-011	0.214	----(exp OH)	0			
benzo [g,h,i] perylene		(OH est)		8.68620E-011	0.123	----(exp OH)	0			
dibenz [a,h] anthracene		(OH est)		5.00000E-011	0.214	----(exp OH)	0			
indeno [1,2,3-c,d] pyrene		(OH est)		6.44740E-011	0.166	----(exp OH)	0			
2,3,7,8-TCDD		(OH est)		2.02120E-012	5.292	----(exp OH)	0			
1,2,3,7,8-PeCDD		(OH est)		1.72152E-012	6.214	----(exp OH)	0			
1,2,3,4,7,8-HxCDD		(OH est)		1.21817E-012	8.781	----(exp OH)	0			
1,2,3,6,7,8-HxCDD		(OH est)		1.42184E-012	7.523	----(exp OH)	0			
1,2,3,7,8,9-HxCDD		(OH est)		1.42184E-012	7.523	----(exp OH)	0			
1,2,3,4,6,7,8-HpCDD		(OH est)		9.18490E-013	11.646	----(exp OH)	0			
OCDD		(OH est)		4.15140E-013	25.767	----(exp OH)	0			
2,3,7,8-TCDF		(OH est)		1.64520E-013	65.018	----(exp OH)	0			
2,3,4,7,8-PeCDF		(OH est)		7.45600E-014	143.465	----(exp OH)	0			
1,2,3,7,8-PeCDF		(OH est)		7.45600E-014	143.465	----(exp OH)	0			
1,2,3,4,7,8-HxCDF		(OH est)		3.03550E-013	35.239	----(exp OH)	0			
1,2,3,6,7,8-HxCDF		(OH est)		3.58920E-013	29.803	----(exp OH)	0			
1,2,3,7,8,9-HxCDF		(OH est)		3.38000E-014	316.471	----(exp OH)	0			
2,3,4,6,7,8-HxCDF		(OH est)		3.03980E-013	35.189	----(exp OH)	0			
1,2,3,4,6,7,8-HpCDF		(OH est)		1.53100E-014	698.675	----(exp OH)	0			
1,2,3,4,7,8,9-HpCDF		(OH est)		1.53000E-014	699.132	----(exp OH)	0			
OCDF		(OH est)		6.94000E-015	1541.314	----(exp OH)	0			
biphenyl	0	(OH est)		6.77470E-012	1.579	----(exp OH)	1	7.20E-012		
2-PCB	1	(OH est)		3.48475E-012	3.070	----(exp OH)	1	2.82E-012		
3-PCB	2	(OH est)		4.87861E-012	2.193	----(exp OH)	1	5.28E-012		
4-PCB	3	(OH est)		3.48475E-012	3.070	----(exp OH)	1	3.86E-012		
2,2'-PCB	4	(OH est)		1.72691E-012	6.194	----(exp OH)	1	2.00E-012		
2,3-PCB	5	(OH est)		2.47319E-012	4.325	----(exp OH)	0			
2,4-PCB	7	(OH est)		2.46678E-012	4.336	----(exp OH)	1	2.60E-012		
2,4'-PCB	8	(OH est)		1.72691E-012	6.194	----(exp OH)	0			
2,5-PCB	9	(OH est)		2.47319E-012	4.325	----(exp OH)	0			
2,6-PCB	10	(OH est)		2.46678E-012	4.336	----(exp OH)	0			
3,3'-PCB	11	(OH est)		3.51132E-012	3.046	----(exp OH)	1	4.10E-012		
3,4-PCB	12	(OH est)		2.47319E-012	4.325	----(exp OH)	0			
3,5-PCB	14	(OH est)		3.45372E-012	3.097	----(exp OH)	1	4.20E-012		

MDC	MDC	**ESTM RXN RATE with HYDROXYL RADICAL**			**Atm Half Life**			**EXPT'L: RXN RATE with OH**		
		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN
		AOPWIN output text indicating that it tried to estm OH rxn	AOPWIN estimated an OH rxn rate of 0.0e-12 for this	Reaction Rate Estimate with Hydroxyl cm3/	estimated half-life (days) assuming 12 hours/day and [OH]= 1.5E+006	AOPWIN output text indicating that it tried to find expt'l OH		**EXPT'L: RXN RATE with OH cm3/(molecule-sec)**		
								AVG Expt'l OH	LOW Expt'l OH	HIGH Expt'l OH
4,4'-PCB	15	(OH est)		1.72691E-012	6.194	----(exp OH)	1	2.00E-012		
2,2',3-PCB	16	(OH est)		1.09075E-012	9.807	----(exp OH)	0			
2,2',5-PCB	18	(OH est)		1.09075E-012	9.807	----(exp OH)	0			
2,3,3'-PCB	20	(OH est)		1.76298E-012	6.067	----(exp OH)	0			
2,3,4-PCB	21	(OH est)		1.25509E-012	8.523	----(exp OH)	0			
2,3',5-PCB	26	(OH est)		1.09075E-012	9.807	----(exp OH)	0			
2,4,4'-PCB	28	(OH est)		1.18556E-012	9.023	----(exp OH)	1	1.10E-012		
2,4,5-PCB	29	(OH est)		1.25509E-012	8.523	----(exp OH)	1	1.30E-012		
2,4,6-PCB	30	(OH est)		1.53687E-012	6.960	----(exp OH)	0			
2,4',5,-PCB	31	(OH est)		1.09080E-012	9.806	----(exp OH)	1	1.20E-012		
2',3,4-PCB	33	(OH est)		1.09075E-012	9.807	----(exp OH)	1	1.00E-012		
3,3',4-PCB	35	(OH est)		1.76300E-012	6.067	----(exp OH)	0			
3,4,4'-PCB	37	(OH est)		1.09080E-012	9.806	----(exp OH)	0			
2,2',3,3'-PCB	40	(OH est)		7.30150E-013	14.650	----(exp OH)	0			
2,2',3,5'-PCB	44	(OH est)		7.30150E-013	14.650	----(exp OH)	1	8.00E-013		
2,2',4,4'-PCB	47	(OH est)		8.13400E-013	13.151	----(exp OH)	1	1.00E-012		
2,2',4,5'-PCB	49	(OH est)		7.71780E-013	13.860	----(exp OH)	0			
2,2',4,6-PCB	50	(OH est)		8.26530E-013	12.942	----(exp OH)	0			
2,2',4,6'-PCB	51	(OH est)		8.13410E-013	13.150	----(exp OH)	0			
2,2,5,5'-PCB	52	(OH est)		7.30150E-013	14.650	----(exp OH)	0			
2,2,5,6'-PCB	53	(OH est)		7.71780E-013	13.860	----(exp OH)	0			
2,2,6,6'-PCB	54	(OH est)		8.13410E-013	13.150	----(exp OH)	0			
2,3,4,4'-PCB	60	(OH est)		5.76590E-013	18.552	----(exp OH)	0			
2,3,4,5-PCB	61	(OH est)		8.05110E-013	13.286	----(exp OH)	0			
2,3,5,6-PCB	65	(OH est)		8.05110E-013	13.286	----(exp OH)	0			
2,3,4,4'-PCB	66	(OH est)		7.71780E-013	13.860	----(exp OH)	0			
2,3',4',5-PCB	70	(OH est)		7.30150E-013	14.650	----(exp OH)	0			
2,4,4',6-PCB	75	(OH est)		8.26530E-013	12.942	----(exp OH)	0			
3,3',4,4'-PCB	77	(OH est)		7.30150E-013	14.650	----(exp OH)	0			
3,3',5,5'-PCB	80	(OH est)		1.75918E-012	6.081	----(exp OH)	0			
3,4,4',5-PCB	81	(OH est)		7.59800E-013	14.078	----(exp OH)	0			
2,2',3,3',5-PCB	83	(OH est)		4.72900E-013	22.619	----(exp OH)	0			
2,2',3,4,5-PCB	86	(OH est)		3.99600E-013	26.769	----(exp OH)	0			
2,2',3,4,5'-PCB	87	(OH est)		3.34810E-013	31.949	----(exp OH)	0			
2,2',3,4,6-PCB	88	(OH est)		4.18010E-013	25.590	----(exp OH)	0			
2,2',3,5,6-PCB	95	(OH est)		3.34810E-013	31.949	----(exp OH)	1	4.00E-013		
2,2',4,4',5-PCB	99	(OH est)		3.99600E-013	26.769	----(exp OH)	0			
2,2',4,4',6-PCB	100	(OH est)		5.66950E-013	18.867	----(exp OH)	0			

MDC	MDC	ESTM RXN RATE with HYDROXYL RADICAL			Atm Half Life			EXPT'L: RXN RATE with OH		
		AOPWIN	AOPWIN	AOPWIN	MDC	AOPWIN	AOPWIN	AOPWIN	AOPWIN	AOPWIN
		AOPWIN output text indicating that it tried to estm OH rxn	AOPWIN estimated an OH rxn rate of 0.0e-12 for this	Reaction Rate Estimate with Hydroxyl cm3/	estimated half-life (days) assuming 12 hours/day and [OH]= 1.5E+006	AOPWIN output text indicating that it tried to find expt'l OH		**EXPT'L: RXN RATE with OH cm3/(molecule-sec)** AVG Expt'l OH	LOW Expt'l OH	HIGH Expt'l OH
2,2',4,5,5'-PCB	101	(OH est)		3.34810E-013	31.949	----(exp OH)	0			
2,2',4,6,6'-PCB	104	(OH est)		5.66950E-013	18.867	----(exp OH)	0			
2,3,3',4,4'-PCB	105	(OH est)		3.34810E-013	31.949	----(exp OH)	0			
2,3,3',4',6-PCB	110	(OH est)		3.34810E-013	31.949	----(exp OH)	1	6.00E-013		
2,3,4,4',5-PCB	114	(OH est)		3.98530E-013	26.840	----(exp OH)	0			
2,3,4,5,6-PCB	116	(OH est)		5.28130E-013	20.254	----(exp OH)	1	9.00E-013		
2,3',4,4',5-PCB	118	(OH est)		3.34810E-013	31.949	----(exp OH)	0			
2',3,4,5,5'-PCB	124	(OH est)		4.72880E-013	22.620	----(exp OH)	0			
3,3',4,4',5-PCB	126	(OH est)		4.72900E-013	22.619	----(exp OH)	0			
2,2',3,3',4,4'-PCB	128	(OH est)		1.64000E-013	65.224	----(exp OH)	0			
2,2',3,3',4,5-PCB	129	(OH est)		2.11000E-013	50.695	----(exp OH)	0			
2,2',3,3',5,6-PCB	134	(OH est)		2.11000E-013	50.695	----(exp OH)	0			
2,2',3,3',6,6'-PCB	136	(OH est)		1.64000E-013	65.224	----(exp OH)	0			
2,2',3,4,4',5'-PCB	138	(OH est)		1.64000E-013	65.224	----(exp OH)	0			
2,2',3,4',5',6-PCB	149	(OH est)		1.64000E-013	65.224	----(exp OH)	0			
2,2',4,4',5,5'-PCB	153	(OH est)		1.64000E-013	65.224	----(exp OH)	0			
2,2',4,4',6,6'-PCB	155	(OH est)		3.95140E-013	27.071	----(exp OH)	0			
2,3,3',4,4',5-PCB	156	(OH est)		2.11000E-013	50.695	----(exp OH)	0			
2,3,3',4,4',5'-PCB	157	(OH est)		2.34000E-013	45.712	----(exp OH)	0			
2,3',4,4',5,5'-PCB	167	(OH est)		2.33990E-013	45.714	----(exp OH)	0			
3,3',4,4',5,5'-PCB	169	(OH est)		3.03980E-013	35.189	----(exp OH)	0			
2,2',3,3',4,4',5-PCB	170	(OH est)		1.04610E-013	102.253	----(exp OH)	0			
2,2',3,3',4,4',6-PCB	171	(OH est)		1.17920E-013	90.712	----(exp OH)	0			
2,2',3,4,4',5,5'-PCB	180	(OH est)		1.04610E-013	102.253	----(exp OH)	0			
2,2',3,4,5,5',6-PCB	185	(OH est)		1.24290E-013	86.063	----(exp OH)	0			
2,2',3,4',5,5',6-PCB	187	(OH est)		1.04610E-013	102.253	----(exp OH)	0			
2,3,3',4,4',5,5'-PCB	189	(OH est)		1.40060E-013	76.372	----(exp OH)	0			
2,2',3,3',4,4',5,5'-PCB	194	(OH est)		5.58700E-014	191.457	----(exp OH)	0			
2,2',3,3',5,5',6,6'-PCB	202	(OH est)		5.58700E-014	191.457	----(exp OH)	0			
2,2',3,3',4,4',5,5',6-PCB	206	(OH est)		3.28900E-014	325.227	----(exp OH)	0			
2,2',3,3',4,4',5,6,6'-PCB	207	(OH est)		4.34900E-014	245.958	----(exp OH)	0			
2,2',3,3',4,5,5',6,6'-PCB	208	(OH est)		3.28900E-014	325.227	----(exp OH)	0			
2,2',3,3',4,4',5,5',6,6'-PCB	209	(OH est)		1.81700E-014	588.702	----(exp OH)	0			

								EXPT'L: RXN RATE with O3 cm3/(molecule-sec)					EXPT'L: RXN RATE with NO3 cm3/(molecule-sec)			
Chemical Name	IUPAC #	Best CAS #	did AOPWIN estimate rxn with ozone?	estimated rxn rate with ozone cm3/ molec.-sec	estimated half-life (days) assuming 24 hours/day and [O3]= 7.0E+011 molec/cm3	estimated half-life (days) assuming 24 hours/day and [O3]= 7.0E+011 molec/cm3	exist?	<?	AVG Expt'l O3 Value	LOW Expt'l O3 Value	HIGH Expt'l O3 Value	exist?	<?	AVG Expt'l NO3 Value	LOW Expt'l NO3 Value	HIGH Expt'l NO3 Value
octachlorostyrene		029082-74-4	1	6.14E-020	186.619	187	0					0				
4-bromophenyl phenyl ether		000101-55-3	0				0					0				
3,3'-dichlorobenzidene		000091-94-1	0				0					0				
1,3-dinitropyrene		075321-20-9	0				0					0				
1,6-dinitropyrene		042397-64-8	0				0					0				
1,8-dinitropyrene		042397-65-9	0				0					0				
2,7-dinitropyrene		117929-15-4	0				0					0				
dinitropyrenes (mixed)		078432-19-6	0				0					0				
hexachloro-1,3-butadiene		000087-68-3	1	7.00E-023		163,725	0					0				
4,4'-methylene bis(2-chloroaniline)		000101-14-4	0				0					0				
pentachlorophenol		000087-86-5	0				0					0				
aldrin		000309-00-2	1	2.00E-016		0.057	0					0				
dieldrin		000060-57-1	1	3.58E-020		320	0					0				
p,p'-DDT		000050-29-3	0				0					0				
p,p'-DDD		000072-54-8	0				0					0				
p,p'-DDE		000072-55-9	1	5.15E-018		2.2	0					0				
heptachlor		000076-44-8	1	2.00E-016		0.057	0					0				
heptachlor epoxide		001024-57-3	1	3.58E-020		320	0					0				
methoxychlor		000072-43-5	0				0					0				
mirex		002385-85-5	0				0					0				
toxaphene		008001-35-2	0				0					0				
endrin		000072-20-8	1	3.58E-020		320	0					0				
alpha-hexachlorocyclohexane		000319-84-6	0				0					0				
beta-hexachlorocyclohexane		000319-85-7	0				0					0				
delta-hexachlorocyclohexane		000319-86-8	0				0					0				
gamma-hexachlorocyclohexane		000058-89-9	0				0					0				
mixed hexachlorocyclohexanes		000319-84-6	0				0					0				
cadmium		007440-43-9	0				0					0				
cadmium carbonate		000513-78-0	0				0					0				
cadmium chloride		010108-64-2	0				0					0				
cadmium oxide		001306-19-0	0				0					0				
cadmium sulfate		010124-36-4	0				0					0				
cadmium sulfide		001306-23-6	0				0					0				
elemental mercury		007439-97-6	0				0					0				
mercury oxide		021908-53-2	0				0					0				
mercuric chloride		007487-94-7	0				0					0				
monomethyl mercury chloride		000115-09-3	0				0					0				
dimethyl mercury		000593-74-8	0				0					0				
tetraethyl lead		000078-00-2	0				0					0				
tetramethyl lead		000075-74-1	0				0					0				
triethyl lead radical (1+ cation)		014570-15-1	0				0					0				
triethyl lead hydride		005224-23-7	0				0					0				
triethyl lead chloride		001067-14-7	0				0					0				
diethyl lead radical (2+ cation)		024952-65-6	0				0					0				
diethyl lead dihydride		081494-11-3	0				0					0				
diethyl lead dichloride		013231-90-8	0				0					0				
trimethyl lead radical (1+ cation)		014570-16-2	0				0					0				
trimethyl lead hydride		007442-13-9	0				0					0				
trimethyl lead chloride		001520-78-1	0				0					0				
dimethyl lead radical (2+ cation)		021774-13-0	0				0					0				
dimethyl lead dihydride		030691-92-0	0				0					0				
dimethyl lead dichloride		001520-77-0	0				0					0				

									EXPT'L: RXN RATE with O3 cm3/(molecule-sec)					EXPT'L: RXN RATE with NO3 cm3/(molecule-sec)		
Chemical Name	IUPAC #	Best CAS #	did AOPWIN estimate rxn with ozone?	estimated rxn rate with ozone cm3/ molec.-sec	estimated half-life (days) assuming 24 hours/day and [O3]= 7.0E+011 molec/cm3	estimated half-life (days) assuming 24 hours/day and [O3]= 7.0E+011 molec/cm3	exist?	<?	AVG Expt'l O3 Value	LOW Expt'l O3 Value	HIGH Expt'l O3 Value	exist?	<?	AVG Expt'l NO3 Value	LOW Expt'l NO3 Value	HIGH Expt'l NO3 Value
bis (tributyltin) oxide		000056-35-9	0				0					0				
tributyl tin		000688-75-3	0				0					0				
tributyltin fluoride		001983-10-4	0				0					0				
tributyltin chloride		001461-22-9	0				0					0				
tributyltin hydroxide		001067-97-6	0				0					0				
tributyltin naphthenate			0				0					0				
tris(tributylstannyl) phosphate		013435-05-7	0				0					0				
1,4-dichlorobenzene		000106-46-7	0				0					0				
1,2,3,4-tetrachlorobenzene		000634-66-2	0				0					0				
1,2,4,5-tetrachlorobenzene		000095-94-3	0				0					0				
1,2,3,5-tetrachlorobenzene		000634-90-2	0				0					0				
pentachlorobenzene		000608-93-5	0				0					0				
hexachlorobenzene		000118-74-1	0				0					0				
naphthalene		000091-20-3	0				1	<	2E-019			1		6.4E-015		
acenaphthene		000083-32-9	0				0					0				
acenaphthylene		000208-96-8	1	2.52E-016		0.045	0					0				
fluorene		000086-73-7	0				0					0				
phenanthrene		000085-01-8	0				0					0				
anthracene		000120-12-7	0				0					0				
pyrene		000129-00-0	0				0					0				
fluoranthene		000206-44-0	0				0					0				
chrysene		000218-01-9	0				0					0				
benz [a] anthracene		000056-55-3	0				0					0				
benzo [b] fluoranthene		000205-99-2	0				0					0				
benzo [j] fluoranthene		000205-82-3	0				0					0				
benzo [k] fluoranthene		000207-08-9	0				0					0				
benzo [a] pyrene		000050-32-8	0				0					0				
benzo [e] pyrene		000192-97-2	0				0					0				
perylene		000198-55-0	0				0					0				
benzo [g,h,i] perylene		000191-24-2	0				0					0				
dibenz [a,h] anthracene		000053-70-3	0				0					0				
indeno [1,2,3-c,d] pyrene		000193-39-5	0				0					0				
2,3,7,8-TCDD		001746-01-6	0				0					0				
1,2,3,7,8-PeCDD		040321-76-4	0				0					0				
1,2,3,4,7,8-HxCDD		039227-28-6	0				0					0				
1,2,3,6,7,8-HxCDD		057653-85-7	0				0					0				
1,2,3,7,8,9-HxCDD		019408-74-3	0				0					0				
1,2,3,4,6,7,8-HpCDD		035822-46-9	0				0					0				
OCDD		003268-87-9	0				0					0				
2,3,7,8-TCDF		051207-31-9	0				0					0				
2,3,4,7,8-PeCDF		057117-31-4	0				0					0				
1,2,3,7,8-PeCDF		057117-41-6	0				0					0				
1,2,3,4,7,8-HxCDF		070648-26-9	0				0					0				
1,2,3,6,7,8-HxCDF		057117-44-9	0				0					0				
1,2,3,7,8,9-HxCDF		072918-21-9	0				0					0				
2,3,4,6,7,8-HxCDF		060851-34-5	0				0					0				
1,2,3,4,6,7,8-HpCDF		067562-39-4	0				0					0				
1,2,3,4,7,8,9-HpCDF		055673-89-7	0				0					0				
OCDF		039001-02-0	0				0					0				
biphenyl	0	000092-52-4	0				1	<	*************			0				
2-PCB	1	002051-60-7	0				0					0				
3-PCB	2	002051-61-8	0				0					0				

								EXPT'L: RXN RATE with O3 cm3/(molecule-sec)					EXPT'L: RXN RATE with NO3 cm3/(molecule-sec)			
Chemical Name	IUPAC #	Best CAS #	did AOPWIN estimate rxn with ozone?	estimated rxn rate with ozone cm3/ molec.-sec	estimated half-life (days) assuming 24 hours/day and [O3]= 7.0E+011 molec/cm3	estimated half-life (days) assuming 24 hours/day and [O3]= 7.0E+011 molec/cm3	exist?	<?	AVG Expt'l O3 Value	LOW Expt'l O3 Value	HIGH Expt'l O3 Value	exist?	<?	AVG Expt'l NO3 Value	LOW Expt'l NO3 Value	HIGH Expt'l NO3 Value
4-PCB	3	002051-62-9	0				0					0				
2,2'-PCB	4	013029-08-8	0				0					0				
2,3-PCB	5	016605-91-7	0				0					0				
2,4-PCB	7	033284-50-3	0				0					0				
2,4'-PCB	8	034883-43-7	0				0					0				
2,5-PCB	9	034883-39-1	0				0					0				
2,6-PCB	10	033146-45-1	0				0					0				
3,3'-PCB	11	002050-67-1	0				0					0				
3,4-PCB	12	002974-92-7	0				0					0				
3,5-PCB	14	034883-41-5	0				0					0				
4,4'-PCB	15	002050-68-2	0				0					0				
2,2',3-PCB	16	038444-78-9	0				0					0				
2,2',5-PCB	18	037680-65-2	0				0					0				
2,3,3'-PCB	20	038444-84-7	0				0					0				
2,3,4-PCB	21	055702-46-0	0				0					0				
2,3',5-PCB	26	038444-85-8	0				0					0				
2,4,4'-PCB	28	007012-37-5	0				0					0				
2,4,5-PCB	29	015862-07-4	0				0					0				
2,4,6-PCB	30	035693-92-6	0				0					0				
2,4',5,-PCB	31	016606-02-3	0				0					0				
2',3,4-PCB	33	038444-86-9	0				0					0				
3,3',4-PCB	35	037680-69-6	0				0					0				
3,4,4'-PCB	37	038444-90-5	0				0					0				
2,2',3,3'-PCB	40	038444-93-8	0				0					0				
2,2',3,5'-PCB	44	041464-39-5	0				0					0				
2,2',4,4'-PCB	47	002437-79-8	0				0					0				
2,2',4,5'-PCB	49	041464-40-8	0				0					0				
2,2',4,6-PCB	50	062796-65-0	0				0					0				
2,2',4,6'-PCB	51	068194-04-7	0				0					0				
2,2,5,5'-PCB	52	035693-99-3	0				0					0				
2,2,5,6'-PCB	53	041464-41-9	0				0					0				
2,2,6,6'-PCB	54	015968-05-5	0				0					0				
2,3,4,4'-PCB	60	033025-41-1	0				0					0				
2,3,4,5-PCB	61	033284-53-6	0				0					0				
2,3,5,6-PCB	65	033284-54-7	0				0					0				
2,3,4,4'-PCB	66	032598-10-0	0				0					0				
2,3',4',5-PCB	70	032598-11-1	0				0					0				
2,4,4',6-PCB	75	032598-12-2	0				0					0				
3,3',4,4'-PCB	77	032598-13-3	0				0					0				
3,3',5,5'-PCB	80	033284-52-5	0				0					0				
3,4,4',5-PCB	81	070362-50-4	0				0					0				
2,2',3,3',5-PCB	83	060145-20-2	0				0					0				
2,2',3,4,5-PCB	86	065510-45-4	0				0					0				
2,2',3,4,5'-PCB	87	038380-02-8	0				0					0				
2,2',3,4,6-PCB	88	055215-17-3	0				0					0				
2,2',3,5,6-PCB	95	038379-99-6	0				0					0				
2,2',4,4',5-PCB	99	038380-01-7	0				0					0				
2,2',4,4',6-PCB	100	039485-83-1	0				0					0				
2,2',4,5,5'-PCB	101	037680-73-2	0				0					0				
2,2',4,6,6'-PCB	104	056558-16-8	0				0					0				
2,3,3',4,4'-PCB	105	032598-14-4	0				0					0				
2,3,3',4',6-PCB	110	038380-03-9	0				0					0				

Chemical Name	IUPAC #	Best CAS #	did AOPWIN estimate rxn with ozone?	estimated rxn rate with ozone cm3/ molec.-sec	estimated half-life (days) assuming 24 hours/day and [O3]= 7.0E+011 molec/cm3	estimated half-life (days) assuming 24 hours/day and [O3]= 7.0E+011 molec/cm3	exist?	<?	AVG Expt'l O3 Value	LOW Expt'l O3 Value	HIGH Expt'l O3 Value	exist?	<?	AVG Expt'l NO3 Value	LOW Expt'l NO3 Value	HIGH Expt'l NO3 Value
									EXPT'L: RXN RATE with O3 cm3/(molecule-sec)					**EXPT'L: RXN RATE with NO3 cm3/(molecule-sec)**		
2,3,4,4',5-PCB	114	074472-37-0	0				0					0				
2,3,4,5,6-PCB	116	018259-05-7	0				0					0				
2,3',4,4',5-PCB	118	031508-00-6	0				0					0				
2',3,4,5,5'-PCB	124	070424-70-3	0				0					0				
3,3',4,4',5-PCB	126	057465-28-8	0				0					0				
2,2',3,3',4,4'-PCB	128	038380-07-3	0				0					0				
2,2',3,3',4,5-PCB	129	055215-18-4	0				0					0				
2,2',3,3',5,6-PCB	134	052704-70-8	0				0					0				
2,2',3,3',6,6'-PCB	136	038411-22-2	0				0					0				
2,2',3,4,4',5'-PCB	138	035065-28-2	0				0					0				
2,2',3,4',5',6-PCB	149	038380-04-0	0				0					0				
2,2',4,4',5,5'-PCB	153	035065-27-1	0				0					0				
2,2',4,4',6,6'-PCB	155	033979-03-2	0				0					0				
2,3,3',4,4',5-PCB	156	038380-08-4	0				0					0				
2,3,3',4,4',5'-PCB	157	069782-90-7	0				0					0				
2,3',4,4',5,5'-PCB	167	052663-72-6	0				0					0				
3,3',4,4',5,5'-PCB	169	032774-16-6	0				0					0				
2,2',3,3',4,4',5-PCB	170	035065-30-6	0				0					0				
2,2',3,3',4,4',6-PCB	171	052663-71-5	0				0					0				
2,2',3,4,4',5,5'-PCB	180	035065-29-3	0				0					0				
2,2',3,4,5,5',6-PCB	185	052712-05-7	0				0					0				
2,2',3,4',5,5',6-PCB	187	052663-68-0	0				0					0				
2,3,3',4,4',5,5'-PCB	189	039635-31-9	0				0					0				
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7	0				0					0				
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4	0				0					0				
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9	0				0					0				
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3	0				0					0				
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1	0				0					0				
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3	0				0					0				

Appendix D.3.

Atmospheric Lifetime Relative to Gas Phase Reaction Rates, Adjusted for Vapor Particle Partitioning

NAME			**ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)**					
common chemical name	IUPAC #	cas # (1)	AVG Expt'l OH Value cm3/ (molec.-sec)	Reaction Rate Estimate with Hydroxyl cm3/ (molecule-sec)	estm OH 1/2-life (days) assuming **12** hours/day and [OH]= **1.5E+006** molecules/cm3	estimated rxn rate with ozone cm3/ molec.-sec	estm O3 1/2-life (days) assuming **24** hours/day and [O3]= **7.0E+011** molecules/cm3	mimimum half-life (rxn w OH or O3) divided by fraction in gas phase (days)
octachlorostyrene		029082-74-4		1.07E-012	9.968	6.14E-020	186.657	9.996
4-bromophenyl phenyl ether		000101-55-3		6.33E-012	1.690			1.691
3,3'-dichlorobenzidene		000091-94-1		3.96E-011	0.270			2.618
1,3-dinitropyrene		075321-20-9		5.46E-013	19.591			30.086
1,6-dinitropyrene		042397-64-8		5.46E-013	19.591			30.086
1,8-dinitropyrene		042397-65-9		5.46E-013	19.591			30.086
2,7-dinitropyrene		117929-15-4		5.46E-013	19.591			30.086
dinitropyrenes (mixed)		078432-19-6						
hexachloro-1,3-butadiene		000087-68-3		3.00E-014	356.320	7.00E-023	163725.241	356.321
4,4'-methylene bis(2-chloroaniline)		000101-14-4		7.75E-011	0.138			0.139
pentachlorophenol		000087-86-5		5.50E-013	19.431			19.444
aldrin		000309-00-2		6.46E-011	0.166	2.00E-016	0.057	0.057
dieldrin		000060-57-1		8.84E-012	1.210	3.58E-020	320.223	1.214
p,p'-DDT		000050-29-3		3.44E-012	3.114			4.371
p,p'-DDD		000072-54-8		4.34E-012	2.462			2.699
p,p'-DDE		000072-55-9		7.43E-012	1.440	5.15E-018	2.224	1.475
heptachlor		000076-44-8		6.13E-011	0.174	2.00E-016	0.057	0.057
heptachlor epoxide		001024-57-3		3.85E-012	2.779	3.58E-020	320.223	2.785
methoxychlor		000072-43-5		5.35E-011	0.200			0.221
mirex		002385-85-5						
toxaphene		008001-35-2		2.50E-012	4.286			4.790
endrin		000072-20-8		8.84E-012	1.210	3.58E-020	320.223	1.212
alpha-hexachlorocyclohexane		000319-84-6		5.73E-013	18.660			18.671
beta-hexachlorocyclohexane		000319-85-7		5.73E-013	18.660			18.689
delta-hexachlorocyclohexane		000319-86-8		5.73E-013	18.660			18.682
gamma-hexachlorocyclohexane		000058-89-9		5.73E-013	18.660			18.713
mixed hexachlorocyclohexanes		000319-84-6		5.73E-013	18.660			18.660

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)

NAME common chemical name	IUPAC #	cas # (1)	AVG Expt'l OH Value cm3/ (molec.-sec)	Reaction Rate Estimate with Hydroxyl cm3/ (molecule-sec)	estm OH 1/2-life (days) assuming **12** hours/day and [OH]= **1.5E+006** molecules/cm3	estimated rxn rate with ozone cm3/ molec.-sec	estm O3 1/2-life (days) assuming **24** hours/day and [O3]= **7.0E+011** molecules/cm3	mimimum half-life (rxn w OH or O3) divided by fraction in gas phase (days)
cadmium		007440-43-9						
cadmium carbonate		000513-78-0						
cadmium chloride		010108-64-2						
cadmium oxide		001306-19-0						
cadmium sulfate		010124-36-4						
cadmium sulfide		001306-23-6						
elemental mercury		007439-97-6						
mercury oxide		021908-53-2						
mercuric chloride		007487-94-7						
monomethyl mercury chloride		000115-09-3		8.16E-012	1.311			1.311
dimethyl mercury		000593-74-8	1.90E-011	1.63E-011	0.655			0.655
tetraethyl lead		000078-00-2	6.00E-011	4.92E-011	0.217			0.217
tetramethyl lead		000075-74-1	6.00E-012	7.07E-012	1.513			1.513
triethyl lead radical (1+ cation)		014570-15-1		3.69E-011	0.290			
triethyl lead hydride		005224-23-7		3.69E-011	0.290			
triethyl lead chloride		001067-14-7		3.69E-011	0.290			
diethyl lead radical (2+ cation)		024952-65-6		2.46E-011	0.434			
diethyl lead dihydride		081494-11-3		2.46E-011	0.434			
diethyl lead dichloride		013231-90-8		2.46E-011	0.434			
trimethyl lead radical (1+ cation)		014570-16-2		5.30E-012	2.017			
trimethyl lead hydride		007442-13-9		5.30E-012	2.017			
trimethyl lead chloride		001520-78-1		5.30E-012	2.017			
dimethyl lead radical (2+ cation)		021774-13-0		3.54E-012	3.025			
dimethyl lead dihydride		030691-92-0						
dimethyl lead dichloride		001520-77-0		3.54E-012	3.025			
bis (tributyltin) oxide		000056-35-9		8.53E-011	0.125			0.239
tributyl tin		000688-75-3						
tributyltin fluoride		001983-10-4		4.27E-011	0.251			
tributyltin chloride		001461-22-9		4.27E-011	0.251			
tributyltin hydroxide		001067-97-6		4.28E-011	0.250			
tributyltin naphthenate								
tris(tributylstannyl) phosphate		013435-05-7						

NAME			**ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)**					
common chemical name	IUPAC #	cas # (1)	AVG Expt'l OH Value cm3/ (molec.-sec)	Reaction Rate Estimate with Hydroxyl cm3/ (molecule-sec)	estm OH 1/2-life (days) assuming **12** hours/day and [OH]= **1.5E+006** molecules/cm3	estimated rxn rate with ozone cm3/ molec.-sec	estm O3 1/2-life (days) assuming **24** hours/day and [O3]= **7.0E+011** molecules/cm3	mimimum half-life (rxn w OH or O3) divided by fraction in gas phase (days)
1,4-dichlorobenzene		000106-46-7	3.20E-013	4.00E-013	26.710			26.710
1,2,3,4-tetrachlorobenzene		000634-66-2		8.23E-014	130.051			130.052
1,2,4,5-tetrachlorobenzene		000095-94-3		8.23E-014	130.051			130.052
1,2,3,5-tetrachlorobenzene		000634-90-2		1.98E-013	53.975			53.975
pentachlorobenzene		000608-93-5		5.79E-014	184.872			184.889
hexachlorobenzene		000118-74-1		1.69E-014	633.317			633.516
naphthalene		000091-20-3	2.16E-011	2.16E-011	0.495			0.495
acenaphthene		000083-32-9	7.85E-011	6.72E-011	0.159			0.159
acenaphthylene		000208-96-8	1.10E-010	7.55E-011	0.142	2.52E-016	0.045	0.045
fluorene		000086-73-7	1.20E-011	9.00E-012	1.188			1.189
phenanthrene		000085-01-8	1.30E-011	1.30E-011	0.823			0.823
anthracene		000120-12-7	4.00E-011	4.00E-011	0.267			0.268
pyrene		000129-00-0	5.00E-011	5.00E-011	0.214			0.215
fluoranthene		000206-44-0	5.00E-011	2.92E-011	0.366			0.370
chrysene		000218-01-9		5.00E-011	0.214			0.384
benz [a] anthracene		000056-55-3		5.00E-011	0.214			0.432
benzo [b] fluoranthene		000205-99-2		1.86E-011	0.577			0.608
benzo [j] fluoranthene		000205-82-3		5.36E-011	0.200			0.575
benzo [k] fluoranthene		000207-08-9		5.36E-011	0.200			4.573
benzo [a] pyrene		000050-32-8		5.00E-011	0.214			1.158
benzo [e] pyrene		000192-97-2		5.00E-011	0.214			1.101
perylene		000198-55-0		5.00E-011	0.214			4.547
benzo [g,h,i] perylene		000191-24-2		8.69E-011	0.123			2.802
dibenz [a,h] anthracene		000053-70-3		5.00E-011	0.214			213.199
indeno [1,2,3-c,d] pyrene		000193-39-5		6.45E-011	0.166			31.840

NAME			**ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)**					
common chemical name	IUPAC #	cas # (1)	AVG Expt'l OH Value cm3/ (molec.-sec)	Reaction Rate Estimate with Hydroxyl cm3/ (molecule-sec)	estm OH 1/2-life (days) assuming **12** hours/day and [OH]= **1.5E+006** molecules/cm3	estimated rxn rate with ozone cm3/ molec.-sec	estm O3 1/2-life (days) assuming **24** hours/day and [O3]= **7.0E+011** molecules/cm3	mimimum half-life (rxn w OH or O3) divided by fraction in gas phase (days)
2,3,7,8-TCDD		001746-01-6		2.02E-012	5.292			12.831
1,2,3,7,8-PeCDD		040321-76-4		1.72E-012	6.214			138.871
1,2,3,4,7,8-HxCDD		039227-28-6		1.22E-012	8.781			541.159
1,2,3,6,7,8-HxCDD		057653-85-7		1.42E-012	7.523			463.641
1,2,3,7,8,9-HxCDD		019408-74-3		1.42E-012	7.523			463.641
1,2,3,4,6,7,8-HpCDD		035822-46-9		9.18E-013	11.646			5910.600
OCDD		003268-87-9		4.15E-013	25.767			23515.495
2,3,7,8-TCDF		051207-31-9		1.65E-013	65.018			93.174
2,3,4,7,8-PeCDF		057117-31-4		7.46E-014	143.465			895.754
1,2,3,7,8-PeCDF		057117-41-6		7.46E-014	143.465			895.754
1,2,3,4,7,8-HxCDF		070648-26-9		3.04E-013	35.239			1070.669
1,2,3,6,7,8-HxCDF		057117-44-9		3.59E-013	29.803			717.409
1,2,3,7,8,9-HxCDF		072918-21-9		3.38E-014	316.471			8548.215
2,3,4,6,7,8-HxCDF		060851-34-5		3.04E-013	35.189			950.489
1,2,3,4,6,7,8-HpCDF		067562-39-4		1.53E-014	698.675			112057.229
1,2,3,4,7,8,9-HpCDF		055673-89-7		1.53E-014	699.132			120715.569
OCDF		039001-02-0		6.94E-015	1541.314			1420877.201

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)

NAME common chemical name	IUPAC #	cas # (1)	AVG Expt'l OH Value cm3/ (molec.-sec)	Reaction Rate Estimate with Hydroxyl cm3/ (molecule-sec)	estm OH 1/2-life (days) assuming **12** hours/day and [OH]= **1.5E+006** molecules/cm3	estimated rxn rate with ozone cm3/ molec.-sec	estm O3 1/2-life (days) assuming **24** hours/day and [O3]= **7.0E+011** molecules/cm3	mimimum half-life (rxn w OH or O3) divided by fraction in gas phase (days)
biphenyl	0	000092-52-4	7.20E-012	6.77E-012	1.579			1.579
2-PCB	1	002051-60-7	2.82E-012	3.48E-012	3.070			3.070
3-PCB	2	002051-61-8	5.28E-012	4.88E-012	2.193			2.193
4-PCB	3	002051-62-9	3.86E-012	3.48E-012	3.070			3.070
count				3	3			3
average				**3.95E-012**	**2.78E+000**			**2.78E+000**
standard deviation				6.57E-013	4.13E-001			4.13E-001
minimum				3.48E-012	2.19E+000			2.19E+000
maximum				4.88E-012	3.07E+000			3.07E+000
2,2'-PCB	4	013029-08-8	2.00E-012	1.73E-012	6.194			6.197
2,3-PCB	5	016605-91-7		2.47E-012	4.325			4.329
2,4-PCB	7	033284-50-3	2.60E-012	2.47E-012	4.336			4.340
2,4'-PCB	8	034883-43-7		1.73E-012	6.194			6.199
2,5-PCB	9	034883-39-1		2.47E-012	4.325			4.328
2,6-PCB	10	033146-45-1		2.47E-012	4.336			4.338
3,3'-PCB	11	002050-67-1	4.10E-012	3.51E-012	3.046			3.051
3,4-PCB	12	002974-92-7		2.47E-012	4.325			4.333
3,5-PCB	14	034883-41-5	4.20E-012	3.45E-012	3.097			3.101
4,4'-PCB	15	002050-68-2	2.00E-012	1.73E-012	6.194			6.206
count				10	10			10
average				**2.45E-012**	**4.64E+000**			**4.64E+000**
standard deviation				6.09E-013	1.12E+000			1.13E+000
minimum				1.73E-012	3.05E+000			3.05E+000
maximum				3.51E-012	6.19E+000			6.21E+000

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)

NAME common chemical name	IUPAC #	cas # (1)	AVG Expt'l OH Value cm3/ (molec.-sec)	Reaction Rate Estimate with Hydroxyl cm3/ (molecule-sec)	estm OH 1/2-life (days) assuming **12** hours/day and [OH]= **1.5E+006** molecules/cm3	estimated rxn rate with ozone cm3/ molec.-sec	estm O3 1/2-life (days) assuming **24** hours/day and [O3]= **7.0E+011** molecules/cm3	mimimum half-life (rxn w OH or O3) divided by fraction in gas phase (days)
2,2',3-PCB	16	038444-78-9		1.09E-012	9.807			9.832
2,2',5-PCB	18	037680-65-2		1.09E-012	9.807			9.825
2,3,3'-PCB	20	038444-84-7		1.76E-012	6.067			6.099
2,3,4-PCB	21	055702-46-0		1.26E-012	8.523			8.568
2,3',5-PCB	26	038444-85-8		1.09E-012	9.807			9.842
2,4,4'-PCB	28	007012-37-5	1.10E-012	1.19E-012	9.023			9.061
2,4,5-PCB	29	015862-07-4	1.30E-012	1.26E-012	8.523			8.550
2,4,6-PCB	30	035693-92-6		1.54E-012	6.960			6.970
2,4',5,-PCB	31	016606-02-3	1.20E-012	1.09E-012	9.806			9.858
2',3,4-PCB	33	038444-86-9	1.00E-012	1.09E-012	9.807			9.861
3,3',4-PCB	35	037680-69-6		1.76E-012	6.067			6.134
3,4,4'-PCB	37	038444-90-5		1.09E-012	9.806			9.924
count				12	12			12
average				**1.28E-012**	**8.67E+000**			**8.71E+000**
standard deviation				2.51E-013	1.43E+000			1.43E+000
minimum				1.09E-012	6.07E+000			6.10E+000
maximum				1.76E-012	9.81E+000			9.92E+000
2,2',3,3'-PCB	40	038444-93-8		7.30E-013	14.650			14.876
2,2',3,5'-PCB	44	041464-39-5	8.00E-013	7.30E-013	14.650			14.823
2,2',4,4'-PCB	47	002437-79-8	1.00E-012	8.13E-013	13.151			13.280
2,2',4,5'-PCB	49	041464-40-8		7.72E-013	13.860			13.984
2,2',4,6-PCB	50	062796-65-0		8.27E-013	12.942			13.514
2,2',4,6'-PCB	51	068194-04-7		8.13E-013	13.150			13.229
2,2,5,5'-PCB	52	035693-99-3		7.30E-013	14.650			14.787
2,2,5,6'-PCB	53	041464-41-9		7.72E-013	13.860			13.934
2,2,6,6'-PCB	54	015968-05-5		8.13E-013	13.150			13.197
2,3,4,4'-PCB	60	033025-41-1		5.77E-013	18.552			19.100
2,3,4,5-PCB	61	033284-53-6		8.05E-013	13.286			13.457
2,3,5,6-PCB	65	033284-54-7		8.05E-013	13.286			13.429
2,3,4,4'-PCB	66	032598-10-0		7.72E-013	13.860			14.205
2,3',4',5-PCB	70	032598-11-1		7.30E-013	14.650			15.072
2,4,4',6-PCB	75	032598-12-2		8.27E-013	12.942			13.050
3,3',4,4'-PCB	77	032598-13-3		7.30E-013	14.650			15.728
3,3',5,5'-PCB	80	033284-52-5		1.76E-012	6.081			6.262
3,4,4',5-PCB	81	070362-50-4		7.60E-013	14.078			14.880
count				18	18			18
average				**8.20E-013**	**1.36E+001**			**1.39E+001**
standard deviation				2.35E-013	2.22E+000			2.31E+000
minimum				5.77E-013	6.08E+000			6.26E+000
maximum				1.76E-012	1.86E+001			1.91E+001

ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)

NAME

common chemical name	IUPAC #	cas # (1)	AVG Expt'l OH Value cm3/ (molec.-sec)	Reaction Rate Estimate with Hydroxyl cm3/ (molecule-sec)	estm OH 1/2-life (days) assuming **12** hours/day and [OH]= **1.5E+006** molecules/cm3	estimated rxn rate with ozone cm3/ molec.-sec	estm O3 1/2-life (days) assuming **24** hours/day and [O3]= **7.0E+011** molecules/cm3	mimimum half-life (rxn w OH or O3) divided by fraction in gas phase (days)
2,2',3,3',5-PCB	83	060145-20-2		4.73E-013	22.619			23.962
2,2',3,4,5-PCB	86	065510-45-4		4.00E-013	26.769			28.321
2,2',3,4,5'-PCB	87	038380-02-8		3.35E-013	31.949			34.217
2,2',3,4,6-PCB	88	055215-17-3		4.18E-013	25.590			26.261
2,2',3,5,6-PCB	95	038379-99-6	4.00E-013	3.35E-013	31.949			32.890
2,2',4,4',5-PCB	99	038380-01-7		4.00E-013	26.769			28.210
2,2',4,4',6-PCB	100	039485-83-1		5.67E-013	18.867			25.102
2,2',4,5,5'-PCB	101	037680-73-2		3.35E-013	31.949			33.463
2,2',4,6,6'-PCB	104	056558-16-8		5.67E-013	18.867			19.987
2,3,3',4,4'-PCB	105	032598-14-4		3.35E-013	31.949			38.137
2,3,3',4',6-PCB	110	038380-03-9	6.00E-013	3.35E-013	31.949			34.753
2,3,4,4',5-PCB	114	074472-37-0		3.99E-013	26.840			30.426
2,3,4,5,6-PCB	116	018259-05-7	9.00E-013	5.28E-013	20.254			21.666
2,3',4,4',5-PCB	118	031508-00-6		3.35E-013	31.949			36.389
2',3,4,5,5'-PCB	124	070424-70-3		4.73E-013	22.620			27.409
3,3',4,4',5-PCB	126	057465-28-8		4.73E-013	22.619			30.830
count				16	16			16
average				**4.19E-013**	**2.65E+001**			**2.95E+001**
standard deviation				8.22E-014	4.87E+000			5.13E+000
minimum				3.35E-013	1.89E+001			2.00E+001
maximum				5.67E-013	3.19E+001			3.81E+001
2,2',3,3',4,4'-PCB	128	038380-07-3		1.64E-013	65.224			98.009
2,2',3,3',4,5-PCB	129	055215-18-4		2.11E-013	50.695			70.288
2,2',3,3',5,6-PCB	134	052704-70-8		2.11E-013	50.695			57.559
2,2',3,3',6,6'-PCB	136	038411-22-2		1.64E-013	65.224			71.571
2,2',3,4,4',5'-PCB	138	035065-28-2		1.64E-013	65.224			86.919
2,2',3,4',5',6-PCB	149	038380-04-0		1.64E-013	65.224			74.853
2,2',4,4',5,5'-PCB	153	035065-27-1		1.64E-013	65.224			81.448
2,2',4,4',6,6'-PCB	155	033979-03-2		3.95E-013	27.071			28.144
2,3,3',4,4',5-PCB	156	038380-08-4		2.11E-013	50.695			91.501
2,3,3',4,4',5'-PCB	157	069782-90-7		2.34E-013	45.712			86.540
2,3',4,4',5,5'-PCB	167	052663-72-6		2.34E-013	45.714			74.620
3,3',4,4',5,5'-PCB	169	032774-16-6		3.04E-013	35.189			136.891
count				12	12			12
average				**2.18E-013**	**5.27E+001**			**7.99E+001**
standard deviation				6.71E-014	1.24E+001			2.45E+001
minimum				1.64E-013	2.71E+001			2.81E+001
maximum				3.95E-013	6.52E+001			1.37E+002

NAME			ATMOSPHERIC HALFLIFE RELATIVE to RXN with OH (with some data for rxn with O3 also included)					
			AVG Expt'l OH Value cm3/ (molec.-sec)	Reaction Rate Estimate with Hydroxyl cm3/ (molecule-sec)	estm OH 1/2-life (days) assuming **12** hours/day and [OH]= **1.5E+006** molecules/cm3	estimated rxn rate with ozone cm3/ molec.-sec	estm O3 1/2-life (days) assuming **24** hours/day and [O3]= **7.0E+011** molecules/cm3	mimimum half-life (rxn w OH or O3) divided by fraction in gas phase (days)
common chemical name	IUPAC #	cas # (1)						
2,2',3,3',4,4',5-PCB	170	035065-30-6		1.05E-013	102.253			321.332
2,2',3,3',4,4',6-PCB	171	052663-71-5		1.18E-013	90.712			177.181
2,2',3,4,4',5,5'-PCB	180	035065-29-3		1.05E-013	102.253			242.250
2,2',3,4,5,5',6-PCB	185	052712-05-7		1.24E-013	86.063			133.420
2,2',3,4',5,5',6-PCB	187	052663-68-0		1.05E-013	102.253			160.382
2,3,3',4,4',5,5'-PCB	189	039635-31-9		1.40E-013	76.372			377.695
count				6	6			6
average				**1.16E-013**	**9.33E+001**			**2.35E+002**
standard deviation				1.32E-014	9.88E+000			8.86E+001
minimum				1.05E-013	7.64E+001			1.33E+002
maximum				1.40E-013	1.02E+002			3.78E+002
2,2',3,3',4,4',5,5'-PCB	194	035694-08-7		5.59E-014	191.457			2010.704
2,2',3,3',5,5',6,6'-PCB	202	002136-99-4		5.59E-014	191.457			254.537
count				2	2			2
average				**5.59E-014**	**1.91E+002**			**1.13E+003**
standard deviation				0.00E+000	0.00E+000			8.78E+002
minimum				5.59E-014	1.91E+002			2.55E+002
maximum				5.59E-014	1.91E+002			2.01E+003
2,2',3,3',4,4',5,5',6-PCB	206	040186-72-9		3.29E-014	325.227			6317.514
2,2',3,3',4,4',5,6,6'-PCB	207	052663-79-3		4.35E-014	245.958			1659.813
2,2',3,3',4,5,5',6,6'-PCB	208	052663-77-1		3.29E-014	325.227			2282.857
count				3	3			3
average				**3.64E-014**	**2.99E+002**			**3.42E+003**
standard deviation				5.00E-015	3.74E+001			2.06E+003
minimum				3.29E-014	2.46E+002			1.66E+003
maximum				4.35E-014	3.25E+002			6.32E+003
2,2',3,3',4,4',5,5',6,6'-PCB	209	002051-24-3		1.82E-014	588.702			8674.359

Appendix D.4.

Information about Atmospheric Photolysis (i.e., Destruction by UV Light)

Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study

Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	**Information Regarding Atmospheric Photolysis** All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
METALS / ORGANOMETALLICS			
Alkylated Lead TEL = Tetraethyl Lead TML = Tetramethyl Lead	I	**0.000002** (TEL) (0.00000007 - 0.00004)	
		0.00000003 (TML) (1e-9 - 0.00004)	
Mercury	I	**0.0005** (Hg) (0.00001 - 0.02)	The main atmospheric transformation process for organomercurials appears to be photolysis (EPA 1984b; Johnson and Bramen 1974; Williston 1968).
		0.0000004 ($HgCl_2$) (0.00000003 - 0.000003)	
		0.000003 ($HgCH_3Cl$ (0.0000002 - 0.00004)	
Cadmium	II	**1** (Cd) (0.8 - 1)	
		1 ($CdCl_2$)	
Tributyltin TBTO = Tributyltin Oxide	II	**0.5** (TBTO) (0.02 -0.98)	[in water:] Tributyltin has been shown to undergo slow photolysis (Maguire et al. 1983). The half-life of the photolysis reaction was estimated to be greater than 89 days. The direct photolysis of tributyltin in water initiates a sequential removal of the butyl groups, leading to inorganic tin as a residual. The reaction was much faster in the presence of fulvic acid (a major component of soil organic matter). The overall half-life of tributyltin (photolysis and biodegradation) in water was estimated to be on the order of months in Canadian lakes. However, the half-life of tributyltin in river waters in Georgia was estimated to be between 3 and 13 days (Lee et al. 1989). The degradation of the chemical was attributed to microalgae whereas direct photolysis did not appear to be important.

Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study

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ORGANOCHLORINE BIOCIDES			
Aldrin / Dieldrin	I	**0.0009** (Aldrin) (0.00004 - 0.02)	While the evidence supports the view that a considerable proportion of the aldrin and dieldrin used in agriculture reaches the atmosphere, it seems probable that atmospheric degradation prevents accumulation of aldrin. In laboratory studies, aldrin is photochemically isomerized and epoxidated by sunlight to photoaldrin, dieldrin, or photodieldrin (Glotfelty 1978). Irradiation of aldrin (5 mg) vapor with ultraviolet light for 45 hours resulted in the formation of photoaldrin (20-30 mg) and dieldrin (50-60 mg). [IN WATER:] Aldrin, irradiated with ultraviolet light in an oxygenated aqueous solution, underwent little change except in the presence of amino acids and humic acids present in natural waters (Ross and Crosby 1975, 1985). In filtered natural field water, aldrin was photooxidized by 75% to dieldrin after 48 hours of irradiation at 238 nm (Ross and Crosby 1985).
		0.003 (Dieldrin) (0.0002 - 0.03)	Irradiation of either photoaldrin (2 mg) or dieldrin (0.5 mg) vapor for 65 hours and 91 minutes, respectively, resulted in a single photoproduct, photodieldrin (20-30 mg), which was resistant to further photolyses (Crosby and Moilanen 1974). **Since photodieldrin no longer contains a chromophore**, it is believed to be a stable photoproduct of aldrin (dieldrin) (Glotfelty 1978). However, results of a laboratory study showed that photolysis of photoaldrin and photodieldrin in the presence of triethylamine gave photometabolites arising from the loss of chlorine atoms (Dureja et al. 1986). Information regarding the persistence of photodieldrin in the atmosphere was not located; however, air samples taken in 1973 in Ireland contained dieldrin, but neither aldrin nor the photoproducts of aldrin or dieldrin were detected (Baldwin et al. 1977). The estimated lifetime of dieldrin in the atmosphere, based on reactions with atmospheric hydroxyl radicals, is approximately 1 day. However, dieldrin may be more stable than implied by this lifetime if it is associated with particulate matter in the atmosphere. Under these conditions, wet and dry deposition may be more important loss processes (Bidleman et al. 1990). [IN WATER:] More than 80% of the initial dieldrin added to natural water (from a drainage canal in an agricultural area) was present after 16 weeks of incubation in the dark (Sharon et al. 1980). Dieldrin exposed to sunlight is converted to photodieldrin, a stereoisomer of dieldrin. It is unlikely that photodieldrin occurs widely in the environment. Microorganisms isolated from lake water and lake-bottom sediments may convert dieldrin to photodieldrin under anaerobic conditions (Fries 1972). Dieldrin has been found to undergo minor degradation to photodieldrin in marine environments. The marine algae of the genus Dunaliella had the maximum degradation activity, degrading 23% of aldrin to dieldrin and 8.5% of dieldrin to photodieldrin (Patil et al. 1972).

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DDT / DDD / DDE	I	**0.3** (DDT) (0.03 - 0.8)	Environmental processes contribute to the degradation and transformation of DDT to different extents. Under simulated atmospheric conditions, both DDT and DDE decompose to form carbon dioxide and hydrochloric acid (WHO 1979). **In air and sunlight, DDT is subject to direct photooxidation and reaction with photochemically produced hydroxyl radicals. The latter process has an estimated half-life of 2 days.** **Since DDT residues are ubiquitous in the atmosphere, it seems likely that photodegradation must occur at a slower rate than this estimated half-life.** DDT which reaches the photochemically active ionosphere may be rapidly destroyed by solar irradiation as indicated under laboratory conditions (Coulston 1985). IN WATER: DDT present in water may be converted by both photodegradation and biodegradation. **DDE in water absorbs short-wavelength ultraviolet sunlight (<320 nm) and undergoes rapid photolysis. The photolysis half-life of DDE ranges from 0.94 to 6.1 days depending on the season.** DDE also undergoes photoisomerization when exposed to sunlight. Photolysis of DDE photoisomers is slower by at least one order of magnitude compared to DDE (Coulston 1985; Zepp et al. 1977). Biodegradation of DDT by aquatic microorganisms is reported to be a minor mechanism of transformation (Johnsen 1976).
		0.09 (DDD) (0.005 - 0.6)	
		0.02 (DDE) (0.001 - 0.3)	

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Mirex	I	**0.00002** (0.000001 - 0.0005)	Little information was found on the degradation of mirex in the atmosphere. Mirex is expected to be stable against photogenerated hydroxyl radicals in the atmosphere (Eisenreich et al. 1981). **(Photolysis of chlordecone in the atmosphere does not appear to be an important degradation pathway for this compound).; While nonvolatile products of photolysis were not monitored, only 1.8% of the chlordecone adsorbed on silica gel and exposed to ultraviolet light (wavelength >290 nm) was photolyzed to carbon dioxide or other volatile compounds (Freitag et al. 1985)).** 5.3.2.2 Water **The degradation of mirex in water occurs primarily by photolysis.** During the photodecomposition of mirex, the chlorine atoms are replaced by hydrogen atoms. The primary photoreduction product of mirex in water is photomirex (Andrade et al. 1975); the rate of this reaction can be increased by the presence of dissolved organic matter (such as humic acids) and was greatest at 265 nm in Lake Ontario water (Mudami and Hassett 1988). In Lake Ontario, Mudambi et al. (1992) reported that the ratio of photomirex to mirex (P/M) increased in the stratified surface layer of the lake from spring until autumn and in water from Oswego Harbor. P/M ratios in the mirex source sediments (the Niagara and Oswego Rivers) were very low (<0.07), whereas higher P/M ratios were seen in the lake bottom sediments (>0.10) and surface waters (>0.30). These findings suggest that photomirex in Lake Ontario is produced by photolysis of mirex present in the surface waters and it is then partitioned between water, sediment, and biota.

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Toxaphene	I	**0.1** (0.004 - 0.8)	5.3.2.1 Air **Direct photolytic degradation of toxaphene in the troposphere apparently does not occur.** **No information was found regarding the susceptibility of toxaphene to free radical oxidation in the atmosphere.** **The worldwide, long-range atmospheric transport of the mixture suggests that toxaphene is relatively resistant to transformation in the atmosphere.** **Since the production of toxaphene involves exposing chlorinated camphenes to UV-radiation, the congeners in the final mixture are resistant to degradation from direct photolysis (EPA 1976a; Korte et al. 1979).** **Rapaport and Eisenreich (1986) cited an atmospheric residence time of 46-70 days for the mixture.** **They noted that the toxaphene found in peat cores taken from remote regions in the northern United States and Canada was deposited from the atmosphere in a relatively untransformed state.** 5.3.2.2 Water **Toxaphene is resistant to chemical and biological transformation in aerobic surface waters. It is not expected to undergo direct photolysis or photooxidation (EPA 1979a). Hydrolysis is also not an important fate process; a hydrolytic half-life of greater than 10 years for pH 5 to 8 and 25øC has been estimated (EPA 1976d).**

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Endrin	II	**0.001** (0.00007 - 0.02)	Laboratory studies have indicated that one common mechanism for the transformation and degradation of endrin in air, water, and soil under field conditions is via **photochemical reactions and rearrangements resulting from ultraviolet irradiation from sunlight** (EPA 1985e; Zabik et al. 1971). Photochemical isomerization of endrin, primarily to the pentacyclic ketone commonly called delta ketoendrin or endrin ketone, was observed after exposure of thin layers of solid endrin on glass to sunlight (Burton and Pollard 1974). Minor amounts of endrin aldehyde were also formed in this reaction. *Results of seasonal studies indicated that this isomerization would proceed with a half-life of 5-9 days in intense summer sunlight, with complete conversion to the pentacyclic ketone in 15-19 days.* Knoevenagel and Himmelreich (1976) reported that photodegradation of solid endrin in the laboratory proceeded with a half-life of 20-40 hours. In laboratory studies conducted by Zabik et al. (1971) on endrin formulations in hexane and cyclohexane (similar to those commonly used for pesticide applications), *endrin was found to undergo photolytic dechlorination when exposed to ultraviolet radiation*, yielding a pentachlorinated half-cage ketone as the major product. This degradation product was also detected in environmental samples. Endrin is also sensitive to transformation by heat, yielding primarily the pentacyclic ketone and endrin aldehyde at temperatures greater than 230øC (EPA 1979g; Phillips et al. 1962). 5.3.2.1 Air **Studies regarding photodegradation of endrin in the atmosphere have not been located.** Based on laboratory experiments on solid endrin (Burton and Pollard 1974) and on endrin in organic solvents (Zabik et al. 1971), it is likely that endrin in air will undergo photoisomerization to a ketoendrin, with minor amounts of endrin aldehyde also being formed. Endrin may also be transformed by heat in the atmosphere to the pentacylic ketone and endrin aldehyde (Phillips et al. 1962). Laboratory studies of the fate of endrin in water samples suggest a significant degree of stability... Studies in which sealed water samples from the Little Miami River were exposed to sunlight and artificial fluorescent light showed no measurable degradation of endrin over an 8-week period (Eichelberger and Lichtenberg 1971).

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Heptachlor / Heptachlor Epoxide	II	**0.0003** Hept. (0.00002 - 0.004)	**Heptachlor may undergo direct photolysis in sunlight and is also susceptible to photosensitized reactions (Graham et al. 1973; Ivie et al. 1972).** Heptachlor is hydrolyzed in surface water and distilled water to 1-hydroxychlordene. When heptachlor was added to a sample of river water maintained at room temperature and exposed to sunlight, only 25% remained after 1 week, and no heptachlor remained after the 2nd week. The 75% loss of heptachlor after 1 week corresponds to a half-life of 3.5 days. The products formed were identified as 1- hydroxychlordene and heptachlor epoxide. It was observed that an equilibrium exists at the end of 4 weeks between 1-hydroxychlordene and heptachlor epoxide, so that approximately 60% of the converted heptachlor remained as 1-hydroxychlordene and 40% was converted to the epoxide. When a 14C-heptachlor-treated model aquatic ecosystem was examined for transformation of heptachlor in water, the relative amounts of various transformation products in water were determined as the percentage of the total 14C label in the water sample. Heptachlor was found to decrease from 100% to approximately 10% of total 14C material in 1 day (Lu et al. 1975). After 1 day, 1-hydroxychlordene epoxide was present as 50% of the total 14C, rose to 70% on day 3, and then remained constant until day 13 of the experiment. The heptachlor hydrolysis product, 1-hydroxychlordene, reached a maximum of 10% of the total 14C at day 1 and decreased thereafter. **A relatively small proportion of heptachlor epoxide was formed**. Heptachlor epoxide was never found to be greater than 10% of the total 14C in the water sample. **The authors concluded that the major pathway of heptachlor in aquatic systems is rapid abiotic hydrolysis of heptachlor to 1-hydroxychlordene followed by metabolism to 1-hydroxychlordene epoxide (Lu et al. 1975).** Loamy soils treated with heptachlor at 25 pounds per 5-inch acre, over a 5-year period from 1958 through 1962, contained about 5% of the applied dosages in the fall of 1968, primarily in the form of heptachlor epoxide. In addition to g-chlordane and nonachlor, which were present in the original heptachlor formulation, two toxic metabolites (heptachlor epoxide and a-chlordane) and three unidentified compounds were detected, thus indicating the breakdown in soils of heptachlor and related compounds (Lichenstein et al. 1970).

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		0.002 Hept. Epox. (0.0001 - 0.02)	Heptachlor epoxide is converted to intermediate and final photoproducts when exposed to sunlight or ultraviolet light on the surface of plants (Podowski et al. 1979). From 40% to 50% conversion occurred in 4 hours on bean leaves treated with rotenone, an insecticide, acting as a photosensitizer. No detectable photoproducts (photoheptachlor epoxide) were formed in the absence of rotenone. The photolysis products were ketones. The intermediate photoproduct has a reduced toxicity in mice as compared to heptachlor epoxide, and it is completely nontoxic to houseflies. The final photoproduct is more toxic to flies and mice than the parent heptachlor epoxide (Ivie et al. 1972). **The photoisomers of heptachlor epoxide are not expected to form in appreciable amounts in the environment unless a potent photosensitizer is present (Ivie et al. 1972).** The photolysis of heptachlor epoxide as a solid (pressed) disk, as a powder, and as 0.5% heptachlor epoxide in a potassium bromide (a photosensitizer) disk was studied. The physical nature of the sample and the intensity of illumination affected the rate of photolysis. After 121 hours of exposure to sunlight in July, 93%, 98%, and 0% heptachlor epoxide remained in the solid disk, powder, and potassium bromide disk, respectively. ***When a powdered sample of heptachlor epoxide was irradiated on a rooftop of an unspecified location from January through mid-September, degradation was almost negligible until May, then increased through July, reaching a maximum decomposition rate of 1% per day at the end of July. By the end of the experiment (8.5 months), 39% of the original sample has decomposed (Graham et al. 1973).*** When heptachlor epoxide was added to a sample of river water (pH 7.3-8) and to distilled water, it remained unchanged for 8 weeks. A half-life of at least 4 years was calculated for heptachlor epoxide (Eichelberger and Lichtenberg 1971).

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Hexachloro-cyclohexane	II	**0.0006** (α) (0.00004 - 0.006)	As mentioned earlier, g-HCH can be present in the air as vapor or sorbed to particulate matter.The widespread global distribution of HCH isomers is indicative of the persistence of g- HCH in the air. It appears that photodegradation or other degradation processes are not significant processes in the removal of g-HCH from air, as compared to rain-out or dry deposition. **The structure of g-HCH and other isomers of HCH are such that the compounds would have very little absorption above the solar spectral region cutoff at 290 nm.**
		0.002 (β) (0.0001 - 0.01)	However, Hamada et al. (1981) found that g-HCH underwent photodegradation to form two isomers of tetrachlorohexene and pentachlorohexane in propanol solution when irradiated with ultraviolet light produced by a low-pressure mercury lamp. Similar transformation of g-HCH and other isomers is thought to occur to some extent in the atmosphere. Water: **Biodegradation is believed to be the dominant degradative process for g-HCH in aquatic systems, although hydrolysis and photolysis do occur.**
		0.001 (δ) (0.00007 - 0.01)	• **Somewhat conflicting information is available on the rate of photolysis of g-HCH in water.** • In the study by Saleh et al. (1982) discussed above, the authors also reported g-HCH first- order photolysis half-lives of 169, 1,791, and 1,540 hours at pH 9.3, 7.3, and 7.8, respectively. The adjusted mid-winter half-life of g-HCH in pure water was reported to be 1,560 hours.
		0.003 (γ) (0.0002 - 0.03)	• However, in another study, g -HCH rapidly disappeared from a sterile aqueous solution when exposed to ultraviolet radiation in atmospheric nitrogen; less than 1% of the original amount was left in solution after 30 hours of exposure (Malaiyandi et al. 1982). • Hydrolysis is not considered an important degradation process for g-HCH in aquatic environments under neutral pH conditions. However, under alkaline conditions, g-HCH is hydrolyzed fairly rapidly. Saleh et al. (1982) tested rates of hydrolysis of g-HCH in sterilized natural waters at 25øC and found that hydrolysis of g-HCH followed first-order kinetics with half- lives of 92 hours at pH 9.3, 648 hours at pH 7.8, and 771 hours at pH 7.3.

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Methoxychlor	II	**0.1** (0.005 - 0.6)	**Data regarding the transformation and degradation of methoxychlor in air were not located.** **It has been estimated that the half-life for photooxidation in air may range from 1 to 11 hours (Howard 1991).** 5.3.2.2 Water Methoxychlor can be degraded in water by chemical, photochemical, and biological processes. Methoxychlor undergoes a spontaneous elimination reaction in aqueous solution to yield dehydrochlorinated products including methoxy-DDE (a proestrogenic derivative of methoxychlor discussed in Section 2.3.5). The half-life for the degradation of methoxychlor by this process was estimated to be approximately 1 year (Wolfe et al. 1977). Methoxychlor may also be oxidized by hydroxyl radicals or ozone in ozonated waters (Haag and Yao 1992; Yao and Haag 1991). The half-life of methoxychlor reaction with ozone under ozonation conditions was estimated to be 2.1 minutes. ***Methoxychlor is photochemically degraded by sunlight through loss of one chlorine atom to form a radical intermediate, which rearranges to the more stable methoxy-DDE (Zepp et al. 1976).*** **A dramatic difference in half-life was observed for the photochemical degradation of methoxychlor in distilled water (4.5 months) and natural water (2-5 hours).** Methoxychlor was found to form adducts extensively with plant materials via a photochemically-induced radical mechanism (Schwack 1988). This observation may explain the dramatic differences in the half-life of methoxychlor in distilled and natural waters.

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Pentachlorophenol	II	**0.0006** (0.00004 - 0.006)	5.3.2.1 Air Atmospheric pentachlorophenol is transformed via photolysis; the compound is not expected to undergo free radical oxidation. **Atmospheric pentachlorophenol is probably photolyzed in the absence of water, although mechanisms for this reaction are not well known (Crosby and Hamadad 1971; Gab et al. 1975).** Photolysis of sorbed or film-state pentachlorophenol in the presence of oxygen has also been observed (Gab et al. 1975). The reaction products were similar to those found in aqueous photolysis. No information was found regarding susceptibility of pentachlorophenol to free radical oxidation in the atmosphere. However, related compounds such as benzene, chlorobenzenes, and phenol have low reactivity with atmospheric hydroxy radicals; therefore, atmospheric oxidation of penta-chlorophenol is not expected. 5.3.2.2 Water **Photolysis and biodegradation are believed to be the dominant transformation processes for pentachlorophenol in aquatic systems.** Hydrolysis and oxidation are not important mechanisms for removal of the compound from surface waters. The molecular structure of pentachlorophenol is indicative of its stability to hydrolysis or oxidation (Callahan et al. 1979). Wong and Crosby (1981) reported no changes in pentachloro-phenol concentration in dark controls during their study of pentachlorophenol photodecomposition in water. Pentachlorophenol apparently did not hydrolyze in aqueous solutions at pH 3.3 or 7.3 when held at 26øC for up to 100 hours. **Wong and Crosby (1981) reported that pentachlorophenol in aqueous solutions was photolyzed under laboratory ultraviolet (UV)-light irradiation with estimated half-lives of about 100 hours at pH 3.3 and 3.5 hours at pH 7.3.** Photolysis of pentachlorophenol in aqueous solution following exposure to sunlight was also rapid; in laboratory experiments, concentrations of pentachloro-phenol in water were reduced from 9.3 ppm to 0.4 ppm in 24 hours and approached zero at the end of 48 hours (Arsenault 1976). In outdoor tests conducted with river water in man-made channels, Pignatello et al. (1983) demonstrated that photolysis of pentachlorophenol was rapid at the water surface (half-life of 0.70 hour at a depth of 0.5 cm). However, photolysis was greatly attenuated with increasing depth of the water column (half-life of 228 hours at a depth of 30 cm). Photolytic degradation accounted for a 5-28% decrease in the initial test concentration of the compound after 3 weeks.

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INDUSTRIAL / MISCELLANEOUS			
Octachloro-styrene	I	**0.003** (0.0001 - 0.04)	
3,3'-Dichloro-benzidene	II	**0.9** (0.3 - 0.99)	5.3.2.1 Air 3,3'-DCB in the atmosphere may be photooxidized with hydroxyl radicals and ozone, but there were no quantitative data on reaction rates. Radding et al. (1977) estimated the persistence of "all benzidines" in the atmosphere by assuming a hydroxyl radical concentration of 8 x 10-15 mole/liter (an average value in a 24-hour day-night cycle). Treating the photooxidation process as a first-order reaction, the rate constant was 7.2 x 1012/mole-hr and the corresponding half-life was 12 hours. This approach was based on data on the rates of reaction of hydroxyl radicals with olefins, aromatics, and alkanes in the atmosphere. The estimated half-life of 3,3'-DCB in air has ranged from 1 to 60 days (Shriner et al. 1978; EPA 1980b). Based on the reaction rate constant of photodegradation in the atmosphere, the half-life may be as little as two hours (DCMA 1989). There was no other information on the fate of atmospheric 3,3'-DCB. 5.3.2.2 Water The limited information that is available suggest that 3,3'-DCB may photolyze yielding benzidine which is more photostable. It does not appear that the chemical is susceptible to other transformations in water. **In a study reported by Sikka et al. (1978) and Banerjee et al. (1978), 3,3'-DCB was found to be extremely photolabile in water. 3,3'-DCB photolyzed yielding monochlorobenzidine, benzidine, and a number of colored, water-insoluble products. In natural sunlight, the half-life of 3,3'-DCB in water was approximately 90 seconds. While 3,3'-DCB is very rapidly photolyzed under environmental conditions, the process may yield benzidine, a relatively photostable carcinogen (Banerjee et al. 1978).** There are no data to suggest that the hydrolysis of 3,3'-DCB is significant (Callahan et al. 1979). Mabey et al. (1982) proposed a hydrolysis-rate constant of 0/mole-hour for 3,3'-DCB. It has been speculated that aromatic amines can be oxidized in solution by organic radicals, but there are no actual data on reaction rates. Based on structural analogs, Radding et al. (1977) estimated that the half-life of such compounds in water is approximately 100 days, assuming a peroxy concentration of 10-10 mole/L in sunlit, oxygenated water. Based on the oxidation rates with similar compounds, Mabey et al. (1982) treated the direct oxidation of 3,3'-DCB by oxygen in solution as a first-order reaction, and estimated a reaction rate constant of less than 4 x 107/mole-hour. The oxidation rate constant with peroxy radicals was estimated to be approximately 4 x 107/mole-hour. However, no information was located that demonstrates that 3,3'-DCB is significantly oxidized in water.

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4,4'-Methylene bis (2-Chloro-aniline) "MBOCA"	II	**0.009** (0.0005 - 0.1)	5.3.2.1 Air The photooxidation half-life of MBOCA in air is estimated to be between 0.290 and 2.90 hours based on reactions with hydroxyl radicals (Howard et al. 1991), suggesting that this may be a significant fate process. 5.3.2.2 Water The estimated photooxidation half-life of MBOCA in surface water is between 1.3 and 72 days; while in groundwaters, MBOCA may have a half-life of 8 weeks to 1 year (Howard et al. 1991). The estimated hydrolysis half-life of MBOCA in water at 25øC and pH 7 is more than 800 years (EPA 1988c).
4-Bromo-phenyl Phenyl Ether "4BPE"	II	**0.0005** (0.00002 - 0.02)	
Hexachloro-1,3-Butadiene "HCBD"	II	**0.000005** (0.0000002 - 0.0001)	5.3.2.1 Air No data were located regarding the transformation and degradation of hexachlorobutadiene in air. Based on the monitoring data, the tropospheric half-life of hexachlorobutadiene was estimated by one author to be 1.6 years in the northern hemisphere (Class and Ballschmiter 1987). However, analogy to structurally similar compounds such as tetrachloroethylene indicates that the half-life of hexachlorobutadiene may be as short as 60 days, predominantly due to reactions with photochemically produced hydroxyl radicals and ozone (Atkinson 1987; Atkinson and Carter 1984). Oxidation constants of <103 and 6 (m • hr)-1 were estimated for reactions with singlet oxygen and peroxy radicals, respectively (Mabey et al. 1982). 5.3.2.2 Water Data concerning the transformation and degradation of hexachlorobutadiene in waters are limited... Data regarding the hydrolysis or photolysis of hexachlorobutadiene in water were not located.

Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study

Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	**Information Regarding Atmospheric Photolysis** All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
CHLOROBENZENES			
1,4-dichloro-benzene "pDCB"	II	**0.0000004** (0.00000003 - 0.000003)	5.3.2.1 Air The main degradation pathway for 1,4-dichlorobenzene in air is reaction with photochemically generated hydroxyl radicals (Cuppitt 1980; EPA 1985). Reactions with ozone or other common atmospheric species are not expected to be significant (Atkinson et al. 1985; Cuppitt 1980). Therefore, the atmospheric lifetime of 1,4-dichlorobenzene may be predicted from an assumed hydroxyl radical concentration in air and the rate of reaction. The reported rate for reaction of hydroxyl radicals with 1,4-dichlorobenzene is 3x10-3 cm3/mol-sec (Atkinson et al. 1985; Singh et al. 1981), and the estimated atmospheric residence time for 1,4- dichlorobenzene is about 39 days (Singh et al. 1981). Since this degradation process is relatively slow, 1,4-dichlorobenzene may become widely dispersed, but is not likely to accumulate in the atmosphere. 5.3.2.2 Water Biodegradation may be an important transformation process for 1,4-dichlorobenzene in water under aerobic, but not anaerobic, conditions (Bouwer and McCarty 1982, 1983, 1984; Spain and Nishino 1987; Tabak et al. 1981). Although volatilization of 1,4-dichlorobenzene may interfere with biodegradation studies, 14C studies indicate that significant biodegradation of 1,4- dichlorobenzene does occur (Spain and Nishino 1987). 5.3.2.3 Soil **Based on its tendency to sublime, volatilization is the most likely fate process for 1,4- dichlorobenzene from surface soil.** Biodegradation by soil organisms and leaching to groundwater from subsurface soils may also occur (EPA 1985). However, no quantitative data on rate or extent of volatilization were located.
Tetrachloro-benzenes 1234 TCB 1245 TCB 1235 TCB	II	**0.000009** (1234TCB) (0.0000006 - 0.0001)	
		0.000008 (1245TCB) (0.0000005 - 0.00006)	
		0.000004 (1235TCB) (0.0000003 - 0.00004)	
Pentachloro-benzene "PeCB"	II	**0.00009** (0.000006 - 0.001)	

Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study

Chemical or Group	**LVL**	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	**Information Regarding Atmospheric Photolysis** All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
Hexachloro-benzene "HCB"	I	**0.0003** (0.00002 - 0.003)	Few studies regarding atmospheric degradation of hexachlorobenzene have been located, probably because the atmosphere is not a significant reservoir of hexachlorobenzene. Photodegradation of hexachlorobenzene in its vapor phase, or as an adsorbable on silica gel, has been reported as **not** occurring when hexachlorobenzene was irradiated with ultraviolet radiation of wavelength 290 nm for 6 days; however, production of HC1 and CO2 was observed when hexachlorobenzene was irradiated at 230 nm (Parlar 1978). **In the troposphere, hexachlorobenzene is probably photochemically stable,** but degradation in the stratosphere by photodissociation by shorter-wavelength, higher-ultraviolet light may be a mechanism for atmospheric degradation. While not highly volatile, hexachlorobenzene can volatilize and is often studied in conjunction with the semi-volatile organochloro compounds (Ballschmiter and Wittlinger 1991; Lane et al. 1992). It is resistant to the types of hydrolysis reactions that can help degrade other organochlorines or organophosphates; and **with a half-life of about 90 days, it is not markedly subject to photolytic decay (EPA 1992b).**

Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study

Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	**Information Regarding Atmospheric Photolysis** All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
POLYCHLORINATED DIBENZO-P-DIOXINS AND DIBENZOFURANS (PCDD/F'S)			
2,3,7,8-TCDD	I	**0.6** (0.08 - 0.9)	5.3.2.1 Air **No data regarding vapor phase photolysis of CDFs were located. In the absence of data, the half-lives of these compounds in the vapor phase have been estimated from aqueous phase photolysis data and it was concluded that photolysis is relatively unimportant, even when compared to reaction with hydroxyl radicals (with the possible exception of 1,3,6,8-tetraCDF) (Atkinson 1991).** The loss of vapor phase CDFs by reactions with HO2 radicals, NO3 radicals and ozone has been estimated to be of negligible importance in the troposphere (Atkinson 1991). The estimated rate constants for the reactions of vapor phase CDFs with OH radicals are as follows (10-12 cm3/molecule-sec): tetraCDFs, 1.4-8.3; pentaCDFs, 1.0-4.3; hexaCDFs, 0.74-2.6; heptaCDFs, 0.53-0.92; and octaCDFs, 0.39. Using a 12-hour average daytime hydroxyl radical concentration of 1.5x106/cm3, the estimated tropospheric lifetimes of tetra-, penta-, hexa-, hepta-, and octaCDF are 1.9-11, 3.6-15, 5.9-22, 17-31, and 39 days, respectively. The vapor phase reaction of CDFs with hydroxyl radicals is the dominant loss process and this loss process is more important for the lower, than the higher, chlorinated congeners, because the lifetimes due to this reaction are shorter for lower chlorinated congeners and the vapor phase concentrations of lower chlorinated congeners are higher. Based on the available information, the reactions of hydroxyl radicals with particulate phase CDFs are insignificant and the principal air removal mechanism for CDFs is wet and dry deposition. Photodegradation of CDFs bound to atmospheric particles is not an important process in removing these compounds from air (Koester and Hites 1992).
2,3,7,8-TCDF	I	**0.3** (0.02 - 0.9)	
PeCDD/F's (penta-chloro-)	I	**0.9** (0.2 - 0.99)	
HxCDD/F's (hexa-chloro-)	I	**0.97** (0.6 - 1)	
HpCDD/F's (hepta-chloro-)	I	**0.99** (0.9 - 1)	
OCDD/F's (octa-chloro-)	I	**1** (0.98 - 1)	
PCDD/F's (as a group)	I		

Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study

Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	**Information Regarding Atmospheric Photolysis** All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
POLYCHLORINATED BIPHENYLS (PCB'S)			
Cl_1-PCB		**0.00007 - 0.00014** (0.000001 - 0.01)	The ability of PCBs to be degraded or transformed in the environment depends on the degree of chlorination of the biphenyl molecule as well as on the isomeric substitution pattern (Callahan et al. 1979; EPA 1988a; Leifer et al. 1983). In general, the persistence of PCB congeners increases as the degree of chlorination increases. 5.3.2.1 Air **In the atmosphere, the vapor-phase reaction of PCBs with hydroxyl radicals (which are photochemically formed by sunlight) may be the dominant transformation process.** **The estimated tropospheric half-lives for this reaction with various PCB isomers are: monochlorobiphenyl, 3.5-7.6 days; dichlorobiphenyl, 5.5-11.8 days; trichlorobiphenyl, 9.7-20.8 days; tetrachlorobiphenyl, 17.3-41.6 days; and pentachlorobiphenyl, 41.6-83.2 days (Atkinson 1987).** **Photochemical studies conducted with a number of chlorobiphenyl congeners and commercial PCB mixtures in aqueous suspension, thin film, or vapor state under simulated and natural sunlight conditions resulted in several degradative reactions that produced dechlorination, polymerization, and polar (hydroxy- and carboxy-) products (Hutzinger et al. 1972). Therefore, photolytic degradation of PCBs in the atmosphere is possible. However, the rates of these reactions with natural sunlight were not reported.** 5.3.2.2 Water ***In water, transformation processes such as hydrolysis and oxidation do not significantly degrade PCBs (Callahan et al. 1979). Photolysis appears to be the only viable chemical degradation process in water. PCBs containing up to six chlorine substitutions do not significantly absorb sunlight, and the estimated photolysis half-lives of mono- through tetrachlorobiphenyls with summer sunlight at shallow water depth (<0.5 m) range from 17 to 210 days. Photolysis rates with sunlight are even slower during winter. Nonetheless, as the number of chlorine substitutions increases, the light absorption band shifts towards longer wavelengths, and the photolysis rate for hepta- through decachlorinated biphenyls increases. The estimated photolysis half-life of Aroclor 1268 with summer sunlight is 0.1 days, compared to 23 days for Aroclor 1232 (Leifer et al. 1983). However, these results must be used with caution since the solvent used was predominantly acetonitrile (75%) and, therefore, the experiment does not correspond with environmental conditions. More reliable photolysis data are needed to estimate rates of photolysis in aqueous media in the presence of sunlight.*** The photolysis rates for PCBs can be enhanced by a factor of 311, in the presence of sodium borohydride (Epling et al. 1988). Therefore, photolysis in the presence of sodium borohydride may be useful as a method for destruction of PCBs in water. The exposure of 0.08 mg/L aqueous solution of Aroclor 1248 to sunlight in the presence of a titanium dioxide suspension (50 g/L) decreased the total PCB concentration to 23% of original in 2 hours and to 13% of original in 4 hours (Zhang et al. 1993). Although the intermediate and final products of photocatalysis were not identified, it was suggested by the authors of other related studies that photolysis resulted in complete mineralization of PCB.
Cl_2-PCB		**0.0004 - 0.0020** (0.000007 - 0.2)	
Cl_3-PCB		**0.001 - 0.012** (0.00002 - 0.6)	
Cl_4-PCB		**0.003 - 0.069** (0.00006 - 0.94)	
Cl_5-PCB		**0.03 - 0.27** (0.0003 - 0.99)	
Cl_6-PCB		**0.04 - 0.74** (0.0005 - 0.999)	
Cl_7-PCB		**0.36 - 0.80** (0.005 - 0.999)	
Cl_8-PCB		**0.25 - 0.91** (0.003 - 1.000)	
Cl_9-PCB		**0.85 - 0.95** (0.05 - 1.000)	
Cl_{10}-PCB		**0.93** (0.09 - 1.00)	
PCB's as a group	I		

Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study

Chemical or Group	**LVL**	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	**Information Regarding Atmospheric Photolysis** All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
POLYCYCLIC AROMATIC HYDROCARBONS			
Naphthalene "Naph"		**0.000002** (0.0000001 - 0.00002)	
Acenaphthene "Acn"		**0.00005** (0.000003 - 0.0006)	
Acenaphthylene "Acl"		**0.00002** (0.000001 - 0.0002)	
Fluorene "Flr"		**0.0001** (0.000007 - 0.001)	
Phenanthrene "Phen"	II	**0.0008** (0.00004 - 0.01)	
Anthracene "Anth"	II	**0.001** (0.00006 - 0.01)	
Pyrene "Pyr"		**0.007** (0.0004 - 0.08)	
Fluoranthene "Fln"		**0.01** (0.0005 - 0.1)	
Chrysene "Chr"		**0.4** (0.04 - 0.9)	
Benz (a) Anthracene "BaA"	II	**0.5** (0.05 - 0.95)	
Benzo (b) Fluoranthene "BbF"		**0.05** (0.002 - 0.5)	
Benzo (j) Fluoranthene "BjF"		**0.7** (0.08 - 0.97)	
Benzo (k) Fluoranthene "BkF"		**0.96** (0.5 - 1)	
Benzo (a) Pyrene "BaP"	I	**0.8** (0.2 - 0.99)	**[HSDB]:** When released to air it may be subject to direct photolysis, although adsorption to particulates apparently can retard this process. It may also be removed by reaction with O3 (half-life 37 min) and NO2 (half-life 7 days), and an estimated half-life for reaction with photochemically produced hydroxyl radicals is 21.49 hr.(SRC) [CITATION] **PEER REVIEWED** **[HSDB]:** Half-life for reaction of a thin film of BaP with 0.19 ppm O3 is 37 min and for reaction of adsorbed BaP with NO2 is 7 days. The estimated half-life for reaction with photochemically produced hydroxyl radicals is 21.49 hr.

Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study

Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	**Information Regarding Atmospheric Photolysis** All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
Benzo (e) Pyrene "BeP"		**0.8** (0.1 - 0.99)	
Perylene "Per"	II	**0.95** (0.5 - 1)	
Benzo (g,h,i) Perylene "BgP"	II	**0.96** (0.5 - 1)	
Dibenz (a,h) Anthracene "dBA"		**1** (0.98 - 1)	
Indeno (1,2,3-c,d) Pyrene "IPyr"		**0.99** (0.9 -1)	
Dinitro-pyrenes "DNPs"	II	**0.4** (0.03 - 0.9)	The processes that transform and degrade PAHs in the atmosphere include photolysis and reaction with NOx, N2O5, OH, ozone, sulfur dioxide, and peroxyacetyl nitrate (Baek et al. 1991; NRC 1983). Possible atmospheric reaction products are oxy-, hydroxy-, nitro- and hydroxynitro-PAH derivatives (Baek et al. 1991). **Photochemical oxidation of a number of PAHs has been reported with the formation of nitrated PAHs**, quinones, phenols, and dihydrodiols (Holloway et al. 1987; Kamens et al. 1986). **Some of these breakdown products are mutagenic** (Gibson et al. 1978). Reaction with ozone or peroxyacetylnitrate yields diones; **nitrogen oxide reactions yield nitro and dinitro PAHs.** Sulfonic acids have also been formed from reaction with sulfur dioxide. The reactions of PAHs, including fluoranthene and pyrene, with the OH radical (in the presence of NOx) and with N2O5 led to the formation of nitroarenes that have been identified in the ambient air. As a class of compounds, the nitrated PAHs have been found to be much more mutagenic than their parent PAHs (Kamens et al. 1993).

Table D.4.-(1). Some Information about Atmospheric Photolysis (i.e., Destruction by UV Light) for Compounds Considered in this Study

Chemical or Group	LVL	Estimated Fraction Adsorbed to Particles in Atm. (App. C) (1)	**Information Regarding Atmospheric Photolysis** All Information Imported Directly from ATSDR Toxicological Profiles (CD ROM version) unless otherwise indicated; References cited are as cited in the original (e.g. ATSDR) document. Time constraints did not allow the inclusion of these references in the bibliography for this report.
PAH's (as a group)	II		The processes that transform and degrade PAHs in the atmosphere include photolysis and reaction with NOx, N2O5, OH, ozone, sulfur dioxide, and peroxyacetyl nitrate (Baek et al. 1991; NRC 1983). Most PAHs in the atmosphere are associated with particulates (Baek et al. 1991). Vu-Duc and Huynh (1991) describe two types of chemical reactions that appear to be the predominant mode of transformation of these PAHs: (1) reactions between PAHs adsorbed on the particle surfaces and oxidant gases like NO2, O3, and SO3 that do not appear to be influenced by exposure to UV irradiation and (2) photooxidation of PAHs irradiated either under solar radiation or simulated sunlight which produces a variety of oxidized derivatives such as quinones, ketones, or acids. **Kamens et al. (1990) estimate that, even in highly polluted air, photolysis is the most important factor in the decay of particle-sorbed PAHs in the atmosphere, followed by reaction with NO2, N2O5, and HNO3.** The rates of homogeneous vapor phase chemical reactions are usually faster than heterogeneous chemical reactions of particulate PAHs with sunlight and oxidants in the atmosphere, particularly due to light shielding and stabilizing (toward both oxidation and photolysis) effects in the adsorbed state (Behymer and Hites 1988). PAHs have a wide range of volatilities and therefore are distributed in the atmosphere between the gas and particle phases. The 2-4 ring PAHs exist, at least partially, in the gas phase. Atkinson et al. (1991) calculated atmospheric lifetimes (1.44 times the half-life) of several gas-phase PAHs due to reactions with measured or estimated ambient concentrations of OH radicals, NO3 radicals, N2O5, and O3. Their laboratory studies showed that, for PAHs not containing cyclopenta-fused rings, the major gas-phase process resulting in atmospheric loss will be reaction with the OH radical. Calculated atmospheric lifetimes for acenaphthene, acenaphthylene, phenanthrene, and anthracene were on the order of a few hours. Nighttime reaction with N2O5 was estimated to be a minor source of atmospheric loss.

References and Notes for above Table

(1) Vapor Particle Partition Estimates Included here for convenience:

- Central Estimate (**bold**) T = 290°K; Aerosol surface area = 3.5e-6 cm^2/cm^3
- RANGE (in parentheses): 310 to 260 °K; 4.2e-7 to 1.1e-5 cm^2/cm^3

Appendix D.5.

Results of a Literature Search for Measurements of Rate Constants for the Reaction of Hydroxyl Radical with Organic Compounds in the Atmosphere Made by Atkinson and Colleagues

(sorted by year: 1983 - 1996)

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