

FINAL REPORT

**AMBIENT MEASUREMENT METHODS AND PROPERTIES OF THE
189 TITLE III HAZARDOUS AIR POLLUTANTS**

by

**Thomas J. Kelly, R. Mukund, Sydney M. Gordon, and Melinda J. Hays
BATTELLE
505 King Avenue
Columbus, Ohio 43201**

March 1994

**Contract Number 68-D0-0007
Work Assignment No. 44**

Project Officer

**William A. McClenny
Atmospheric Research and Exposure Assessment Laboratory
U.S. Environmental Protection Agency
MD-44
Research Triangle Park, North Carolina 27711**

FINAL REPORT

**AMBIENT MEASUREMENT METHODS AND PROPERTIES OF THE
189 TITLE III HAZARDOUS AIR POLLUTANTS**

by

**Thomas J. Kelly, R. Mukund, Sydney M. Gordon, and Melinda J. Hays
BATTELLE
505 King Avenue
Columbus, Ohio 43201**

March 1994

**Contract Number 68-D0-0007
Work Assignment No. 44**

Project Officer

**William A. McClenny
Atmospheric Research and Exposure Assessment Laboratory
U.S. Environmental Protection Agency
MD-44
Research Triangle Park, North Carolina 27711**

EPA DISCLAIMER

The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under Contract 68-D0-0007 to Battelle Memorial Institute. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

BATTELLE DISCLAIMER

This report is a work prepared for the United States Environmental Protection Agency by Battelle Memorial Institute. In no event shall either the United States Environmental Protection Agency or Battelle Memorial Institute have any responsibility or liability for any consequences of any use, misuse, inability to use, or reliance upon the information contained herein, nor does either warrant or otherwise represent in any way the accuracy, adequacy, efficacy, or applicability of the contents hereof.

FOREWORD

Measurement and monitoring research efforts are designed to anticipate environmental problems, to support regulatory actions by developing an in-depth understanding of the nature of processes that impact health and the ecology, to provide innovative means of monitoring compliance with regulations, and to evaluate the effectiveness of health and environmental protection efforts through the monitoring of long-term trends. The Atmospheric Research and Exposure Assessment Laboratory, Research Triangle Park, North Carolina, has responsibility for assessment of environmental monitoring technology and systems for air, implementation of agency-wide quality assurance programs for air pollution measurement systems, and supplying technical support to other groups in the Agency, including the Office of Air and Radiation, the Office of Toxic Substances, and the Office of Solid Waste.

The 189 Hazardous Air Pollutants (HAPs) listed in the 1990 Clear Air Act Amendments were so designated because of concerns about human health risks from the presence of those HAPs in air. Determination of human health risks, confirmation of mandated reductions in those risks, and evaluation of emission control efforts all require ambient measurements of the 189 HAPs. The survey of measurement methods for HAPs described in this report is an important resource with which HAP measurement methods may be identified and implemented.

Jay J. Messer
Acting Director
Atmospheric Research and Exposure
Assessment Laboratory
Research Triangle Park,
North Carolina 27711

ABSTRACT

This is the final report on a study conducted by Battelle to identify ambient air measurement methods for the 189 Hazardous Air Pollutants (HAPs) designated in Title III of the 1990 Clean Air Act Amendments. The main objective of this work was to document the state of development of measurement methods for each of the 189 HAPs in ambient air. This was accomplished by identifying and reviewing pertinent literature on applicable methods for each HAP. A secondary objective of this work was to compile data on the chemical and physical properties of the HAPs, as the basis for selecting and evaluating measurement methods. The results of both the HAP properties and HAP methods surveys are presented in this report.

The 189 HAPs are an extremely diverse group of chemicals, including a few compounds unlikely to exist in ambient air, and several mixtures or chemical groups spanning wide ranges of physical and chemical properties. The physical and chemical properties of the HAPs were surveyed by first distinguishing the 166 organic and 23 inorganic chemicals on the HAPs list. For all 189 HAPs, vapor pressure and boiling point data were compiled. Both the organic and inorganic HAPs were then separated into four volatility classes, based on quantitative vapor pressure criteria. Listings of the HAPs assigned to each volatility class are provided in Appendix D of this report. For the volatile and very volatile HAPs, further properties were then compiled, including water solubility, electronic polarizability, aqueous reactivity, and estimated lifetime in the atmosphere. These properties were used to assess the chemical and physical characteristics of the HAPs, and the similarities and differences between HAPs, as a guide in selecting measurement methods. The data on HAPs properties are tabulated in Appendices A and B of this report.

The survey of measurement methods for the 189 HAPs drew upon standard methods published by EPA, NIOSH, OSHA, and other organizations, and upon wide-ranging literature searches and reviews of recent publications. A total of 168 distinct measurement methods were identified, some applicable to several HAPs, and others applicable to a single HAP. The identified methods were assigned to one of three categories according to their degree of development, i.e.:

Demonstrated methods, established and documented to a reasonable degree for measurement of the target HAP in ambient air. (This definition does not necessarily imply that all issues have been fully resolved regarding the sampling and analysis of the HAP in the atmosphere. An overly optimistic view of the state of HAPs measurement methods could result if these reservations are overlooked.)

Likely methods, established for the target HAP or for a closely similar HAP in (e.g.) workplace air, but needing further development before application to ambient air.

Potential methods, needing extensive further development before measurements in ambient air could be considered.

For each HAP, all identified methods were tabulated, so that for many HAPs methods in more than one of the above-named categories were listed. Quantitative detection limits were also tabulated, for at least the most fully developed methods for each HAP. Pertinent literature was also cited, to allow the reader to obtain details of each method if needed. The full data base resulting from the HAPs methods survey is presented in Appendix C of this report.

For 126 of the HAPs, ***Demonstrated*** methods of measurement were identified. For 53 other HAPs, ***Likely*** methods, but no ***Demonstrated*** methods, were found. These two results combined suggest that ambient measurements should be achievable for most of the 189 HAPs, with a reasonable further method development effort. However, that method development must include both ***Demonstrated*** and ***Likely*** methods, since methods currently identified as ***Demonstrated*** may not all be fully proven for all ambient conditions and for the full range of HAPs properties and reactivity. In addition, for 6 HAPs only ***Potential*** methods were found, implying

extensive further development before ambient measurements are achievable, and for 4 HAPs no methods were found at any stage of development.

The primary recommendation of this study is that method development be focussed on the 53 HAPs for which *Likely* methods were found. This approach is likely to produce the greatest return for the resources invested. The 10 HAPs with little or no current measurement capability should also be the subject of methods development, but that effort should be prioritized based on the likely presence and importance of these HAPs in the atmosphere.

This report is submitted in fulfillment of Contract No. 68-D0-0007 (Work Assignment 44) by Battelle under the sponsorship of the U.S. Environmental Protection Agency. It covers the period from March 1, 1993 to March 31, 1994, and all work was completed as of March 31, 1994.

CONTENTS

Foreword	iii
Abstract	iv
Figures	viii
Tables	ix
Acknowledgment	x
1. Introduction	1
2. Conclusions	4
3. Recommendations	5
4. Survey Methods	6
HAPs Properties	6
HAPs Measurement Methods	7
5. Survey Results	13
HAPs Properties	13
HAPs Measurement Methods	16
References	29
Appendices	
A. Results of the Survey of Chemical and Physical Properties of the 189 HAPs	33
B. Physical and Chemical Properties of VOCs on the HAPs List	45
C. Results of the Survey of Ambient Air Measurement Methods for the 189 HAPs	54
D. Listings of the 189 HAPs by Volatility Classes	94

FIGURES

<u>Number</u>		<u>Page</u>
1	Example of a few entries from Table A-1	15
2	Example of a few entries from Table B-1	17
3	Example of a few entries from Table C-1	18
4	Distribution of the 189 HAPs by the most developed type of ambient measurement method currently available for each compound	24

TABLES

<u>Number</u>		<u>Page</u>
1	Summary of HAP categories with corresponding vapor pressure ranges and properties reviewed	8
2	Numbers of HAPs in each volatility class	14
3	Most developed ambient measurement method identified for each of the 189 HAPs	20
4	Type of measurement methods currently available for each of the 189 HAPs, by volatility class	26
5	Identification of the ten HAPs for which ambient methods are least developed	28

ACKNOWLEDGMENT

The involvement and technical insight of Drs. William A. McClenny and Robert G. Lewis of U.S. EPA in this work are gratefully acknowledged.

SECTION 1

INTRODUCTION

The presence of toxic contaminants in air has been a public health issue for many years. However, the 1990 Clean Air Act Amendments (CAAA) greatly accelerated the pace of designating and regulating air contaminants by defining a list of 189 Hazardous Air Pollutants (HAPs).¹ The 189 HAPs are remarkably diverse, consisting of industrial chemicals and intermediates, pesticides, chlorinated and hydrocarbon solvents, metals, combustion byproducts, chemical groups such as polychlorinated biphenyls, and mixed chemicals such as coke oven emissions. Some of the HAPs are common air pollutants, such as volatile organic compounds (VOCs), but many other HAPs were assigned to the list based on their recognized toxicity in workplace environments, and had not previously been considered as ambient air contaminants. Some of the HAPs are not single compounds, but rather complex mixtures or groups of chemicals spanning broad ranges of chemical and physical properties. A few HAPs, such as titanium tetrachloride, phosphorus, and diazomethane, are unlikely to exist in ambient air because of their reactivity.

Title III of the CAAA is aimed at reducing the public health risks from HAPs in ambient air, and includes mandated risk reduction goals. For example, a 75 percent reduction in cancer incidence due to area sources of HAPs is a stated goal of Title III.¹ However, determining the current health risks from HAPs, or quantifying reductions in health risks, requires knowledge of the ambient concentrations of the HAPs. Partly because of the diversity of the HAPs, ambient measurements are severely lacking for many HAPs. For example, only 70 of the 189 HAPs are included in the U.S. EPA's National VOC Data Base.²⁻⁴ A recent survey of ambient HAPs data conducted for U.S. EPA showed no ambient data for 74 of the 189 HAPs,⁵⁻⁷ and furthermore found

less than 100 ambient measurements for 116 of the HAPs. These findings indicate that currently available information may be insufficient to conduct health risk assessments for many HAPs.⁵⁻⁷

The main reason suggested for the absence of ambient data for many HAPs is the lack of suitable sampling and analysis methods.⁵⁻⁷ As a result, reviews have been conducted of possible measurement methods for the 189 HAPs.^{8,9} However, those reviews have generally considered only long-established standard methods, to the exclusion of novel research methods, and have generally taken optimistic views of the effectiveness of standard methods for measuring the diverse HAPs.^{8,9} The chemical and physical properties of the individual HAPs have not been carefully considered in previous studies. Instead, the approach generally taken has been to suggest measurement methods for HAPs based on the perceived similarity of one HAP to another. The diversity of the HAPs makes this approach suspect. The present study was intended to avoid the shortcomings of previous surveys in identifying measurement methods for the HAPs.

This document is the final report on a survey of measurement methods for the 189 HAPs in ambient air. This work was conducted by Battelle under EPA Contract No. 68-D0-0007, Work Assignment 44. The goal of this project was to identify documented measurement methods for the 189 HAPs that could be applied at Superfund sites where the presence of such compounds was suspected, or in ambient air in urban areas. This survey differed from previous efforts in four important ways:

- (1) It includes a detailed review of physical and chemical properties of the HAPs. Those properties were the basis for selection of measurement methods, and also constitute a valuable product of this study in themselves. The HAPs properties compiled in this survey are included in this report.
- (2) Grouping of HAPs into classes, and ranking of HAPs within those classes, was based on the physical and chemical properties noted above. Identification of measurement methods was based on the properties of individual HAPs and not simply on apparent similarities in chemical composition. As a result, the

identification of methods in this survey is likely to be more realistic than in previous surveys.

- (3) The survey was not limited to compilations of standard methods, but included extensive literature searches to identify research methods applicable to HAPs in ambient air. The research methods identified include (e.g.) several from foreign language journals. This detailed search assures that the most recent and novel approaches have been identified.
- (4) The measurement methods identified for the HAPs have been categorized by the degree of development of the method. Thus, for example, a method which is proven in ambient measurements is distinguished from one proven only at higher concentration levels, as in workplace air. This approach provides a wider range of information to the user of this survey, and results in methods being identified for nearly all the HAPs, albeit at varying levels of development. This approach avoids the all-or-nothing results characteristic of previous method surveys.⁹

The work detailed in this report was conducted between March 1993 and March 1994. Subsequent sections describe the Conclusions, Recommendations, Methods, and Results of this survey. Appendices to this report present extensive tabulations of the properties and measurement methods identified for the HAPs, and the associated literature citations.

SECTION 2

CONCLUSIONS

1. For 126 of the 189 HAPs, measurement methods designed for use in ambient air were identified. Most, but not all, of these methods have actually been used for ambient measurements of the pertinent HAPs.
2. For 53 other HAPs, measurement methods were identified which are likely to be applicable to ambient air after some further development.
3. Based on the two conclusions above, ambient measurement methods appear to be achievable for the great majority of the 189 HAPs.
4. For 6 HAPs, existing measurement methods would require extensive further development before application to ambient air can be considered.
5. For 4 HAPs, no measurement methods in any state of development were identified.
6. The 10 HAPs noted in conclusions 4 and 5 comprise the greatest gap in measurement capabilities for the HAPs.

SECTION 3

RECOMMENDATIONS

1. High priority should be given to further development of measurement methods for the 53 HAPs for which such effort is likely to lead to ambient air measurement capabilities.
2. Development of methods should be initiated for the 10 HAPs for which existing methods are most lacking. However, prioritization of that effort should be based on the reactivity, emitted quantities, and potential products of these HAPs.
3. Method verification efforts should continue for all HAPs, with the aim of consolidating or simplifying the wide variety of measurement methods currently identified.

SECTION 4

SURVEY METHODS

This section describes the methods used to obtain and compile information on the properties and measurement methods of the 189 HAPs. It should be noted that in conducting this study we relied on a list of the 189 HAPs that included (in draft form) the latest corrections and clarifications from the U.S. EPA.¹⁰

HAPs PROPERTIES

The chemical and physical properties of interest in this survey are those that affect the sampling and measurement of HAPs in the atmosphere.¹¹ To organize the compilation of properties, the HAPs were divided into groups. As a starting point, the 189 HAPs were first divided into organic compounds and inorganic compounds (designated OC and INC, respectively). This initial distinction was based largely on the designation of chemicals in the CRC Handbook of Chemistry and Physics,¹² and on the known nature of the HAPs. The primary properties then obtained for all the HAPs were vapor pressure (in mm of Hg at 25°C) and boiling point temperature. The vapor pressure data were the primary factor used to categorize the HAPs further, since vapor pressure indicates the likely physical state of a chemical in the atmosphere. The 189 HAPs were ranked in order of vapor pressure, with boiling point a secondary ranking factor.

Once ranked according to vapor pressure, the HAPs were grouped according to ranges in vapor pressure. Quantitative vapor pressure criteria were set up defining very volatile organic and inorganic compounds (i.e., VVOC and VVINC), volatile compounds (VOC and VINC), semivolatile compounds (SVOC and SVINC), and

nonvolatile compounds (NVOC and NVINC). The vapor pressure criteria corresponding to each of these HAPs volatility classes are shown in Table 1. The vapor pressure criteria shown are the same as those used in previous such categorizations,¹³ except for the very volatile categories (VVOC and VVINC). This study denoted as very volatile any compound with a vapor pressure greater than 380 mm Hg (i.e., half an atmosphere); previous categorizations used a somewhat lower criterion of 10 kPa (i.e., 0.099 atm). The vapor pressure criteria are somewhat arbitrary, and compounds with vapor pressures near the criterion values generally fall into "gray areas" that define gradual transitions from one volatility class to the next. For the volatile and very volatile HAPs, further chemical and physical properties were compiled, consisting of electronic polarizability, water solubility, aqueous reactivity, and estimated lifetime relative to chemical reaction or deposition in the atmosphere. These properties were compiled because they determine the effectiveness with which a HAP may be sampled in the atmosphere,¹¹ and the extent to which atmospheric processes may obscure emissions of HAPs to the atmosphere. Table 1 summarizes the properties reviewed for the various volatility classes of HAPs.

The primary information sources used for the HAPs properties survey were handbooks and data bases of chemical and physical properties,¹²⁻¹⁸ including an EPA computer data base specifically addressing the 189 HAPs.¹⁴ Whenever possible, inconsistencies and errors were corrected by comparisons of data from various sources, and by consultation with EPA staff.

The chemical and physical property data compiled in this study are summarized in Section 5, and presented in detail in Appendix A, for the full list of 189 HAPs. Additional properties are shown in Appendix B, for the VVOCs and VOCs on the HAPs list. Appendix D provides a separate list identifying the organic and inorganic HAPs in each of the volatility ranges.

**TABLE 1. SUMMARY OF HAP CATEGORIES WITH CORRESPONDING VAPOR PRESSURE RANGES
AND PROPERTIES REVIEWED**

Volatility Class ^a	Range of Vapor Pressures (mm Hg at 25°)	Properties Reviewed
VVOC	> 380	Vapor pressure; boiling point; polarizability; water solubility; aqueous reactivity; atmospheric lifetime
VVINC	> 380	Vapor pressure; boiling point; polarizability; water solubility; aqueous reactivity; atmospheric lifetime
VOC	0.1 to 380	Vapor pressure; boiling point; polarizability; water solubility; aqueous reactivity; atmospheric lifetime
VINC	0.1 to 380	Vapor pressure; boiling point; polarizability; water solubility; aqueous reactivity; atmospheric lifetime
SVOC	1×10^{-7} to 0.1	Vapor pressure; boiling point
SVINC	1×10^{-7} to 0.1	Vapor pressure; boiling point
NVOC	$< 1 \times 10^{-7}$	Vapor pressure; boiling point
NVINC	$< 1 \times 10^{-7}$	Vapor pressure; boiling point

- a:
- | | | |
|-------|---|-----------------------------------|
| VVOC | = | very volatile organic compounds |
| VVINC | = | very volatile inorganic compounds |
| VOC | = | volatile organic compounds |
| VINC | = | volatile inorganic compounds |
| SVOC | = | semivolatile organic compounds |
| SVINC | = | semivolatile inorganic compounds |
| NVOC | = | nonvolatile organic compounds |
| NVINC | = | nonvolatile inorganic compounds. |

HAPs MEASUREMENT METHODS

The search for measurement methods for the HAPs was intended to be as wide-ranging as possible. Information sources included standard compilations of air sampling methods, such as EPA Screening Methods, EPA Contract Laboratory Program (CLP) and Compendium (i.e., TO-) methods, as have been used in previous surveys.^{8,9} However, this study also reviewed standard methods designated by the Intersociety Committee on Methods of Air Sampling and Analysis, the National Institute of Occupational Safety and Health (NIOSH), the Occupational Safety and Health Administration (OSHA), and the American Society for Testing and Materials (ASTM). Although not necessarily targeted for ambient air measurements, these methods are well documented and might serve as the starting point for an ambient air method. EPA solid waste (SW 846) methods were also consulted. Another resource was the EPA database on measurement methods for HAPs,⁸ which includes primarily established EPA methods. Additional sources of information were the two surveys recently conducted by Battelle for EPA on the ambient concentrations⁵⁻⁷ and atmospheric transformations^{7,19,20} of the HAPs. The ambient concentrations survey⁵⁻⁷ was especially useful as a guide to measurement methods for HAPs, and assured that methods were identified for all HAPs that have been measured in ambient air. In addition, reports, journal articles, and meeting proceedings known to contain information on HAPs methods were obtained and reviewed. In general, highly complex and expensive spectroscopic research methods were considered unsuitable for widespread monitoring and were not included in this survey.

The aim of the methods survey was to provide information on methods immediately applicable to HAPs measurements, and on those still in development. As a result, measurement methods for the 189 HAPs were organized into three categories, depending on the degree of development of the method. Those categories are:

Demonstrated - A *Demonstrated* method was defined as one which has been reasonably established and documented for measurement of the target HAP in ambient air. In most cases, methods identified as *Demonstrated* have actually been used for

ambient measurements, i.e., ambient data are available illustrating the effectiveness of the method. A good example of a *Demonstrated* method is EPA Compendium Method TO-14,²¹ which has been widely used for VOC measurements. In other cases, a method was identified as *Demonstrated* for a specific HAP because of the degree of documentation and standardization of the method, even though no ambient data were found. The primary examples of this are a few CLP and TO- methods. Although such methods are targeted for a number of HAPs, for a few of those HAPs no ambient measurements were found, and further development may be needed to achieve ambient measurement capabilities. It must be stressed that the existence of a *Demonstrated* method does not guarantee adequate measurement of the pertinent HAP(s) under all circumstances. Further development and evaluation may be needed to assure sensitivity, freedom from interferences, stability of samples, precision, accuracy, etc. under the range of conditions found in ambient measurements.

Likely - Two types of *Likely* measurement methods were defined. The most common type is a method which has been clearly established and used for the target HAP in air, but not in ambient air. The presumption is that further development (such as an increase in sensitivity or sampled volume) would allow measurements in ambient air. The primary examples of this type of *Likely* method are NIOSH or OSHA methods established for HAPs in workplace air. A specific example is OSHA Method No. 21, stated to have a detection limit of 1.3 ppbv in workplace air, and designated as a *Likely* method for acrylamide. In a few cases, such methods have been applied to ambient air, but in such limited conditions or time periods that demonstration of the method is judged to be incomplete. The second type of *Likely* method consists of techniques identified as *Demonstrated* for one HAP, and consequently inferred as *Likely* for another HAP, based on close similarity of chemical and physical properties. An example of an inferred *Likely* method is TO-14 for 1,2-dibromo-3-chloropropane, based on the similarity of this compound to other VOCs in terms of volatility, water solubility, and reactivity.

Potential - A ***Potential*** method was defined as one which needs extensive further development before application to ambient air measurements will be justified. Many ***Potential*** methods have been evaluated under laboratory conditions, or for the target HAP in sample matrices other than air (e.g., water, soil). ***Potential*** methods were inferred for some HAPs, based on ***Demonstrated*** or ***Likely*** methods found for other HAPs of somewhat similar chemical and physical properties. The degree of similarity of properties between HAPs was used as the guide in designating ***Potential*** methods in those cases.

For HAPs for which no ***Demonstrated*** or ***Likely*** methods were found, further searches were conducted beyond the reviews outlined above. For such HAPs, detailed literature searches were conducted using the files of Chemical Abstracts Service (CAS) and the National Technical Information Service (NTIS). Such searches targeted the chemical name and CAS number of the HAP of interest, and used successive sets of keywords such as air; trace or ambient or workplace; and detect or measure or monitor. Abstracts obtained in such searches were reviewed, and whole papers were obtained for review if the abstracts appeared promising. These additional searches were not restricted to English language publications. Several ***Likely*** and ***Potential*** methods reported in foreign language publications were identified by these searches.

In all method searches and reviews, the chemical and physical properties compiled in this study were valuable. The quantitative similarity of properties such as vapor pressure, solubility, and reactivity of HAPs was used to suggest ***Likely*** and ***Potential*** methods, and the degree of similarity of properties determined the choice between designation as a ***Likely*** or ***Potential*** method.

A key characteristic of an ambient air measurement method is the detection limit. As part of this methods survey, ambient air detection limits were indicated whenever they were reported in method documentation. The various units in which detection limits were reported include parts-per-million by volume (ppmv), parts-per-billion by volume (ppbv), parts-per-trillion by volume (pptv), milligrams per cubic meter (mg/m³), micrograms per cubic meter (μg/m³), nanograms per cubic meter

(ng/m³), and picograms per cubic meter (pg/m³). Detection limits were reported in this review as they were stated in the respective methods. Detection limits for certain CLP methods were reported as a Contract Required Quantitation Limits (CRQL) in mass units only (e.g., ng), or as a range of applicable concentrations. In such cases the detection limit was reported as stated in the method, along with needed supporting information such as the approximate sampled air volume. An effort was made to indicate the detection limit for at least the most fully developed method(s) for each HAP. Estimation of detection limits, when they were not explicitly stated in the material reviewed, was generally not done. The detection limits reported should be considered primarily a guide to the relative capabilities of the various methods, rather than an absolute statement of method performance.

Citation of literature in the methods survey was aimed at providing the user of the survey enough information to review at least the basics of the identified method, and to locate further information if needed. No effort was made to compile all possible information on each method.

The results of the HAPs measurement method survey are summarized in Section 5, and are presented in detail in Appendix C for the full list of 189 HAPs.

SECTION 5

SURVEY RESULTS

This section of the report summarizes the data obtained on properties and measurement methods for the 189 HAPs. Complete tables of the information compiled in these surveys are presented in Appendices A and B, for the properties, and Appendix C, for the measurement methods, respectively. For convenience, Appendix D provides a listing of the HAPs by volatility classes. Chemical structure and formula information is presented for all the HAPs in the recent HAPs transformation survey,¹⁹ and for selected HAPs in various handbooks and data bases.^{12,15,16}

HAPs PROPERTIES

The initial result of the survey of HAPs properties was the assignment of HAPs to the various volatility classes. That result is shown in Table 2, which lists the number of HAPs in each compound class. Table 2 shows that the largest classes are the volatile and semivolatile compounds. Organic compounds (166 chemicals) predominate over inorganic compounds (23 chemicals) on the HAPs list as a whole. Inorganic elements and compounds comprise the majority of the non-volatile class of HAPs, i.e., those compounds found exclusively in the particulate phase in the atmosphere.

This report presents the full results of the properties survey, in two different tabular forms. Table A-1 in Appendix A lists the 189 HAPs in the same order as in the CAAA, along with the CAS number and properties compiled for each HAP. An example listing from that table is shown in Figure 1. The successive columns in the example in Figure 1 list the HAP name, CAS number, molecular weight, volatility

TABLE 2. NUMBERS OF HAPs IN EACH VOLATILITY CLASS

Volatility Class ^a	Number of HAPs in Class
VVOC	15
VVINC	6
VOC	82
VINC	3
SVOC	64
SVINC	2
NVOC	5
NVINC	<u>12</u>
Total	189

a: VVOC = very volatile organic compounds
 VVINC = very volatile inorganic compounds
 VOC = volatile organic compounds
 VINC = volatile inorganic compounds
 SVOC = semivolatile organic compounds
 SVINC = semivolatile inorganic compounds
 NVOC = nonvolatile organic compounds
 NVINC = nonvolatile inorganic compounds.

Figure 1. Example of a few entries from Table A-1 on physical properties of the 189 HAPs.

Compound	CAS No.	MW	Compound Class ¹	vp ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Acetaldehyde; C ₂ H ₄ O	75-07-0	44.0	VVOC	952	21	33.0 / 25	
Acetamide; C ₂ H ₅ NO	60-35-5	59.0	SVOC	7.2E-02	222	>100 / 22	
Acetonitrile; C ₂ H ₃ N	75-05-8	41.0	VOC	74.0	82	>100 / 22	
Acetophenone; C ₈ H ₈ O	98-86-2	120.0	VOC	1.0	202	6.3 / 25	
2-Acetylaminofluorene; C ₁₅ H ₁₃ NO	53-96-3	223.3	NVOC	1.1E-12 (?)	444	<0.1 / 20.5	
Acrolein; C ₃ H ₄ O	107-02-8	56.0	VOC	220.0	53	>100 / 21	Reactive ⁵

class, vapor pressure, boiling point, and water solubility. A column for comments is also shown. The second tabular form is Table B-1 in Appendix B, which lists properties for VVOCs and VOCs only. An example from Table B-1 is shown in Figure 2. This example shows that Table B-1 includes some of the information from Table A-1, but also includes information on electronic polarizability, aqueous reactivity, and lifetime in ambient air. The reader is referred to Appendices A and B for the full presentation of results on HAP properties. Appendix B also includes a discussion of polarizability and water solubility as defining characteristics of polar VOCs.

HAPs MEASUREMENT METHODS

The primary product of this study was the identification of methods for ambient measurements of the HAPs. In this subsection the complete data set as presented in Appendix C is described, followed by summary descriptions and comments.

The HAPs method survey is presented in Appendix C in the form of a comprehensive table that presents the 189 HAPs in the same order as they appear in the CAAA. An example portion of that table is shown in Figure 3. For each HAP, the name, CAS number, and major volatility class are shown. The ambient methods information is listed in successive columns for *Demonstrated*, *Likely*, and *Potential* methods. Within each column, the identified methods are indicated by standard method designations (e.g., TO-5, CLP-2, NIOSH 5514), or by citations to the pertinent literature (e.g., R-1, R-2, etc.). The final two columns of the Table show the limits of detection for selected methods, and provide explanatory comments on the entries, respectively.

The methods and literature compiled in conducting the methods survey are cited in a reference list in Appendix C, following the methods table exemplified in Figure 3. Standard methods, such as NIOSH, OSHA, or TO- methods, are listed by title under a general reference heading. Research methods are listed in numerical order (R-1, R-2, etc.). For each research method, the citation includes a brief description of the method, and one or more literature citations pertinent to the method. In all, this survey identified 51 NIOSH methods, 31 OSHA methods; 15 TO- methods, 3 EPA screening

Figure 2. Example of a few entries from Table B-1 on physical and chemical properties of VOCs in the HAPs list.

Compound	CAS No.	Sub-category ¹	VP ² (mm Hg at 25°C)	Polarizability ³ (cm ³ /mole)	Water Solubility ⁴ (g/L at °C)	Reactivity & t _{1/2} range ⁵			Other ⁷
						Aqueous ⁶		Air	
Acetaldehyde	75-07-0	VVOC	952	11.6	33.0 / 25	--	--	--	Polar
Acetonitrile	75-05-8	VOC	74	11.0	>100 / 22	aab	7-28d	54-541d	Polar
Acetophenone	98-86-2	VOC	1	36.3	6.3 / 25	--	--	--	Polar
Acrolein	107-02-8	VOC	220	16.2	>100 / 21	aab	7-28d	3-34h	Polar
Acrylamide	79-06-1	VOC	0.53	--	>100 / 22	--	--	--	Polar
Acrylic acid	79-10-7	VOC	3.2	17.4	>100 / 17	aab	1-7d	3-24h	Polar
Acrylonitrile	107-13-1	VOC	100	15.6	716.0 / 258	aab	1-23d	0.6-8d	Polar
Allyl chloride	107-05-1	VOC	340	20.5	19.5 / 208	ah	7-14d	3-29h	Non-Polar

Figure 3. Example of a few entries from Table C-1 (Ambient Measurement Methods for the 189 HAPs).

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Acetaldehyde	75-07-0	VOC	TO-5 TO-11	R-4 [14]		TO-5: 1 ppbv; TO-11: 1 ppbv; [14]: 30 ppmv	
Acetamide	60-35-5	SVOC			OSHA CIM [A625]; R-37; R-47		[A625]: not a validated method; R-47: method developed for analysis of water
Acetonitrile	75-05-8	VOC	R-1, CLP-1A, R-3	TO-15		R-1: 1 ppbv	
Acetophenone	98-86-2	VOC	CLP-2		TO-15	CLP-2 ⁴ : 37 ng/m ³ (0.007 ppbv)	
2-Acetylaminofluorene	53-96-3	NVOC			OSHA CIM [0065]		[0065]: not a validated method

methods, 4 CLP methods, and 64 reference methods pertinent to the HAPs. The reader is referred to Appendix C for the full results of the methods survey. However, some general comments on the findings of this study are of interest here.

Table 3 is a summary listing of the methods survey results, indicating whether the most fully developed methods for each HAP fall within the definition of *Demonstrated*, *Likely*, or *Potential*. Table 3 lists the HAPs in the same order as in the original Title III list. Table 3 shows the name and volatility class assignment for each HAP, and the status of methods identified for that HAP. This table serves as a quick reference guide, with details presented in Appendix C. Table 3 includes brief definitions for each of the types of methods found (*Demonstrated*, *Likely*, *Potential*). For the *Likely* and *Potential* methods, separate columns are provided for methods inferred on the basis of HAP chemical and physical properties, as opposed to those established for the HAP in question. At the end of Table 3, the total number of HAPs falling in each method development column is indicated.

In considering Table 3, the definition of a *Demonstrated* method must be stressed. A *Demonstrated* method is one which is targeted for the indicated HAP in ambient air, and which has been developed and documented to a reasonable degree. This does not mean that all *Demonstrated* methods have actually been used for ambient measurements of the indicated HAPs, or that all sampling and analysis difficulties have been solved. An overly optimistic view of the state of HAPs measurement methods could result if the summary in Table 3 is taken without these reservations.

Figure 4 is a graphical overview of the results in Table 3 for the 189 HAPs. Figure 4 shows that for 126 HAPs (two-thirds of the HAPs list), *Demonstrated* ambient measurement methods were found. Note that Table 3 and Figure 4 show only the most developed state of methods found; for some of these 126 HAPs, *Likely* and *Potential* methods were also found. Figure 4 also shows that for 53 HAPs, *Likely* methods were found, but no *Demonstrated* methods. Most of these *Likely* methods were specific for the HAP in question, but for 7 HAPs the identification of *Likely* methods was inferred based on HAP properties. For 6 HAPs only *Potential* methods could be identified, and of those, 3 were inferred on the basis of chemical and physical properties. For 4 HAPs

Table 3. Most Developed Ambient Measurement Method Identified for Each of the 189 HAPs.

		Most Developed Ambient Method Identified					
		Demonstrated	Likely		Potential		None
COMPOUND	CLASS	Applied in ambient air	Applied in non-ambient air	Inferred	Applied for compound in other media	Inferred	No methods found
Acetaldehyde	VVOC	X					
Acetamide	SVOC				X		
Acetonitrile	VOC	X					
Acetophenone	VOC	X					
2-Acetylaminofluorene	NVOC				X		
Acrolein	VOC	X					
Acrylamide	VOC		X				
Acrylic acid	VOC						X
Acrylonitrile	VOC	X					
Allyl chloride	VOC	X					
4-Aminobiphenyl	SVOC	X					
Aniline	VOC	X					
o-Anisidine	SVOC		X				
Asbestos	NVINC	X					
Benzene	VOC	X					
Benzidine	SVOC	X					
Benzotrichloride	SVOC				X		
Benzyl chloride	VOC	X					
Biphenyl	SVOC	X					
Bis (2-ethylhexyl)phthalate	SVOC	X					
Bis (chloromethyl) ether	VOC	X					
Bromoform	VOC	X					
1,3-Butadiene	VVOC	X					
Calcium cyanamide	NVINC		X				
Caprolactam	SVOC		X				
Captan	SVOC	X					
Carbaryl	SVOC	X					
Carbon disulfide	VOC	X					
Carbon tetrachloride	VOC	X					
Carbonyl sulfide	VVOC	X					
Catechol	VOC			X			
Chloramben	SVOC					X	
Chlordane	SVOC	X					
Chlorine	VVINC	X					
Chloroacetic acid	VOC		X				
2-Chloroacetophenone	SVOC		X				
Chlorobenzene	VOC	X					
Chlorobenzilate	SVOC		X				
Chloroform	VOC	X					
Chloromethyl methyl ether	VOC		X				
Chloroprene	VOC	X					
Cresol/Cresylic acid (mixed isomers)	VOC	X					
o-Cresol	VOC	X					
m-Cresol	SVOC	X					
p-Cresol	SVOC	X					
Cumene	VOC	X					
2,4-D (2,4-Dichloro phenoxyacetic acid) (incl. salts and esters)	SVOC	X					
DDE	SVOC	X					

Table 3. (continued)

		Most Developed Ambient Method Identified					
		<i>Demonstrated</i>	<i>Likely</i>		<i>Potential</i>		<i>None</i>
COMPOUND	CLASS	Applied in ambient air	Applied in non-ambient air	Inferred	Applied for compound in other media	Inferred	No methods found
Diazomethane	VVOC		X				
Dibenzofurans	SVOC	X					
1,2-Dibromo-3-chloropropane	VOC	X					
Dibutyl phthalate	SVOC	X					
1,4-Dichlorobenzene	VOC	X					
3,3'-Dichlorobenzidine	SVOC		X				
Dichloroethyl ether (Bis[2-chloroethyl]ether)	VOC	X					
1,3-Dichloropropene	VOC	X					
Dichlorvos	SVOC	X					
Diethanolamine	SVOC		X				
Diethyl sulfate	VOC		X				
3,3'-Dimethoxybenzidine	NVOC		X				
4-Dimethylaminoazobenzene	NVOC		X				
N,N-Dimethylaniline	VOC		X				
3,3'-Dimethylbenzidine	SVOC			X			
Dimethylcarbamoyl chloride	VOC		X				
N,N-Dimethylformamide	VOC	X					
1,1-Dimethylhydrazine	VOC		X				
Dimethyl phthalate	SVOC	X					
Dimethyl sulfate	VOC	X					
4,6-Dinitro-o-cresol (including salts)	SVOC	X					
2,4-Dinitrophenol	SVOC	X					
2,4-Dinitrotoluene	SVOC	X					
1,4-Dioxane	VOC	X					
1,2-Diphenylhydrazine	SVOC					X	
Epichlorohydrin	VOC	X					
1,2-Epoxybutane	VOC			X			
Ethyl acrylate	VOC	X					
Ethylbenzene	VOC	X					
Ethyl carbamate	VOC						X
Ethyl chloride	VVOC	X					
Ethylene dibromide	VOC	X					
Ethylene dichloride	VOC	X					
Ethylene glycol	SVOC		X				
Ethyleneimine	VOC		X				
Ethylene oxide	VVOC	X					
Ethylene thiourea	SVOC		X				
Ethylidene dichloride	VOC	X					
Formaldehyde	VVOC	X					
Heptachlor	SVOC	X					
Hexachlorobenzene	SVOC	X					
Hexachlorobutadiene	VOC	X					
1,2,3,4,5,6-Hexachloro cyclohexane (all stereo isomers, including Lindane)	SVOC	X					
Hexachlorocyclopentadiene	SVOC	X					
Hexachloroethane	VOC	X					
Hexamethylene diisocyanate	SVOC		X				
Hexamethylphosphoramide	SVOC						X
Hexane	VOC	X					

Table 3. (continued)

		Most Developed Ambient Method Identified					
		Demonstrated	Likely		Potential		None
COMPOUND	CLASS	Applied in ambient air	Applied in non-ambient air	Inferred	Applied for compound in other media	Inferred	No methods found
Hydrazine	VINC		X				
Hydrochloric acid (Hydrogen chloride)	VINC	X					
Hydrogen fluoride (Hydrofluoric acid)	VVINC	X					
Hydroquinone	SVOC		X				
Isophorone	VOC	X					
Maleic anhydride	SVOC		X				
Methanol	VOC	X					
Methoxychlor	SVOC	X					
Methyl bromide	VVOC	X					
Methyl chloride	VVOC	X					
Methyl chloroform	VOC	X					
Methyl ethyl ketone	VOC	X					
Methylhydrazine	VOC		X				
Methyl iodide	VVOC		X				
Methyl isobutyl ketone	VOC		X				
Methyl isocyanate	VOC		X				
Methyl methacrylate	VOC	X					
Methyl tert-butyl ether	VOC	X					
4,4'-Methylenebis(2-chloroaniline)	NVOC		X				
Methylene chloride	VOC	X					
4,4'-Methylenediphenyl diisocyanate	SVOC		X				
4,4'-Methylenedianiline	NVOC		X				
Naphthalene	SVOC	X					
Nitrobenzene	VOC	X					
4-Nitrobiphenyl	SVOC	X					
4-Nitrophenol	SVOC	X					
2-Nitropropane	VOC		X				
N-Nitroso-N-methylurea	VOC					X	
N-Nitrosodimethylamine	VOC	X					
N-Nitrosomorpholine	VOC			X			
Parathion	SVOC	X					
Pentachloronitrobenzene	SVOC		X				
Pentachlorophenol	SVOC	X					
Phenol	VOC	X					
p-Phenylenediamine	SVOC		X				
Phosgene	VVOC	X					
Phosphine	VVINC	X					
Phosphorus	SVINC		X				
Phthalic anhydride	SVOC		X				
Polychlorinated biphenyl	SVOC	X					
1,3-Propane sulfone	VOC	X					
beta-Propiolactone	VOC		X				
Propionaldehyde	VOC	X					
Propoxur (Baygon)	SVOC	X					
Propylene dichloride	VOC	X					
Propylene oxide	VVOC			X			
1,2-Propylenimine	VOC			X			
Quinoline	SVOC	X					
Quinone	SVOC		X				

Table 3. (continued)

		Most Developed Ambient Method Identified					
		Demonstrated	Likely		Potential		None
COMPOUND	CLASS	Applied in ambient air	Applied in non-ambient air	Inferred	Applied for compound in other media	Inferred	No methods found
Styrene	VOC	X					
Styrene oxide	VOC		X				
2,3,7,8-Tetrachloro dibenzo-p-dioxin	SVOC	X					
1,1,2,2-Tetrachloroethane	VOC	X					
Tetrachloroethylene	VOC	X					
Titanium tetrachloride	VINC						X
Toluene	VOC	X					
Toluene-2,4-diamine	SVOC		X				
2,4-Toluene diisocyanate	SVOC		X				
o-Toluidine	SVOC		X				
Toxaphene (chlorinated camphene)	SVOC	X					
1,2,4-Trichlorobenzene	VOC	X					
1,1,2-Trichloroethane	VOC	X					
Trichloroethylene	VOC	X					
2,4,5-Trichlorophenol	SVOC	X					
2,4,6-Trichlorophenol	SVOC	X					
Triethylamine	VOC		X				
Trifluralin	SVOC	X					
2,2,4-Trimethylpentane	VOC	X					
Vinyl acetate	VOC	X					
Vinyl bromide	VVOC			X			
Vinyl chloride	VVOC	X					
Vinylidene chloride	VVOC	X					
Xylene (mixed isomers)	VOC	X					
o-Xylene	VOC	X					
m-Xylene	VOC	X					
p-Xylene	VOC	X					
Antimony Compounds	NVINC	X					
Arsenic Compounds (Inorganic including arsine)	VVINC/NVINC	X					
Beryllium Compounds	NVINC	X					
Cadmium Compounds	NVINC	X					
Chromium Compounds	NVINC	X					
Cobalt Compounds	NVINC	X					
Coke Oven Emissions	SVOC/NVOC	X					
Cyanide Compounds	VVINC/NVINC		X				
Glycol ethers	SVOC		X				
Lead Compounds	NVINC	X					
Manganese Compounds	NVINC	X					
Mercury Compounds	SVINC/NVINC	X					
Fine mineral fibers	NVINC		X				
Nickel Compounds	NVINC	X					
Polycyclic Organic Matter	SVOC/NVOC	X					
Radionuclides (including radon)	VVINC/NVINC	X					
Selenium Compounds	NVINC	X					
All HAPs: 189 Compounds		126	46	7	3	3	4

Note: HAPs that can be categorized in more than one compound class, e.g. mercury compounds in vapor and particulate forms (SVINC and NVINC), have been addressed in this table on the basis of the vapor pressure of the most volatile species present in ambient air. For example, the methods entry for mercury compounds reflects that for the SVINC category (mercury vapor)

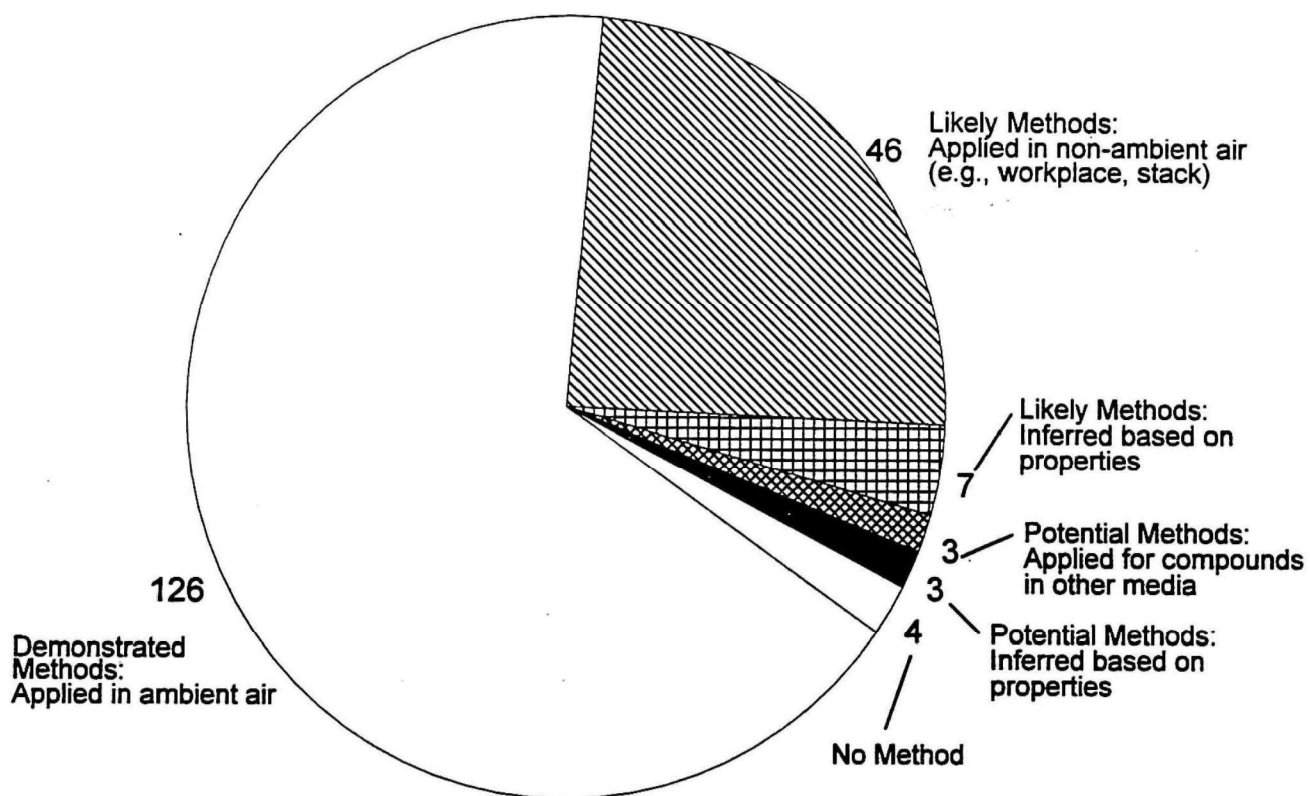


Figure 4. Distribution of the 189 HAPs by the most developed type of ambient measurement method currently available for each compound.

no measurement methods could be identified at any level of development. The finding of 126 HAPs with *Demonstrated* methods is consistent with a recent survey⁵⁻⁷ which disclosed ambient data for 115 of the HAPs.

A more detailed look at the study results is shown in Table 4, which presents the state of methods found for each of the volatility classes of HAPs. Each entry in Table 4 is the number of HAPs in the indicated volatility class, for which the most developed method falls in the indicated method category. For most of the volatility classes, *Demonstrated* methods are identified for the majority of the HAPs. In total, *Demonstrated* methods were identified for 109 of the 166 organic compounds, and for 17 of the 23 inorganic compounds. However, for the 5 NVOCs and 2 of the 3 VINCs, no *Demonstrated* methods were found. Table 4 also shows that in all volatility classes, most compounds with no *Demonstrated* methods could be associated with one or more *Likely* methods. This result indicates that for the great majority of the HAPs, promising methods at least exist from which ambient methods may be developed. However, for 6 HAPs (all organic compounds) only *Potential* methods could be identified, and for 4 HAPs (3 organic, 1 inorganic) no methods of any kind were identified.

In terms of method development needs for the HAPs, the most cost-effective approach would probably be further development of the *Likely* methods that exist for the 53 HAPs with no *Demonstrated* methods. The definition of a *Likely* method means that a reasonable degree of further development should result in a method applicable to ambient air. Of the 53 HAPs with only *Likely* methods, 44 are VVOCs, VOCs, or SVOCs (see Table 4). These three groups are the largest classes of HAPs, so further development of methods for such compounds would be particularly beneficial. In addition, the large number of *Demonstrated* methods already available for volatile and semi-volatile organics should enhance development of methods for additional compounds. A good example is the current effort to extend canister sampling and analysis, as embodied in EPA Compendium Method TO-14,²¹ to a broader range of volatile compounds, including HAPs. Activities toward extension of the TO-14 method include evaluations of the utility of canister sampling for polar HAPs;^{e.g., 22-26}

Table 4. Type of Measurement Methods Currently Available for Each of the 189 HAPs, by Volatility Class.

		Most Applicable Ambient Method Identified					
		<i>Demonstrated</i>	<i>Likely</i>		<i>Potential</i>		<i>None</i>
VOLATILITY CLASS	Total in Class	Applied in ambient air	Applied in non-ambient air	Inferred	Applied for compound in other media	Inferred	No methods found
VVOC	15	11	2	2	0	0	0
VOC	82	60	15	4	0	1	2
SVOC	64	38	20	1	2	2	1
NVOC	5	0	4	0	1	0	0
VVINC	6	5	1	0	0	0	0
VINC	3	1	1	0	0	0	1
SVINC	2	1	1	0	0	0	0
NVINC	12	10	2	0	0	0	0
Totals	189	126	46	7	3	3	4

Note: HAPs that can be categorized in more than one compound class, e.g. mercury compounds in vapor and particulate forms (SVINC and NVINC), have been assigned in this table based on the vapor pressure of the most volatile species present in ambient air. For example, mercury compounds have been assigned to the SVINC category using this rationale.

modelling of the adsorptive behavior of VOCs in canisters;^{11,27} and preparation of a more broadly applicable canister method, designated TO-15.²⁸

Continued evaluation of measurement methods for all the HAPs would be worthwhile. An important goal of that effort should be to consolidate and simplify the variety of methods available into a smaller number of well-characterized and broadly applicable methods. Although some of the standard EPA methods cited in this survey are intended to be broadly applicable, the diversity of the 189 HAPs calls for further work in this area. Development of a TO-15 canister-based method of broad applicability to the volatile HAPs is one opportunity for such consolidation.²⁸ Another area of opportunity for consolidation of methods is the NIOSH and OSHA workplace methods, many of which are cited in this survey as *Likely* methods for various HAPs. Although generally targeted for a single chemical or a small group of chemicals, the workplace methods often share very similar operational and analytical procedures. Combination or consolidation of these methods thus would seem feasible. Finally, further verification of HAPs methods is needed, even for *Demonstrated* methods. The existence of *Demonstrated* methods for 126 of the HAPs may present an optimistic picture of the state of HAPs measurement capabilities. However, the absence of ambient data from some *Demonstrated* methods, the reactivity of some HAPs, the variability of ambient sampling conditions, and the complexity of air composition that can be encountered in ambient measurements suggest that for many methods further testing is needed. The 64 research methods identified here, which have generally been applied only to a limited extent by a small number of investigators, are particularly appropriate candidates for further evaluation.

The 10 HAPs for which only *Potential* methods or no methods were found would seem to indicate the greatest current need for ambient method development. Those 10 compounds are identified in Table 5, which also indicates their respective volatility classes. These 10 HAPs are relatively unusual compounds, not normally regarded as ambient air contaminants, and some are highly reactive and not likely to be present for long in the atmosphere.^{7,19,20} There are no ambient air concentration data for these 10 HAPs,⁵⁻⁷ and virtually no information on potential atmospheric reaction

**TABLE 5. IDENTIFICATION OF THE TEN HAPs FOR WHICH
AMBIENT METHODS ARE LEAST DEVELOPED**

Compound	CAS No.	Volatility Class
<u>Potential Methods Identified</u>		
Acetamide	60-35-5	SVOC
2-Acetylaminofluorene	53-96-3	NVOC
Benzotrichloride	98-07-7	SVOC
Chloramben	133-90-4	SVOC
1,2-Diphenylhydrazine	122-66-7	SVOC
N-nitroso-N-methyl urea	684-93-5	VOC
<u>No Methods Identified</u>		
Acrylic acid	79-10-7	VOC
Ethyl carbamate (urethane)	51-79-6	VOC
Hexamethyl phosphoramide	680-31-9	SVOC
Titanium tetrachloride	7550-45-0	VINC

products,^{19,20} so it is difficult to determine whether they or their reaction products cause a significant health risk in ambient air. Method development should be pursued for these 10 HAPs. However, because of the very inadequate state of current methods, such method development should be prioritized based on information on the emissions, reactivity, and products of these HAPs. This approach will avoid spending time and resources on method development for a HAP or HAPs that are, for example, too reactive (e.g., titanium tetrachloride) or emitted in quantities too small to be present at measurable levels in the atmosphere. This linkage of method development with other information should be valuable for all HAPs, but especially so for the 10 HAPs shown in Table 5.

REFERENCES

- (1) Clean Air Act Amendments of 1990, Conference Report to Accompany S. 1630, Report No. 101-952, U.S. Government Printing Office, Washington, D.C., 1990, pp 139-162.
- (2) Shah, J.J., Heyerdahl, E.K. National Ambient Volatile Organic Compounds (VOCs) Data Base Update, Report EPA-600/3-88/010(a), U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, 1988.
- (3) Shah, J.J., Singh, H.B. Distribution of Volatile Organic Chemicals in Outdoor and Indoor Air: A National VOCs Data Base, Environ. Sci. Technol., 1988, 22, 1381-1388.
- (4) Shah, J.J., Joseph, D.W. National Ambient VOC Data Base Update: 3.0, report to U.S. Environmental Protection Agency, Contract No. 68-D8-0082, by G₂ Environmental, Inc., Washington, D.C., under subcontract from Battelle, Columbus, Ohio, May 1993.
- (5) Kelly, T.J., Mukund, R., Pollack, A.J., Spicer, C.W. Ambient Concentration Summaries for Clean Air Act Title III Hazardous Air Pollutants, Final Report to U.S. Environmental Protection Agency, Contract No. 68-D8-0082, Battelle, Columbus, Ohio, July 1993.
- (6) Kelly, T.J., Mukund, R., Pollack, A.J., Spicer, C.W., Shah, J., Joseph, D.W., Cupitt, L.T. Surveys of the 189 CAAA Hazardous Air Pollutants: I. Atmospheric Concentrations in the U.S., in Measurement of Toxic and Related Air Pollutants, Proceedings of the 1993 EPA/AWMA International Symposium, EPA Report No. EPA/600/A93/024, Publication VIP-34, Air and Waste Management Association, Pittsburgh, Pennsylvania, pp 161-166, 1993.
- (7) Kelly, T.J., Mukund, R., Spicer, C.W., Pollack, A.J. The Hazardous Air Pollutants: Their Concentrations, Transformations, and Fate in Urban Air, Environ. Sci. Technol., in press, March 1994.
- (8) Keith, L.H., Walker, M.M. EPA's Clean Air Act Air Toxics Database, Volume I: Sampling and Analysis Methods Summaries, ISBN-0-87371-819-4, Lewis Publishers, Boca Raton, Florida, 1992.

- (9) Winberry, W.T., Jr. Sampling and Analysis Under Title III, Environmental Lab., June/July 1993, pp 46-58.
- (10) List of Section 112 Hazardous Air Pollutants, update obtained from the U.S. Environmental Protection Agency, Office of Air Quality Planning and Standards, Technology Transfer Network (TTN) computer bulletin board, National Air Toxics Information Clearinghouse (NATICH) subsection, September 15, 1993.
- (11) Coutant, R.W., McClenny, W.A. Competitive Adsorption Effects and the Stability of VOC and PVOC in Canisters, in Proceedings of the 1991 EPA/AWMA Symposium on Measurement of Toxic and Related Air Pollutants, EPA-600/9-91/018, Publication No. VIP-21, Air and Waste Management Association, Pittsburgh, Pennsylvania, pp 382-388, 1991.
- (12) CRC Handbook of Chemistry and Physics, R.C. Weast, ed., 59th Edition, CRC Press, Boca Raton, Florida, 1979.
- (13) Clements, J.B., Lewis, R.G., Sampling for Organic Compounds, in Principles of Environmental Sampling, L.H. Keith, ed., American Chemical Society, Washington, D.C., pp 287-296, 1987.
- (14) Keith, L.H., Walker, M.M. EPA's Clean Air Act Air Toxics Database, Volume II: Air Toxics Chemical and Physical Properties, ISBN-0-87371-820-8, Lewis Publishers, Boca Raton, Florida, 1993.
- (15) Mackay, D., Shiu, W.Y., Ma, K.C. Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals, Volume III: Volatile Organic Chemicals, ISBN-0-83731-973-5, Lewis Publishers, Chelsea, Michigan, 1993.
- (16) Howard, P.H., Boethling, R.S., Jarvis, W.F., Meylan, W.M., Michalenko, E.M. Handbook of Environmental Degradation Rates, ISBN-0-87371-358-3, Lewis Publishers, Chelsea, Michigan, 1991.
- (17) Jones, D.L., Bursey, J. Simultaneous Control of PM-10 and Hazardous Air Pollutants, II: Rationale for Selection of Hazardous Air Pollutants as Potential Particulate Matter, EPA-452/R-93/013, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, October 1992.
- (18) Weber, R.C., Parker, P.A., Bowser, M. Vapor Pressure Distribution of Selected Organic Chemicals, EPA-600/2-81/021, U.S. Environmental Protection Agency, Cincinnati, Ohio, February 1981.

- (19) Spicer, C.W., Pollack, A.J., Kelly, T.J., Mukund, R. A Literature Review of Atmospheric Transformation Products of Clean Air Act Title III Hazardous Air Pollutants, Final Report to U.S. Environmental Protection Agency, Contract No. 68-D80082, Battelle, Columbus, Ohio, July 1993.
- (20) Kelly, T.J., Pollack, A.J., Mukund, R., Spicer, C.W., Cupitt, L.T. Surveys of the 189 CAAA Hazardous Air Pollutants: II. Atmospheric Lifetimes and Transformation Products, in Measurement of Toxic and Related Air Pollutants, Proceedings of the 1993 EPA/AWMA International Symposium, EPA Report No. EPA/600/A93/024, Publication VIP-34, Air and Waste Management Association, Pittsburgh, Pennsylvania, pp 167-172, 1993.
- (21) McClenny, W.A., Pleil, J.D., Evans, G.F., Oliver, K.D., Holdren, M.W., Winberry, W.T. Canister-Based Method for Monitoring Toxic VOCs in Ambient Air, J. Air Waste Manage. Assoc., 1991, 41: 1308-1318.
- (22) McClenny, W.A., Evans, G.F., Oliver, K.D., Daughtery, E.H., Jr., Winberry, W.T., Decker, D.L. Status of VOC Methods Development to Meet Monitoring Requirements for the Clean Air Act Amendments of 1990, in Measurement of Toxic and Related Air Pollutants, Proceedings of the 1991 U.S. EPA/AWMA International Symposium, Report No. EPA-600/9-91/018, Publication VIP-21, Air and Waste Management Assoc., Pittsburgh, Pennsylvania, pp 367-374, 1991.
- (23) Kelly, T.J., Holdren, M.W. Applicability of Canister Sampling for Hazardous Air Pollutants, Final Report to U.S. Environmental Protection Agency, Contract No. 68-D0-0007, Work Assignment 45, Subtask 4, Battelle, Columbus, Ohio, March 1994.
- (24) Kelly, T.J., Callahan, P.J., Pleil, J.D., Evans, G.E. Method Development and Field Measurements for Polar Volatile Organic Compounds in Ambient Air, Environ. Sci. Technol., 1993, 27: 1146-1153.
- (25) Oliver, K.D. Sample Integrity of Trace Level Polar VOCs in Ambient Air Stored in Summa-Polished Canisters, Technical Note TN-4420-93-03, submitted to U.S. EPA under Contract No. 68-D0-0106, by ManTech Environmental Technology, Inc., Research Triangle Park, North Carolina, November, 1993.
- (26) Pate, B., Jayanty, R.K.M., Peterson, M.R., Evans, G.F. Temporal Stability of Polar Organic Compounds in Stainless Steel Canisters, J. Air Waste Manage. Assoc., 1992, 42: 460-462.

- (27) Coutant, R.W. Theoretical Evaluation of Stability of Volatile Organic Chemicals and Polar Volatile Organic Chemicals in Canisters, Final Report to U.S. EPA, Contract No. 68-D0-0007, Work Assignment No. 45, Subtask 2, Battelle, Columbus, Ohio, September 1993.
- (28) Holdren, M.W. and Winberry, W.T. Method TO-15: The Determination of Volatile Organic Compounds (VOCs) in Air Collected in Summa Canisters and Analyzed by Gas Chromatography/Mass Spectrometry (GC/MS), Final Report to U.S. EPA, Contract No. 68-D0-0007, Work Assignment No. 40, Battelle, Columbus, Ohio, March 1994.

APPENDIX A
RESULTS OF THE SURVEY OF CHEMICAL AND PHYSICAL PROPERTIES
OF THE 189 HAPs

Table A-1. Physical Properties of the 189 Compounds in the HAPs List.

Compound	CAS No.	MW	Compound Class ¹	Vp ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Acetaldehyde; C ₂ H ₄ O	75-07-0	44.0	VVOC	952.0	21	33.0 / 25	
Acetamide; C ₂ H ₅ NO	60-35-5	59.0	SVOC	7.2E-02	222	>100 / 22	
Acetonitrile; C ₂ H ₃ N	75-05-8	41.0	VOC	74.0	82	>100 / 22	
Acetophenone; C ₈ H ₈ O	98-86-2	120.0	VOC	1.0	202	6.3 / 25	
2-Acetylaminofluorene; C ₁₅ H ₁₃ NO	53-96-3	223.3	NVOC	1.1E-12 (?)	444	<0.1 / 20.5	
Acrolein; C ₃ H ₄ O	107-02-8	56.0	VOC	220.0	53	>100 / 21	Reactive ⁵
Acrylamide; C ₃ H ₅ NO	79-06-1	71.0	VOC	0.53	125/25 mm	>100 / 22	Reactive ⁵
Acrylic acid; C ₃ H ₄ O ₂	79-10-7	72.0	VOC	3.2	141	>100 / 17	
Acrylonitrile; C ₃ H ₃ N	107-13-1	53.0	VOC	100.0	77	716.0 / 25 ⁴	
Allyl chloride; C ₃ H ₅ Cl	107-05-1	76.5	VOC	340.0	45	19.5 / 20 ⁴	
4-Aminobiphenyl; C ₁₂ H ₁₁ N	92-67-1	169.0	SVOC	6.0E-05	302	<0.1 / 19	
Aniline; C ₆ H ₇ N	62-53-3	93.0	VOC	0.67	184	1.0 / 25*	
o-Anisidine; C ₇ H ₉ NO	90-04-0	123.0	SVOC	0.1	224	<0.1 / 19	Reactive ⁶
Asbestos	1332-21-4	--	NVINC	Very low	Decomposes at 1112°C	Insoluble	
Benzene; C ₆ H ₆	71-43-2	78.0	VOC	76.0	80	1-5 / 18	
Benzidine; C ₁₂ H ₁₂ N ₂	92-87-5	184.2	SVOC	1.0E-05	402	< 1 / 22	
Benzotrichloride; C ₇ H ₅ Cl ₃	98-07-7	195.5	SVOC	7.6E-02	213	Reacts	Reactive ⁵
Benzyl chloride; C ₇ H ₇ Cl	100-44-7	126.6	VOC	1.0	179	Reacts	Reactive (?) ⁸
Biphenyl; C ₁₂ H ₁₀	92-52-4	154.0	SVOC	3.9E-04	254	Insoluble	
Bis(2-ethylhexyl) phthalate; C ₂₄ H ₃₈ O ₄	117-81-7	390.5	SVOC	1.4E-07	384	<0.1 / 22	

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	vp ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Bis(chloromethyl) ether; C ₂ H ₄ Cl ₂ O	542-88-1	115.0	VOC	30.0	104	Reacts	Reactive ⁷
Bromoform; CHBr ₃	75-25-2	252.8	VOC	5.6	149	<0.1 / 22.5	
1,3-Butadiene; C ₄ H ₆	106-99-0	54.0	VVOC	2000.0	-5	Insoluble	Reactive (?) ⁸
Calcium cyanamide; CaCN ₂	156-62-7	80.0	NVINC	<<1.0E-10	1175	Insoluble	Reactive ⁵
Caprolactam; C ₆ H ₁₁ NO	105-60-2	113.0	SVOC	1.0E-03	139/12 mm	>100 / 20.5	
Captan; C ₉ H ₈ Cl ₃ NO ₂ S	133-06-2	300.6	SVOC	9.7E-07	479	<1 / 20	Pesticide
Carbaryl; C ₁₂ H ₁₁ NO ₂	63-25-2	201.2	SVOC	1.4E-06	331	40 /	Pesticide
Carbon disulfide; CS ₂	75-15-0	76.0	VOC	260.0	47	<1 / 20	
Carbon tetrachloride; CCl ₄	56-23-5	153.8	VOC	90.0	77	<1 / 21	
Carbonyl sulfide; COS	463-58-1	60.1	VVOC	3700.0	-50	>100 / 20	
Catechol; C ₆ H ₆ O ₂	120-80-9	110.0	VOC	0.2	240	>100 / 21.5	
Chloramben; C ₇ H ₅ Cl ₂ NO ₂	133-90-4	206.0	SVOC	4.7E-06	350	<0.1 / 22	Pesticide
Chlordane; C ₁₀ H ₆ Cl ₈	57-74-9	409.8	SVOC	9.8E-6	175/2 mm	<1 / 23	Pesticide - mixture of compds; VP for α- or γ- chlordane
Chlorine; Cl ₂	7782-50-5	70.9	VVINC	4000.0	-34	>100 / 0	
Chloroacetic acid; C ₂ H ₃ ClO ₂	79-11-8	94.5	VOC	0.7	189	>100 / 20	
2-Chloroacetophenone; C ₈ H ₇ ClO	532-27-4	154.6	SVOC	1.2E-02	245	<1 / 19	
Chlorobenzene; C ₆ H ₅ Cl	108-90-7	112.6	VOC	8.8	132	<1 / 20	
Chlorobenzilate; C ₁₆ H ₁₄ Cl ₂ O ₃	510-15-6	325.2	SVOC	2.2E-06	415	<0.1 / 22	Pesticide
Chloroform; CHCl ₃	67-66-3	119.0	VOC	160.0	61	0.85 / 20 - 24 ⁴	
Chloromethyl methyl ether; C ₂ H ₅ ClO	107-30-2	80.5	VOC	224.0	59	Reacts	Reactive ⁷

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	VP ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Chloroprene (2-chloro-1,3-butadiene); C ₄ H ₅ Cl	126-99-8	88.5	VOC	226.0	59	Slightly soluble	
Cresol/Cresylic acid (isomer mixture); C ₇ H ₈ O	1319-77-3	108.0	VOC	0.3	202		
o-Cresol; C ₇ H ₈ O	95-48-7	108.0	VOC	0.2	191	25.9 / 25	
m-Cresol; C ₇ H ₈ O	108-39-4	108.0	SVOC	4.0E-02	202	10-50 / 20	
p-Cresol; C ₇ H ₈ O	106-44-5	108.0	SVOC	4.0E-02	202	<1 / 21	
Cumene; C ₉ H ₁₂	98-82-8	120.0	VOC	3.2	153	Insoluble	
2,4-D (2,4-dichlorophenoxyacetic acid, incl salts & esters); C ₈ H ₆ Cl ₂ O ₃	—	—	SVOC/NVOC	1.0E-04 to 1.0E-10	135 / 1 mm		Pesticide; VP range for acid, esters, and salts; BP for acid
DDE (1,1-dichloro-2,2-bis(p-chlorophenyl) ethylene); C ₁₄ H ₈ Cl ₄	72-55-9	318.0	SVOC	2.4E-05	350	<0.1 / 22	Pesticide
Diazomethane; CH ₂ N ₂	334-88-3	42.1	VVOC	2800.0	-23	Reacts	Highly reactive ⁵
Dibenzofurans:							
Dibenzofuran; C ₁₂ H ₈ O	132-64-9	168.0	SVOC	4.4E-03	287	Slightly	Higher chlorinated species (e.g., octa) are SVOCs to NVOCs
Tetrachlorodibenzofuran; C ₁₂ H ₄ Cl ₄ O	5120-31-9	306.0	SVOC	1.1E-06	429	<1 / 20	
1,2-Dibromo-3-chloropropane; C ₃ H ₅ Br ₂ Cl	96-12-8	236.4	VOC	0.8	196	<0.1 / 18	
Dibutylphthalate; C ₁₆ H ₂₂ O ₄	84-74-2	278.4	SVOC	4.2E-05	340	<1 / 20	
1,4-Dichlorobenzene (p-); C ₆ H ₄ Cl ₂	106-46-7	147.0	VOC	0.6	173	<1 / 23	
3,3'-Dichlorobenzidine; C ₁₂ H ₁₀ Cl ₂ N ₂	91-94-1	253.0	SVOC	2.6E-06	402	Insoluble	
Dichloroethyl ether (Bis[2-Chloroethyl]ether); C ₄ H ₈ Cl ₂ O	111-44-4	143.0	VOC	0.7	178	Reacts	Reactive (?) ⁸
1,3-Dichloropropene; C ₃ H ₄ Cl ₂ (cis)	542-75-6	111.0	VOC	27.8	112	<0.1 / 16.5	
Dichlorvos; C ₄ H ₇ Cl ₂ O ₄ P	62-73-7	221.0	SVOC	5.3E-02	140/20 mm	0.01 /	Pesticide
Diethanolamine; C ₄ H ₁₁ NO ₂	111-42-2	105.0	SVOC	1.0E-02	269	>100 / 14	Reactive (?) ⁸ ; strong base
Diethyl sulfate; C ₄ H ₁₀ O ₄ S	64-67-5	154.0	VOC	0.29	208	Reacts	Reactive (?) ⁸

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	VP ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
3,3'-Dimethoxybenzidine; C ₁₄ H ₁₆ N ₂ O ₂	119-90-4	244.0	NVOC	3.2E-13	458	<0.1 / 20	
4-Dimethyl aminoazobenzene; C ₁₄ H ₁₅ N ₃	60-11-7	225.3	NVOC	6.8E-10	407	<1 / 22	
N,N-Dimethylaniline; C ₈ H ₁₁ N	121-69-7	121.0	VOC	0.5	192	<1 / 21	
3,3'-Dimethylbenzidine; C ₁₄ H ₁₆ N ₂	119-93-7	212.3	SVOC	2.9E-07	300	<1 / 19	
Dimethylcarbamoylchloride; C ₃ H ₆ ClNO	79-44-7	107.6	VOC	4.9	166	Reacts	Highly reactive ⁷
N,N-Dimethylformamide; C ₃ H ₇ NO	68-12-2	73.0	VOC	2.7	153	>100 / 22	
1,1-Dimethylhydrazine; C ₂ H ₈ N ₂	57-14-7	60.0	VOC	157.0	63	Reacts	Reactive (?) ⁸
Dimethyl phthalate, C ₁₀ H ₁₀ O ₂	131-11-3	194.0	SVOC	8.9E-03	282	<1 / 20	
Dimethyl sulfate; C ₂ H ₆ O ₄ S	77-78-1	126.1	VOC	1.0	188	>100 / 20	Reactive (?) ⁸
4,6-Dinitro-o-cresol & salts; C ₇ H ₆ N ₂ O ₅	534-52-1	198.1	SVOC	8.3E-05	312	slightly soluble	Pesticide; VP, BP for the cresol; salts are probably NVOCs
2,4-Dinitrophenol; C ₆ H ₄ N ₂ O ₅	51-28-5	184.0	SVOC	1.0E-05	Sublimes on heating	<1 / 19.5	
2,4-Dinitrotoluene; C ₇ H ₆ N ₂ O ₄	121-14-2	182.0	SVOC	3.7E-03	300	<0.1 / 17	
1,4-Dioxane (1,4-Diethylene oxide); C ₄ H ₈ O ₂	123-91-1	88.0	VOC	37.0	101	>100 / 20	
1,2-Diphenylhydrazine; C ₁₂ H ₁₂ N ₂	122-66-7	184.3	SVOC	8.0E-02	220	Insoluble	Reactive (?) ⁸
Epichlorohydrin (1-chloro-2,3-epoxy propane); C ₃ H ₅ ClO	106-89-8	92.5	VOC	12.0	117	50-100 / 22	Highly reactive ⁶
1,2-Epoxybutane; C ₄ H ₈ O	106-88-7	72.0	VOC	163.0	63	>100 / 17	Reactive ⁶
Ethyl acrylate; C ₅ H ₈ O ₂	140-88-5	100.0	VOC	29.3	100	4.2 / 20 ⁴	
Ethylbenzene; C ₈ H ₁₀	100-41-4	106.0	VOC	7.0	136	<1 / 23	
Ethyl carbamate (urethane); C ₃ H ₇ NO ₂	51-79-6	89.0	VOC	0.54	183	>100 / 22	
Ethyl chloride; C ₂ H ₅ Cl	75-00-3	64.5	VVOC	1000.0	13	>100 / 20	

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	VP ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Ethylene dibromide; C ₂ H ₄ Br ₂	106-93-4	187.9	VOC	11.0	132	<1 / 21	Pesticide
Ethylene dichloride; C ₂ H ₄ Cl ₂	107-06-2	99.0	VOC	61.5	84	5-10 / 19	Pesticide
Ethylene glycol; C ₂ H ₆ O ₂	107-21-1	62.0	SVOC	5.0E-02	198	>100 / 17.5	
Ethylenimine; C ₂ H ₅ N	151-56-4	43.0	VOC	160.0	56	Miscible	Reactive (?) ⁸
Ethylene oxide; C ₂ H ₄ O	75-21-8	44.0	VVOC	1100.0	11	Miscible	Reactive ⁸
Ethylene thiourea; C ₃ H ₆ N ₂ S	96-45-7	102.0	SVOC	1.5E-06	450	1-5 / 18	
Ethylidene dichloride; C ₂ H ₄ Cl ₂	75-34-3	99.0	VOC	230.0	57	<1 / 20	
Formaldehyde; CH ₂ O	50-00-0	30.0	VVOC	2700.0	-20	>100 / 20.5	
Heptachlor; C ₁₀ H ₅ Cl ₇	76-44-8	373.3	SVOC	2.3E-04	145/1.5 mm	<0.1 / 18	Pesticide
Hexachlorobenzene; C ₆ Cl ₆	118-74-1	284.8	SVOC	9.5E-04	324	<1 / 20	Pesticide
Hexachlorobutadiene; C ₄ Cl ₆	87-68-3	260.8	VOC	0.4	215	<0.1 / 22	
1,2,3,4,5,6- Hexachlorocyclohexane (Lindane) (all isomers); C ₆ H ₆ Cl ₆	58-89-9	290.8	SVOC	5.6E-05	323	<1 / 24	Pesticide
Hexachlorocyclopentadiene; C ₅ Cl ₆	77-47-4	272.8	SVOC	4.0E-02	234	<0.1 / 21.5	Reactive (?) ⁸
Hexachloroethane; C ₂ Cl ₆	67-72-1	236.7	VOC	0.4	Sublimes at 186	<1 / 21	
Hexamethylene-1,6-diisocyanate; C ₆ H ₁₂ N ₂ O ₂	822-06-0	168.2	SVOC	1.9E-03	255		Reactive (?) ⁸
Hexamethylphosphoramide; C ₆ H ₁₈ N ₃ OP	680-31-9	179.2	SVOC	9.0E-02	233	>100 / 18	
Hexane; C ₆ H ₁₄	110-54-3	86.2	VOC	120.0	69	<1 / 16.5	
Hydrazine; H ₄ N ₂	302-01-2	32.1	VINC	16.0	113	Miscible	
Hydrogen chloride; HCl	7647-01-0	36.5	VINC	23.5	110	>100 / 20	
Hydrogen fluoride; HF	7664-39-3	20.0	VVINC	900.0	20	Very soluble	
Hydroquinone; C ₆ H ₆ O ₂	123-31-9	110.0	SVOC	7.2E-06	218	10-50 / 20	

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	vp ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Isophorone; C ₉ H ₁₄ O	78-59-1	138.2	VOC	0.38	215	0.1-1 / 18	
Maleic anhydride; C ₄ H ₂ O ₃	108-31-6	98.0	SVOC	5.0E-05	202	Soluble	Reactive ⁵
Methanol; CH ₄ O	67-56-1	32.0	VOC	92.0	65	>100 / 21	
Methoxychlor; C ₁₆ H ₁₅ Cl ₃ O ₂	72-43-5	345.7	SVOC	1.4E-06	447	<1 / 23	Pesticide
Methyl bromide; CH ₃ Br	74-83-9	94.9	WVOC	1800.0	4	Slightly soluble	Pesticide
Methyl chloride; CH ₃ Cl	74-87-3	50.5	WVOC	3800.0	-24	Slightly soluble	
Methyl chloroform (1,1,1-trichloroethane); C ₂ H ₃ Cl ₃	71-55-6	133.4	VOC	100.0	74	<1 / 20	
Methyl ethyl ketone (2-butanone); C ₄ H ₈ O	78-93-3	72.0	VOC	77.5	80	>100 / 19	
Methylhydrazine; CH ₆ N ₂	60-34-4	46.1	VOC	49.6	88	<1 / 24	Highly reactive ⁷
Methyl iodide (iodomethane); CH ₃ I	74-88-4	141.9	WVOC	400.0	42	10-50 / 18	
Methyl isobutyl ketone (hexone); C ₆ H ₁₂ O	108-10-1	100.2	VOC	6.0	117	1-5 / 21	
Methyl isocyanate; C ₂ H ₃ NO	624-83-9	57.1	VOC	348.0	60	Reacts	Highly reactive ⁷
Methyl methacrylate; C ₅ H ₈ O ₂	80-62-6	100.1	VOC	28.0	101	15.9 / 20	
Methyl ter-butyl ether; C ₅ H ₁₂ O	1634-04-4	86.0	VOC	249.0	55	Soluble	
4,4'-Methylenebis(2-chloroaniline); C ₁₃ H ₁₂ Cl ₂ N ₂	101-14-4	267.2	NVOC	3.9E-16	517	<1 / 25	
Methylene chloride; CH ₂ Cl ₂	75-09-2	84.9	VOC	349.0	40	10-50 / 21	
4,4'-Methylenediphenyl diisocyanate (MDI); C ₁₅ H ₁₀ N ₂ O ₂	101-68-8	250.3	SVOC	1.0E-03	538	Insoluble	Reactive (?) ⁸
4,4'-Methylenedianiline; C ₁₃ H ₁₄ N ₂	101-77-9	198.3	NVOC	1.7E-10	393	<1 / 19	
Naphthalene; C ₁₀ H ₈	91-20-3	128.2	SVOC	4.9E-02	218	<1 / 22	PAH
Nitrobenzene; C ₆ H ₅ NO ₂	98-95-3	123.0	VOC	0.15	211	1.9 / 25	
4-Nitrobiphenyl; C ₁₂ H ₉ NO ₂	92-93-3	199.2	SVOC	4.0E-07	340	Insoluble	

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	VP ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
4-Nitrophenol; C ₆ H ₅ NO ₃	100-02-7	139.0	SVOC	1.3E-06	279	<0.1 / 21	
2-Nitropropane; C ₃ H ₇ NO ₂	79-46-9	89.0	VOC	10.0	120	1.7 / 20	
N-Nitroso-N-methylurea; C ₂ H ₅ N ₃ O ₂	684-93-5	103.0	VOC	10.0	124	<1 / 18	Reactive ⁷
N-Nitrosodimethylamine; C ₂ H ₈ N ₂ O	62-75-9	74.0	VOC	3.7	152	>100 / 19	Reactive ⁷
N-Nitrosomorpholine; C ₄ H ₈ N ₂ O ₂	59-89-2	116.1	VOC	0.32	225	>100 / 19	
Parathion; C ₁₀ H ₁₄ NO ₅ PS	56-38-2	291.3	SVOC	9.7E-06	375	<1 / 23	Pesticide
Pentachloronitrobenzene (quintobenzene); C ₆ Cl ₅ NO ₂	82-68-8	295.3	SVOC	2.4E-03	328	<1 / 22	
Pentachlorophenol; C ₆ Cl ₅ OH	87-86-5	266.3	SVOC	1.1E-04	310	<1 / 20	Pesticide
Phenol; C ₆ H ₆ O	108-95-2	94.0	VOC	0.2	182	50-100 / 19	
p-Phenylenediamine; C ₆ H ₈ N ₂	106-50-3	108.2	SVOC	2.6E-04	267	Soluble	
Phosgene; CCl ₂ O	75-44-5	99.0	WVOC	1200.0	8	Slightly soluble	Reactive (?) ⁸
Phosphine; PH ₃	7803-51-2	34.0	VVINC	2000.0	-88	Slightly soluble	Pesticide
Phosphorus; P	7723-14-0	124.0	SVINC	2.6E-02	280	0.0003%	Highly reactive (red and white forms)
Phthalic anhydride; C ₈ H ₄ O ₃	85-44-9	148.0	SVOC	2.2E-04	285	Reacts	Reactive ⁵
Polychlorinated biphenyls (PCBs): 1-chlorobiphenyl; C ₁₂ H ₉ Cl 2,4,6-trichlorobiphenyl; C ₁₂ H ₇ Cl ₃		188.6	SVOC	1.1E-02	297	Insoluble	Higher chlorinated species (upto deca-) are NVOCs
	1336-36-3	257.5	SVOC	7.8E-05	423	Insoluble	
1,3-Propane sultone; C ₃ H ₆ O ₃ S	1120-71-4	122.1	VOC	2.0	180/30 mm	0.1	Reactive (?) ⁸
Beta-Propiolactone; C ₃ H ₄ O ₂	57-57-8	72.0	VOC	3.4	Decomposes at 162	37.0 / 20	
Propionaldehyde; C ₂ H ₅ CHO	123-38-6	58.1	VOC	235.0	49	50-100 / 18	
Propoxur (Baygon); C ₁₁ H ₁₅ NO ₃	114-26-1	209.2	SVOC	7.8E-07	400	Slightly soluble	Pesticide

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	VP ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Propylene dichloride (1,2-dichloropropane); C ₃ H ₆ Cl ₂	78-87-5	113.0	VOC	42.0	97	<0.1 / 21.5	Pesticide
Propylene oxide; C ₃ H ₆ O	75-56-9	58.0	VVOC	445.0	34	400 / 20	Reactive ⁶
1,2-Propyleneimine (2-methylaziridine); C ₃ H ₇ N	75-55-8	57.1	VOC	112.0	66	>100 / 19	Highly Reactive (?) ⁸
Quinoline; C ₈ H ₇ N	91-25-5	129.2	SVOC	9.5E-02	238	<0.1 / 22.5	
Quinone; C ₆ H ₄ O ₂	106-51-4	108.0	SVOC	1.0E-02	201	Slightly soluble	
Styrene; C ₈ H ₈	100-42-5	104.0	VOC	6.6	145	<1 / 19	
Styrene oxide; C ₈ H ₈ O	96-09-3	120.2	VOC	0.3	194	<1 / 19.5	Highly reactive ⁷
2,3,7,8-Tetrachlorodibenzo-p-dioxin; C ₁₂ H ₄ Cl ₄ O ₂	1746-01-6	322.0	SVOC	3.6E-06	495	<1 / 25	
1,1,2,2-Tetrachloroethane; C ₂ H ₂ Cl ₄	79-34-5	167.9	VOC	5.0	146	<0.1 / 22	
Tetrachloroethylene; C ₂ Cl ₄	127-18-4	165.8	VOC	14.0	121	<0.1 / 17	
Titanium tetrachloride; TiCl ₄	7550-45-0	154.2	VINC	0.3	136	Soluble	Highly reactive in air; forms TiO ₂
Toluene; C ₇ H ₈	108-88-3	92.0	VOC	22.0	111	<1 / 18	
2,4-Toluenediamine; C ₇ H ₁₀ N ₂	95-80-7	122.2	SVOC	3.2E-05	292	1-5 / 21	
2,4-Toluene diisocyanate; C ₈ H ₈ N ₂ O ₂	584-84-9	174.2	SVOC	1.0E-02	251	Reacts	Reactive ⁵
o-Toluidine; C ₇ H ₉ N	95-53-4	107.2	SVOC	0.1	200	5-10 / 15	
Toxaphene (chlorinated camphene); C ₁₀ H ₁₀ Cl ₈	8001-35-2	413.8	SVOC	1.1E-05	155/0.4 mm	<1 / 19	Pesticide; complex mixture of isomers
1,2,4-Trichlorobenzene; C ₆ H ₃ Cl ₃	120-82-1	181.5	VOC	0.2	213	<1 / 21	
1,1,2-Trichloroethane; C ₂ H ₃ Cl ₃	79-00-5	133.4	VOC	19.0	114	1-5 / 20	
Trichloroethylene; C ₂ HCl ₃	79-01-6	131.4	VOC	20.0	87	<1 / 21	
2,4,5-Trichlorophenol; C ₆ H ₃ Cl ₃ O	95-95-4	197.5	SVOC	2.2E-02	252	<0.1 / 18	Pesticide
2,4,6-Trichlorophenol; C ₆ H ₃ Cl ₃ O	88-06-2	197.5	SVOC	1.1E-03	245	<1 / 21	Pesticide

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	VP ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Triethylamine; C ₆ H ₁₅ N	121-44-8	101.2	VOC	54.0	90	Soluble	Reactive (?) ⁸ ; strong base
Trifluralin; C ₁₃ H ₁₆ F ₃ N ₃ O ₄	1582-09-8	335.3	SVOC	1.0E-04	140/4.2 mm	<0.1 / 22.5	Pesticide
2,2,4-Trimethyl pentane; C ₈ H ₁₈	540-84-1	114.0	VOC	40.6	99	Insoluble	
Vinyl acetate; C ₄ H ₈ O ₂	108-05-4	86.0	VOC	83.0	72	Insoluble	
Vinyl bromide (bromoethene); C ₂ H ₃ Br	593-60-2	107.0	WVOC	1100.0	16	Insoluble	
Vinyl chloride (chloroethene); C ₂ H ₃ Cl	75-01-4	62.5	WVOC	3200.0	-14	Slightly soluble	
Vinylidene chloride (1,1-dichloroethylene); C ₂ H ₂ Cl ₂	75-35-4	97.0	WVOC	500.0	32	5-10 / 21	
Xylene (isomer mixture); C ₈ H ₁₀	1330-20-7	106.2	VOC	6.7	142	<1 / 22	
o-Xylene; C ₈ H ₁₀	95-47-6	106.2	VOC	5.0	144	Insoluble	
m-Xylene; C ₈ H ₁₀	108-38-3	106.2	VOC	6.0	139	Insoluble	
p-Xylene; C ₈ H ₁₀	106-42-3	106.2	VOC	6.5	138	Insoluble	
Antimony Compounds: particulate	--	--	NVINC	1 mm / 574°C	656 °C (mp)	Insoluble	VP and MP for antimony trioxide ^{2c} ; Volatile forms exist, e.g., stibene, SbH ₃
Arsenic compounds: Arsine, AsH ₃ Particulate	7784-42-1	78.0	VVINC	> 760	-63	20 mL / 100 cc cold water	
	--	--	NVINC	1 mm / 212°C	313 (mp)	Insoluble	VP and MP given for arsenic trioxide ^{2c}
Beryllium compounds: particulate	--	--	NVINC			Insoluble	
Cadmium compounds: particulate	--	--	NVINC	1 mm / 1000°C		Insoluble	VP given for cadmium oxide ^{2c}
Chromium compounds: particulate	--	--	NVINC			Insoluble	Semi-volatile forms can also exist in air, e.g., Cr(CO) ₆
Cobalt compounds: particulate	--	--	NVINC			Insoluble	Semi-volatile forms can also exist in air, e.g., Co(CO) ₄

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	VP ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Coke Oven Emissions Naphthalene; C ₁₀ H ₁₈	91-20-3	128.2	SVOC	8.7E-02	218	Insoluble	Emissions include VOCs, e.g., benzene, toluene, xylenes
	Coronene 191-07-1	300.4	NVOC	1.5E-12	525	Insoluble	
Cyanide Compounds Hydrogen Cyanide; HCN	74-90-8	27.0	VVINC	630.0	26	Soluble	
	Particulate --	--	NVINC			Insoluble	
Glycol ethers	--	76.1 - 206.3	SVOC/VOC	0.022 to 10.9	120 - 249	10 - 100 / 22 °C	
Lead compounds: particulate	--	--	NVINC	1 mm / 943°C	890 (mp)	Insoluble	VP and MP given for lead oxide ^{2c}
Manganese compounds: particulate	--	--	NVINC			Insoluble	
Mercury Compounds Mercury Vapor	7439-97-6	200.6	SVINC	0.0012 mm/ 20°C	356		
	Particulate --	--	NVINC			Insoluble	
Fine mineral fibers (incl. glass)	--	--	NVINC			Insoluble	
Nickel compounds: particulate	--	--	NVINC			Insoluble	Volatile forms can also exist briefly in air, e.g., Ni(CO) ₄
Polycyclic Organic Matter (POM): Naphthalene; C ₁₀ H ₁₈	91-20-3	128.2	SVOC	8.7E-02	218	Insoluble	PAH
	Coronene 191-07-1	300.4	NVOC	1.5E-12	525	Insoluble	PAH

Table A-1. (continued)

Compound	CAS No.	MW	Compound Class ¹	VP ² (mm Hg/ 25°C)	BP ² (°C)	Water Solubility ³ (g/L at °C)	Comment
Radionuclides							
Various (particulate and gaseous)	10043-92-2	—	NVINC				Reactive (?) ⁸
Radon; Rn-222	14859-67-7	222.0	WVINC	—	-62	224 cc	Noble gas
Selenium compounds: particulate	—	—	NVINC	1 mm / 157°C	340 (mp)	Insoluble	VP and MP given for selenium dioxide ^{2c}

Footnotes:¹ Compound Classes:

- WVOC = Very Volatile Organic Compounds (Vapor Pressure at 25°C >380 mm Hg)
 WVINC or Gases = Very Volatile Inorganic Compounds (Vapor Pressure at 25°C >380 mm Hg)
 VOC = Volatile Organic Compounds (1.0E-01 < Vapor Pressure at 25°C <380 mm Hg)
 VINC or Gases = Volatile Inorganic Compounds (1.0E-01 < Vapor Pressure at 25°C <380 mm Hg)
 SVOC = Semi-Volatile Organic Compounds (1.0E-07 < Vapor Pressure at 25°C <1.0E-01 mm Hg)
 SVINC = Semi-Volatile Inorganic Compounds (1.0E-07 < Vapor Pressure at 25°C <1.0E-01 mm Hg)
 NVOC = Non-Volatile Organic Compounds (Vapor Pressure at 25°C < 1.0E-07 mm Hg)
 NVINC = Non-Volatile Inorganic Compounds (Vapor Pressure at 25°C < 1.0E-07 mm Hg)

² Vapor Pressure (VP) and Boiling Point (BP)/Melting Point (MP) data from:

- (a) D.L. Jones and J. Bursey, "Simultaneous Control of PM-10 and Hazardous Air Pollutants II: Rationale for Selection of Hazardous Air Pollutants as Potential Particulate Matter," Report EPA-452/R-93/013, U.S. Environmental Protection Agency, Research Triangle Park, NC, October 1992.
 (b) R.C. Weber, P.A. Parker, and M. Bowser, Vapor Pressure Distribution of Selected Organic Chemicals, Report EPA-600/2-81-021, U.S. Environmental Protection Agency, Cincinnati, OH, February 1981.
 (c) R.C. Weast, ed., "CRC Handbook of Chemistry and Physics," 59th edition, CRC Press, Boca Raton, 1979.

³ Solubility data from (unless otherwise indicated):

D. Mackay, W.Y. Shui, and K.C. Ma, "Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals: Volume III Volatile Organic Chemicals," Lewis Publishers, Ann Arbor, MI, 1993.

⁴ Obtained from the STN International computer database (BEILSTEIN file)⁵ The Merck Index, 11th Edition, S. Budavari, ed., Merck & Co., Inc., Rahway, NJ, 1989.⁶ R.T. Morrison and R.N. Boyd, "Organic Chemistry," 2nd Edition, Allyn and Bacon, Inc., Boston, MA, 1966.⁷ From reactivity data in Table B-1.⁸ Reactive (?) or Highly Reactive (?) indicates judgment based on properties, personal communication from Robert G. Lewis, U.S. EPA, March 1994.

APPENDIX B

PHYSICAL AND CHEMICAL PROPERTIES OF THE VOLATILE ORGANIC COMPOUNDS ON THE HAPs LIST

1. **Table of Physical and Chemical Properties (Table B-1).**
2. **Discussion of Polarizability and Water Solubility Characteristics of VOCs.**

Table B-1. Physical and Chemical Properties of Volatile Organic Compounds in the HAPs List.

Compound	CAS No.	Sub-category ¹	VP ² (mm Hg at 25°C)	Polarizability ³ (cm ³ /mole)	Water Solubility ⁴ (g/L at °C)	Reactivity & t _{1/2} range ⁵			Other ⁷
						Aqueous ⁶		Air	
Acetaldehyde	75-07-0	VVOC	952.0	11.6	33.0 / 25	--	--	--	Polar
Acetonitrile	75-05-8	VOC	74.0	11.0	>100 / 22	aab	7-28d	54-541d	Polar
Acetophenone	98-86-2	VOC	1.0	36.3	6.3 / 25	--	--	--	Polar
Acrolein	107-02-8	VOC	220.0	16.2	>100 / 21	aab	7-28d	3-34h	Polar
Acrylamide	79-06-1	VOC	0.53	--	>100 / 22	--	--	--	Polar
Acrylic acid	79-10-7	VOC	3.2	17.4	>100 / 17	aab	1-7d	3-24h	Polar
Acrylonitrile	107-13-1	VOC	100.0	15.6	716.0 / 25 ⁸	aab	1-23d	0.6-8d	Polar
Allyl chloride	107-05-1	VOC	340.0	20.5	19.5 / 20 ⁸	ah	7-14d	3-29h	Non-Polar
Aniline	62-53-3	VOC	0.67	30.6	1.0 / 25 ⁸	--	--	--	Polar
Benzene	71-43-2	VOC	76.0	26.2	1-5 / 18	aab	5-16d	2-21d	Non-Polar
Benzyl chloride	100-44-7	VOC	1.0	36.0	Reacts	ah	12d	1-9d	Non-Polar
Bis(chloromethyl) ether	542-88-1	VOC	30.0	22.8	Reacts	ah	0.01-0.1h	0.2-2h	Polar
Bromoform	75-25-2	VOC	5.6	29.8	<0.1 / 22.5	aab	28-180d	54-541d	Non-Polar
1,3-Butadiene	106-99-0	VVOC	2000.0	22.4	Insoluble	aab	7-28d	1-8h	Non-Polar
Carbon disulfide	75-15-0	VOC	260.0	21.5	<1 / 20	--	--	--	Non-Polar
Carbon tetrachloride	56-23-5	VOC	90.0	26.5	<1 / 21	aab	0.5-1y	2-18y	Non-Polar
Carbonyl sulfide	463-58-1	VVOC	3700.0	12.6	>100 / 20	--	--	--	Polar
Catechol	120-80-9	VOC	0.22	32.9	>100 / 21.5	aab	1-7d	3-26h	Polar
Chloroacetic acid	79-11-8	VOC	0.69	17.6	>100 / 20	aab	1-7d	9-86d	Polar
Chlorobenzene	108-90-7	VOC	8.80	31.1	<1 / 20	aab	68-150d	3-30d	Non-Polar
Chloroform	67-66-3	VOC	160.0	21.4	0.85 / 20-24 ⁸	aab	28-168d	26-260d	Non-Polar
Chloromethyl methyl ether	107-30-2	VOC	224.0	18.2	Reacts	ah	0.01-0.03h	1-10d	Polar
Chloroprene	126-99-8	VOC	226.0	25.2	Slightly soluble	aab	28-180d	3-28h	Non-Polar
Cresol/Cresylic acid	1319-77-3	VOC	0.26	32.5		aab	0.04-29d	1-16h	Polar
o-Cresol	95-48-7	VOC	0.24	32.2	25.9 / 25	aab	1-7d	2-16h	Polar
Cumene	98-82-8	VOC	3.20	40.5	Insoluble	aab	3-22d	10-97h	Non-Polar
Diazomethane	334-88-3	VVOC	2800.0	--	Reacts	--	--	--	Polar
1,2-Dibromo-3-chloropropane	96-12-8	VOC	0.80	36.3	<0.1 / 18	aab	14-180d	6-61d	Non-Polar
1,4-Dichlorobenzene	106-46-7	VOC	0.60	36.3	<1 / 23	aab	28-180d	8-84d	Non-Polar
Dichloroethyl ether	111-44-4	VOC	0.71	32.0	Reacts	aab	28-180d	10-97h	Polar

Table B-1. (continued)

Compound	CAS No.	Sub-category ¹	VP ² (mm Hg at 25°C)	Polarizability ³ (cm ³ /mole)	Water Solubility ⁴ (g/L at °C)	Reactivity & t _{1/2} range ⁵			Other ⁷
						Aqueous ⁶		Air	
1,3-Dichloropropene	542-75-6	VOC	27.8	25.5	<0.1 / 16.5	ah	5-11d	5-80h	Non-Polar
Diethyl sulfate	64-67-5	VOC	0.29	31.6	Reacts	ah	2-12h	4-36h	Polar
N,N-Dimethylaniline	121-69-7	VOC	0.50	40.8	<1 / 21	aab	17-180d	3-21h	Polar
Dimethylcarbonyl chloride	79-44-7	VOC	4.9	—	Reacts	ah	0.05h	1-10h	Polar
N,N-Dimethylformamide	68-12-2	VOC	2.7	19.9	>100 / 22	—	—	—	Polar
1,1-Dimethylhydrazine	57-14-7	VOC	157.0	18.7	Reacts	aab	8-24d	1-8h	Non-Polar
Dimethyl sulfate	77-78-1	VOC	1.0	—	>100 / 20	ah	1-12h	2-15d	Polar
1,4-Dioxane	123-91-1	VOC	37.0	21.4	>100 / 20	aab	28-180d	0.3-3d	Polar
Epichlorohydrin	106-89-8	VOC	12.0	20.5	50-100 / 22	aab	7-28d	6-61d	Polar
1,2-Epoxybutane	106-88-7	VOC	163.0	20.3	>100 / 17	ah	12d	1-13d	Polar
Ethyl acrylate	140-88-5	VOC	29.3	26.6	4.2 / 20 ⁸	aab	1-7d	2-23h	Polar
Ethylbenzene	100-41-4	VOC	7.0	35.7	<1 / 23	aab	3-10d	9-86h	Non-Polar
Ethyl carbamate	51-79-6	VOC	0.54	22.6	>100 / 22	aab	1-7d	3-30h	Polar
Ethyl chloride	75-00-3	VVOC	1000.0	16.2	>100 / 20	aab	7-28d	7-67d	Non-Polar
Ethylene dibromide	106-93-4	VOC	11.0	27.0	<1 / 21	aab	28-180d	11-107d	Non-Polar
Ethylene dichloride	107-06-2	VOC	61.5	21.0	5-10 / 19	aab	100-180d	12-122d	Non-Polar
Ethyleneimine	151-56-4	VOC	160.0	—	Miscible	aab	7-28d	11-105h	Polar
Ethylene oxide	75-21-8	VVOC	1100.0	11.2	Miscible	ah	11d	38-382d	Polar
Ethylidene dichloride	75-34-3	VOC	230.00	21.1	<1 / 20	aab	32-150d	10-103d	Non-Polar
Formaldehyde	50-00-0	VVOC	2700.0	8.4	>100 / 20.5	aab	1-7d	1-6h	Polar
Hexachlorobutadiene	87-68-3	VOC	0.40	49.8	<0.1 / 22	aab	28-180d	0.3-3y	Non-Polar
Hexachloroethane	67-72-1	VOC	0.40	—	<1 / 21	aab	28-180d	7-73y	Non-Polar
Hexane	110-54-3	VOC	120.0	29.9	<1 / 16.5	—	—	—	Non-Polar
Isophorone	78-59-1	VOC	0.38	42.1	0.1-1 / 18	aab	7-28d	0.4-3h	Polar
m-Xylene	108-38-3	VOC	6.0	36.0	Insoluble	aab	7-28d	3-26h	Non-Polar
Methanol	67-56-1	VOC	92.0	8.2	>100 / 21	aab	1-7d	3-30d	Polar
Methyl bromide	74-83-9	VVOC	1800.0	15.0	Slightly soluble	aab	28-180d	68-680d	Non-Polar
Methyl chloride	74-87-3	VVOC	3800.0	11.5	Slightly soluble	ah	292d	61-613d	Non-Polar
Methyl chloroform	71-55-6	VOC	100.0	26.2	<1 / 20	aab	0.4-0.5y	0.6-6y	Non-Polar
Methyl ethyl ketone	78-93-3	VOC	77.5	20.7	>100 / 19	aab	1-7d	3-27d	Polar
Methylhydrazine	60-34-4	VOC	49.6	13.7	<1 / 24	aab	13-24d	0.1-0.4h	Non-Polar

Table B-1. (continued)

Compound	CAS No.	Sub-category ¹	VP ² (mm Hg at 25°C)	Polarizability ³ (cm ³ /mole)	Water Solubility ⁴ (g/L at °C)	Reactivity & t _{1/2} range ⁵			Other ⁷
						Aqueous ⁶		Air	
Methyl iodide	74-88-4	VVOC	400.0	19.3	10-50 / 18	aab	7-28d	22-223d	Non-Polar
Methyl isobutyl ketone	108-10-1	VOC	6.0	30.0	1-5 / 21	aab	1-7d	5-46h	Polar
Methyl isocyanate	624-83-9	VOC	348.0	14.0	Reacts	ah	0.14-0.33h	2-19h	Polar
Methyl methacrylate	80-62-6	VOC	28.0	26.5	15.9 / 20	aab	7-28d	1-10h	Polar
Methyl ter-butyl ether	1634-04-4	VOC	249.0	26.2	Soluble	aab	28-180d	1-11d	Polar
Methylene chloride	75-09-2	VOC	349.0	16.4	10-50 / 21	aab	7-28d	19-191d	Non-Polar
Nitrobenzene	98-95-3	VOC	0.15	32.7	1.9 / 25	aab	13-200d	0.5-5h	Polar
2-Nitropropane	79-46-9	VOC	10.0	21.6	1.7 / 20	aab	28-180d	5-49h	Polar
N-Nitroso-N-methylurea	684-93-5	VOC	10.0	—	<1 / 18	ah	0.01-3.5h	0.5-5h	Polar
N-Nitrosodimethylamine	62-75-9	VOC	3.7	19.3	>100 / 19	aab	21-180d	0.5-1h	Polar
N-Nitrosomorpholine	59-89-2	VOC	0.32	—	>100 / 19	aab	28-180d	0.9-18h	Polar
Phenol	108-95-2	VOC	0.20	28.0	50-100 / 19	aab	6-84h	2-23h	Polar
Phosgene	75-44-5	VVOC	1200.0	—	Slightly soluble	aab	7-28d	113->>y	Polar
1,3-Propane sultone	1120-71-4	VOC	2.0	—	100 /	ah	0.4-28d	4-40h	Polar
Beta-Propiolactone	57-57-8	VOC	3.4	15.7	37 / 20	ah	3-22d	8-75d	Polar
Propionaldehyde	123-38-6	VOC	235.0	16.1	50-100 / 18	aab	1-7d	3-33h	Polar
Propylene dichloride	78-87-5	VOC	42.0	25.7	<0.1 / 21.5	aab	0.5-4y	3-27d	Non-Polar
Propylene oxide	75-56-9	VVOC	445.0	15.7	400 / 20	ah	7-13d	—	Polar
1,2-Propyleneimine	75-55-8	VOC	112.0	17.6	>100 / 19	aab	7-28d	1-11h	Polar
Styrene	100-42-5	VOC	6.6	36.4	<1 / 19	aab	14-28d	0.9-7h	Non-Polar
Styrene oxide	96-09-3	VOC	0.3	35.5	<1 / 19.5	ah	0.004-28h	0.5-5d	Polar
1,1,2,2-Tetrachloroethane	79-34-5	VOC	5.0	30.7	<0.1 / 22	ah	45d	9-89d	Non-Polar
Tetrachloroethylene	127-18-4	VOC	14.0	30.3	<0.1 / 17	aab	180-360d	16-160d	Non-Polar
Toluene	108-88-3	VOC	22.0	31.0	<1 / 18	aab	4-22d	10-104h	Non-Polar
1,2,4-Trichlorobenzene	120-82-1	VOC	0.18	41.0	<1 / 21	aab	28-180d	5-54d	Non-Polar
1,1,2-Trichloroethane	79-00-5	VOC	19.0	25.9	1-5 / 20	aab	100-180d	8-82d	Non-Polar
Trichloroethylene	79-01-6	VOC	20.0	25.4	<1 / 21	aab	180-360d	1-11d	Non-Polar
Triethylamine	121-44-8	VOC	54.0	33.8	Soluble	—	—	—	Polar
2,2,4-Trimethyl pentane	540-84-1	VOC	40.6	39.2	Insoluble	—	—	—	Non-Polar
Vinyl acetate	108-05-4	VOC	83.0	22.2	Insoluble	aab	1-7d	—	Polar
Vinyl bromide	593-60-2	VVOC	1100.0	18.9	Insoluble	aab	28-180d	9-94h	Non-Polar

Table B-1. (continued)

Compound	CAS No.	Sub-category ¹	VP ² (mm Hg at 25°C)	Polarizability ³ (cm ³ /mole)	Water Solubility ⁴ (g/L at °C)	Reactivity & t _{1/2} range ⁵			Other ⁷
						Aqueous ⁶		Air	
Vinyl chloride	75-01-4	VVOC	3200.0	15.5	Slightly soluble	aab	28-168d	10-97h	Non-Polar
Vinylidene chloride	75-35-4	VVOC	500.0	20.4	5-10 / 21	aab	28-168d	10-99h	Non-Polar
Xylenes (isomer mixture)	1330-20-7	VOC	6.7	36.1	<1 / 22	aab	7-28d	3-44h	Non-Polar
o-Xylene	95-47-6	VOC	5.0	35.8	Insoluble	aab	7-28d	4-44h	Non-Polar
p-Xylene	106-42-3	VOC	6.5	36.0	Insoluble	aab	7-28d	4-42h	Non-Polar

Footnotes:

¹ VVOC = Very Volatile Organic Compounds (Vapor Pressure at 25°C >380 mm Hg);

VOC = Volatile Organic Compounds (0.1 < Vapor Pressure at 25°C <380 mm Hg)

² Vapor Pressure (VP) data from (with some exceptions):

(a) D.L. Jones and J. Bursey, "Simultaneous Control of PM-10 and Hazardous Air Pollutants II: Rationale for Selection of Hazardous Air Pollutants as Potential Particulate Matter," Report EPA-452/R-93/013, U.S. Environmental Protection Agency, Research Triangle Park, NC, October 1992.

(b) R.C. Weber, P.A. Parker, and M. Bowser, Vapor Pressure Distribution of Selected Organic Chemicals, Report EPA-600/2-81-021, U.S. Environmental Protection Agency, Cincinnati, OH, February 1981.

³ Electronic Polarizability = $(MW/\rho)[n^2 - 1]/[n^2 + 2]$

from: E.B. Sansone, Y.B. Tewari, and L.A. Jonas, Prediction of Removal of Vapors from Air by Adsorption on Activated Carbon, Environ. Sci. Technol., 13, 1511-1513 (1979). Values for molecular weight (MW), density (ρ), and refractive index (n) are taken from:

(a) R.C. Weast, ed., "CRC Handbook of Chemistry and Physics," 59th edition, CRC Press, Boca Raton, 1979.

(b) L.H. Keith and M.M. Walker, eds., "EPA's Clean Air Act Air Toxics Database: Air Toxics Chemical and Physical Properties," Vol. II, Lewis Publishers, Boca Raton, 1993.

⁴ Solubility data from (unless otherwise indicated):

D. Mackay, W.Y. Shiu, and K.C. Ma, "Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals: Volume III Volatile Organic Chemicals," Lewis Publishers, Ann Arbor, MI, 1993.

⁵ Reactivity and Half-Life data from:

(a) P.H. Howard, R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko, "Handbook of Environmental Degradation Rates," Lewis Publishers, Boca Raton, 1991.

(b) C.W. Spicer, A.J. Pollack, T.J. Kelly and R. Mukund, "A Literature Review of Atmospheric Transformation Products of Clean Air Act Title III Hazardous Air Pollutants, Final Report to U.S. EPA, Contract No. 68-D80082, Battelle, Columbus, Ohio, July 1993.

⁶ aab = aqueous aerobic biodegradation; ah = aqueous hydrolysis

⁷ Customary classification of VOCs as either Nonpolar or Polar.

⁸ Obtained from the STN International computer database (BEILSTEIN File)

Discussion of Polarizability and Water Solubility Characteristics of Polar Volatile Organic Compounds

Volatile organic compounds (VOCs) in air consist largely of hydrocarbons and oxygenated hydrocarbons, as well as some nitrogen- and sulfur-containing compounds. The oxygenated hydrocarbons, in turn, consist of several compound classes, including alcohols, aldehydes, ketones, ethers, carboxylic acids, etc. For analytical purposes, airborne organic compounds may be considered as either nonpolar (i.e., hydrocarbons) or polar (i.e., compounds containing oxygen, sulfur, nitrogen, etc.).

Nonpolar VOCs can be characterized at the part-per-billion by volume (ppbv) level using currently available methods. However, polar VOCs tend to be difficult to sample and analyze at trace levels because of their chemical reactivity, affinity for metal and other surfaces, and solubility in water. Because polar VOCs include compound classes generally associated with higher polarizabilities, we have investigated the general classification of the VOCs of interest as a function of electronic polarizability (molar refractivity). Polarizabilities were calculated from the relationship:

$$\text{Molar Refractivity} = \frac{MW}{\rho} \frac{n^2 - 1}{n^2 + 2}$$

where MW = molecular weight; ρ = density; and n = refractive index. Figure B-1 shows the data generated in this way for the VOCs. This plot ranks the VOCs that are customarily identified as either nonpolar (N) or polar (P) compounds as a function of their electronic polarizability. Figure B-1 shows that the N and P compounds are well mixed in the ranking by polarizability. It is clear from this plot that there is no clear distinction between the N and P compounds, based on polarizability, as both groups of compounds are distributed over the entire polarizability range. *

Because of the collection and analysis problems known to be associated with the water solubility of certain VOCs, we also ranked the VOCs on the basis of their solubility in water at 25°C. The most useful literature compilations found were those of Keith and Walker (1993) and Mackay et al. (1993) (see references 14 and 15 in the body of this report). As Coutant has already noted (references 11 and 27), in many cases values reported for the same compound in the literature differ widely; in many other cases, only solubility ranges are available. As a result, we have been forced to group several compounds or make selections based on chemical similarity with other compounds on the target compound list. We have also conducted several literature searches, using the STN computer data base, for solubility data on individual VOCs. Figure B-2 shows a plot ranking the VOCs as a function of their water solubility.

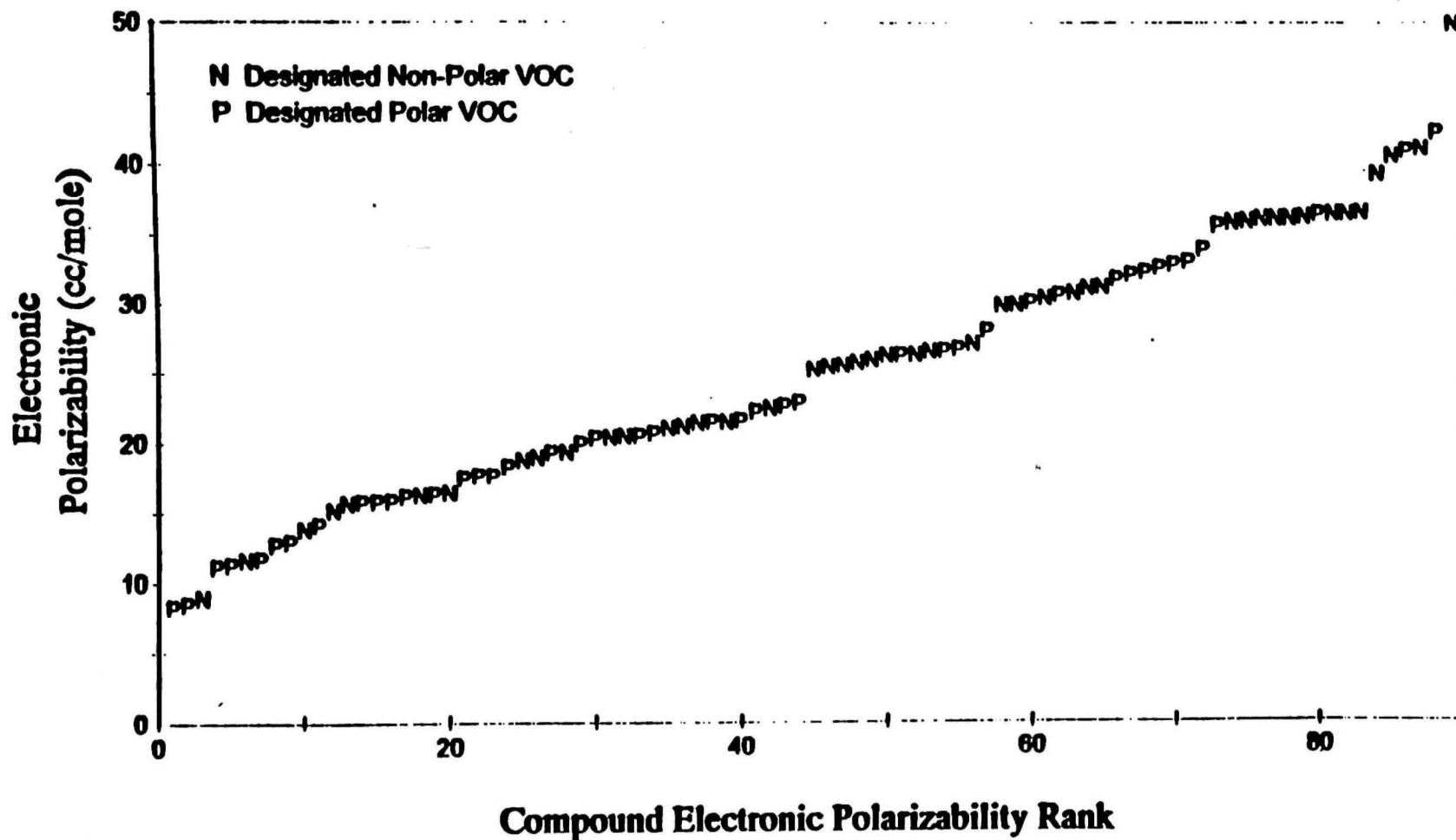


Figure B-1. Distribution of electronic polarizabilities for Volatile Organic Compounds (VOCs) on the HAPs list.

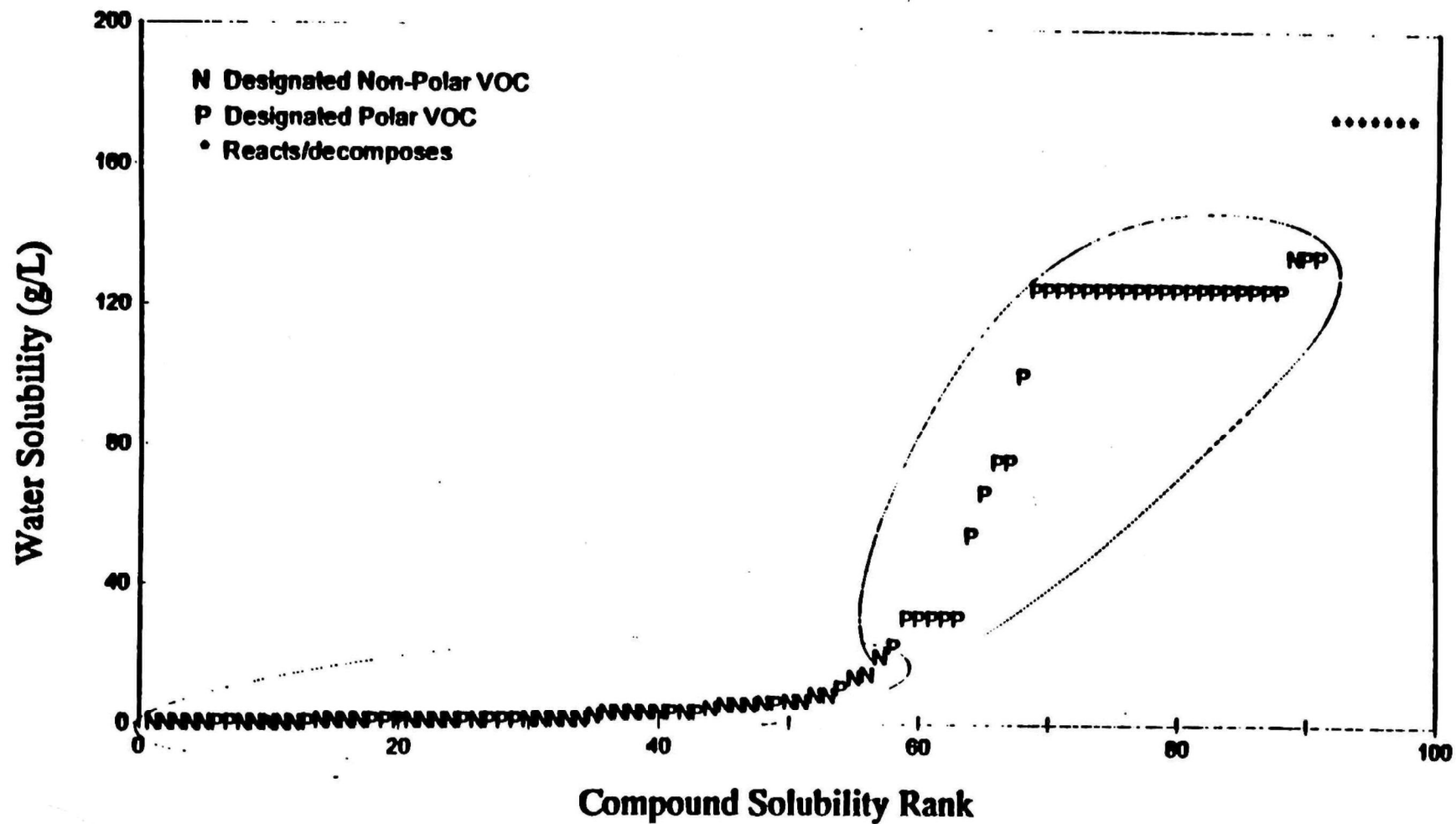


Figure B-2. Distribution of water solubilities for Volatile Organic Compounds (VOCs) on the HAPs list.

Here, it is seen that compounds that have conventionally been identified as nonpolar VOCs are characterized by relatively low water solubilities, whereas compounds that are generally regarded as polar VOCs are characterized by relatively high water solubilities. Classifying VOCs on the basis of their solubility in water therefore provides a more realistic distinction between polar and nonpolar compounds than does classification on the basis of polarizability.

APPENDIX C

RESULTS OF THE SURVEY OF AMBIENT AIR MEASUREMENT METHODS FOR THE 189 HAPS

1. Table of Measurement Methods Identified (Table C-1).
2. List of References Associated with Table C-1.

Table C-1. Available Ambient Measurement Methods for the 189 HAPs.

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Acetaldehyde	75-07-0	VVOC	TO-5 TO-11	R-4 [14]		TO-5: 1 ppbv; TO-11: 1 ppbv; [14]: 30 ppmv	
Acetamide	60-35-5	SVOC			OSHA CIM [A625]; R-37; R-47		[A625]: not a validated method; R-47: method developed for analysis of water
Acetonitrile	75-05-8	VOC	R-1, CLP-1A, R-3	TO-15		R-1: 1 ppbv	
Acetophenone	98-86-2	VOC	CLP-2		TO-15	CLP-2 ⁴ : 37 ng/m ³ (0.007 ppbv)	
2-Acetylaminofluorene	53-96-3	NVOC			OSHA CIM [0065]		[0065]: not a validated method
Acrolein	107-02-8	VOC	TO-5 TO-11 CLP-1A	NIOSH III [#2501]		CLP-1A ⁴ : 5 ppbv; TO-5: 1 ppbv; TO-11: 1 ppbv	
Acrylamide	79-06-1	VOC		OSHA [#21]		[#21]: 1.3 ppbv	
Acrylic acid	79-10-7	VOC					
Acrylonitrile	107-13-1	VOC	TO-2, R-1, CLP-1A, R-3	R-4 [14]; TO-15		R-1: 1 ppbv	
Allyl chloride	107-05-1	VOC	TO-14, TO-2, CLP 1A,B, R-3			TO-14: ≥ 0.1 ppbv	
4-Aminobiphenyl	92-67-1	SVOC	CLP-2	R-36	R-37	CLP-2 ⁴ : 183 ng/m ³ ; R-36: 0.1 ng/m ³	R-36: evaluated for particulate phase only

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Aniline	62-53-3	VOC	CLP-2			CLP-2 ⁴ : 73 ng/m ³ (0.02 ppbv)	Current concern exists that CLP-2 methodology is inadequate for collection of this compound.
o-Anisidine	90-04-0	SVOC		NIOSH III [#2514]	OSHA CIM [0225]		[#2514]: working range = 0.06 - 0.8 mg/m ³ (200-L sample volume)
Asbestos	1332-21-4	NVINC	R-21	NIOSH III [#7400] & [#7402]; OSHA [ID160]; R-63		R-21: < 0.1 ng/m ³ (i.e., < 0.01 fibers/cc)	[#7400] & [#7402]: working range = 0.04 - 0.5 fiber/cc (1000-L sample volume)
Benzene	71-43-2	VOC	TO-14; TO-1; TO-2; TO-3; R-1; CLP 1A,B; R-3; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.03 ppbv ¹	
Benzidine	92-87-5	SVOC	CLP-2	R-36	R-37	CLP-2 ⁴ : 73 ng/m ³ ; R-36: 1 ng/m ³	R-36: Evaluated for particulate phase only
Benzotrichloride	98-07-7	SVOC			OSHA CIM [B408]		[B408]: not a validated method
Benzyl chloride	100-44-7	VOC	TO-14, CLP-1A, R-3			TO-14: ≥ 0.1 ppbv	
Biphenyl	92-52-4	SVOC	R-50; R-51	NIOSH III [#2530]		R-50: 14 - 16 ng/m ³	[#2530]: working range = 0.13 - 4 mg/m ³ (30-L sample volume); R-50: LOD is range of ambient data.
Bis (2-ethylhexyl)phthalate (DEHP)	117-81-7	SVOC	CLP-2; R-28; R-57			CLP-2 ⁴ : 37 ng/m ³ ; R-28: 0.77 - 3.60 ng/m ³	R-28: LOD shown is range of reported ambient data
Bis (chloromethyl) ether	542-88-1	VOC	CLP-2			CLP-2 ⁴ : 37 ng/m ³ (0.006 ppbv)	
Bromoform	75-25-2	VOC	CLP-1B	TO-15			CLP-1B minimum quantifiable level of 28 ng
1,3-Butadiene	106-99-0	VVOC	R-1, CLP-1A, R-3	NIOSH III [#1024]; TO-14; TO-15		R-1: 1 ppbv	[#1024]: working range = 0.02 - 8.4 ppmv (25-L sample volume)

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Calcium cyanamide	156-62-7	Particulate		R-32		R-32: 0.08 mg/m ³	R-32: recommended range in air = 0.24 mg/m ³ (240-L sample volume)
Caprolactam	105-60-2	SVOC		R-43; R-44	OSHA CIM [0524]	R-43: 0.1 mg/m ³ ; R-44: 5 µg/m ³	R-43: LOD for GC analysis (100-L sample volume); R-44: evaluated for particle-phase samples only
Captan	133-06-2	SVOC	TO-10; CLP-2; R-27	TO-4		TO-10: 0.01 - 50 µg/m ³ ; R-27: 1.6 - 14 ng/m ³	
Carbaryl	63-25-2	SVOC	R-27	NIOSH III [#5006]; OSHA [63]		[63]: 0.028 mg/m ³ ; R-27: 8 - 42 ng/m ³	[#5006]: working range = 0.5 - 20 mg/m ³ (200-L sample volume); [63]: sample volume = 60 L
Carbon disulfide	75-15-0	VOC	R-11	NIOSH III [#1600], EPA-15, R-4 [14]	TO-15	R-11: 0.02 ppbv; EPA-15: 0.5 ppmv MDQ; [14]: 20 ppmv	LOD of R-11 estimated; range of ambient data 0.025 - 0.34 ppbv; [15]: listed as target compound for EPA 15
Carbon tetrachloride	56-23-5	VOC	TO-14; TO-1; CLP 1A,B; R-3; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.03 ppbv ¹	
Carbonyl sulfide	463-58-1	VVOC	R-10	EPA-15 R-4 [14]		R-10: 0.03 ppbv; EPA-15: 0.5 ppmv MDQ; [14]: 1 ppmv	LOD for R-10 estimated based on calibration data; range of ambient data 0.4 - 0.7 ppbv; [15]: listed as a target compound for EPA 15
Catechol	120-80-9	VOC		R-2; TO-8; R-25			R-2 and TO-8 indicated by analogy with phenol based on similar properties; R-2: 0.02 ppbv (estimated); R-2: 0.02 ppbv (estimated); R-25: 1 ppbv (estimated)
Chloramben	133-90-4	SVOC			R-27		R-27 indicated based on applicability of method for other pesticides
Chlordane	57-74-9	SVOC	TO-4; TO-10; CLP 2; R-27 to R-31			TO-4: >1 ng/m ³ ; TO-10: 0.01-50 µg/m ³ ; R-27: 4 - 50 ng/m ³ ; R-29: < 5 µg/m ³	
Chlorine	7782-50-5	VVINC	R-4 [805]	OSHA [ID101]; NIOSH III [#6011]		[ID101]: 14 ppbv	[805]: LOD not established; [6011]: working range = 7 - 500 ppbv (90-L sample volume); [ID101]: sample volume = 15 L

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Chloroacetic acid	79-11-8	VOC		R-42		R-42: 0.2 mg/m ³ (51 ppbv)	
2-Chloroacetophenone	532-27-4	SVOC		NIOSH II [#P & CAM 291]	OSHA CIM [0618]	[#291]: 0.16 - 0.62 mg/m ³	[#291]: sample volume = 12 L (measurement range shown as LOD)
Chlorobenzene	108-90-7	VOC	TO-14, TO-3, CLP 1A,B, R-3			TO-14: ≥ 0.1 ppbv	
Chlorobenzilate	510-15-6	SVOC		R-46; CLP-2; TO-4; TO-10	R-27		R-46: No LOD's or air concentrations reported (workplace exposure measurements)
Chloroform	67-66-3	VOC	TO-14; TO-1; TO-2; TO-3; CLP-1A,B; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.04 ppbv ¹	
Chloromethyl methyl ether	107-30-2	VOC		NIOSH II(1) [P&CAM #220]; R-56		[#220]: 0.5 ppbv; R-56: 1 ppbv	[#220]: sample volume = 10 L (measurement range shown as LOD)
Chloroprene	126-99-8	VOC	R-7	NIOSH III [#1002]; TO-15		R-7: 0.06 ppbv	
Cresol/Cresylic acid (mixed isomers)	1319-77-3	VOC	TO-8	R-60		TO-8: 1-5 ppbv	Current concern exists that TO-8 sampling technique has not been field validated.
o-Cresol	95-48-7	VOC	TO-8	R-2; R-25; R-60	R-59	TO-8: 1-5 ppbv	R-2: 0.02 ppbv (estimated); See also Cresol/Cresylic acid note above
m-Cresol	108-39-4	SVOC	TO-8	R-2; R-3; R-60	R-59	TO-8: 4.5 - 22.5 µg/m ³ ; R-2: 4.5 µg/m ³ ; R-3: 0.09 µg/m ³	See also Cresol/Cresylic acid note above
p-Cresol	106-44-5	SVOC	TO-8	R-2; R-3; R-59; R-60		TO-8: 4.5 - 22.5 µg/m ³ ; R-2: 4.5 µg/m ³ ; R-3: 0.09 µg/m ³	See also Cresol/Cresylic acid note above
Cumene	98-82-8	VOC	TO-14; R-6	NIOSH III [#1501]		TO-14: ≥ 0.1 ppbv	

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
2,4-D (2,4-Dichloro phenoxyacetic acid) (incl. salts and esters)		SVOC	TO-10; R-27	NIOSH III [#5001]; CLP-2; TO-4	R-38	TO-10: 0.01 - 50 µg/m ³ ; R-27: < 0.8 ng/m ³	T-10 only for esters; 2,4-acid and salts would require filter for particulate; see R-38; [#5001]: working range = 1.5 - 20 mg/m ³ (100-L sample volume); R-27: esters only
DDE (1,1-dichloro-2,2-bis(p-chlorophenyl) ethylene)	72-55-9	SVOC	TO-4; TO-10; CLP 2; R-29; R-27; R-28			TO-4: >1 ng/m ³ ; TO-10: 0.01- 50 ng/m ³ ; R-29: < 5 pg/m ³ ; R-27: 1.4 - 3.6 ng/m ³	
Diazomethane	334-88-3	VVOC		NIOSH III [#2515]			[#2515]: working range = 0.11 - 0.57 ppmv (10-L sample volume)
Dibenzofurans	132-64-9	SVOC Dibenzofuran	R-50	R-4 [836]	EPA 23; OSHA CIM [D639]	[836]: 3.3 ng/m ³ ; R-50: 13 - 26 ng/m ³	[836]: sample volume = 1500 m ³ , method is for total particulate aromatic hydrocarbons; [D639]: not a validated method; [23]: not a target compound for EPA 23; R-50: LOD is range of ambient data
		SVOC Tetrachloro-dibenzofuran	R-5; R-51	TO-9		R-5: 0.02 pg/m ³ ; R-51: < 0.01 pg/m ³	Not a target analyte in TO-9; Higher chlorinated species (e.g., octa-) are probably NVOC
1,2-Dibromo-3-chloropropane	96-12-8	VOC	R-12	TO-14; TO-3; TO-15		R-12: < 2 ng/m ³ (< 0.2 pptv)	TO-14, TO-15 and TO-3 indicated by analogy with VOC's having similar properties; R-12: range of ambient data 2 - 21 ng/m ³
Dibutyl phthalate		SVOC	CLP-2; R-28; R-57			CLP-2 ⁴ : 37 ng/m ³ ; R-28: 0.48 - 3.6 ng/m ³ ; R-57: 5 - 370 ng/m ³	R-28: LOD shown is range of reported ambient data; R-57: LOD shown is range of ambient data for separate vapor and particulate measurements of various isomers.
1,4-Dichlorobenzene	106-46-7	VOC	TO-14, TO-1, CLP 1A,B, R-3			TO-14: ≥ 0.1 ppbv; TO-1: 0.02 ppbv ¹	
3,3'-Dichlorobenzidine	91-94-1	SVOC		NIOSH III [#5509]; OSHA [65]; R-36	R-37	[65]: 40 ng/m ³ ; R-36: 0.1 ng/m ³	[#5509]: working range = 4 - 200 µg/m ³ (50-L sample volume); [65]: sample volume = 100 L; R-36: evaluated for particulate phase only
Dichloroethyl ether (Bis[2-chloroethyl]ether)	111-44-4	VOC	CLP-2		TO-15	CLP-2 ⁴ : 37 ng/m ³ (0.006 ppbv)	Current concern exists that CLP-2 methodology is inadequate for collection of this compound.

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
1,3-Dichloropropene	542-75-6	VOC	TO-14, CLP-1A, R-3			TO-14: ≥ 0.1 ppbv	
Dichlorvos	62-73-7	SVOC	TO-10; CLP-2; R-27	TO-4		TO-10: $0.01 - 50 \mu\text{g}/\text{m}^3$	
Diethanolamine	111-42-2	SVOC		NIOSH III [#3509]	OSHA CIM [D129]		[#3509]: working range = $0.4 - 3 \text{ mg}/\text{m}^3$ (100-L sample volume)
Diethyl sulfate	64-67-5	VOC		R-40; R-8		R-40: 8 pptv	R-40: not applied to ambient air analysis; Indication of R-8 based on similarity of properties with dimethyl sulfate
3,3'-Dimethoxybenzidine	119-90-4	NVOC		R-36	R-37	R-36: $1 \text{ ng}/\text{m}^3$	R-36: Evaluated for particulate phase only
4-Dimethylaminoazobenzene	60-11-7	NVOC		NIOSH II [#P & CAM 284]		[#284]: $4 - 2000 \mu\text{g}/\text{m}^3$	[#284]: sample volume = 50 L (measurement range shown as LOD)
N,N-Dimethylaniline	121-69-7	VOC		NIOSH III [#2002]; CLP-2			[#2002]: measurement range = $0.05 - 3.0 \text{ mg}/\text{sample}$ (unknown sample volume); CLP-2 indicated by similarity of properties with aniline
3,3'-Dimethylbenzidine	119-93-7	SVOC		R-36	R-37	R-36: $1 \text{ ng}/\text{m}^3$	R-36: evaluated for particulate phase only
Dimethylcarbamoyl chloride	79-44-7	VOC		R-39		R-39: 0.05 ppbv	R-39: sample volume = 48 L
N,N-Dimethylformamide	68-12-2	VOC	R-9	NIOSH III [#2004] R-4 [14]		R-9: $0.6 - 50$ ppbv	R-9: reports four separate methods
1,1-Dimethylhydrazine	57-14-7	VOC		NIOSH II(3) [#S143]; R-22		R-22: 4 ppbv	[#S143]: working range = $0.04 - 4 \text{ ppmv}$ (100-L sample volume); R-22: sample volume = 2 L

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Dimethyl phthalate	131-11-3	SVOC	CLP-2	R-26; R-28		CLP-2 ⁴ : 37 ng/m ³ ; R-26: 60 ng/m ³	R-28 suggested by analogy with di-n-butyl phthalate
Dimethyl sulfate	77-78-1	VOC	R-8	NIOSH III [#2524]		R-8: 0.05 ppbv	LOD for R-8 estimated based on ranges of sampling durations, sampling rates, and analytical capabilities
4,6-Dinitro-o-cresol (including salts)	534-52-1	SVOC	CLP-2		R-3	CLP-2 ⁴ : 183 ng/m ³	R-3 suggested by analogy to other phenols
2,4-Dinitrophenol	51-28-5	SVOC	CLP-2			CLP-2 ⁴ : 73 ng/m ³	
2,4-Dinitrotoluene	121-14-2	SVOC	CLP-2			CLP-2 ⁴ : 37 ng/m ³	
1,4-Dioxane (1,4-Diethyleneoxide)	123-91-1	VOC	CLP-1B	R-4 [14]	TO-15	[14]: 2 ppmv	CLP-1B minimum quantifiable level of 13 ng
1,2-Diphenylhydrazine	122-66-7	SVOC			R-22		Suggestion of R-22 based on chemical similarity to volatile hydrazines
Epichlorohydrin (1-Chloro-2,3-epoxypropane)	106-89-8	VOC	CLP-1B	R-4 [14]		[14]: 20 ppmv	CLP-1B minimum quantifiable level of 26 ng
1,2-Epoxybutane	106-88-7	VOC		NIOSH III [#1614]; R-3			R-3 and NIOSH methods indicated by similarity of properties with ethylene oxide
Ethyl acrylate	140-88-5	VOC	R-1 R-3	TO-15		R-1: 0.2 ppbv	
Ethylbenzene	100-41-4	VOC	TO-14; TO-1; CLP 1A,B; R-3; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.005 ppbv ^{1*}	
Ethyl carbamate (urethane)	51-79-6	VOC					

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Ethyl chloride	75-00-3	VVOC	TO-14, CLP-1A, R-3	R-4 [14]		TO-14: ≥ 0.1 ppbv; [14]: 10 ppmv	
Ethylene dibromide	106-93-4	VOC	TO-14 CLP-1A,B			TO-14: ≥ 0.1 ppbv	
Ethylene dichloride	107-06-2	VOC	TO-14, TO-2, TO-3, CLP-1A,B, R-3			TO-14: ≥ 0.1 ppbv	
Ethylene glycol	107-21-1	SVOC		NIOSH III [#5500]	OSHA CIM [1911]		[#5500]: working range = 7 - 330 mg/m ³ (3-L sample volume)
Ethyleneimine	151-56-4	VOC		NIOSH II(5) [P&CAM #300]; R-4 [14]		[14]: 15 ppmv	[P&CAM #300]: working range = 0.01 - 8.9 ppmv (50-L sample volume)
Ethylene oxide	75-21-8	VVOC	R-13	NIOSH III [#1614]; R-3	TO-15	R-13: 0.001 - 0.1 ppbv	[#1614]: working range = 0.04 - 4.5 ppmv (24-L sample volume); R-13 evaluated five different methods
Ethylene thiourea	96-45-7	SVOC		NIOSH III [#5011]			[#5011]: working range = 0.05 - 75 mg/m ³ (200-L sample volume)
Ethylidene dichloride	75-34-3	VOC	TO-14; CLP-1A,B; R-3			TO-14: ≥ 0.1 ppbv	
Formaldehyde	50-00-0	VVOC	TO-5 TO-11			TO-5: 1 ppbv; TO-11: 1 ppbv	
Heptachlor	76-44-8	SVOC	TO-10; CLP-2; R-29; R-30; R-27	TO-4		TO-10: 0.01 - 50 $\mu\text{g}/\text{m}^3$; R-29: 0.04 - 0.1 pg/m^3 ; R-30: 1 ng/m^3	
Hexachlorobenzene	118-74-1	SVOC	TO-10; CLP-2; R-29; R-28			TO-10: 0.01 - 50 $\mu\text{g}/\text{m}^3$; R-29: 0.04 - 0.1 pg/m^3	
Hexachlorobutadiene	87-68-3	VOC	TO-14, CLP-1A, R-3			TO-14: ≥ 0.1 ppbv	

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
1,2,3,4,5,6-Hexachlorocyclohexane (all stereo isomers, including Lindane)		SVOC	TO-10; CLP-2; R-28; R-29; R-27	R-30; TO-4		TO-10: 0.01 - 50 µg/m ³ (g-BHC); R-30: 1 ng/m ³ ; R-29: < 5 pg/m ³	
Hexachlorocyclopentadiene	77-47-4	SVOC	CLP-2			CLP-2 ⁴ : 37 ng/m ³	
Hexachloroethane	67-72-1	VOC	CLP-2	TO-14; TO-3; TO-15		CLP-2 ⁴ : 37 ng/m ³ (0.004 ppbv)	TO-14 and TO-3 indicated by analogy with VOC's having similar properties
Hexamethylene diisocyanate	822-06-0	SVOC		OSHA [42]; R-23	NIOSH III [#5521]; R-4 [837]; R-62	[42]: 2.3 µg/m ³ ; R-23: 1 µg/m ³	[42]: sample volume = 15 L
Hexamethylphosphoramide	680-31-9	SVOC					
Hexane	110-54-3	VOC	CLP-1A; TO-14; R-6			TO-14: ≥ 0.1 ppbv; R-6: 0.03 ppbv	TO-14 by analogy to other VOC's with similar properties on TO-14 list
Hydrazine	302-01-2	VINC		NIOSH III [#3503]; OSHA [20]; R-22	R-55	[20]: 1.2 ppbv; R-22: 4 ppbv	[#3503]: working range = 0.07 - 3 ppmv (100-L sample volume); [20]: sample volume = 20 L; R-22: sample volume = 2 L
Hydrochloric acid (Hydrogen chloride)	7647-01-0	VINC	R-19	NIOSH III [#7903]; OSHA [ID174SG]		R-19: 0.22 ppbv	[#7903]: working range = 0.0066 - 3.3 ppmv (50-L sample volume)
Hydrogen fluoride (Hydrofluoric acid)	7664-39-3	VVINC	R-20	R-4[809/205]; NIOSH III [#7903]		R-20: 0.08 ppbv	[#7903]: working range = 0.012 - 6.02 ppmv (50-L sample volume)
Hydroquinone	123-31-9	SVOC		NIOSH III [#5004]			[#5004]: working range = 2 - 25 mg/m ³ (30-L sample volume)
Isophorone	78-59-1	VOC	CLP-2	NIOSH III [#2508]; TO-15		CLP-2 ⁴ : 37 ng/m ³ (0.006 ppbv)	[#2508]: working range = 0.35 - 70 ppmv (12-L sample volume)

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Maleic anhydride	108-31-6	SVOC		NIOSH III [#P & CAM 302]; OSHA [25] & [86]		[86]: 33 µg/m ³ ; [25]: 0.005 mg/m ³	[#P & CAM 302]: working range = 0.5 - 2.14 mg/m ³ ; [25]: sample volume = 20 L; [86]: sample volume = 60 L (method not yet published)
Methanol	67-56-1	VOC	R-1, CLP-1A, R-3	R-64; TO-15		R-1: 1 ppbv	
Methoxychlor	72-43-5	SVOC	TO-10; CLP-2; R-27; R-29	TO-4		TO-10: 0.01 - 50 µg/m ³ ; R-27: 1 - 8 ng/m ³ ; R-29: < 5 pg/m ³	
Methyl bromide (Bromomethane)	74-83-9	VVOC	TO-14, CLP-1A, R-3			TO-14: ≥ 0.1 ppbv	
Methyl chloride (Chloromethane)	74-87-3	VVOC	TO-14, CLP-1A, R-3			TO-14: ≥ 0.1 ppbv	
Methyl chloroform (1,1,1-Trichloroethane)	71-55-6	VOC	TO-14; TO-1; TO-2; TO-3; CLP-1A,B; R-3; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.03 ppbv ¹	
Methyl ethyl ketone (2-Butanone)	78-93-3	VOC	TO-5, R-1, CLP-1A, R-3	R-58; TO-15		R-1: 0.2 ppbv; TO-5: 1 ppbv	
Methylhydrazine	60-34-4	VOC		NIOSH II(3) [#S149]; R-22	R-55	R-22: 4 ppbv	[#S149]: working range = 0.018 - 0.55 ppmv (20-L sample volume); R-22: sample volume = 2 L
Methyl iodide (Iodomethane)	74-88-4	VVOC		NIOSH III [#1014], TO-14	TO-15		
Methyl isobutyl ketone (Hexone)	108-10-1	VOC		NIOSH III [#1300]; R-4 [14]; R-1; R-58; TO-15		[14]: 10 ppmv; R-58: < 1ppbv	[#1300]: measurement range = 2.1 - 8.3 mg/sample (1 - 10-L sample volumes); R-1 suggested by similarity of properties with methyl ethyl ketone
Methyl isocyanate	624-83-9	VOC		OSHA [#54]	R-62	[54]: 1.9 ppbv	

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Methyl methacrylate	80-62-6	VOC	CLP-1A	R-4 [14]; R-1; R-3; TO-15		CLP-1A ⁴ : 2 ppbv; [14]: 1 ppmv	R-1 and R-3 indicated by similarity of properties with ethyl acrylate
Methyl tert-butyl ether	1634-04-4	VOC	R-1 R-3	R-64; TO-15		R-1: 1 ppbv	
4,4'-Methylenebis-(2-chloroaniline)	101-14-4	NVOC		OSHA [71] & [24]	NIOSH III [8302]	[71]: 440 ng/m ³ ; [24]: 3.6 µg/m ³	[24]: sample volume = 100 L; [8320]: urine matrix
Methylene chloride (Dichloromethane)	75-09-2	VOC	TO-14, TO-2, CLP 1A, R-3			TO-14: ≥ 0.1 ppbv	
4,4'-Methylenediphenyl diisocyanate	101-68-8	SVOC		NIOSH III [#5521]; R-23; R-4 [831]	R-62	[831]: 3 - 1040 µg/m ³ ; R-23: 1 µg/m ³	[831]: sample volume = 20 L
4,4'-Methylenedianiline	101-77-9	NVOC		NIOSH III [#5029]; OSHA [57]		[57]: 81 ng/m ³	[#5029]: working range = 0.0002 - 10 mg/m ³ (100-L sample volume); [57]: sample volume = 100 L
Naphthalene	91-20-3	SVOC	TO-13; CLP-2; R-7			TO-13: <100 pg/m ³	R-7: range of measured ambient concentrations = 5.5 - 182 ng/m ³ ; Volatility presents collection problems with PUF/XAD at high sample volume
Nitrobenzene	98-95-3	VOC	CLP-2	NIOSH III [#2005], R-53	TO-15		[#2005]: working range = 0.59 - 2.34 ppmv (55-L sample volume); R-53 by analogy to nitrotoluenes.
4-Nitrobiphenyl	92-93-3	SVOC	CLP-2; R-53	R-52		CLP-2 ⁴ : 183 ng/m ³ ; R-53: 0.01 ng/m ³	R-52 reports ambient data for 3-nitrobiphenyl
4-Nitrophenol	100-02-7	SVOC	CLP-2; R-53	R-2; R-54		CLP-2 ⁴ : 183 ng/m ³ ; R-53: 0.04 ng/m ³	R-2 by analogy with 2- and 3-Nitrophenol; R-54 by analogy with 2-nitrophenol
2-Nitropropane	79-46-9	VOC		NIOSH III [#2528] R-4 [14]; TO-15		[14]: 10 ppmv	[#2528]: working range = 1.4 - 27 ppmv (2 L sample volume)

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
N-Nitroso-N-methylurea	684-93-5	VOC			TO-7		Based on similarity of properties with N-nitroso-dimethylamine
N-Nitrosodimethylamine	62-75-9	VOC	TO-7	NIOSH III [#2522]		TO-7: < 0.32 ppbv	
N-Nitrosomorpholine	59-89-2	VOC		TO-7			Based on similarity of properties with N-Nitroso-dimethylamine
Parathion	56-38-2	SVOC	CLP-2	R-4 [835]; TO-4; TO-10		CLP-2 ⁴ : 146 ng/m ³	
Pentachloronitrobenzene (Quintobenzene)	82-68-8	SVOC		R-48; R-49	CLP-2	R-48: 0.1 - 10 ng/m ³ ; R-49: 10.7 - 1560 ng/m ³	R-48 and R-49: measurement range shown as LOD
Pentachlorophenol	87-86-5	SVOC	TO-10; CLP-2	R-50; R-61	R-3	TO-10: 0.01 - 50 µg/m; R-3: 0.2 µg/m ³ ; R-50: < 1 ng/m ³	Use of TO-10 would require filter for particulate material
Phenol	108-95-2	VOC	TO-8; R-2; R-54	R-25; R-60	R-53	TO-8: 1-5 ppbv; R-2: 0.02 ppbv; R-54: 56 - 110 pptv	TO-8: Current concern exists that sampling technique has not been field validated; R-54: LOD shown is range of ambient data.
p-Phenylenediamine	106-50-3	SVOC		OSHA [87]		[87]: 0.44 µg/m ³	[87]: sample volume = 100 L (method not yet published)
Phosgene	75-44-5	VVOC	TO-6			TO-6: 0.1 ppbv	
Phosphine	7803-51-2	VVINC	R-33	OSHA [ID180]		R-33: 0.15 ppbv; [ID180]: 9 ppbv	R-33: LOD derived from reference abstract; [ID180]: sample volume = 36 L
Phosphorus	7723-14-0	SVINC		NIOSH III [#7300] & [#7905]			[#7300]: working range= 0.005 - 2 mg/m ³ (500-L sample volume); [#7905]: working range= 0.04 - 0.8 mg/m ³ (12-L sample volume)

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			<i>Demonstrated</i>	<i>Likely</i>	<i>Potential</i>		
Phthalic anhydride	85-44-9	SVOC		NIOSH II [#S179]; OSHA [90]	R-26; R-28; R-9	[#S179]: 1 - 36 ng/m ³ ; [90]: 0.048 mg/m ³	[#S179]: sample volume = 100 L (measurement range shown as LOD); [90]: sample volume = 75 L (method not yet published)
Polychlorinated biphenyl (Aroclors)	1336-36-3	SVOC 1-Chloro- biphenyl	CLP-2; R-29; R- 28	TO-4		CLP-2 ⁴ : 146 ng/m ³ ; R-29: 0.04 - 0.1 pg/m ³	
		SVOC 2,4,6-Trichlo- robiphenyl	TO-10; CLP-2; R- 29; R-28	TO-4		TO-10: 0.01 - 50 µg/m ³ ; R- 29: 0.04 - 0.1 pg/m ³	Note: Higher chlorinated species, up to decachloro, are probably NVOC
1,3-Propane sultone	1120-71-4	VOC		R-41			
beta-Propiolactone	57-57-8	VOC		T-40	TO-15	R-40: 1.2 pptv	R-40: not applied to ambient air analysis
Propionaldehyde	123-38-6	VOC	TO-5, TO-11			TO-5: 1 ppbv; TO-11: 1 ppbv	
Propoxur (Baygon)	114-26-1	SVOC	CLP-2; R-27	TO-4; TO-10		CLP-2 ⁴ : 183 ng/m ³	R-27: LOD shown is range of reported ambient data
Propylene dichloride (1,2-Dichloropropane)	78-87-5	VOC	TO-14; CLP- 1A,B; R-3			TO-14: ≥ 0.1 ppbv	
Propylene oxide	75-56-9	VVOC		R-1, R-3, R-13, NIOSH III [#1614]		R-1: 1 ppbv	R-1, R-3, R-13, and NIOSH methods indicated by similarity of properties with ethylene oxide
1,2-Propylenimine (2-Methylaziridine)	75-55-8	VOC		NIOSH II(5) [#P & CAM 300]			NIOSH method indicated by similarity of properties with ethyleneimine
Quinoline	91-22-5	SVOC	R-6	R-57		R-6: 0.78 - 1100 ng/m ³	R-6: LOD is range of measured concentrations

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Quinone (p-Benzoquinone)	106-51-4	SVOC		NIOSH II [#S181]	OSHA CIM [2222]; R-57	[#S181]: 0.17 - 0.75 mg/m ³	[#S181]: sample volume = 24 L (measurement range shown as LOD)
Styrene	100-42-5	VOC	TO-14; TO-1; CLP 1A,B; R-3; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.02 ppbv ¹	
Styrene oxide	96-09-3	VOC		R-40	R-3; NIOSH III [#1614]	R-40: 0.41 pptv	R-40: not applied to ambient air analysis; R-3, [#1614]: Based on comparison of properties with ethylene oxide and 1,2-epoxybutane
2,3,7,8-Tetrachloro dibenzo-p-dioxin	1746-01-6	SVOC	TO-9; R-5; R-51			TO-9: 1-5 pg/m ³ ; R-5: 0.02 pg/m ³ ; R-51: < 0.01 pg/m ³	
1,1,2,2-Tetrachloroethane	79-34-5	VOC	TO-14; CLP-1A,B; R-3			TO-14: ≥ 0.1 ppbv	CLP-1B minimum quantifiable level of 22 ng
Tetrachloroethylene (Perchloroethylene)	127-18-4	VOC	TO-14; TO-1; TO-3; CLP-1A,B; R-3; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.007 ppbv ¹	
Titanium tetrachloride	7550-45-0	VINC					Hydrolyzes extremely rapidly in the ambient atmosphere
Toluene	108-88-3	VOC	TO-14; TO-1; TO-2; R-1; CLP-1A,B; R-3; R-6			TO-14: ≥ 0.1 ppbv; R-1: 0.2 ppbv	
Toluene-2,4-diamine	95-80-7	SVOC		NIOSH III [#5516]; OSHA [65]			[#5516]: working range = 3 - 30 µg/m ³ (100-L sample volume)
2,4-Toluene diisocyanate	584-84-9	SVOC		NIOSH III [#2535] & [#5521]; R-4 [837]; R-23; R-24	R-62	R-23: 1 µg/m ³ ; R-24: 7.24 µg/m ³ ; [837]: 0.05 - 1.01 mg/m ³	[#2535]: working range = 0.03 - 2.5 mg/m ³ (10-L sample volume); [837]: sample volume = 20 L
o-Toluidine	95-53-4	SVOC		NIOSH III [#2002]; OSHA [73]		[73]: 0.97 µg/m ³	[#2002]: working range = 5 - 60 mg/m ³ (55-L sample volume); [73]: sample volume = 100 L

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Toxaphene (chlorinated camphene)	8001-35-2	SVOC	R-31; R-28	NIOSH III [#S67]	OSHA CIM [0612]	R-31: < 0.1 ng/m ³	[#S67]: working range = 0.05 - 1.5 mg/m ³ (15-L sample volume); R-31: LOD estimated
1,2,4-Trichlorobenzene	120-82-1	VOC	TO-14, CLP-1A, R-3			TO-14: ≥ 0.1 ppbv	
1,1,2-Trichloroethane	79-00-5	VOC	TO-14 R-3			TO-14: ≥ 0.1 ppbv	
Trichloroethylene	79-01-6	VOC	TO-14; TO-1; TO-3; CLP-1A,B; R-8			TO-14: ≥ 0.1 ppbv; TO-1: 0.02 ppbv ¹	
2,4,5-Trichlorophenol	95-95-4	SVOC	TO-10; CLP-2; R-50	R-54	R-3	TO-10: 0.01 - 50 µg/m ³ ; R-50: 0.07 ng/m ³	Use of T-10 would require filter for particulate-phase material; R-54 reprot's sum of 2,4,5- and 2,4,6- isomers
2,4,6-Trichlorophenol	88-06-2	SVOC	CLP-2; R-50	TO-10; R-54	R-3	CLP-2 ⁴ : 183 ng/m ³ ; R-3: 0.2 µg/m ³ ; R-50: 0.07 ng/m ³	TO-10 by analogy with 2,4,5-TCP. Use of TO-10 would require filter for particulate material; R-54 reports sum of 2,4,5- and 2,4,6- isomers
Triethylamine	121-44-8	VOC		NIOSH II(3) [#S152]; R-9		[#S152]: 2 - 71 ppbv	[#S152]: sample volume = 100 L (measurement range shown as LOD); R-9 indicated by comparison of properties with dimethylformamide
Trifluralin	1582-09-8	SVOC	R-29	TO-4; CLP-2; TO-10	OSHA CIM [T338]	R-29: < 100 pg/m ³	
2,2,4-Trimethylpentane	540-84-1	VOC	R-8	TO-14; TO-15		R-6: 0.025 ppbv	TO-14 and TO-15 indicated by analogy with other VOC's having similar properties, and based on canister stability data.
Vinyl acetate	108-05-4	VOC	R-1, CLP-1A, R-3	TO-15		R-1: 1 ppbv	
Vinyl bromide	593-60-2	VVOC		TO-14; TO-15			TO-14 and TO-15 indicated by analogy to other VVOC's with similar properties

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Vinyl chloride	75-01-4	VVOC	TO-14, TO-2, CLP 1A, R-3			TO-14: ≥ 0.1 ppbv	
Vinylidene chloride (1,1-Dichloroethylene)	75-35-4	VVOC	TO-14, TO-2, TO-3, CLP-1A,B, R-3			TO-14: ≥ 0.1 ppbv	
Xylene (mixed isomers)	1330-20-7	VOC	TO-14; CLP-1A,B; R-3			TO-14: ≥ 0.1 ppbv	CLP-1B minimum quantifiable level of 2 ng
o-Xylene	95-47-6	VOC	TO-14; TO-1; CLP 1A,B; R-3; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.02 ppbv ¹	
m-Xylene	108-38-3	VOC	TO-14; TO-1; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.014 ppbv ¹	
p-Xylene	106-42-3	VOC	TO-14; TO-1; R-6			TO-14: ≥ 0.1 ppbv; TO-1: 0.014 ppbv ¹	
Antimony Compounds		NVINC	CLP-3; R-4 [301]	R-4 [804 & 822B]		[301]: 0.05 $\mu\text{g}/\text{m}^3$; [804]: 4 $\mu\text{g}/\text{m}^3$; [822B] ² : 17.5 ng/ m^3	[301]: sample volume= 20 m^3 ; [804]: sample volume= 60 L
Arsenic Compounds (Inorganic including arsine)		VVINC Arsine		NIOSH III [#6001]; OSHA [ID105]; R-34		R-34: 1 ppbv	[#6001]: working range = 0.3 - 62 ppbv (10-L sample volume); [ID105]: validated range = 1.85 - 12.4 ppbv; R-34: chemiluminescence methods
		NVINC	CLP-3; R-4 [302]	R-4 [804 & 822B]		[302]: 0.1 $\mu\text{g}/\text{m}^3$; [804]: 0.4 $\mu\text{g}/\text{m}^3$; [822B] ² : 10 ng/ m^3	
Beryllium Compounds		NVINC	CLP-3; R-4 [822]			[822]: 0.08 $\mu\text{g}/\text{m}^3$	[822]: sample volume = 0.24 m^3
Cadmium Compounds		NVINC	CLP-3; R-4 [822]	R-4 [822B]		[822]: 0.03 $\mu\text{g}/\text{m}^3$; [822B] ² : 22.5 ng/ m^3	[822]: sample volume = 0.24 m^3

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Chromium Compounds		NVINC	CLP-3; R-4 [822]	R-4 [822B]		[822]: 0.2 µg/m ³ ; [822B] ² : 25 ng/m ³	[822]: sample volume = 0.24 m ³
Cobalt Compounds		NVINC	CLP-3; R-4 [822]	R-4 [822B]		[822]: 0.3 µg/m ³ ; [822B] ² : 12.5 ng/m ³	[822]: sample volume = 0.24 m ³
Coke Oven Emissions		SVOC Naphthalene	TO-13; CLP-2; R-7			TO-13: <100 pg/m ³	R-7: range of measured ambient concentrations = 5.5 - 182 ng/m ³
(see also VOCs, e.g., benzene, toluene, xylene)		NVOC Coronene	R-14	R-4 [836]		R-14: 0.09 - 1.4 ng/m ³	R-14: LOD shown is range of measured ambient concentrations
Cyanide Compounds		VVINC Hydrogen cyanide		NIOSH III [#6010]; R-35			[#6010]: working range = 0.893 - 232 ppmv (3-L sample volume); R-35: 1 pg quantitation limit
		NVINC		NIOSH III [#7904]			[#7904]: working range (as CN ⁻) = 0.5 - 15 mg/m ³ (sample volume = 90 L)
Glycol ethers		SVOC		R-45		R-45: > 0.74 mg/m ³	See also ethylene glycol; R-45: developed for 9 different glycol ethers, LOD calculated for ethylene glycol monobutyl ether
Lead Compounds		NVINC	CLP-3; R-4 [822]	R-4 [822B]		[822]: 0.8 µg/m ³ ; [822B] ² : 10 ng/m ³	[822]: sample volume = 0.24 m ³
Manganese Compounds		NVINC	CLP-3; R-4 [822]	R-4 [822B]		[822]: 0.1 µg/m ³ ; [822B] ² : 20 ng/m ³	[822]: sample volume = 0.24 m ³
Mercury Compounds		SVINC Mercury vapor	R-4 [317]; R-18			[317]: 0.002 - 0.06 ppbv; R-18: 0.001 - 0.06 pptv	
		NVINC	R-18	R-4 [822B]		R-18: 0.01 ng/m ³	
Fine mineral fibers		NVINC		NIOSH III [#7400]; R-21		[#7400]: 7 fibers/mm ² filter area	[#7400]: working range = 0.04 - 0.5 fiber/cc (1000-L sample volume)

Table C-1. (continued)

Compound	CAS No.	Compd. Class ^A	Ambient Measurement Method			Limit of Detection ^{1,2,3,4,5}	Comment
			Demonstrated	Likely	Potential		
Nickel Compounds		NVINC	CLP-3; R-4 [822]	R-4 [822B]		[822]: 0.3 µg/m ³ ; [822B] ² : 10 ng/m ³	[822]: sample volume = 0.24 m ³
Polycyclic Organic Matter		SVOC Naphthalene	TO-13; CLP-2; R-7			TO-13: <100 pg/m ³	R-7: range of measured ambient concentrations = 5.5 - 182 ng/m ³
		NVOC Coronene	R-14	R-4 [836]		R-14: 0.09 - 1.4 ng/m ³	R-14: LOD shown is range of measured ambient concentrations
Radionuclides (including radon)		VVINC Radon	R-4 [606, A & B]			[606B]: 0.1 pCi/L	
		NVINC/ VINC	R-16; R-17	OSHA CIM [2560]; EPA 114		Varies depending on radionuclide	Long-lived radionuclides in air include: ²²² Rn, ²²⁰ Rn, ¹³¹ I, ⁸⁵ Kr, ³ H (gases); ²¹⁰ Po, ²¹⁰ Pb, ⁷ Be, ²³⁸ Pu, ²³⁹ Pu, ¹⁴⁴ Ce, ¹³⁷ Cs, ⁹⁰ Sr (particles); [114]: ²²² Rn and ²¹⁰ Po listed as target compounds for EPA 114
Selenium Compounds		NVINC	CLP-3	R-4 [804 & 822B]		[804]: 0.4 µg/m ³ ; [822B] ² : 10 ng/m ³ ; CLP-3 ³ : 83 ng/m ³	[804]: sample volume= 60 L

^A Compound Classes:

VVOC = Very Volatile Organic Compounds (Vapor Pressure at 25°C >380 mm Hg)

VVINC or Gases = Very Volatile Inorganic Compounds (Vapor Pressure at 25°C >380 mm Hg)

VOC = Volatile Organic Compounds (1.0E-01 < Vapor Pressure at 25°C <380 mm Hg)

VINC or Gases = Volatile Inorganic Compounds (1.0E-01 < Vapor Pressure at 25°C <380 mm Hg)

SVOC = Semi-Volatile Organic Compounds (1.0E-07 < Vapor Pressure at 25°C <1.0E-01 mm Hg)

SVINC = Semi-Volatile Inorganic Compounds (1.0E-07 < Vapor Pressure at 25°C <1.0E-01 mm Hg)

NVOC = Non-Volatile Organic Compounds (Vapor Pressure at 25°C < 1.0E-07 mm Hg)

NVINC or Particulate = Non-Volatile Inorganic Compounds (Vapor Pressure at 25°C < 1.0E-07 mm Hg)

Limit of Detection:

¹ Sampling and analytical procedures similar to TO-1 (Tenax sorbent bed and thermal desorption-injection capillary GC/MS); 18-L sampling volume used; method LODs for target compounds reported in µg/m³.² R-4 (822B): Concentrations in ng/cm² of filter converted to ng/m³ of air using the factor 4 m³/cm² (typical for 24-h Hi-Vol Sample)³ CLP-3: Contract Required Quantitation Limits (CRQL) assume 2500 m³ air volume per Hi-Vol filter and 40 mL final extraction volume⁴ CLP-2: LODs shown are Contract Required Quantitation Limits (CRQL), not absolute detection limits. For VOCs, CRQLs are shown in ppbv, converted from reported CRQLs in ng/m³ at 20°C and 1 atm.⁵ MDQ = Minimum Detectable Quantity

REFERENCES

Measurement Methods

TO-1 to 14

"Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air", PB90-127374, EPA/600/4-89/017, June 1988, USEPA, Research Triangle Park, NC.

- TO-1 Determination of Volatile Organic Compounds in Ambient Air Using Tenax-Adsorption and Gas Chromatography (GC/MS) - collection using Tenax and analysis using GC/MS
- TO-2 Determination of Volatile Organic Compounds in Ambient Air by Carbon Molecular Sieve Adsorption and Gas Chromatography/Mass Spectrometry (GC/MS) - collection by molecular sieve adsorption and analysis by GC/MS
- TO-3 Determination of Volatile Organic Compounds in Ambient Air Using Cryogenic Preconcentration Techniques and Gas Chromatography with Flame Ionization and Electron Capture Detection - collection by cryogenic preconcentration and analysis by GC/FID and GC/ECD
- TO-4 Determination of Organochlorine Pesticides and Polychlorinated Biphenyls in Ambient Air - sampling on glass fiber filter and polyurethane foam, soxhlet extraction, and analysis by GC/ECD
- TO-5 Determination of Aldehydes and Ketones in Ambient Air Using High Performance Liquid Chromatography (HPLC) - sampling using midjet impinger (hydrochloric acid/ 2,4-dinitrophenylhydrazine/ isooctane) and analysis by HPLC
- TO-6 Determination of Phosgene in Ambient Air Using High Performance Liquid Chromatography (HPLC) - sampling using midjet impinger (aniline/ toluene), solvent exchange to acetonitrile, and analysis by HPLC
- TO-7 Determination of N-Nitrosodimethylamine in Ambient Air Using Gas Chromatography - collection on sorbent cartridge (Thermosorb/N), extraction by dichloromethane, and analysis by GC/MS
- TO-8 Determination of Phenol and Methylphenols (Cresols) in Ambient Air Using High Performance Liquid Chromatography (HPLC) - sampling using two midjet impingers (sodium hydroxide) and analysis by reverse phase HPLC

- TO-9 Determination of Polychlorinated Dibenzo-p-Dioxins (PCDDs) in Ambient Air Using High Resolution Gas Chromatography/High Resolution Mass Spectrometry - collection on inlet filter and polyurethane foam cartridge, extraction with benzene, and analysis by GC/MS
- TO-10 Determination of Organochlorine Pesticides in Ambient Air Using Low Volume Polyurethane Foam (PUF) Sampling with Gas Chromatography/Electron Capture Detector (GC/ECD) - collection by PUF and analysis by GC/ECD
- TO-11 Determination of Formaldehyde in Ambient Air Using Adsorbent Cartridge Followed by High Performance Liquid Chromatography (HPLC) - collection by silica gel adsorbent and analysis by HPLC
- TO-12 Determination of Nonmethane Organic Compounds (NMOC) in Ambient Air Using Cryogenic Preconcentration and Direct Flame Ionization Detection (PDFID) - collection by cryogenic preconcentration and analysis by FID
- TO-13 Determination of Polynuclear Aromatic Hydrocarbons (PAHs) in Ambient Air Using High Volume Sampling with Gas Chromatography/Mass Spectrometry (GC/MS) and High Performance Liquid Chromatography Analysis - collection on sorbent (XAD-2) and polyurethane foam cartridge, and analysis by GC/FID, GC/MS, or HPLC
- TO-14 Determination of Volatile Organic Compounds (VOCs) in Ambient Air Using SUMMA Polished Canister Sampling and Gas Chromatographic (GC) Analysis - collection by passivated pre-evacuated canister and analysis by GC/ECD, NPD, or FID

TO-15

Method TO-15: The Determination of Volatile Organic Compounds (VOCs) in Air Collected in Summa Canisters and Analyzed by Gas Chromatography/Mass Spectrometry (GC/MS), EPA Contract No. 68-D0-0007 (WA-40), in progress. Collection is by canister, with analysis by GC/MS.

CLP-1A, 1B, 2, and 3

USEPA Contract Laboratory Program Statement of Work for Analysis of Ambient Air, Rev. IAIR01.2, US EPA, Research Triangle Park, NC, October 1993.

- CLP-1A: Tenax adsorbent collection and GC/MS/SCAN analysis
- CLP-1B: Summa canister sampling and GC/MS/SCAN analysis
- CLP-2: Collection on filter and XAD-2/polyurethane foam and GC/MS/SCAN analysis
- CLP-3: Collection on glass fiber filter and inductively coupled argon plasma spectroscopy or graphite furnace atomic adsorption analysis

NIOSH Methods

NIOSH Manual of Analytical Methods, 2nd edition, Vol. 1-7, Department of Health and Human Services, U.S. Government Printing Office, Washington, D.C., 1977-1982 (available from NTIS).

- S143: Visible absorption spectrophotometry using midget bubbler (HCl) for 1,1-dimethylhydrazine
- S149: Visible absorption spectrophotometry using midget bubbler (HCl) for methylhydrazine
- S152: Gas Chromatography using bubbler (sulfuric acid), followed by basification for triethylamine
- S179: HPLC-UV using cellulose membrane filter for collection, followed by extraction and hydrolysis with ammonia for phthalic anhydride
- S181: HPLC using XAD-2 resin in tube for collection of quinone
- P & CAM 220: GC-ECD using glass impingers' (methanolic solution of the sodium salt of 2,4,6-trichlorophenol) for collection of chloromethyl methyl ether
- P & CAM 284: Gas Chromatography using glass fiber filter and Gas-Chrom P for collection of 4-dimethyl aminoazobenzene
- P & CAM 291: GC-FID using Tenax GC in glass tube for collection of α -chloroacetophenone
- P & CAM 300: HPLC-UV using midget bubbler (Folin's Reagent) for aziridine and 2-methyl aziridine

NIOSH Manual of Analytical Methods, 3rd edition, Vol. 1-2, U.S. Department of Health and Human Services, U.S. Government Printing Office, Washington, D.C., February 1984 (available from NTIS).

- S67: GC-ECD using cellulose ester membrane filter for chlorinated camphene
- P & CAM 302: RPHPLC-UV using glass midget bubbler (distilled water) for maleic anhydride
- 1002: GC-FID using solid sorbent tube (coconut shell charcoal) for chloroprene
- 1014: GC-FID using solid sorbent tube (coconut shell charcoal) for methyl iodide
- 1024: GC-FID using solid sorbent tube (coconut shell charcoal) for 1,3-butadiene
- 1300: GC-FID using solid sorbent tube (coconut shell charcoal) for methyl isobutyl ketone
- 1501: GC-FID using solid sorbent tube (coconut shell charcoal) for cumene
- 1600: GC-Sulfur FPD using solid sorbent tube (coconut shell charcoal) + drying tube (sodium sulfate) for carbon disulfide
- 1614: GC-ECD using solid sorbent tube (HBr-coated petroleum charcoal) for ethylene oxide and propylene oxide
- 2002: GC-FID using solid sorbent tube (silica gel) for o-toluidine and N,N-dimethyl formamide
- 2004: GC-FID using solid sorbent tube (silica gel) for N,N-dimethyl formamide
- 2005: GC-FID using solid sorbent tube (silica gel) for nitrobenzene

- 2501: GC-Nitrogen-specific detector using solid sorbent tube (2-(hydroxymethyl)piperidine on XAD-2) for acrolein
- 2508: GC-FID using solid sorbent tube (petroleum-based charcoal) for isophorone
- 2514: HPLC-UV using solid sorbent tube (XAD-2) for o-anisidine
- 2515: GC-FID using solid sorbent tube (octanoic acid-coated XAD-2 resin) for diazomethane
- 2522: GC-TEA using solid sorbent tube (Thermosorb/NTM air sampler) for N-nitrosodimethylamine
- 2524: GC-electrolytic conductivity detector using solid sorbent tube (Porapak P) for dimethyl sulfate
- 2528: GC-FID using solid sorbent tube (Chromosorb) for 2-nitropropane
- 2530: GC-FID using solid sorbent tube (Tenax) for biphenyl
- 2535: HPLC-UV using tube with reagent-coated glass wool (N-[(4-nitrophenyl)methyl]-propylamine) for 2,4-toluene diisocyanate
- 3503: Visible absorption spectrophotometry using bubbler (HCl) for hydrazine
- 3509: Ion chromatography, ion pairing using impinger (hexanesulfonic acid) for diethanolamine
- 5001: HPLC-UV using glass fiber filter for 2,4-D diethylamine
- 5004: HPLC-UV using cellulose ester membrane filter for hydroquinone
- 5006: Visible absorption spectrophotometry using glass fiber filter for carbaryl
- 5011: Visible absorption spectrophotometry using PVC or mixed cellulose ester membrane for ethylene thiourea
- 5029: HPLC-UV/Electrochemical detector using acid-treated glass fiber filter for 4,4'-methylenedianiline
- 5500: GC-FID using glass fiber filter + silica gel sorbent for ethylene glycol
- 5509: HPLC-UV using glass fiber filter + silica gel sorbent tube for 3,3'-dichlorobenzidine
- 5516: HPLC-UV using impinger (1-(2-methoxyphenyl)-piperazine in toluene) for 2,4-toluenediamide
- 5521: HPLC-UV/Electrochemical detector using impinger (1-(2-methoxyphenyl)-piperazine in toluene) for 2,4-toluene diisocyanate and 4,4'-methylenediphenyl diisocyanate
- 6001: Atomic absorption with graphite furnace using solid sorbent tube (coconut shell charcoal) for arsine
- 6010: Visible absorption spectrophotometry using solid sorbent tube (soda lime) for HCN
- 6011: Ion chromatography, conductivity detection using silver membrane filter for bromine and chlorine
- 7300: Inductively coupled argon plasma, atomic emission spectroscopy using cellulose ester membrane filter for phosphorous
- 7400: Phase contrast light microscopy using cellulose ester membrane filter for asbestos
- 7402: Transmission electron microscopy using cellulose ester membrane filter for asbestos

- 7903: Ion chromatography using washed silica gel sorbent tube (with glass fiber filter plug) for HF and HCl
- 7904: Ion-specific electrode using filter (cellulose ester membrane) + bubbler (sodium hydroxide) for cyanides, aerosol and gas
- 7905: GC-phosphorous FPD using Tenax sorbent tube for phosphorous
- 8302: For 4,4'-Methylenebis(2-chloroaniline) in urine matrix

OSHA Methods

"OSHA Analytical Methods Manual", Second Edition, Parts I and II, U.S. Department of Labor, Occupational Safety and Health Administration, Salt Lake City, Utah, January 1990.

- [10]: GC-ECD using two bubblers (2,4,6-trichlorophenol and sodium methoxide in methanol) for bis(chloromethyl)ether
- [20]: Spectrophotometry or HPLC-UV using sulfuric acid-coated Glass Chrom R collection tubes for hydrazine
- [21]: GC-nitrogen/phosphorous detector using glass fiber filter and silica gel for acrylamide
- [24]: HPLC-UV using bubbler (hydrochloric acid) for 4,4'-methylenebis(2-chloroaniline)
- [25]: HPLC-UV using two adsorption tubes (p-anisidine-coated XAD-2, untreated XAD) for maleic anhydride
- [42]: HPLC-UV or fluorescence detection using coated glass fiber filters (1-(2-pyridyl)piperazine) for hexamethyl-1,6-diisocyanate
- [54]: HPLC-UV or fluorescence detection using coated XAD-7 tubes (1-(2-pyridyl)piperazine) for methyl isocyanate
- [57]: GC-ECD using sulfuric acid-treated glass fiber filters for 4,4'-methylenedianiline
- [63]: HPLC-UV using glass fiber filter and XAD-2 adsorbent in OSHA versatile sampler tubes for carbaryl
- [65]: GC-ECD using sulfuric acid-treated glass fiber filters for 2,4-toluenediamine and 3,3'-dichlorobenzidine
- [71]: GC-ECD using sulfuric acid-treated glass fiber filters for 4,4'-methylenebis(2-chloroaniline)
- [73]: GC-ECD using sulfuric acid-treated glass fiber filters for o-toluidine
- [86]: HPLC-UV using coated glass fiber filters (3,4-dimethoxybenzylamine) for maleic anhydride
- [90]: HPLC-UV coated glass fiber filters (3,4-dimethoxybenzylamine) for phthalic anhydride
- [ID101]: Ion-specific electrode using midget glass bubbler (sulfamic acid) for chlorine
- [ID105]: Atomic absorption spectroscopy with heated graphite atomizer using mixed-cellulose ester filter for arsine
- [ID160]: Phase contrast microscopy using mixed-cellulose ester filter for asbestos
- [ID174SG]: For hydrogen chloride

[ID180]: Ion chromatography using potassium hydroxide-impregnated beaded carbon for phosphine

"Chemical Information Manual" (CIM), U.S. Department of Labor, Occupational Safety and Health Administration, Washington, D.C., July 1991.

- [0065]: HPLC-UV using glass fiber filter for 2-acetylaminofluorene
- [P129]: HPLC-UV using coated XAD-2 tube (1-naphthyl isothiocyanate) for diethanolamine
- [0225]: HPLC-UV using XAD-2 tube for o-anisidine
- [T338]: HPLC-UV using glass fiber filter with Chromosorb 102 tube for trifluralin
- [B408]: GC-FID using Tenax GC tube for benzotrichloride
- [0524]: HPLC-UV using OSHA versatile sampler containing XAD-7 tube with glass fiber filter for caprolactam
- [0612]: GC-ECD using mixed-cellulose ester filter for toxaphene
- [0618]: HPLC-UV using two Tenax tubes for 2-chloroacetaphenone
- [A625]: GC-NPD using silica gel tube for acetamide
- [D639]: HPLC-UV using bulk sample media for dibenzofuran
- [1911]: GC-FID using glass fiber filter and silica gel tube for ethylene glycol
- [2222]: HPLC-UV using XAD-2 tube for quinone

EPA Methods

"Screening Methods for the Development of Air Toxics Emission Factors", PB92-108778, EPA-450/4-91-021, September 1991, USEPA, Research Triangle Park, NC.

- EPA 15: "Detection of Hydrogen Sulfide, Carbonyl Sulfide, and Carbon Disulfide from Stationary Sources", Standards of Performance for New Stationary Sources. Compilation U.S. Environmental Protection Agency, EPA-340/1-77-015. Gas sample drawn through heated sample probe followed by a particulate filter. Analysis is by GC/FPD.
- EPA 23: "Determination of Polychlorinated Dibenzo-p-dioxins (PCDDs) and Polychlorinated Dibenzofurans (PCDFs) from Stationary Sources" Federal Register, February 13, 1991 (56 FR 5758). To be included in 40 CFR Part 60, Appendix A. Sample is drawn through a probe, a glass fiber filter, and a XAD-2 trap. Extraction is by toluene and analysis by GC/MS.
- EPA 114: "Test Methods for Monitoring Radionuclide Emissions from Stationary Sources" Standards of Performance for New Stationary Sources. Compilation. U.S. Environmental Protection Agency, EPA-340/1-77-015. Particulate sampling is by a filter that has a high efficiency for submicrometer particles. Gaseous sampling is by various media: silica gel, charcoal, caustic solution. Analysis is by alpha, beta, and gamma analysis.

R-1

Collection of whole air in canisters, separation of co-collected water using a two-stage sorbent trap, thermal desorption, and analysis by GC with ion trap MS detection.

Kelly, T.J., Callahan, P.J., Pleil, J.P., Evans, G.F., Method Development and Field Measurements for Polar Volatile Organic Compounds in Ambient Air, Environ. Sci. Technol., 1993, 27(6), 1146-53.

R-2

Sampling at 10 LPM using a Teflon microfiber matrix (4-in.-dia. filter) impregnated with 5 μ m particles of AG-1 anion exchange resin; analyzed using BSTFA derivatization and EI-GC/MS.

H. Burkholder, M. Brinkman, M. Nishioka, J. Hodgeson, and J. Pleil, Anion Exchange Resins for Collection of Phenols from Air and Water, in Proceedings of the 16th Annual EPA Conference on Analysis of Pollutants in the Environment, Norfolk, VA, May 1993.

Nishioka, M.G., Burkholder, H.M., Evaluation of an Anion Exchange Resin for Sampling Ambient Level Phenolic Compounds, Final Report for EPA Contract No. 68-02-4127/WA-69 and -80, Battelle, Columbus, Ohio, April 1990.

R-3

Collection using three-stage tubes packed with Carbosieve S-III, Carbotrap, and Carbotrap C; desorption and refocusing onto an electrically cooled Carbosieve-III and Carbotrap sorbent bed; analysis by GC/FID and ECD.

Pollack, A.J., Gordon, S.M., Moschandreas, D.J., Evaluation of Portable Multisorbent Air Samplers for Use with an Automated Multitube Analyzer, Final Report for EPA Contract No.. 68-D0-0007/WA-27, September 1992.

R-4

Methods of Air Sampling and Analysis, 3rd Ed., Lodge, J.P. Jr., editor, Intersociety Committee on Methods of Air Sampling and Analysis, Lewis Publishers, Inc., Chelsea, Michigan, 1989.

- [14] Infrared Absorption Spectroscopy (using Saran or Mylar plastic bag sampler or silica gel) for VOCs
- [205]: Determination of Fluoride Content of Plant Tissues (Potentiometric Method)
- [301]: Determination of Particulate Antimony Content in the Atmosphere (using membrane, cellulose or glass fiber filters and visible absorption spectrophotometry)
- [302]: Determination of Arsenic Content of Atmospheric Particulate Matter (using membrane or glass fiber filters and visible absorption spectrophotometry)

- [317]: Determination of Elemental Mercury in Ambient and Workroom Air by Collection on Silver Wool and Atomic Absorption Spectroscopy
- [606A]: Estimation of Airborne Radon-222 by Filter Paper Collection and Alpha Activity Measurements of Its Daughters (Thomas Method or Modified Kusnetz Method)
- [606B]: Determination of Airborne Radon-222 by Its Absorption from the Atmospheric and Gamma Measurement (using charcoal adsorbent)
- [804]: As, Se, and Sb in Urine and Air by Hydride Generation and Atomic Absorption Spectrometry (using cellulose acetate membrane filter)
- [805]: Determination of Chlorine in Air (using midget impinger with sodium acetate and potentiometric analysis)
- [809]: Determination of Fluorides and Hydrogen Fluoride in Air (using impingers with sodium hydroxide)
- [822]: General Atomic Absorption Procedure for Trace Metals in Airborne Material Collected on Filters (using membrane filters) for particulate inorganics
- [822B]: X-Ray Fluorescence Spectrometry for Multielemental Analysis of Airborne Particulate and Biological Material
- [829]: Determination of Chloromethyl Methyl Ether (CMME) and Bis-Chloromethyl Ether (Bis-CME) in Air (using GC-ECD and impingers with a methanolic solution of the sodium salt of 2,4,6-trichlorophenol)
- [831]: Determination of p,p-Diphenylmethane Diisocyanate (MDI) in Air (using midget impingers with hydrochloric and acetic acids and visible absorption spectrophotometry)
- [835]: Determination of EPN, Malathion and Parathion in Air (using glass fiber filters and GC-flame photometric detection)
- [836]: Determination of Total Particulate Hydrocarbons (TpAH) in Air: Ultrasonic Extraction Method (using glass fiber filters and HPLC-UV)
- [837]: Determination of 2,4-Toluene Diisocyanate (TDI) in Air (using midget impingers with hydrochloric and acetic acids and visible absorption spectrophotometry)

R-5

High volume air sampling with glass fiber filter and polyurethane foam sorbent; solvent extraction and chromatographic cleanup; analysis by high resolution gas chromatography and high resolution mass spectrometry (HRGC/HRMS), with multiple isotopically labelled internal surrogate standards. Analysis based on guidelines of EPA Methods 8280 and 8290.

Hunt, G.T., Maisel, B.E., Atmospheric Concentrations of PCDDs/PCDFs in Southern California, J. Air Waste Mgt. Assoc., 1992, 42:672-680.

R-6

Automated gas chromatography with detection by ECD and FID. Sample collection performed hourly using a three-stage sorbent trap, with refocusing on a cryogenic (-186°C) trap for analysis.

Purdue, L.J., Reagan, J.A., Lonneman, W.A., Lawless, T.C., Drago, R.J., Zalaquet, G.M., Holdren, M.W., Smith, D.L., Pate, A.D., Buxton, B.E., Spicer, C.W., Atlanta Ozone Precursor Monitoring Study Data Report, EPA/600/R-92/157, U.S. Environmental Protection Agency, Washington, D.C., September 1992.

R-7

Canister collection of whole air samples; analysis by gas chromatography/multiple detector (ECD, FID, PID) method.

McAllister, R., Bowles, E., DeGarmo, J., Rice, J., Jongleux, R.F., Merrill, R.G., Jr., and Bursey, J., 1990 Urban Air Toxics Monitoring Program. Report No. EPA-450/4-91-024, prepared for U.S. Environmental Protection Agency by Radian Corporation, Research Triangle park, NC, June 1991.

R-8

Sampling with denuder/filter/XAD resin combinations, extraction, and analysis by ion chromatography.

Eatough, D.J., White, V.F., Hansen, L.D., Eatough, N.L., Cheney, J.L., Identification of Gas-Phase Dimethyl Sulfate and Monomethyl Hydrogen Sulfate in the Los Angeles Atmosphere, Environ. Sci. Technol., 1986, 20:867-872.

Hansen, L.D., White, V.F., Eatough, D.J., Determination of Gas-Phase Dimethyl Sulfate and Monomethyl Hydrogen Sulfate, Environ. Sci. Technol., 1986, 20:872-878.

R-9

Four distinct methods: 1) collection on Thermosorb A, solvent extraction, and analysis by GC with nitrogen-selective detector; 2) collection on Tenax, thermal desorption, and GC/MS analysis; 3) grab sampling with analysis by portable GC/FID; 4) atmospheric pressure ionization quadrupole MS.

Clay, P.F. (NUS Corp., Bedford, Mass), Spittler, T.M. (U.S. EPA, Region I, Lexington, Mass), Determination of airborne volatile nitrogen compounds using four independent techniques. Proceedings of Natl. Conf. Manage. Uncontrolled Hazard Waste Sites. Hazard. Mater. Control Res. Inst.: Silver Spring, Maryland, 1983, pp 100-104.

R-10

Cryogenic trapping, thermal desorption, and GC analysis with flame photometric detection

Maroulis, P.J., Torres, A.L., Bandy, A.R., Atmospheric concentrations of carbonyl sulfide in the southwestern and eastern United States, Geophys. Res. Lett., 1977, 4:510-512.

Torres, A.L., Maroulis, P.J., Goldberg, A.B., Bandy, A.R., Atmospheric OCS measurements on Project Gametag, J. Geophys. Res., 1980, C12:7357-7360.

R-11

Cryogenic trapping, thermal desorption, and sequential GC analysis of two samples collected simultaneously with flame photometric detection.

Maroulis, P.J., Bandy, A.R., Measurements of atmospheric concentrations of CS₂ in the eastern United States, Geophys. Res. Lett., 1980, 7:681-684.

R-12

Collection on Tenax sorbent, thermal desorption to a cryogenic focussing trap, and GC/MS analysis.

Pellizzari, E.D., Bunch, J.E., Ambient air carcinogenic vapors: improved sampling and analytical techniques and field studies, EPA-600/2-79-081, NTIS No. PB-297-932, U.S. Environmental Protection Agency, Research Triangle Park, NC, May 1979.

R-13

Collection in canisters or cryogenically, with four detection methods. (1) Ion Trap GC/MS - detection limit of 1 pptv. (2) Quadrupole GC/MS with Selective Ion Monitoring - detection limit of 10 pptv. (3) Gas Chromatography with Photoionization Detection - detection limit 10 pptv. (4) Quadrupole GC/MS with Full Scan Monitoring - detection limit of 0.1 ppbv. Also Portable Gas Chromatograph with Photoionization Detection - detection limit of 0.1 ppbv.

Havlicek, S.C., Hilpert, L.R., Dai, G., Pierotti, D., Assessment of Ethylene Oxide Concentrations and Emissions from Sterilization and Fumigation Processes (PB93-216793; available NTIS). Final report by Coast-to-Coast Analytical Services, Inc., San Luis Obispo, CA, to California Air Resources Board, Sacramento, CA, Contract No. ARB-A832-125, 78 pp, May 1992.

R-14

Collection on XAD-4 resin Soxhlet extraction in dichloromethane and then in ethylacetate, analysis by GC/MS with positive chemical ionization.

Chuang, J.C., Mack, G.A., Kuhlman, M.R., Wilson, N.K., Polycyclic Aromatic Hydrocarbons and Their Derivatives in Indoor and Outdoor Air in an Eight-Home Study, Atmos. Envir., 1991, 25(3): 369-380.

R-15

Collection on XAD-2 or PUF, Soxhlet extraction in 10 percent ether/hexane or methylene chloride, analysis by GC/MS.

Chuang, J.C., Hannan, S.W., Wilson, N.K., Field Comparison of Polyurethane Foam and XAD-2 Resin for Air Sampling for Polynuclear Aromatic Hydrocarbons, *Envir. Sci. Tech.*, 1987, 21(8): 798-804.

R-16

Air sampling methods discussed with references; minimum detectable levels provided for a number of particulate and gaseous radionuclides in air presented, assuming standard gamma-scan-400 to 512 multichannel analyzer - 4 x 4-inch NaI (Te) detector or liquid scintillation counting, with references.

CRC Handbook of Environmental Radiation, Ed. Alfred W. Clement, Jr., CRC Press, Inc., Boca Raton, FL, 1982.

R-17

Background information on radioactivity detectors, measurement procedures, quality assurance, and statistical analysis of radioactivity measurements.

Handbook of Radioactivity Measurements Procedures, NCRP Report No. 58, National Council on Radiation Protection and Measurements, Bethesda, MD, 1985.

R-18

Collection on Teflon filter and iodated activated carbon, acid digestion, and analysis by cold vapor atomic absorption.

Lindbergh, S.E., Turner, R.R., Meyers, T.P., Taylor, G.E., Jr., Schroeder, W.H., Atmospheric concentrations and deposition of Hg to a deciduous forest at Walker Branch Watershed, Tennessee, USA, *Water, Air, Soil Poll.*, 1991, 56:577-594.

Turner, R.R., Bogle, M.A., Heidel, L., McCain, L., Mercury in ambient air at the Oak Ridge Y-12 plant July 1986 through December 1990, Y-12 report Y/TS-574, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 1991.

R-19

Collection on alkaline-impregnated glass fiber filters, aqueous extraction, and ion chromatographic analysis using "negative" UV photometric detection with a strongly UV-absorbing eluent.

Grosjean, D., Liquid chromatography analysis of chloride and nitrate with "negative" ultraviolet detection: ambient levels and relative abundance of gas-phase inorganic and organic acids in southern California, *Environ. Sci. Technol.*, 1990, 24:77-81.

R-20

Revision of ASTM Method D-3266, involving collection of HF on alkaline-impregnated tape, aqueous extraction, and analysis by ion-selective electrode.

Zankel, K.L., McGirr, R., Romm, M., Campbell, S.A., Miller, R., Measurement of ground-level concentrations of hydrogen fluoride, J. Air Poll. Control Assoc., 1987, 37:1191-1196.

R-21

Collection on Nuclepore (i.e., polycarbonate) filters, carbon coating by vapor deposition, and electron microscopic examination.

Samudra, A.U., Harwood, C.F., Stockhalm, J.D., Electron microscope measurement of airborne asbestos concentration. EPA-600/1-77-178, U.S. Environmental Protection Agency, Research Triangle Park, NC, 1977.

See also discussion in:

Asbestiform Fibers: Nonoccupational Health Risks, published by National Academy Press, National Academy of Sciences, Washington, D.C., pp 82-96, 1984.

R-22

Sampling using a chilled acetone collection medium to trap hydrazines and convert to stable derivatives; acetone solution analyzed directly for derivatives using a gas chromatograph with nitrogen-specific detectors.

Holtzclaw, J.R., Rose, S.L., Wyatt, J.R., Ronnbehler, D.P., Fine, D.H., Simultaneous Determination of Hydrazine, Methylhydrazine, and 1,1-Dimethyl Hydrazine in Air by Derivatization/Gas Chromatography, Anal. Chem., 1984, 56: 2952-2956.

R-23

Collection and derivatization in toluene solution containing N-(4-nitrobenzyl)-N-n-propylamine hydrochloride (NBPA); analysis by HPLC and UV detection.

Holdren, M.W., Spicer, C.W., Riggan, R.M., Gas phase reaction of toluene diisocyanate with water vapor, Am. Ind. Hygiene Assoc. J., 1984, 45:626-633.

Dunlap, K.L., Sandridge, R. L., Keller, J., Determination of isocyanates in working atmospheres by high-speed liquid chromatography, Anal. Chem., 1976, 48:497-499.

R-24

Continuous real-time monitoring based on color formation in a substrate-impregnated tape, with electro-optical measurement of color intensity. The unit has a useful range up to 200 ppbv of TDI, with a detection limit of 1 ppbv.

The monitor is sold as the TLD-1 by MDA Scientific, Inc., Lincolnshire, Illinois.

R-25

Sampling at 0.1 LPM using 200-400 mesh granular AG-1 anion exchange resin; analyzed using EI-GC/MS and/or GC/FID; methylation and GC/ECD for chlorinated phenols.

Nishioka, M.G., Burkholder, H.M., Evaluation of an Anion Exchange Resin for Sampling Ambient Level Phenolic Compounds, Final Report for EPA Contract No. 68-02-4127/WA-69 and -80, Battelle, Columbus, Ohio, April 1990.

R-26

Passive sampling using commercial samplers with activated carbon as sorbent; solvent extraction and concentration; analysis by GC/MS.

Shields, H.C., Weschler, C.J., Analysis of ambient concentrations of organic vapors with a passive sampler, J. Air. Poll. Control Assoc., 1987, 37:1039-1045.

R-27

Collection on polyurethane foam (sampling for 24 hours at 3.8 L/min), solvent extraction and evaporative concentration, analysis by GC/ECD and GC/MS (multiple ion mode).

Immerman, F.W., Schaum, J.L., Final Report of the Nonoccupational Pesticide Exposure Study (NOPES), EPA-600/3-90-003, U.S. Environmental Protection Agency, Research Triangle Park, NC, 1990.

Whitmore, R.W., Immerman, F.W., Camann, D.E., Bond, A.E., Lewis, R.G., Schaum, J.L., Nonoccupational Exposures to Pesticides for Residents of Two U.S. Cities, Arch. Environ. Contam. Toxicol., 1994, 26:47-59.

R-28

Collection on glass fiber filters and polyurethane foam or Florisil sorbents. Solvent extraction, cleanup on Florisil, evaporative concentration, and analysis by GC/ECD.

Atlas, E., Giam, C.S., Ambient concentration and precipitation scavenging of atmospheric organic pollutants, Water Air Soil Poll., 1988, 38:19-36.

Chang, L.W., Atlas, E., Giam, C.S., Chromatographic separation and analysis of chlorinated hydrocarbons and phthalic acid esters from ambient air samples, Int. J. Environ. Anal. Chem., 1985, 19:145-153.

R-29

Collection with glass fiber filters and polyurethane foam; solvent extraction, cleanup on Florisil, evaporative concentration; analysis by GC/ECD and GC/MS.

Hoff, R.M., Muir, D.C.G., Grift, N.P., Annual cycle of polychlorinated biphenyls and organohalogen pesticides in air in southern Ontario 1. Air concentration data, Environ. Sci. Technol., 1992, 26:266-275, and references therein.

R-30

High volume or low volume sampling of ambient air. Collection on glass fiber filters and polyurethane foam, solvent extraction, evaporative concentration, and analysis by GC/ECD or GC/MS.

Lewis, R.G., Bond, A.E., Johnson, D.E., Hsu, J.P., Measurement of atmospheric concentrations of common household pesticides: a pilot study, Environ. Monitoring and Assessment, 1988, 10:59-73.

R-31

Collection on glass fiber filters and on any of three sorbents: polyurethane foam, XAD-2 resin, or Tenax GC. Solvent extraction, cleanup, and analysis by GC/ECD.

Billings, W.N., Bidleman, T.F., High volume collection of chlorinated hydrocarbons in urban air using three solid sorbents, Atmos. Environ., 1983, 17:383-393.

R-32

Filter sampling at 1.5 LPM, total sampling volume of 240-L using PVC filters; extraction using buffer solution, pH = 4.5; trisodium pentacyanoaminoferrate reagent; colorimetric analysis in 30 min at 475 nm in 1-cm glass cells; paper provides sampling conditions, extraction solvents, reagents, analytical conditions, and detection ranges for colorimetric determination.

Freixa, A., Magti, A., Application of colorimetric techniques to the measurement of air pesticide content, Pergamon Ser. Environ. Sci., 1982, 7: 297-298.

R-33

Gas chromatography with flame photometric detection (GC-FPD) using a column (0.5 m x 2.5 mm i.d.) packed with GDX-101. Phosphene retention time 19 s at 80 C; ratio of H to O of 10:3.

Qi, Xiaofei, Quantitative determination of trace phosphine in ambient air by gas chromatography with a flame photometric detector, Sepn, 1987, 5(4): 243-5 (in Chinese).

R-34

Chemiluminescence emission from arsine due to reaction of sampled air with ozone.

Inoue, K., Suzuki, M., Kawabayashi, O., Method and Apparatus for Chemiluminescence Analyses, Ger. Offen., DE 3525700/A1/860206 (German patent), 1986 (reports detection limit of 1 ppb for arsine).

Fraser, M. E., Stedman, D. H., Henderson, M. J., Gas-phase Chemiluminescence of Arsine Mixed with Ozone, *Anal. Chem.*, 1982, 54(7): 1200-1.

R-35

Analysis using gas chromatography and an alkali flame ionization detector (N-detector); acidified aqueous solutions directly injected on the column.

Donike, M., Gas chromatographic trace analysis of hydrocyanic acid in the nano- and picogram range, *Mitteilungsbl. GDCh-Fachgruppe Lebensmittelchem. Gerichtl. Chem.*, 1974, 28(1-2): 46-52 (in German).

R-36

Collection of particulate material from air, analysis by HPLC with electrochemical detection.

Riggin, R.M., Howard, C.C., Scott, D.R., Hedgecock, R.L., Determination of benzidine, related congeners, and pigments in atmospheric particulate matter, *J. Chromatogr. Sci.*, 1983, 21:321-325.

R-37

Derivatization of amines to the corresponding amides by reaction with a perfluoro-acid anhydride, gas chromatographic separation, and analysis by N-selective thermionic detection.

Skarping, G., Renman, L., Dalene, M., Trace analysis of amines and isocyanates using glass capillary gas chromatography and selective detection. II. Determination of aromatic amines as perfluorofatty acid amides using nitrogen-selective detection, *J. Chromatogr.*, 1983, 270:207-218.

R-38

GC/ECD method for 2,4-D salts and acid.

Nishioka, M., Burkholder, H., Brinkman, M., Gordon, S., Lewis, R., "Simulation of track-in of lawn-applied herbicide acids from turf to home: Comparison of dislodgeable turf residues with carpet dust and carpet surface residues, prepared for submission to *Environ. Sci. Technol.*, 1993.

R-39

Collection on Tenax-GK sorbent, thermal desorption, gas chromatography with Hall electrolytic chlorine-sensitive detection.

Matienzo, L.J., Hensler, C.J., Determination of N,N-dimethylcarbamoyl chloride (DMCC) in air, *Am. Indus. Hygiene Assoc. J.*, 1982, 43:838-844.

R-40

Collection with glass fiber filter and Tenax GC sorbent, thermal desorption, cryogenic concentration, and analysis by GC/MS.

Krost, K.J., Pellizzari, E.D., Wlaburn, S.G., Hubbard, S.A., Collection and analysis of hazardous organic emissions, *Anal. Chem.*, 1982, 54:810-817.

R-41

Collection in methylisobutyl ketone, gas chromatography with sulfur-selective detection. Alternatively, collection and derivatization on the pre-coated walls of a diffusion denuder tube, and determination by HPLC with UV detection.

Oldeweme, J., Klockow, D., Chromatographic procedures for the determination of 1,3-propanesultone in workplace air, *Fresenius Z. Anal. Chem.*, 1986, 325:57-63.

R-42

Collection in aqueous KOH solution containing methanol and hydroxyl amine, to form a derivative. The iron complex of that derivative is determined quantitatively by absorbance of 530 nm.

Jozwicka, J., Spectrophotometric method for determination of monochloroacetic acid vapors in workplace air, *Wlokn Chem.*, 1990, 16:394-401.

R-43

Workplace air monitoring of caprolactam; collection on filter and XAD-2 tubes or XAD-2 tubes only; desorption with methanol containing 2 percent water, or with MeCN; analysis by GC or HPLC. Sampled air volume of 100 L yields detection limit of 0.20 mg/m³ using HPLC analysis, and 0.10 mg/m³ using GC analysis.

Nau, D.R., Darr, R.W., Gad, S.C., Pai, S.V., Validation study of a method for monitoring personnel exposure to caprolactam, *Proc Symp. Ind. Approach Chem. Risk Assess.: Caprolactam Relat. Compd. Case Study*, 275-91. Ind. Health Found.: Pittsburgh, PA, 1984.

R-44

Detection of caprolactam in workplace air and toxicol. studies; aerosols sampled on filter AFA-KhA-20 at 2 L/min, extracted with di-Et ether or a 1:1 EtOH/ether mixture; evaporated, and chromatographic drying in Cl, analysis by thin-layer chromatography with a mobile alcohol solvent system; and development with o-tolidine solution or fresh KI-starch reagent. Detection limit is 0.005 mg/m³; cyclohexanone, hydroxylamine, and NH₃ stated not to interfere with method.

Ledovskikh, N.G., Sensitive method for the determination of caprolactam in air, *Gig. r. Prof. Zabol.*, 1982, 10: 52-3 (in Russian).

R-45

Collection by charcoal adsorbent tube (or silica gel tube under high humidity conditions); desorption using distilled water then carbon disulfide; analysis of both layers by GC-FID.

Langhorst, M.L., Glycol Ethers Validation Procedures for Tube/Pump and Dosimeter Monitoring Methods, Am. Ind. Hyg. Assoc. J., 1984, 45:416-424.

R-46

Personal air sampling through polyurethane foam plug; extraction in hexane; solvent transfer to toluene; analysis by GLC.

Nigg, H.N., Stamper, J.H., Exposure of Spray Applicators and Mixer-Loaders to Chlorobenzilate Miticide in Florida Citrus Groves, Arch. Environ. Contam. Toxicol., 1983, 12:477-482.

R-47

Headspace gas chromatography is applied for the analysis of water in liquid and solid samples with the preferred quantitation technique being standard addition.

Kolb, B., Auer, M., Analysis for Water in Liquid and Solid Samples by Headspace Gas Chromatography. Part I: Liquid and Soluble Solid Samples, Fresenius. Z. Anal. Chem., 1990, 336:291-6.

R-48

Sampling via an activated carbon fiber felt put between quartz filters and determination by gas chromatography-mass spectroscopy.

Suzuki, S., Simultaneous Determination of Airborne Pesticides by GC/MS, Bunseki Kagaku, 1992, 41:115-24 (in Japanese).

R-49

Collection on XAD resins and determination by gas chromatography-mass spectroscopy and a nitrogen-phosphorous detector.

Yeboah, P.O., Kilgore, W.W., Analysis of Airborne Pesticides in a Commercial Pesticide Storage Building, Bull. Environ. Contam. Toxicol., 1984, 32:629-34.

R-50

High volume sampling with collection on a cartridge containing PUF/Tenax/PUF. Multiple extraction, derivation, and analysis by GC/MS or GC/ECD.

McConnell, L.L., Patton, G.W., Zaranski, M.T., Bidleman, T.F., Development of a collection method for chlorophenolic compounds in air, in Proceedings of the 1989

EPA/AWMA Symposium on Measurement of Toxic and Related Air Pollutants, Publication VIP-13, EPA-600/9-89-060, Air and Waste Mgt. Assoc., Pittsburgh, pp 623-628, 1989.

R-51

Collection with glass fiber filters and polyurethane foam sorbent. Solvent extraction after spiking with ^{13}C -labelled isomers, chromatographic cleanup of the extracts, and evaporative concentration. Analysis by GC/MS using electron impact or electron capture negative ion modes.

Eitzer, B.D., Hites, R.A., Polychlorinated dibenzo-p-dioxins and dibenzofurans in the ambient atmosphere of Bloomington, Indiana, Environ. Sci. Technol., 1989, 23:1389-1395.

Edgerton, S.A., Czuczwa, J.M., Rench, J.D., Hodanbosi, R.F., Koval, P.J., Ambient air concentrations of polychlorinated dibenzo-p-dioxins and dibenzofurans in Ohio: Sources and health risk assessment, Chemosphere, 1989, 18:1713-1730.

R-52

High volume sampling with a Teflon-impregnated glass fiber filter and three PUF sorbent plugs in series; addition of deuterated internal standards; solvent extraction and evaporative concentration; analysis by HPLC with UV detection.

Arey, J., Zielinska, B., Atkinson, R., Winer, A.M., Polycyclic aromatic hydrocarbon and nitroarene concentrations in ambient air during a wintertime high- NO_x episode in the Los Angeles basin, Atmos. Environ., 1987, 21:1437-1444.

R-53

Collection on Teflon-impregnated glass fiber filters and XAD-2 resin sorbent; multiple solvent extractions with addition of deuterated internal standards, and separation of acid and base/neutral fractions by HPLC. Analysis by negative chemical ionization GC/MS.

Nishioka, M.G., Lewtas, J., Quantification of nitro- and hydroxylated nitro-aromatic/polycyclic aromatic hydrocarbons in selected ambient air daytime winter samples, Atmos. Environ., 1992, 26A:2077-2087.

R-54

Sampling with glass fiber filters and Tenax-GC and polyurethane foam sorbent traps; solvent extraction with addition of deuterated internal standards; analysis by GC/MS with electron impact ionization.

Leuenberger, C., Ligocki, M.P., Pankow, J.F., Trace organic compounds in rain. 4. Identities, concentrations, and scavenging mechanisms for phenols in urban air and rain, Environ. Sci. Technol., 1985, 19:1053-1058.

R-55

Continuous monitoring in air using ion mobility mass spectrometry.

Leasure, C.S., Eiceman, G.A., Continuous detection of hydrazine and monomethylhydrazine using ion mobility spectrometry, *Anal. Chem.*, 1985, 57:1890-1894.

R-56

Derivatization on-column with an alkali metal salt of 2,4,6-trichlorophenol to form a derivative, which is determined immediately by GC with electron capture detection.

Kallos, G.J., Albe, W.R., Solomon, R.A., On-column reaction gas chromatography for determination of chloromethyl methyl ether at one part-per-billion level in ambient air, *Anal. Chem.*, 1977, 49:1817-1820.

R-57

Collection with glass fiber filters and Tenax-GC sorbent; solvent extraction, evaporative concentration, and analysis by GC/MS.

Cautreels, W., van Cauwenberghe, K., Experiments on the distribution of organic pollutants between airborne particulate matter and the corresponding gas phase, *Atmos. Environ.*, 1978, 12:1133-1141.

R-58

Low volume collection on Tenax-GC, thermal desorption, cryofocusing, and GC/MS analysis in a mobile field sampling laboratory.

Haggert, B., Havkov, R., Design and implementation of a mobile monitoring unit (MMU) to measure ambient volatile organic compounds, paper 84-17.2, presented at the 77th Annual Meeting, Air Pollution Control Association, San Francisco, CA, June 1984.

R-59

Method stated to be collection of whole air in sampling bags, with analysis by GC with photoionization detection.

Hunt, W.F., Jr., Faoro, R.B., Freas, W., Report on the Interim Data Base for State and Local Air Toxic Volatile Organic Chemical Measurements, Report No. EPA-450/4-86-012, U.S. Environmental Protection Agency, Research Triangle Park, NC, 1986.

R-60

Modified version of Compendium Method TO-8, using C₁₈ Sep-Pak cartridges coated with NaOH for sampling, with analysis by HPLC. The resolution of the HPLC analysis is improved by changing the pH of the acetate buffer, and by using a sequential bonding end-capped column.

Bratton, S.A., Sampling and measurement of phenol and methylphenols (cresols) in air by HPLC using a modified Method TO-8, in Measurement of Toxic and Related Air Pollutants, proceedings of the 1992 EPA/AWMA International Symposium, EPA Report No. EPA-600/R-92/131, Publication VIP-25, Air and Waste Mgt. Assoc., Pittsburgh, PA, pp. 719-724 (1992).

R-61

Adsorption of pentachlorophenol (PCP) onto OV-17 stationary phase, with collection /thermal desorption on a 2-minute cycle. Analysis of desorbed PCP by atmospheric pressure chemical ionization tandem mass spectrometry. Detection limit 40 ng/m³.

DeBrou, G.B., Ng, A.C., Karellas, N.S., Near real-time measurements of pentachlorophenol in ambient air by mobile mass spectrometry, in Measurement of Toxic and Related Air Pollutants, proceedings of the 1992 EPA/AWMA International Symposium, EPA Report No. EPA-600/R-92/131, Publication VIP-25, Air and Waste Mgt. Assoc., Pittsburgh, PA, pp. 838-843 (1992).

R-62

Collection of 2,4-toluene diisocyanate in a derivatizing solution of 1-(2-pyridyl)piperazine in toluene, in impingers. The stable TDI/urea derivative is determined by HPLC. Limit of detection for TDI is 116 ng/m³, limit of quantitation is 351 ng/m³.

Wilshire, F.W., Knoll, J.E., Foster, S.C., McGaughey, J.F., Development and validation of a source test method for 2,4-toluene diisocyanate, in Measurement of Toxic and Related Air Pollutants, proceedings of the 1993 EPA/AWMA International Symposium, EPA Report No. EPA-600/A93/024, Publication VIP-34, Air and Waste Mgt. Assoc., Pittsburgh, PA, pp. 399-407 (1993).

R-63

Collection of airborne asbestos on a polycarbonate or mixed cellulose ester filter, deposition of carbon under vacuum, and dissolution of the original filter material. Analysis and counting is conducted by analytical electron microscopy, with identification by electron diffraction and energy dispersive x-ray spectroscopy.

Doom, S.S., Burris, S.B., Airborne asbestos analysis by analytical electron microscopy, in Measurement of Toxic and Related Air Pollutants, proceedings of the 1991 EPA/AWMA International Symposium, EPA Report No. EPA/600/9-91/018, Publication VIP-21, Air and Waste Mgt. Assoc., Pittsburgh, PA, pp. 226-230 (1991).

R-64

Cryogenic concentration of a 100 mL air sample, separation by two dimensional gas chromatography, with flame ionization detection.

Fung, K., A method for the measurement of alcohols and MTBE in ambient air, in Measurement of Toxic and Related Air Pollutants, proceedings of the 1991 EPA/AWMA International Symposium, EPA Report No. EPA/600/9-91/018, Publication VIP-21, Air and Waste Mgt. Assoc., Pittsburgh, PA, pp.770-775 (1991).

APPENDIX D

LISTINGS OF THE 189 HAPs BY ASSIGNED VOLATILITY CLASSES

Table D-1. HAPs grouped by class of compounds, listed in alphabetical order.

<u>VVOCs</u> (VP _{25°C} > 380 mm Hg)	<u>VOCs</u> (0.1 mm Hg < VP _{25°C} < 380 mm Hg)	
Acetaldehyde 1,3-Butadiene Carbonyl sulfide Diazomethane Ethyl chloride Ethylene oxide Formaldehyde Methyl bromide Methyl chloride Methyl iodide Phosgene Propylene oxide Vinyl bromide Vinyl chloride Vinylidene chloride <i>(Total of 15 HAPs)</i>	Acetonitrile Acetophenone Acrolein Acrylamide Acrylic acid Acrylonitrile Allyl chloride Aniline Benzene Benzyl chloride Bis (chloromethyl) ether Bromoform Carbon disulfide Carbon tetrachloride Catechol Chloroacetic acid Chlorobenzene Chloroform Chloromethyl methyl ether Chloroprene Cresol/Cresylic acid (mixed isomers) o-Cresol Cumene 1,2-Dibromo-3-chloropropane 1,4-Dichlorobenzene Dichloroethyl ether (Bis[2-chloroethyl]ether) 1,3-Dichloropropene Diethyl sulfate N,N-Dimethylaniline Dimethylcarbamoyl chloride N,N-Dimethylformamide 1,1-Dimethylhydrazine Dimethyl sulfate 1,4-Dioxane Epichlorohydrin 1,2-Epoxybutane Ethyl acrylate Ethylbenzene Ethyl carbamate Ethylene dibromide	Ethylene dichloride Ethyleneimine Ethylidene dichloride Hexachlorobutadiene Hexachloroethane Hexane Isophorone Methanol Methyl chloroform Methyl ethyl ketone Methylhydrazine Methyl isobutyl ketone Methyl isocyanate Methyl methacrylate Methyl tert-butyl ether Methylene chloride Nitrobenzene 2-Nitropropane N-Nitroso-N-methylurea N-Nitrosodimethylamine N-Nitrosomorpholine Phenol 1,3-Propane sultone beta-Propiolactone Propionaldehyde Propylene dichloride 1,2-Propylenimine Styrene Styrene oxide 1,1,2,2-Tetrachloroethane Tetrachloroethylene Toluene 1,2,4-Trichlorobenzene 1,1,2-Trichloroethane Trichloroethylene Triethylamine 2,2,4-Trimethylpentane Vinyl acetate Xylene (mixed isomers) o-Xylene m-Xylene p-Xylene <i>(Total of 82 HAPs)</i>

Table D-1. (continued)

SVOCs (10^{-7} mm Hg < $VP_{25^{\circ}C}$ < 0.1 mm Hg)		NVOCs ($VP_{25^{\circ}C}$ < 10^{-7} mm Hg)
Acetamide	Hexamethylphosphoramide	2-Acetylaminofluorene
4-Aminobiphenyl	Hydroquinone	3,3'-Dimethoxybenzidine
o-Anisidine	Maleic anhydride	4-Dimethylaminoazobenzene
Benzidine	Methoxychlor	4,4'-Methylenebis-(2-chloroaniline)
Benzotrichloride	4,4'-Methylenediphenyl diisocyanate	4,4'-Methylenedianiline
Biphenyl	Naphthalene	(Total of 5 HAPs)
Bis (2-ethylhexyl)phthalate	4-Nitrobiphenyl	
Caprolactam	4-Nitrophenol	
Captan	Parathion	
Carbaryl	Pentachloronitrobenzene	
Chloramben	Pentachlorophenol	
Chlordane	p-Phenylenediamine	
2-Chloroacetophenone	Phthalic anhydride	
Chlorobenzilate	Polychlorinated biphenyl	
m-Cresol	Propoxur (Baygon)	
p-Cresol	Quinoline	
2,4-D (2,4-Dichloro phenoxyacetic acid) (incl. salts and esters)	Quinone	
DDE	2,3,7,8-Tetrachlorodibenzo-p-dioxin	
Dibenzofurans	Toluene-2,4-diamine	
Dibutyl phthalate	2,4-Toluene diisocyanate	
3,3'-Dichlorobenzidine	o-Toluidine	
Dichlorvos	Toxaphene (chlorinated camphene)	
Diethanolamine	2,4,5-Trichlorophenol	
3,3'-Dimethylbenzidine	2,4,6-Trichlorophenol	
Dimethyl phthalate	Trifluralin	
4,6-Dinitro-o-cresol (including salts)	Coke Oven Emissions	
2,4-Dinitrophenol	Glycol ethers	
2,4-Dinitrotoluene	Polycyclic Organic Matter	
1,2-Diphenylhydrazine	(Total of 64 HAPs)	
Ethylene glycol		
Ethylene thiourea		
Heptachlor		
Hexachlorobenzene		
1,2,3,4,5,6-Hexachloro cyclohexane (all stereo isomers, including Lindane)		
Hexachlorocyclo pentadiene		
Hexamethylene diisocyanate		

Table D-1. (continued)

<p>VVINC_s ($VP_{25^{\circ}C} > 380 \text{ mm Hg}$)</p> <p>Chlorine Hydrogen fluoride (Hydrofluoric acid) Phosphine Arsenic Compounds (Inorganic including arsine) Cyanide Compounds Radionuclides (including radon) (Total of 6 HAPs)</p>	<p>VINC_s ($0.1 \text{ mm Hg} < VP_{25^{\circ}C} < 380 \text{ mm Hg}$)</p> <p>Hydrazine Hydrochloric acid (Hydrogen chloride) Titanium tetrachloride (Total of 3 HAPs)</p>
<p>SVINC_s ($10^{-7} \text{ mm Hg} < VP_{25^{\circ}C} < 0.1 \text{ mm Hg}$)</p> <p>Phosphorus Mercury Compounds (Total of 2 HAPs)</p>	<p>NVINC_s ($VP_{25^{\circ}C} < 10^{-7} \text{ mm Hg}$)</p> <p>Asbestos Calcium cyanamide Antimony Compounds Beryllium Compounds Cadmium Compounds Chromium Compounds Cobalt Compounds Lead Compounds Manganese Compounds Fine mineral fibers Nickel Compounds Selenium Compounds (Total of 12 HAPs)</p>

Note: A number of HAPs can be categorized in more than one compound class, e.g. mercury compounds in vapor and particulate forms (SVINC and NVINC). In such cases, the HAPs have been assigned in this table based on the vapor pressure of the most volatile species present in ambient air. Thus, for example, mercury compounds have been assigned to the SVINC category using this rationale, although they are present in ambient air in both SVINC and NVINC forms.