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OTS INFORMATION ARCHITECTURE

NOTEBOOK

Prepared by:

Henry Lau (Project Manager)

Loren Hall

Geri Nowak

Doug Sellers

The matrices included in this document were prepared by:

Tracor Jitco, Inc.

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Project Officer: Doug Sellers

Technical Monitor: Geri Nowak

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1. The first part of the report is devoted to a general survey of the situation in the country. It is based on the data collected during the last year.

2. The second part of the report is devoted to a detailed analysis of the economic situation. It is based on the data collected during the last year.

3. The third part of the report is devoted to a detailed analysis of the social situation. It is based on the data collected during the last year.

4. The fourth part of the report is devoted to a detailed analysis of the political situation. It is based on the data collected during the last year.

5. The fifth part of the report is devoted to a detailed analysis of the cultural situation. It is based on the data collected during the last year.

6. The sixth part of the report is devoted to a detailed analysis of the scientific situation. It is based on the data collected during the last year.

7. The seventh part of the report is devoted to a detailed analysis of the sports situation. It is based on the data collected during the last year.

8. The eighth part of the report is devoted to a detailed analysis of the health situation. It is based on the data collected during the last year.

The OTS Information Architecture Notebook was prepared to identify sources of information available to the OTS staff. Users of this document may not be aware of where to obtain these services. MSD maintains two facilities to guide people in the acquisition of information.

- o Non-CBI Information - For assistance in obtaining literature searches, ready reference, library services, article acquisition, or translations, people should contact:

Chemical Information Center (CIC)  
Elain Suriano  
Room 447 East Tower  
Phone 382-3524

- o CBI Information - Confidential Business Information including TDIS, CICIS, and PMN material, is included in the responsibilities of the-

CBI Information Center  
Delores Evans  
Room 227 East Tower  
Phone: 382-7694

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## I. INTRODUCTION

The purpose of the OTS TSCA Information Architecture Notebook is to document and analyze OTS scientific and technical information requirements for the successful implementation of the Toxic Substances Control Act (TSCA). Under TSCA, OTS is required to assess the potential risks and possible benefits of commercial chemicals not covered under other Federal authorizations. The investigation of chemical risks and benefits and the development of regulatory or non-regulatory decisions constantly require the effective gathering and utilization of pertinent information for in-depth review and analysis of the effects of the chemical substances on human health and the environment.

While TSCA provides a mechanism for OTS to collect certain specific data from industry by rulemaking or to develop data by conducting testing of chemicals, OTS needs supporting scientific and technical information from a wide variety of existing data sources. The supporting data are often available in the open literature, in Government owned or commercially available computerized data banks and data bases, as well as in manual or unpublished sources.

This Notebook represents an attempt to assess OTS information requirements and to identify the major information sources in which pertinent data are accessible. The ultimate objective is to identify major information gaps, based on identified requirements and system coverage, and to recommend a cost-effective mechanism to obtain or to develop such information. Since both information requirements and system coverage are likely to change with the passage of time, the Notebook must be used as a working document and will be updated periodically.

The Notebook is organized into ten sections, as outlined under the Table of Contents. Section II of the Notebook presents a summary of the major functions of OTS (e.g. Health Effects Analysis, Economic Analysis, etc.) and the major information resources needed in support of these functions. Section III describes the three major processes of OTS (i.e. New Chemicals Review, Existing Chemicals Review, Chemical Testing). In Section IV of the Notebook, the major data categories and sub-categories and their definitions are presented. Section V presents a Matrix matching a set of resource attributes, i.e., search and system attributes, against the major computerized information resources containing pertinent information in support of OTS functions and processes. This section also includes a listing of definitions for the resources attributes to facilitate understanding of the matrix.



In Section VI of the Notebook, there is a presentation of the OTS analytical capabilities for estimating physical chemical properties and predicting environmental fate and exposure of chemical substances. Two matrices are also included, depicting how the different classes of models and tools are used to support the various OTS functions and processes. Section VII presents a series of matrices, matching data categories and data sub-categories against the major information resources identified in this Notebook. In Section VIII, matrices matching data sub-categories against OTS functions are presented. Section IX is a discussion of the relationship between OTS processes and data categories and sub-categories. Finally, Section X summarizes and analyzes the major findings, and discusses major information gaps.

The matrices developed for this Notebook are intended to highlight information requirements for the OTS functions/processes and indicate whether such requirements are being satisfied by currently available information resources. By including resource attributes in the matrices, an attempt was made to depict the quality as well as the accessibility of the available data. As a result, this should provide the readers with a better picture of information availabilities and major information gaps, and of the qualitative and quantitative aspects of the information available.

It is hoped that the TSCA Information Architecture Notebook will be a useful document for OTS. Specifically, the Notebook should be used as follows:

1. It should provide top OTS managers with a better understanding about how and what information is being used to support the OTS functions and processes. It should also provide sufficient knowledge in determining priorities and resource commitments for developing or obtaining data where information gaps are shown, and for analyzing and determining priorities for data base development.
2. For the OTS scientific & technical staff, the Notebook should be a handy reference describing the availabilities and accessibilities of different types of data from a variety of sources. Furthermore, the resource attributes will provide a better understanding of the usefulness and limitations of the information resources.
3. For information managers and information specialists, this should be used as a working document that highlights OTS information requirements and resources. By identifying and understanding the requirements for information and the availabilities of resources, better

information support services can be provided. Furthermore, efforts can be taken to develop information for those areas where gaps are identified and to improve the efficiency and cost-effectiveness of information retrieval. This Notebook also provides a continuing mechanism for communication between the service units (i.e. MSD) and the user community. Such a dialogue will lead to a better understanding of user requirements.

4. For system development managers and specialists, the information strategy should be used to determine needs and priorities for developing new OTS data bases. Information needs and data base needs could be significantly different. In determining needs for data base development, other factors besides information needs must be considered. These factors include frequency of use, cost for system development, and need for computerized retrieval and data manipulations, etc.

This Notebook is a working document. As information requirements and resource capabilities change, the Notebook will be updated periodically.

## II. OTS FUNCTIONS & INFORMATION RESOURCES

This section describes the major OTS functions under TSCA and their relationship with the major information resources. For purposes of this Notebook, seven OTS functions are identified below:

- o Chemical Analysis
- o Control Technology Analysis
- o Economic Analysis
- o Health Effects Analysis
- o Environmental Effects Analysis
- o Exposure Analysis
- o Regulatory Options Analysis

No attempts are made to either associate these functions with OTS organizational units or to establish any sequential relationship of the functions.

Risk assessment, a function routinely performed by OTS, is not included here. From an organization standpoint, risk assessment integrates the hazard evaluations of the other functions except regulatory options analysis. Therefore, risk assessment utilizes the information gathered in support of the other functions and additional information requirements are minimal.

To a large extent, regulatory options analysis is similar to risk assessment in terms of additional information requirements. Like risk assessment, regulatory options analysis integrates the evaluative results of the other functions. However, it also needs information regarding other federal regulations, statutes and standards. This additional information does not come directly from the evaluative results of the other functions. For this reason, regulatory options analysis is included here as a function.

For each of the aforementioned functions, there is a descriptive statement about that function. This statement describes the various steps that are involved in a function. Following each functional statement, there is a listing of the major steps, i.e., sub-functions for that function, and the major information resources that are frequently used to support the sub-functions. No attempt is made here to associate an information resource with a sub-function, since such a relationship may sometimes be misleading.



## Chemical Analysis Functional Statement

Chemical analysis mainly provides broad technical support in the area of chemistry for both regulatory and non-regulatory decision making under the Toxic Substances Control Act. This analysis includes such areas as: validation of chemical identity; evaluation of chemical reactions during manufacturing, processing, and use; identification of impurities, by-products, solvents, and catalysts; estimation of physical and chemical properties relevant to manufacturing, processing and use; identification of chemical constraints on manufacturing, processing, and use conditions; identification of functional groups or structural features responsible for chemical reactivity; development of chemical data for TDIS; and, other aspects of chemical data that may be of interest to further reviewers. This analysis also identifies substructures of molecules that are important for identification of use analogues; classifies substances by use and reactivity; and, identifies structural and use analogues based on knowledge of chemical technology and the physical/chemical properties of molecules. Chemical analysis is used to support all of the other functions listed below; products of chemical analysis include initial and detailed assessments of premanufacture notices (PMN's), analyses to support section 5(h)(4) exemptions and follow-up activities, section 6 regulatory analyses, and analysis to support any other regulatory or non-regulatory decision making.

## Chemical Analysis

Major Sub-functions

- o Verify generic name
- o Ensure description matches:  
chemical name,  
CAS Registry Number,  
molecular formula,  
molecular weight,  
chemical structure,  
synonyms.
- o Define physical-chemical properties of chemicals
- o Identify structural analogs
- o Identify by-products/impurities (i.e., catalysts, solvents) used in the manufacture of the chemical
- o Develop a literature search strategy
- o Prepare detailed in-depth use analysis based on economic and market analysis
- o From known properties of chemicals, identify potential new uses of the chemical

Information Resources1. Computerized Data Bases (Non-bibliographic)

- o CAS ONLINE
- o Chemical Abstracts Service (Contract)
- o CHEMLINE (MEDLARS)
- o CHEMDEX (SDC)
- o CHEMLAB (CIS)
- o CHEMNAME (DIALOG)
- o CHEMSEARCH (DIALOG)
- o CHEMSIS (DIALOG)
- o CHEMZERO (DIALOG)
- o CTCP (CIS)
- o DARC (Questel)
- o SANSS (CIS)
- o TSCA Inventory (CISIS)
- o TDIS
- o UVCB

2. Computerized Models

- o CHEMEST (VAX)

3. Manual Data Bases

- o ICB Card File on Carcinogens

4. Other Sources

- o Chemical Dictionaries/Handbooks

### Control Technology Analysis Functional Statement

Control technology analysis provides support for studies and analyses of exposure to new chemical and technological alternatives for reducing human and environmental exposure including personal protective devices and other industrial hygiene measures, process changes, and effluent controls. It provides a review and evaluation of production technology and alternative technologies, and estimates the effects on release and worker exposure resulting from use of alternative control measures. This function performs control effectiveness analysis for specific projects according to the goals, scope, technical approach, and resource requirements planned for the project.

## Control Technology Analysis

Major Sub-functions

- o Determine methods of manufacture, processing or use, and related worker activities,
- o Determine potential for and quantities of environmental release during manufacture,
- o Determine scenarios for worker activities and possible levels of exposure,
- o Describe workplace, engineering exposure controls, personal protective equipment commonly employed in industrial processing,
- o Describe environmental release controls (i.e., waste control process) commonly used.

Information Resources1. Computerized Data Bases (Bibliographic)

- o BHRA FLUID OCCUPATIONAL HAZARD (DIALOG)
- o CA SEARCH (DIALOG)
- o CHEMICAL INDUSTRY NOTES (DIALOG)
- o COMPENDEX (DIALOG)
- o DOE ENERGY (DIALOG)
- o ELECTRIC POWER (DIALOG)
- o EIS INDUSTRIAL PLANTS (DIALOG)
- o ENVIROLINE (DIALOG)
- o INSPEC (DIALOG)
- o ISMEC (DIALOG)
- o MEDLINE (MEDLARS)
- o METADEX (DIALOG)
- o NIOSHTIC (DIALOG)
- o NTIS (DIALOG)
- o PAPERCHEM (DIALOG)
- o POLLUTION ABSTRACTS (DIALOG)
- o PTS F&S INDEXES (DIALOG)
- o PTS PROMPT (DIALOG)
- o RAPRA (DIALOG)
- o SCISEARCH (DIALOG)
- o SURFACE COATINGS (DIALOG)
- o TEXTILE TECHNOLOGY DIGEST (DIALOG)
- o TOXICOLOGY DATA BANK (MEDLARS)
- o TOXLINE (MEDLARS)
- o WORLD TEXTILES (DIALOG)

2. Computerized Data Bases (Non-bibliographic)

- o Industry File
- o Inventory
- o TDIS

3. Other Sources

- o Chemical Manufacturers National Inspection Summary Report (OSHA)
- o Document Information Directory System (NIOSH) SRI
- o Process Economic Profiles (SRI)
- o Chemical Economic Handbook (SRI)
- o Handbooks
- o Kirk Othmer Encyclopedia
- o National Occupational Hazard Survey (NIOSH)

Economic Analysis  
Functional Statement

The main objective of economic analysis is the determination of potential economic costs and socioeconomic benefits of any regulatory and non-regulatory control actions on chemical substances for purposes of the Toxic Substances Control Act. This function involves analyses of the chemical market, industry trends, price, price trends, chemical uses, use trends, potential uses for new chemicals, chemical substitutes and their uses, etc. It provides economic policy studies as required by TSCA; provides economic and market studies of chemical compounds; estimates the economic and socioeconomic impacts of actions taken under section 4, 5, 6 and 8 of TSCA to gather information on, require testing of, and to control the manufacture, import, processing, use and distribution of chemical substances; prepares Regulatory Impact Analysis, Regulatory Flexibility Analysis and other economic analyses as required by statute or executive order; develops scenarios of incentive programs as alternatives to regulatory options and performs cost-benefit and cost-effectiveness analyses of alternative regulatory options.

## Economic Analysis

Major Sub-functions

- o Determine present and potential uses for chemical,
- o Describe historic market patterns,
- o Identify manufacturers, location of plants, and production volumes, prepare manufacturers profile,
- o Identify import/export patterns, U.S. and international market conditions and trends,
- o Identify market growth pattern,
- o Evaluate economic feasibility of potential substitute chemicals,
- o Evaluate economic impact of substitute chemicals,
- o Determine potential substitutes for end product(s) the chemical is used to manufacture,
- o Analyze effect of TSCA rulings on market, or report burden of cost and economic impact of testing.

Information Resources1. Computerized Data Bases: (Non-bibliographic)

- o CHEMICAL INDUSTRY NOTES (DIALOG)
- o CICIS
- o CLAIMS/CLASS (DIALOG)
- o CLAIMS/PAT (DIALOG)
- o Dun & Bradstreet
- o DISCLOSURE (DIALOG)
- o EIS INDUSTRIAL PLANTS (DIALOG)
- o FIND/SVP REPORTS & STUDIES INDEX (DIALOG)
- o FOREIGN TRADERS INDEX (DIALOG)
- o HARFAX (DIALOG)
- o Inventory (CAS)
- o MILLION DOLLAR DIRECTORY (DIALOG)
- o PAPERCHEM (DIALOG)
- o PREDICASTS (DIALOG)
- o PTS INDEXES (DIALOG)
- o PTS PROMPT (DIALOG)
- o Section 8(a) Level A Data Base
- o TRADE & INDUSTRY INDEX (DIALOG)
- o Toxic Economic Data Base
- o X-Market



2. Manual Data Bases

- o PMN Case History Files
- o RIB Use Code Data Base

3. Other Sources

- o 1977 Census of Manufacturers
- o 1980 Census of Manufacturers
- o International Trade Commission Report
- o Interagency Testing Committee Reports
- o Kirk-Othmer Encyclopedia
- o Personal Contacts with Industry
- o Chemical Economics Handbook (SRI)
- o Directory of Chemical Producers (SRI)
- o Specialty Chemicals (SRI)
- o Process Economics Program (SRI)
- o Reference & Textbooks
- o Trade Journals

### Health Effects Analysis Functional Statement

Health effects analysis focuses on assessing the nature and biological significance of the hazards that chemicals may pose to human health. This function reviews, validates, and evaluates test data submitted by industry, along with other relevant research results, and determines chemical toxicity or other harmful effects in accordance with agency policy. This function identifies, evaluates, and applies new methods and techniques for epidemiological and laboratory testing in support of OTS programs. Specific areas of concern include acute, subchronic and chronic toxicity, onocogenicity, mutagenicity, teratogenicity, neurotoxicity, reproductive effects, and other health end points.

## Health Effects Analysis

Major Sub-functions

- o Relate chemical structure to potential health effects (i.e., acute and chronic toxicity, oncogenicity, teratogenicity, etc.)
- o Substantiate health effects and list uncertainties of prediction
- o Determine adequacy of testing procedures for chemicals for risk assessment; including evaluation and application of new test methods
- o Screen for potential health effects

Information Resources1. Computerized Data Bases: (Bibliographic)

- o BIOSIA (DIALOG)
- o CA ABSTRACTS (DIALOG)
- o CANCERLINE (MEDLARS)
- o EMIC (ORNL)
- o ETIC (ORNL)
- o EXCERPTA MEDICA (DIALOG)
- o LIFE SCIENCES (DIALOG)
- o MEDLINE (MEDLARS)
- o NIOSHTIC
- o NTIS (DIALOG)
- o RTECS (MEDLARS)
- o SCI SEARCH (DIALOG)
- o TOXICOLOGY DATA BANK (MEDLARS)
- o TOXLINE (MEDLARS)

2. Computerized Data Bases (Non-bibliographic):

- o DARC (Questel)
- o DERMAL ABSORPTION (SPHERE)
- o GENE-TOX (SPHERE)
- o SANSS (CIS)
- o TERA-TOX (SPHERE)
- o TDIS

3. Manual Data Bases

- o Chemicals Identified in Human Biological Media
- o ITC Profiles
- o ITC Reviews
- o OPP Registration Data
- o Phthalate Clearing House
- o Section 8(d) Studies
- o TRDB Documents

4. Computerized Models

- o ARTHUR (VAX)
- o CHEMLAB (VAX)
- o Dose Response and Low-Dose Extrapolation Models
- o SAS (VAX)

5. Tracking Systems

- o CECATS
  - Section 8(e) Notices
  - Pre-Chip Hazard Information Profile
  - Chip Documents
  - FYI Submissions

6. Other Sources

- o Contract Reports
- o Industry Studies

Environmental Effects Analysis  
Functional Statement

Environmental effects analysis focuses on assessing the hazards which specific chemicals may pose to the environment. This function reviews and evaluates test data submitted by industry, along with other relevant research results. It estimates the acute potential and chronic effects that chemicals may have on aquatic and terrestrial organisms and ecological systems. This function includes identification of natural populations at risk and the effects on individual ecological components, and abiotic environmental systems such as the atmosphere. It identifies and evaluates new laboratory and field methods that can be used to more reliably and accurately predict potential environmental effects.

## Environmental Effects Analysis

### Major Sub-functions

- o Determine acute and chronic environmental toxicity and bioconcentration potential of chemicals based on test and research results, or predict on basis of structure and knowledge of similar chemicals.
- o Define affected ecological components, and natural and agricultural resources, and populations at risk.
- o Develop methods for integrated, interdisciplinary environmental effect assessment procedures.
- o Evaluate methods for field and laboratory studies of interest to TSCA.
- o Screen for potential ecological effects.

### Information Resources

#### 1. Computerized Data Bases (Bibliographic)

- o AGRICOLA (DIALOG)
- o APTIC (DIALOG)
- o AQUATIC SCIENCE & FISHERIES (DIALOG)
- o AQUALINE (DIALOG)
- o ENVIROLINE (DIALOG)
- o ENVIRONMENTAL BIBLIOGRAPHY (DIALOG)
- o EXCEPTA MEDICA (DIALOG)
- o LIFE SCIENCES (DIALOG)
- o NTIS (DIALOG)
- o OCEANIC ABSTRACTS (DIALOG)
- o POLLUTION ABSTRACTS (DIALOG)
- o TOXLINE (MEDLARS)

#### 2. Computerized Data Bases (Non-bibliographic)

- o ACQUIRE (SPHERE)
- o AQUATOX (SPHERE)
- o CICIS
- o DENVER WILDLIFE RESEARCH CENTER (SPHERE)
- o EPA Database & Environmental Model Index (Information Clearinghouse)
- o FISH REPRODUCTIVE (CHIB)
- o IEO/GAGE (GEMS)
- o ISHOW (SPHERE)
- o Needs Survey Data Base (VAX)
- o 1977 Census of Manufacturers (GEMS)
- o OAQPS Human Activity Patterns (GEMS)
- o PEST
- o PHYTODOX (HERD)
- o RTECS (CIS)

- o SANSS (CIS)
- o STAR (GEMS)
- o STORET
- o SYMN
- o TERATOX
- o TDIS (Exposure File)
- o UVCB
- o Wholesale Trade Data (GEMS)

3. Computerized Models

- o CLOGP (VAX)

4. Manual Data Bases

- o ITC Profiles
- o ITC Reviews

Exposure Analysis  
Functional Statement

Exposure analysis uses laboratory and field monitoring data, as well as data from predictive models to generate, as quantitatively as possible, assessments of the levels and durations of environmental, occupational and consumer exposures to chemical substances. The data used include factors such as chemical transport and transformation, persistence, as well as data on physical or chemical factors which may affect exposure levels and duration. This function provides OTS with estimates of chemical quantities released to the environment subsequent to treatment and of the exposures of the population and environmental biota. This function identifies the ranges of exposure and the exposure to specific populations or subpopulations. This function also provides OTS with new procedures to identify potentially exposed populations or subpopulations, and for conducting exposure assessments; identifies or develops new techniques for chemical fate and exposure modeling and physiochemical property estimation; and examines production release and workplace exposure based on outputs of the control technology analysis.



## Exposure Analysis

Major Sub-functions

- o Substance identification and analysis
- o Estimate physical/chemical properties
- o Screen chemicals for potential human exposure or nature and extent of exposure
- o Determine materials balances
- o Characterize releases after treatment
- o Conduct fate analyses/fate modeling
- o Identify and characterize human and nonhuman receptor populations
- o Estimate exposures
- o Conduct integrated exposure assessments
- o Perform control options exposure analysis
- o Develop models, test and validate them
- o Acquire data for models
- o Implement models, data and data analysis programs
- o Develop exposure methodologies
- o Develop and compile data for exposure assessments
- o Develop physical/chemical property and environmental fate test methods
- o Design monitoring studies
- o Collect and analyze chemical monitoring data

Information Sources1. Computerized Data Bases (Non-bibliographic)

- o CHEMFATE
- o CICIS
- o cLogP (VAX)
- o Federal Reporting Data System (FRDS)
- o Gauging Station File ("Hydrologically Linked Data System" -- HLDS)
- o Geoecology (GEMS)
- o Hazardous & Trace Substances Emissions Systems (AEROS)
- o Hazardous Waste Data Management System
- o IEO/GAGE (GEMS)
- o Industrial Facilities Discharge File (4 WDMS)
- o National Emissions Data System (AEROS)
- o National Occupational Hazard Survey (OTS)
- o Needs Survey Data Base (VAX)
- o 1977 Census of Manufacturers (GEMS)
- o OAQPS Human Activity Patterns (GEMS)
- o OHM-TADS (CIS)
- o OSHA (DIPS)
- o Reach File (HLDS)
- o STAR (GEMS)
- o Source Test Data System (AEROS)
- o Storage & Retrieval of Aerometric Data (AEROS)
- o STORET
- o Water Supply Data Base (HLDS)

- o Water Quality Monitoring Station File (HLDS)
- o Wholesale Trade Data (GEMS)

2. Computerized Models

- o ATM (GEMS)
- o CHEMEST (GEMS)
- o ENPART (GEMS)
- o EXAMS (GEMS)
- o CLOGP (VAX)
- o PTMAX (GEMS)
- o SESOIL (GEMS)

3. Other Sources

- o NPDES Permits

Regulatory Options Available  
Functional Statement

Regulatory options analysis evaluates alternative remedial control measures under TSCA, other federal statutes, and non-regulatory approaches to achieving control of chemical risk. This function enables OTS to keep abreast of regulatory and non-regulatory chemical control programs in all sectors of industry. Specifically, this function is responsible for the identification and analysis of regulatory and non-regulatory remedial options for reducing unreasonable risk of injury to health and the environment from new and existing chemicals under Sections 4,5,6,7,8 and 21 of TSCA. This function prepares development plans for general or specific regulatory and non-regulatory projects to prohibit, limit, or control the manner or method of manufacture, processing, distribution, use, or disposal of new and existing chemical substances, and for needed testing of new or existing chemicals. It provides policy options analyses in support of unreasonable risk determinations in coordination with the chemical analysis, control technology, chemical economics, and risk assessment functions, coordinates with the chemical economics function on the economic analysis and technological impacts of control programs. It also provides regulatory support for individual PMN's, TME's and exemption notices, and drafts 5(e) orders for chemicals which may cause unreasonable adverse effects. Finally, this function ensures that regulatory and non-regulatory analyses are accomplished within current and accepted practice and are in consonance with OTS and EPA policies including Executive Order 12291, and the Regulatory Flexibility Act.

## Regulatory Options Analysis

### Major Sub-functions

- o Evaluate alternative remedial control measures under TSCA and other federal statutes.
- o Prepare development for needed testing of new and existing chemicals.
- o Develop plans for regulatory and non-regulatory projects to prohibit, limit or control the manufacture, method of manufacture, processing, distribution, or use of new and existing chemicals.
- o Analyze policy options to support unreasonable risk determinations in coordination with program findings.
- o Provides policy option analysis support for PMN's, TME's exemption notices, and 5(c) orders.
- o Ensure accomplishment of above functions within accepted practice in consonance with OTS and EPA policies and the Regulatory Flexibility Act.

### Information Resources

#### 1. Computerized Data Bases (Bibliographic)

- o CHEMLAW (DIALOG)
- o CRGS (DIALOG)
- o FEDREG (ORBIT)
- o FRSS (CIS)

#### 2. Other Sources

- o Federal Register
- o Legislative History
- o U.S. Codes
- o PMN Case History Files
- o PMS
- o TDIS

### III. OTS PROCESSES & INFORMATION RESOURCES

The Office of Toxic Substances is organized around three major programs or processes. These are:

- o New Chemicals Review
- o Existing Chemicals Review
- o Chemical Testing

In order to implement a process, which is mandated by a specific section or sub-section of TSCA, various functions and sub-functions (as discussed in Section II of this Notebook) must be performed in support of that process.

This section discusses the three major processes in detail. In each of these processes, a descriptive statement and a flow diagram about that process are presented. For each process, the major milestones are identified in the corresponding flow diagram. In Section IX of this Notebook, the major interim products from each milestone and the final product for a process are identified. For each of these products, the pertinent information requirements are discussed.

Following the functional statements and the flow diagrams for the three OTS processes is a table listing the major information resources that are specifically designed or used in support of a process. A brief description about each of these systems and its capabilities are also included. For more detailed information about these information resources, please refer to the OTS Directory of Information Resources or the OTS Data Directory.

It must be pointed out that the information resources described in this section of the Notebook are different from the bibliographic or non-bibliographic scientific and technical data bases discussed under Section II or Section V. Since it is believed that these bibliographic and non-bibliographic data bases are used to support the various OTS functions which in turn support the processes, they are therefore not included in this section. (This will be discussed in detail in Section IX.) The information resources that are discussed in this section include indexing or tracking systems or information systems or files that are specifically designed to provide direct support to the three processes.

For purposes of this Notebook, the New Chemicals Review Process includes Premanufacture Notification Review and PMN follow-up. (Section 5(h)(4) exemption notices review is not included here, since it is not in implementation. It appears, however, that this review process may have information requirements similar to those for the PMN initial review). The Existing Chemicals Review Process covers both Chemical Hazard

Identification and Special Chemical Review. The Chemical Testing Process covers only Test Rules Development, since there is no obvious information requirement for the development of Test Guidelines.

New Chemicals Review Process

The New Chemicals Review Process has three highly interrelated components:

- o Premanufacture notification review
- o Follow-up
- o Section 5(h)(4) exemption

Among these three components, only the first two have been in implementation. Since limited PMN's will still be submitted to EPA by manufacturers who wish to have their chemicals considered for 5(h)(4) exemptions, it is believed that information requirements for processing the exemption notices will closely resemble those for the initial review stage of a regular PMN submission. Information requirements for the exemption activity will be discussed in future updates of this Notebook.

The functional statements for the Premanufacture Notification Review and the Follow-up components of the New Chemicals Review Program are presented in the following pages. Descriptions for the major information, indexing and tracking systems used, and flow diagrams follow the functional statement.

New Chemicals Review Process  
I. Premanufacture Notification Review  
Functional Statement

The Premanufacture Notification Review Program is responsible for the receipt, evaluation, and disposition of TSCA section 5 premanufacture notices, test market exemptions and 5(h)(4) exemption notifications, within the time constraints imposed by TSCA or by regulation. The program is managed by CCD while the technical efforts in the program are carried out by other OTS divisions. The Premanufacture Notification Review Program: (1) receives, interprets and validates data submitted with each PMN; (2) gathers and reviews additional data; (3) prepares risk assessments; (4) communicates with the submitting company as necessary for clarification or for additional data; (5) determines either dropping or referring chemicals for more detailed risk and benefit/cost analysis, after preliminary risk screening; (6) recommends appropriate measures, informal or regulatory, to control and reduce risks; and (7) makes recommendations after appropriate analysis and review to follow up on new chemical uses.

The Premanufacture Notification Review Program: (1) is responsible for identifying and implementing needed action to ensure compliance with TSCA intent including actions for limitations or injunctions under TSCA section 5(e) or 5(f), in coordination with the Office of the General Counsel, and arranges for hearings, as necessary; (2) identifies new chemicals that require control, and recommends control alternatives; (3) negotiates for appropriate controls; (4) identifies new chemicals which may be controlled or otherwise affected by other EPA programs, or other Federal regulatory Agencies. The Premanufacture Review Program manages the development, evaluation, and revision of reporting procedures and forms for new chemical premanufacture review, and oversees public hearings on rules, procedures, and reporting forms associated with premanufacture review. (For more detailed information about the PMN process, see Description of PMN Review Process prepared by the OTS Chemical Control Division).



New Chemicals Review Process  
II. Follow-Up Process  
Functional Statement

The Follow-Up Process manages the development of specific rules under TSCA Section 5, negotiated control actions and other actions that may be necessary to achieve the reduction of unreasonable risk for chemicals with new uses. Recommends and implements OTS policy on TSCA section 5 exemptions, early exits, and significant new use rules (SNURS). Considers requests for exemptions, e.g., site-limited rule, low volume rule, polymer rule, and specific manufacturing exemptions. Manages the development and promulgation of all follow-up actions on chemicals not on the TSCA Initial Inventory (i.e., rules under 5(a)(2); rules for significant new uses of chemicals; development of section 8(a) follow-up rules). Manages the review and revision of general program rules as appropriate to program implementation, coordinating resources with the Premanufacture Notification Review Program and other OTS and EPA offices. Performs liaison with EPA headquarters and regional enforcement activities in establishing and maintaining an effective program of monitoring compliance with TSCA section 5 rules.

More specifically, this process evaluates chemicals using the following procedures:

- o Follow-up focus meeting
- o Toxicity validation
- o Initial new use exposure analysis
- o Technical integration reports

Determines whether regulatory action under section 5(a)(2) or 8(a) is warranted. OTS Division Directors review regulatory recommendations for each candidate and decide if regulatory analysis is required. If regulatory action is appropriate, regulatory development is initiated. SNURS, 8(d) rules are drafted, sent for Agency review, and proposed as final rules.

Existing Chemical Review Program  
Functional Statement

The Existing Chemical Review process develops, oversees, and manages projects to define specific existing chemical problems warranting detailed evaluation and possible risk reduction action by OTS. This process performs the initial evaluation of data and petitions submitted to EPA under TSCA Section 4, 8(a), 8(c), 9(d), 8(e) and 21, and similar data submitted by other routes to determine whether the data indicate a significant risk to human health and environment. It determines whether the submitted data, in conjunction with other available information, pose a definite potential "problem" in terms of identifying a specific chemical, activity, exposed population, and adverse effect which warrant referral to the appropriate program for further TSCA action. Where current information is strongly indicative of a potential problem but inadequate to fully define the problem, the Existing Chemical Review process identifies appropriate mechanisms to obtain additional information needed to reach a disposition such as encouraging voluntary data submission, using TSCA Section 8 authorities, using EPA chemical testing resources, or referring chemicals to the Interagency Testing Committee through the EPA member. It oversees the evaluation of regulatory and non-regulatory control alternatives and makes recommendations for the most appropriate mechanisms to reduce risk. Existing Chemical Review plans and manages programs to encourage use of specific exposure reduction practices by the chemical industry through informational programs and development of Risk Management Advisories. Where rulemaking under Section 5 (Significant New Use Rule) or Section 6 is necessary, this process refers to other OTS processes as appropriate.

Chemical Testing Process  
Functional Statement

The Chemical Testing Process is responsible for the development of criteria and procedures for evaluating whether chemical substances or categories of chemical substances should be subject to test rules under section 4 of TSCA. While many technical efforts in support of the program are carried out by other OTS divisions, the Program reviews and makes appropriate recommendations on negotiated or regulatory actions on the chemical substances, mixtures, and categories recommended for testing consideration by the TSCA Interagency Testing Committee and others. The program, in coordination with the above-mentioned technical representatives, is also responsible for:

- (1) developing test guidelines and protocols for testing and developing Good Laboratory Practice requirements;
- (2) assessing the availability of adequate testing facilities and personnel;
- (3) preparing test rules or decisions not to test as required under section 4 and holding public hearings on such rules after proposal; and
- (4) developing rules and procedures for granting exemptions from testing and for reimbursement under section 4(c);
- (5) reviewing and responding to requests for exemptions; and
- (6) negotiating with industry to achieve testing through negotiation.

Major Information Resources  
Specifically Designed or Frequently  
Used in Support of OTS Processes

New Chemicals Review Process

- o PMN Analog Card File
- o PMN Card File
- o PMN Case Files
- o PMN Tracking System
- o Technical Data Indexing System (TDIS)
- o TSCA Master Inventory File

Existing Chemicals Review Process

- o Chemical Regulations and Guidelines System (CRGS)
- o CHIP Existing Chemicals Tracking System (CECATS)

Chemical Testing Process

- o Global Indexing System (For Section 8(d) submissions)
- o ITC Hazard Information Profiles\*
- o ITC Hazard Information Reviews\*
- o ITC Tracking System\*
- o Section 8(a) Level A Information System
- o Test Rules Development Support Documents

\* Used by the Interagency Testing Committee

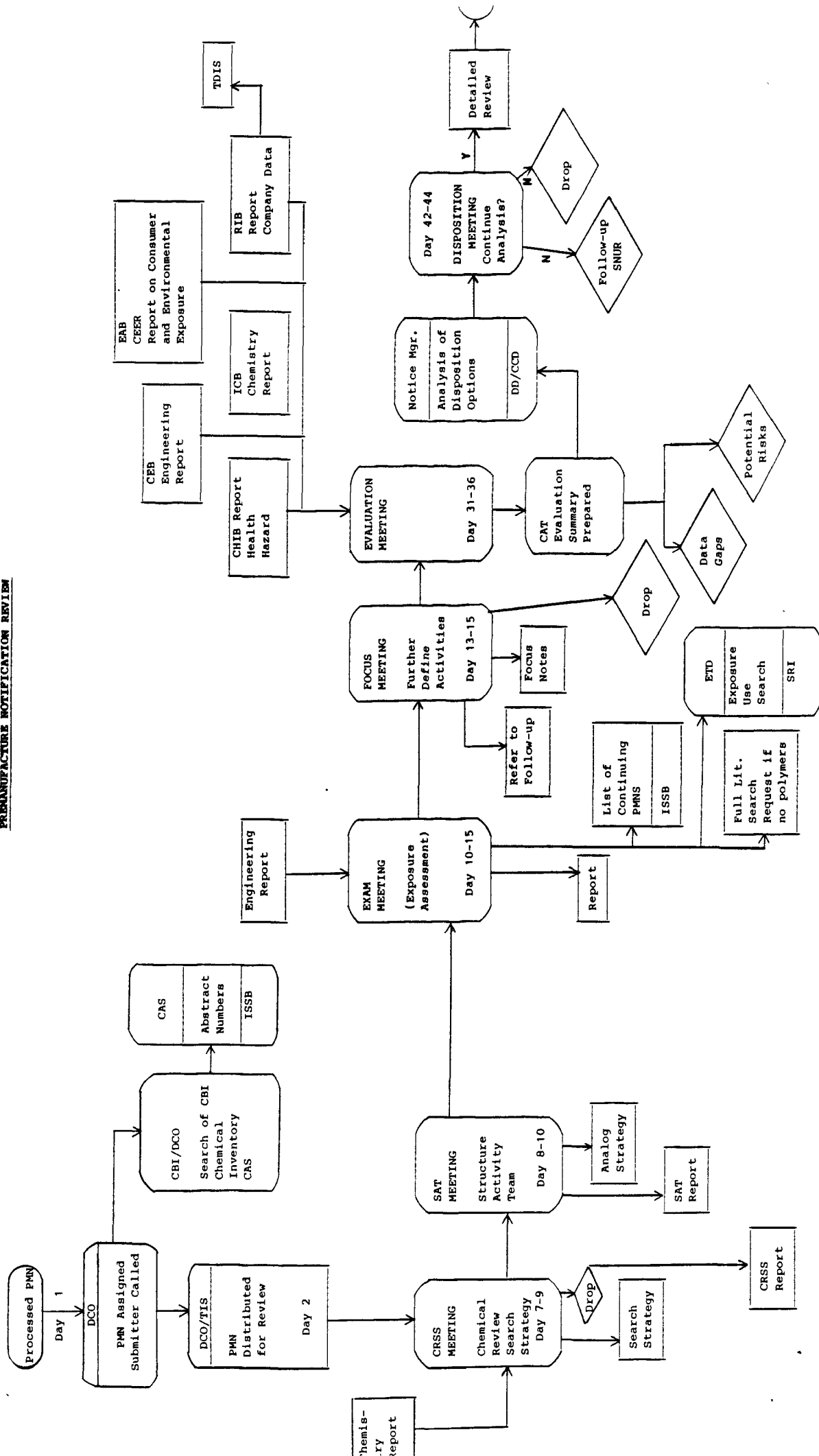
Brief Summaries About the  
Information Resources Designed or  
Used in Support of OTS Processes

1. Chemical Regulations and Guidelines System (CRGS): An automated on-line system covering Federal statutes, promulgated regulations, and Federal guidelines and standards related to the control of chemical substances. Each chemical cited in a regulatory document is indexed by chemical name, CAS Registry Number, and a context in which the substance appears in the document. Each document is described in terms of publication date, title, abstract, index terms, and chemical identifiers.
2. CHIP Existing Chemicals Tracking System (CECATS): An automated document tracking system for existing chemicals, including all CHIP and pre-CHIP compounds, and those substances submitted under section 8(e) of TSCA or on an FYI basis. CECATS is organized into seven interconnected files. The user can use the system to document decisions and types of information included and determine status of the substance within OTS.
3. Global Indexing System (In Section 8(d) Submissions): A general indexing system designed to facilitate retrieval of documents. For 8(d) submissions, the user can search by chemical identifiers or by submitting company.
4. ITC Hazard Information Profiles: A manual file of brief and concise summaries of chemical, physical, health and environmental effects data on a chemical derived from limited review of readily available information sources. The Interagency Testing Committee uses it for supporting TSCA Section 4 test rules development.
5. ITC Hazard Information Reviews: A manual file containing detailed information on exposure, chemical/physical properties, biochemistry, toxicity and environmental effects for specific chemicals and categories of chemicals selected for study by the Interagency Testing Committee.
6. ITC Tracking System: An automated system that provides quick tracking of chemicals studied by the Interagency Testing Committee and the decisions on each chemicals.
7. PMN Analog Card File: A manual file of chemicals that have been searched as analogs for PMN chemicals, including, for each substance, the CAS Registry Number, chemical nomenclature, and PMN number.
8. PMN Card File: A manual file of PMN and TME chemical names and structures, filed by both PMN number and chemical substructures. This file is used to identify previous PMN's that relate to ongoing reviews.

9. PMN Tracking System: An automated tracking system with statistical capability that is used in support of PMN review. It tracks the status of each PMN or TME submission from date of submission through notice of commencement of manufacture. It is used to prepare monthly and weekly reports to the PMN program.
10. Section 8(a) Level A Information System: An automated system containing the data collected under the Preliminary Assessment Information Rule under Section 8(a) of TSCA. This system provides such information as chemical identity, plant site location, plant site activities, manufacturer products and consumer uses of chemical substances designated for testing by the Interagency Testing Committee. The system provides a tracking capability to monitor form submissions under the reporting rule.
11. Technical Data Indexing System (TDIS): An automated system designed specifically for supporting the PMN review process by indexing PMN data and thereby providing quick referrals to historical analyses of chemicals similar to the subject chemical under review. Chemicals can be searched by name fragments and special functional codes. This system also allows for statistical analysis of trends in PMN decision-making.
12. Test Rules Development Support Documents: A manual file of review documents prepared to assist in evaluating the health and/or environmental effects of chemicals nominated for testing by the Interagency Testing Committee.
13. TSCA Master Inventory File: A collection of automated as well as manual files maintained by the Chemical Abstracts Service under contract with OTS. This file contains 60,000 chemicals and represents the most up-to-date file of substances reported for the Inventory and of substances that have been introduced into U.S. commerce after completing Section 5 PMN review. This file is used for supporting the PMN review process by conclusively determining whether a substance is on the Inventory.

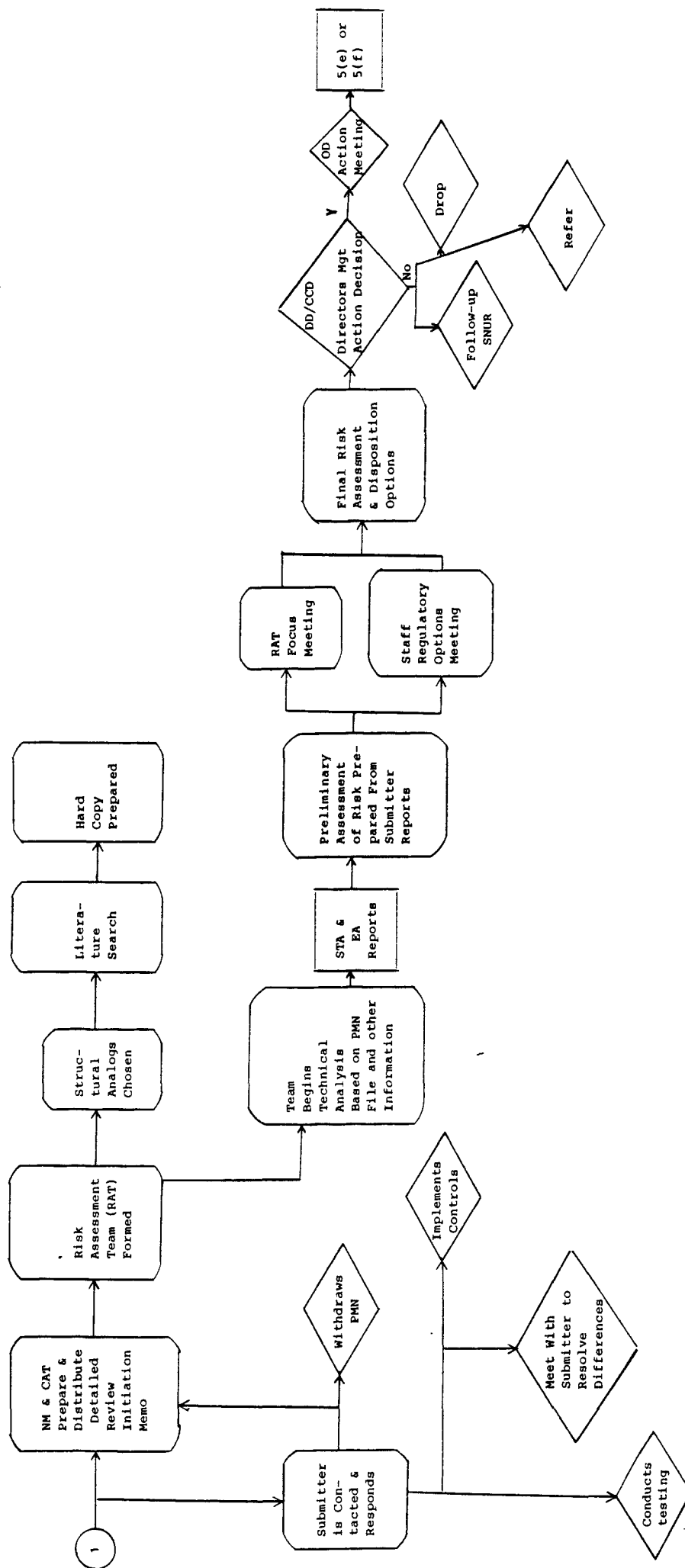
PROCESS FLOW DIAGRAMS

**NEW CHEMICAL REVIEW PROCESS  
PREMANUFACTURE NOTIFICATION REVIEW**



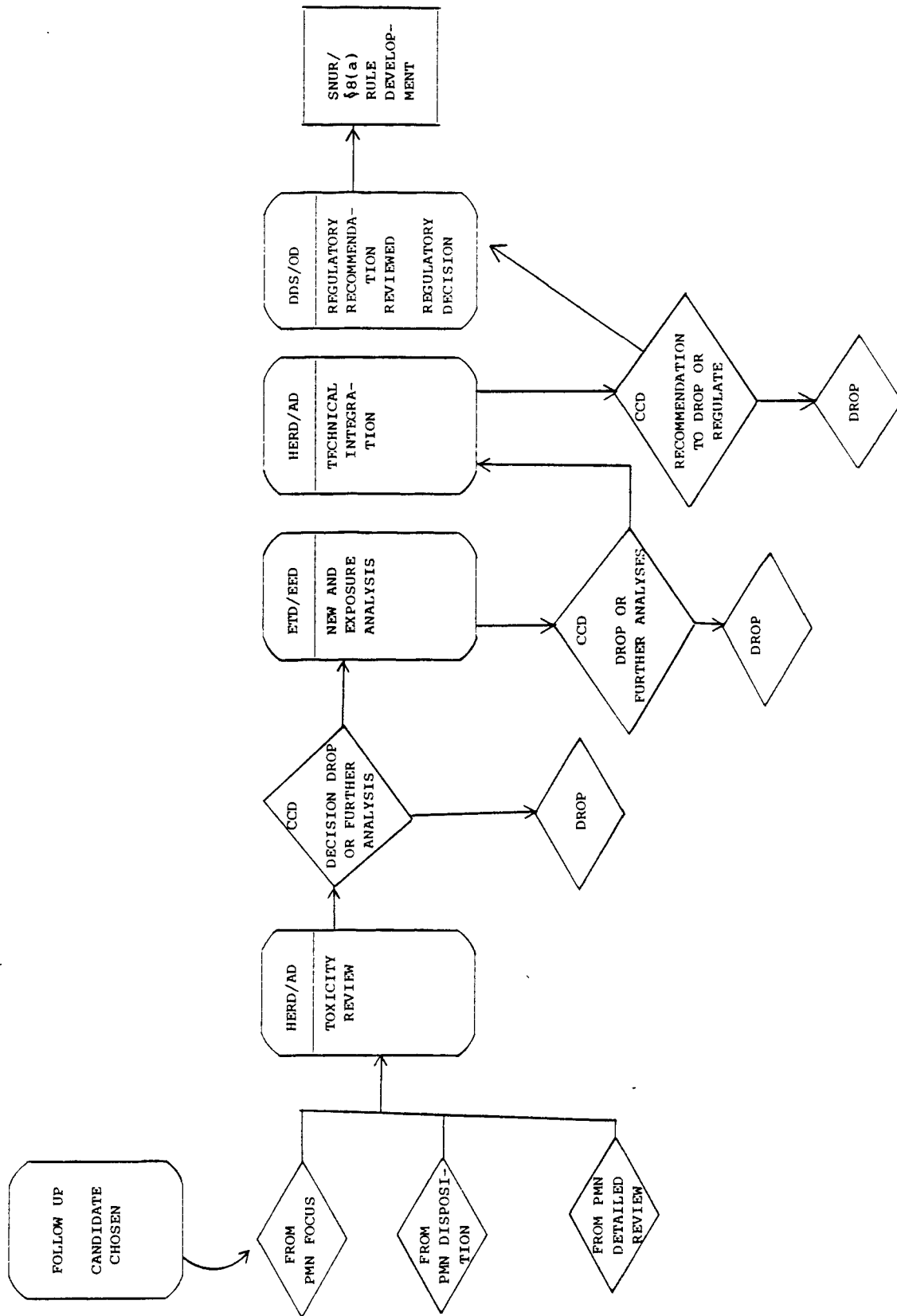


NEW CHEMICAL REVIEW PROCESS  
PREMANUFACTURE NOTIFICATION REVIEW (continued)

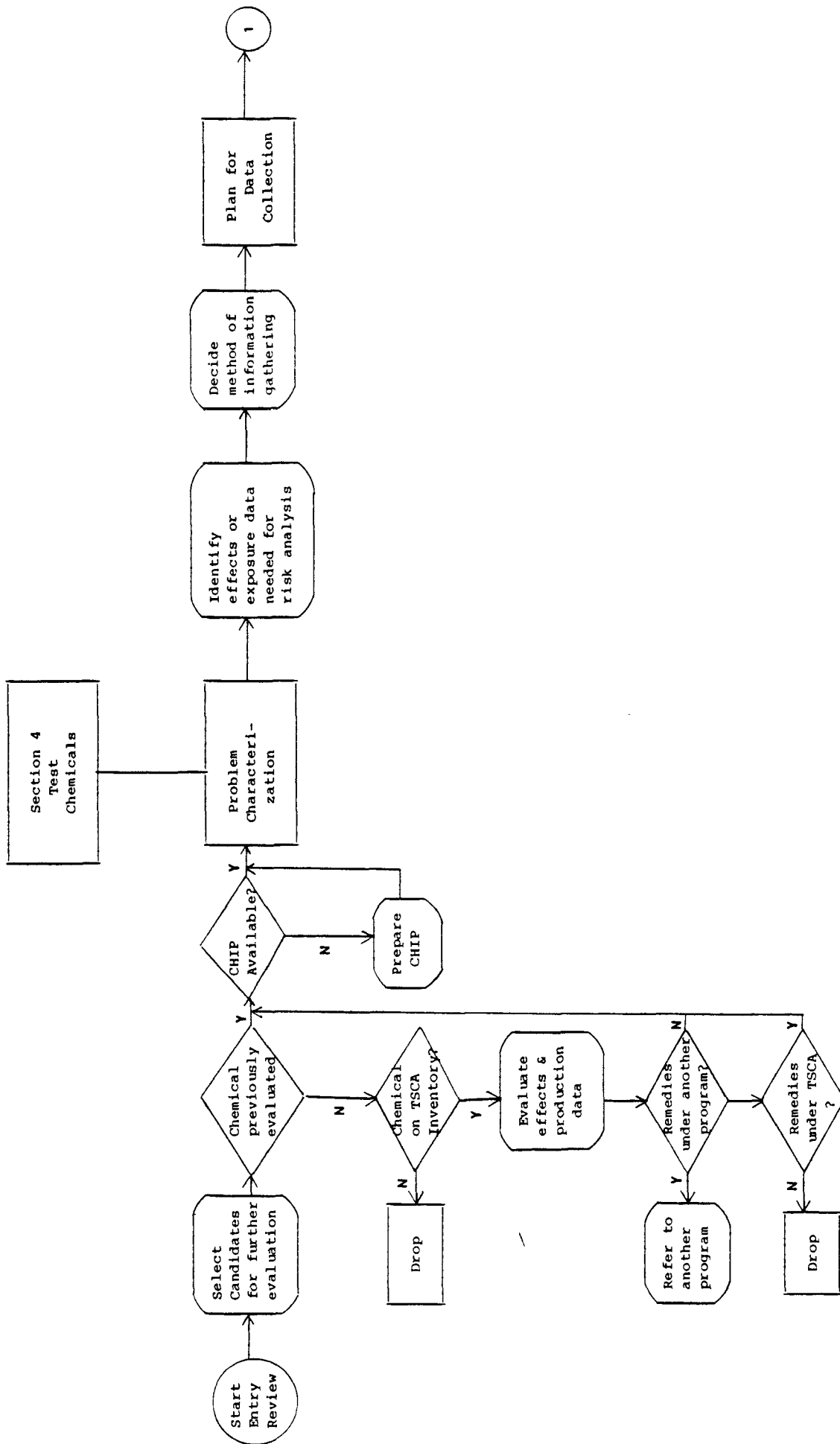


# NEW CHEMICAL REVIEW PROCESS

## Follow-Up



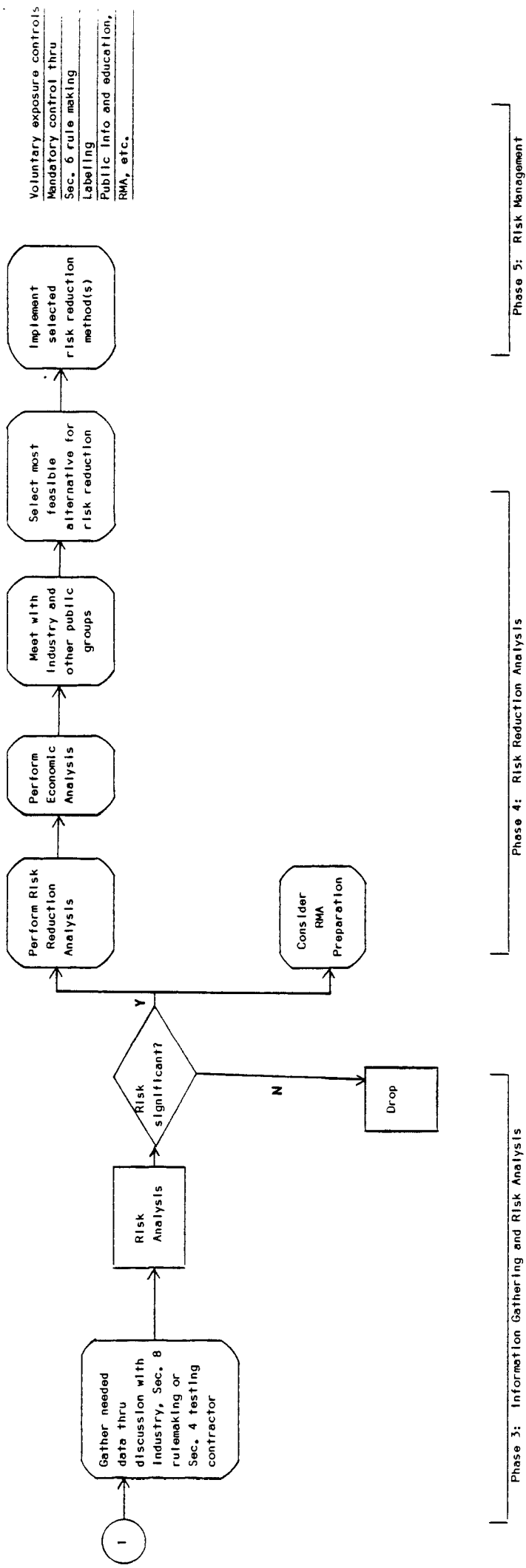
EXISTING CHEMICALS REVIEW PROCESS



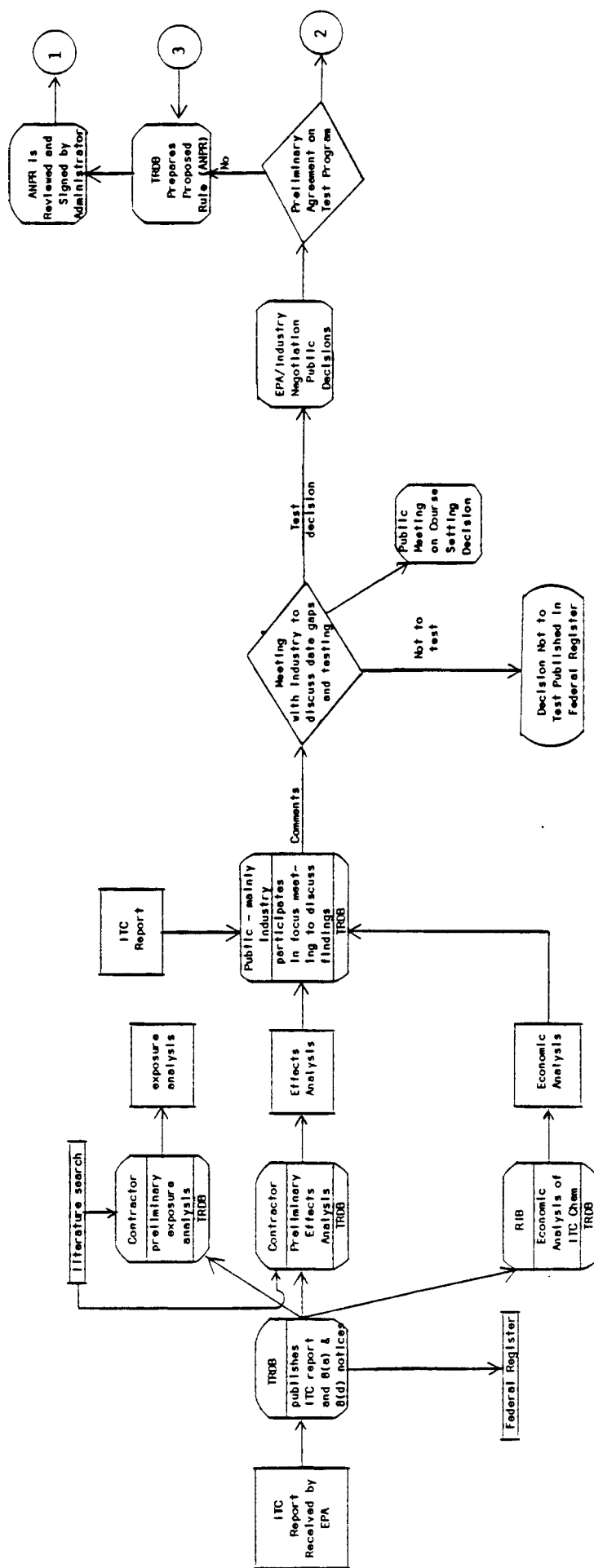
Phase 1: Entry Review

Phase 2: Problem Characterization & Information Identification

EXISTING CHEMICALS REVIEW PROCESS (cont.)

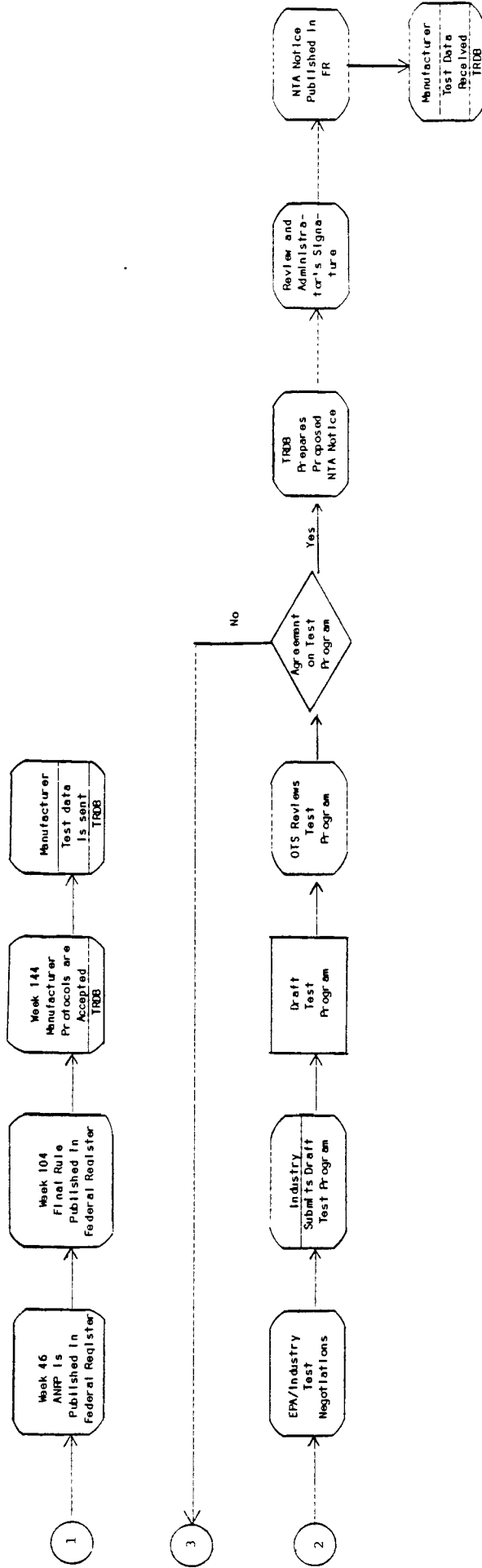


CHEMICAL TESTING PROCESS  
TEST RULES DEVELOPMENT



# CHEMICAL TESTING PROCESS

## TEST RULES DEVELOPMENT (cont.)



#### IV. DATA CATEGORIES, SUB-CATEGORIES & DEFINITIONS

This section classifies the currently known OTS user information requirements into the following nine major data categories:

- o Substance Identification
- o Physical Chemical Properties
- o Health Effects
- o Environmental Effects
- o Production/Processing
- o Use/Disposal
- o Exposure
- o Chemical Economics
- o Regulations/Controls

Within each of the nine major data categories, sub-categories are identified. A sub-category is not necessarily a data element; it may, in some cases, represent a group of data elements.

The classification of data categories and sub-categories is a complex and difficult task. There is probably no one single "correct" way of categorizing the types of technical data that OTS needs in support of the implementation of TSCA. Therefore, some of the data categories were developed partially based on specific information requirements for certain OTS functions, e.g., Health Effects (for Health Effects Analysis), Environmental Effects (for Environmental Effects Analysis), or Chemical Economics (for Economic Analysis). However, certain data categories, e.g., Physical Chemical Properties, Use, etc. may reflect the traditional grouping of data elements from an information management standpoint, and do not necessarily align themselves with specific OTS functions. Physical Chemical Properties data, for example, are used in support of such OTS functions as Chemical Analysis, Exposure Analysis, and Environmental Effects Analysis.

In determining how certain sub-categories should be listed under a specific data category, two factors were taken into consideration. First, a sub-category is placed under a data category which, from a hierarchical standpoint, is the most logical parent of that sub-category. Therefore, for example, CA Index Name (a sub-category) is listed under Substance Identification (a major category). Second, if a sub-category can be logically placed under more than one major category, that sub-category is then listed under the more appropriate category. For example, Method of Manufacture (a sub-category) is listed under Substance Identification (a major category) instead of Production/Processing (another major category), since this information is often needed in establishing the identity of a substance.

To facilitate use and understanding of the data categories and their sub-categories, several data organization techniques are used. First, a scope note is included for each major data category, describing the scope or special features of that category. (A scope note is, nevertheless, not a definition and, therefore, does not define a category). Second, a definition (in some cases, a scope note) is developed for each sub-category. Third, where a sub-category may be logically placed under more than a single major category, the more appropriate category is chosen to incorporate that sub-category and its definition. The same term is repeated under the less appropriate category without a definition, and a "See" reference is used referring the reader to the more appropriate category. For example, Method of Manufacture is listed under Substance Identification with a definition. The same term is repeated under Production with a "See Substance Identification" cross reference. Fourth, for related sub-categories, "See also" references are used. For example, a "See also Production/Processing" cross reference is included for Method of Manufacture (under Substance Identification), alerting the reader that there is a related term, i.e., Production Technology, listed under Production/Processing. This will allow the reader to consult the related term if necessary.

In using this section of the Notebook, the following must be taken into consideration:

1. For each data category, only those sub-categories that are needed by OTS are included. Therefore, a category may not include all of the possible sub-categories.
2. Some of the sub-categories represent the types of information that are not readily available in either the open literature or existing information resources.
3. The definitions for the sub-categories are not necessarily the types of definitions that can be found in a text book or a dictionary. Many of the definitions are scope notes describing what is covered under a sub-category.



A. SUBSTANCE IDENTIFICATION  
Sub-Categories

(Note: The data sub-categories included are those that are needed in establishing the identity of a chemical substance as defined by TSCA. Data elements for identifying Class II substances are also included.)

1. CA Index Name
2. CAS Registry Number
3. Synonym
4. Molecular formula
5. Chemical description/composition
6. Method of Manufacture (See Substance Identification: Synthetic Reactions and Constraints)
7. Synthetic reactions and constraints (See also Production/Processing: Production Technology)
8. Structural diagram
9. Method of identification
10. Indices of structure
11. Linked substances\*

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\*For purposes of this Notebook, this sub-category is not included in the matrices presented. From an informational standpoint, this sub-category is included under the other sub-categories of the Substance Identification category.

A. SUBSTANCE IDENTIFICATION  
Definitions

1. CA Index Name: A unique, fully systematic name assigned by the Chemical Abstracts Service (CAS) in accordance with a set of rigorous and comprehensive nomenclature rules to ensure that a single preferred name can be developed for each chemical substance. The CA Index Name is sometimes referred to as the CAS Preferred Name. A CA Index Name may be made up of several parts, each playing a specific role in describing a chemical substance. The principal portion is the "heading parent" which describes the most significant feature(s) of the substance. Additional parts of the name are appended to the heading parent to describe substituent groups, derivative information, and stereochemistry.
2. CAS Registry Number: A number consisting of up to 9 digits is assigned by the Chemical Abstracts Service to represent only one chemical substance, insofar as that substance has been elucidated and defined. The CAS Registry Number is usually separated into 3 portions by hyphens. The first portion, starting from the left, has up to 6 digits; the second portion has 2 digits and the last portion consists of a single check digit which is used to validate of the entire Registry Number.
3. Synonym: A synonymous chemical name which may be a non-systematic chemical name, a common name, a trade name, a class name, a code, or a trivial name. Care must be exercised in using the synonymous names since they often do not uniquely describe a chemical substance.
4. Molecular Formula: A systematic summation of the actual numbers and kinds of atoms present in a molecule of a chemical substance. For Class II substances and polymers, the molecular formula often identifies only the kinds of atoms present, as the number of atoms is unknown or variable.
5. Chemical Description/Composition: In certain Class II substances and polymers, where the CAS Index/Preferred Name may not be sufficiently detailed, a chemical description is required to identify the substances completely. The definition may include descriptions of the synthetic reaction or reaction pathway, the relative amounts of precursors or reactants, composition, and certain physical/chemical properties.
6. Method of Manufacture: (See Substance Identification: Synthetic Reactions and Constraints)

7. Synthetic Reactions and Constraints: A description of the reactants, the synthetic reaction(s) used, and any chemical constraints on the reaction(s) that must be taken into account when the substance of interest is produced. Typical chemical constraints include the use of high pressure or heat and the exclusion of oxygen or water vapor. Synthetic reactions often include the mechanism of the reaction if this is unusual, or the identification of side-reactions if these are significant. A complete group of synthetic reactions and side-reactions should elucidate the origin of impurities, by-products, and co-products. (See also Production/Processing: Production Technology.)
8. Structural Diagram: A 2-dimensional representation of the bonds and atoms, their connections, and stereochemical relationships in a molecule of chemical substance. For Class II substances, this diagram will be illustrative only and may be incomplete. In the case of polymers, the range and average degree of polymerization may be included.
9. Method of Identification: The analytical technique and/or protocol used in establishing the identity of a chemical substance.
10. Indices of Structure: This section includes such things as codes for functional groups, rings, degree of complexity, and categories of Class II substances.
11. Linked Substances:
  - (a) By-products: Chemical substances "produced without separate commercial intent during manufacture or processing of another chemical substance(s) or mixture(s)." FEDERAL REGISTER (42 FR 64575) Inventory Reporting Regulations (40 CFR 710.2)
  - (b) Co-products: Chemical substances "produced for a commercial purpose during the manufacture, processing use, or disposal of another chemical substance(s) or mixture(s)." FEDERAL REGISTER (44 FR 2264) Premanufacture Notification Requirements and Review Procedures (40 CFR 720.2)
  - (c) Impurities: Chemical substances "unintentionally present with another chemical substance." FEDERAL REGISTER (42 FR 64576) Inventory Reporting Regulations (40 CFR 710.2).
  - (d) Stabilizers, emulsifiers, catalysts, and other additives, that are intentionally present. Not defined here.

B. PHYSICAL/CHEMICAL PROPERTIES  
Sub-Categories

(Note: The listing of physical chemical properties covers only those that are frequently used by OTS for TSCA purposes.)

1. Melting Point
2. Boiling Point
3. Vapor Pressure
4. Partition Coefficient (Log P)
5. Solubility
6. Density
7. Relative Vapor Density
8. Henry's Law Constant
9. Adsorption Coefficient
10. Dissociation Constant ( $k_a$  or  $k_b$ )
11. Flash Point
12. Flammable Limits
13. Molecular Weight
14. Color
15. Odor
16. Physical State
17. Particle Size
18. Chemical Incompatibility
19. pH
20. Extractability
21. Hydrolysis Rate
22. Viscosity
23. Decomposition Temperature
24. Sublimation Temperature

B. PHYSICAL CHEMICAL PROPERTIES  
Definitions

1. Melting Point: The melting point is the temperature at which a substance changes from the solid to the liquid state. It indicates at what temperature solid substances liquify.
2. Boiling Point: The boiling point is the temperature at which a liquid under standard atmospheric pressure (or other specified pressure) changes from the liquid to the gaseous state. It is an indication of the volatility of a substance. The distillation range in a separation process, the temperature at which the more volatile liquid of a mixture forms a vapor, is used for mixtures in the absence of a boiling point.
3. Vapor Pressure: The vapor pressure of a substance is the pressure which a vapor, in a closed container and in equilibrium with its solid or liquid form, exerts on the enclosing walls. It is a function of the substance and, if it reaches the prevailing atmospheric pressure, the liquid boils or sublimes. It provides an indication of the relative tendency of a substance to volatilize.
4. Partition Coefficient (log P): The n-octanol/water partition coefficient is the ratio of a substance's concentration in water-saturated octanol divided by its concentration in octanol-saturated water at equilibrium. The n-octanol/water partitioning system provides an indication of a substance's ability to bioconcentrate in aquatic and other organisms. The information is frequently reported as the common logarithm of the partition coefficient, log P, rather than as the partition coefficient itself.
5. Solubility: The solubility of a substance in water (or other solvent) is the weight of the dissolved substance per volume water of solution in water (or other solvent) when the solution is at equilibrium with an excess of the substance, i.e., saturated at a specific temperature. This definition is limited to homogeneous materials.
6. Density: Density is the mass of a liquid, solid or gas per unit volume of that substance, i.e., the mass in grams contained in 1 cubic centimeter of a substance at 20°C and 1 atmosphere pressure.
7. Relative Vapor Density: Relative Vapor Density is the ratio of the weight of a gas to the weight of an equal quantity of air. Air, the standard, is given the value of 1.

8. Henry's Law Constant: The Henry's Law Constant quantitatively expresses the effect pressure has on the solubility of gas. The Law states that the mass of a slightly soluble gas that dissolves in a definite mass of liquid at a given temperature is very nearly directly proportional to the partial pressure of that gas. This assumes that the gas does not unite chemically with the solvent.
9. Adsorption Coefficient: This coefficient, e.g., the Freundlich Adsorption Coefficient, attempts to quantify the adherence of a substance to a surface. The transport, degradation and bioavailability of a substance are greatly affected by its adsorption properties.
10. Dissociation Constant ( $K_a$ ,  $K_b$ ): The dissociation constant ( $K_a$  or  $K_b$ ) represents the degree of ionization of Brønsted acids and bases in solution. Usually reported as the negative logarithm ( $pK_a$  or  $pK_b$ ) of the dissociation constant.
11. Flash Point: The Flash Point is the temperature at which a liquid or volatile solid gives off a vapor sufficient to form an ignitable mixture with the air near the surface of the liquid or within the test vessel.
12. Flammable Limits: Flammable Limits denote the concentration range, of a vapor or gas in a mixture with air, at which the flammable or explosive mixture will ignite and continue burning on its own after ignition.
13. Molecular Weight: A summation of the individual atomic weights based on the numbers and kinds of atoms present in a molecule of a chemical substance. For polymers and certain Class II substances, this may include molecular weight distributions, ranges, and averages.
14. Color: The aspect of objects (including chemical substances) that may be described in terms of hue, lightness, and saturation. Includes both qualitative (e.g., buff-colored) and quantitative (e.g., absorption maximum at 5800 Angstroms) description of color.
15. Odor: A description of the smell of a chemical substance.
16. Physical State: Whether a chemical substance is a gas, liquid, or solid under ambient or other given conditions.
17. Particle Size: The average diameter of the individual particles in a particular solid. Often both average particle size and range of particle size are used.

18. Chemical Incompatibility: The capacity of a chemical substance for facile reaction with another chemical substance to produce an undesired product. For example, isocyanates are chemically incompatible with aqueous solutions, which hydrolyze the isocyanate groups.
19. pH: A value taken to represent the acidity or alkalinity of an aqueous solution; it is defined as the logarithm of the reciprocal of the hydrogen ion concentration of a solution:

$$\text{pH} = \log \frac{1}{[\text{H}^+]}$$

20. Extractability: This includes extractability by water or other solvents as reported according to various sources (ASTM, etc.).
21. Hydrolysis Rate: The rate of reaction of a chemical substance with water to form a new substance or substances. Usually not applied to reactions where oxidation or reduction of water is involved.
22. Viscosity: The internal resistance to flow exhibited by a fluid. A liquid has a viscosity of one poise if a force of one dyne per square centimeter causes two parallel liquid surfaces one square centimeter in area and one centimeter apart to move past one another at a velocity of one centimeter per second. Viscosity in poises divided by the liquid density at the same temperature gives kinematic viscosity in stokes.
23. Decomposition Temperature: The temperature at which heat causes the chemical degradation of a substance into two or more substances, which may differ from each other and from starting materials. The decomposition temperature of a substance is often of interest if it is below the melting point of the substance.
24. Sublimation Temperature: The temperature at which the partial pressure of a vapor in equilibrium with a solid substance is equal to one atmosphere. At this temperature, the solid passes directly into the vapor state without appearing in the intermediate liquid state.

C. HEALTH EFFECTS  
Definitions

(Note: The sub-categories listed below represent the different types of human/animal toxicity data that OTS needs in evaluating the health effects of chemical substances for purposes of implementing TSCA. Headings in parenthesis are included for easy understanding of the sub-categories; they should not be used as sub-categories.)

(General Toxicity)

1. Acute/Subchronic Toxicity
2. Chronic Toxicity

(Local Toxicity)

3. Eye Irritation
4. Skin Irritation

(Specific Toxicity)

5. Mutagenicity
6. Neurotoxicity
7. Oncogenicity
8. Sensitization
9. Reproductive Toxicity
10. Teratogenicity

(ADME)

11. Absorption
12. Distribution
13. Metabolism
14. Excretion

(Epidemiology)

15. Epidemiology



C. HEALTH EFFECTS  
Definitions

(Generalized Toxicity)

1. Acute/Subchronic Toxicity: Immediate or short term response of an organism to a single dose of a chemical substance through various routes of exposure. Refers to generalized toxic response with lethality usually being the observed endpoint. Includes LD<sub>50</sub>, LC<sub>50</sub>, LD<sub>Lo</sub> and other quantitative endpoints.
2. Chronic Toxicity: Response of an organism to repeated, long-term exposure to a chemical substance. Length of exposure and time of response varies with the organism. Observed endpoints may be on sublethal or lethal effects.

(Local Toxicity)

3. Eye Irritation: Reactions produced in the eye after exposure to a chemical substance. Damage may be assessed by changes in the cornea, iris, and conjunctiva, in the intraocular pressure, in capillary permeability, and in other in vivo and in vitro conditions.
4. Skin Irritation: Local inflammatory response of the skin observed after exposure to a chemical substance. Exposure can be a single, repeated, or prolonged contact. Manifestations include erythema, edema, ulceration, necrosis, and formation of scar tissue. Skin irritation does not involve the immune mechanism.

(Specific Toxicity)

5. Mutagenicity: Inheritable changes in the linear structure of DNA caused by exposure to a chemical substance.
6. Neurotoxicity Behavior: Observed effects to the nervous system caused by exposure to a chemical substance. Includes effects to neuromuscular transmissions and pathological changes in nerves, spinal cord, or brain. Behavioral effects are also included under this category.
7. Oncogenicity: Tumor formation observed in organisms in response to exposure to a chemical substance. May include number, type, site, growth rate and ability to metastasize of tumor.
8. Sensitization: A response of the immune system (an allergic reaction) of an organism caused by its being exposed to a chemical substance.

9. Reproductive Toxicity: Observed effects on reproductive organs or reproductive performance of an organism caused by exposure to a chemical substances. Includes egg laying, fertilization, number of offspring, and sexual and asexual reproduction. Excludes teratogenic effects on offspring (See Teratogenicity).
10. Teratogenicity: Abnormalities observed in offspring of females exposed in utero via chemical substance, and changes in birth weight, developmental delays, or fetal death.

(ADME)

11. Absorption: The uptake of a chemical substance through a membrane, by an organism. Absorption may be represented quantitatively sometimes as rate.
12. Distribution: The internal transport and deposition of a chemical substance in body fluids, tissues, and organs. Distribution can be reported quantitatively.
13. Metabolism: The physical or chemical alteration of a chemical substance by an organism.
14. Excretion: Elimination of a chemical substance or its metabolites by an organism. Excretion can be represented quantitatively and may include rate.

(Epidemiology)

15. Epidemiology: Study of the exposure and toxic responses of human and animal populations to chemical substances. Can include frequency and geographic distribution.

D. ENVIRONMENTAL EFFECTS  
Sub-Categories

(Note: The sub-categories listed below represent the different types of data that OTS needs in evaluating the environmental effects of chemical substances for purposes of implementing TSCA. Although some of the terminologies used are identical or similar to those listed under the Health Effects category, they nevertheless have different meanings and may be defined differently. Headings in parentheses are included for easy understanding of the sub-categories; they should not be used as sub-categories.)

(Aquatic Effects)

1. Acute Toxicity
2. Chronic Toxicity
3. Sublethal Toxicity
4. Bioconcentration/Biomagnification
5. Field Studies

(Terrestrial Effects)

6. Acute Toxicity
7. Chronic Toxicity
8. Behavioral Toxicity
9. Reproductive Toxicity/Teratogenicity
10. Absorption, Distribution, Metabolism, Excretion
11. Field Studies

D. ENVIRONMENTAL EFFECTS  
Definitions

(Aquatic Effects: Includes effects of chemical substances on aquatic vertebrates and invertebrates as well as vascular and non-vascular aquatic plants.)

1. Acute Toxicity: Immediate, or short term response of an organism upon exposure to a chemical substance. Refers to generalized toxic response with lethality usually being the observed endpoint. Includes LD<sub>50</sub>, LC<sub>50</sub>, LD<sub>LO</sub> and other quantitative endpoints.
2. Chronic Toxicity: Response of an organism to repeated, long-term exposure to a chemical substance. Length of exposure and time of response varies with the organism. Observed endpoints may be based on sublethal or lethal effects.
3. Sublethal Effects: Response of an organism exposed to a chemical substance that results in effects other than mortality including: behavioral, reproductive, growth and physiological effects.
4. Bioconcentration/Biomagnification: The uptake and retention of a chemical substance in an organism or in organs or tissues of an organism (bioconcentration). An increase in the tissue concentration of organisms higher in the food chain (biomagnification).
5. Field Studies: An experiment in which organisms are exposed to a chemical substance in a body of water that is located outside the laboratory and is influenced by natural conditions.

(Terrestrial Effects: Includes the effects of chemical substances on terrestrial vertebrates and invertebrates as well as vascular and non-vascular terrestrial plants.)

6. Acute Toxicity: Immediate, or short term response of an organism to a single dose of a chemical substance through various routes of exposure. Refers to generalized toxic response with lethality usually being the observed endpoint. Includes LD<sub>50</sub>, LC<sub>50</sub>, LD<sub>LO</sub> and other quantitative endpoints.
7. Chronic Toxicity: Response of an organism to repeated, long-term exposure to a chemical substance. Length of exposure and time of response varies with the organism. Observed endpoints may be based on sublethal or lethal effects.
8. Behavioral Effects: Behavioral manifestations of a organism's response to a toxic chemical substance. May include avoidance, effects on motor activity, appetite and other behavioral characteristics specific to the organism.

9. Reproductive Effects: Observed effects on reproductive organs or reproductive performance of an organism caused by exposure to a chemical substance. Includes egg laying, fertilization, number of offspring, and sexual and asexual reproduction. (For teratogenicity, see Health Effects.)
10. Absorption, Distribution, Metabolism, Excretion: The uptake, by an organism, of a chemical substance through a membrane, may be represented as a rate value. The internal transport and deposition of a chemical substance in fluids, tissues and organs. The physical or chemical breakdown of a chemical substance by an organism, possibly including metabolites. The elimination of a chemical substance or its metabolites by an organism.
11. Field Studies: An experiment in which organisms are exposed to a chemical substance in a natural habitat or in an artificial habitat that is located outside the laboratory and operated under natural conditions.

E. PRODUCTION/PROCESSING  
Sub-Categories

(Note: Production and processing are two of the several important stages in the flow of a chemical substance through the environment. The other stages are use and disposal which are covered under a separate category).

1. Manufacturer/Importer
2. Processor
3. Plant site (See also Exposure)
4. Method of manufacture (See Substance Identification)
5. Production technology
6. Processing technology
7. By-product (See Substance Identification)
8. Co-product (See Substance Identification)
9. Production volume
10. Amount by site
11. Production loss (See also Exposure)
12. Import volume
13. Export volume
14. Production trend
15. Production capacity by site (See Chemical Economics)
16. Sales volume

E. PRODUCTION/PROCESSING  
Definitions

1. Manufacturer/Importer: The complete identification, i.e., name and address, of a chemical manufacturer or importer.
2. Processor: The complete identification, i.e., name and address, of a person who processes chemical substance.
3. Plant Site: The name and address of a specific manufacturing plant site for a chemical substance.
4. Method of Manufacture: (See Substance Identification)
5. Production Technology: The engineering process(es) employed by industry that yields the chemical substance in question.
6. Processing Technology: The group of unit operations utilized for processing a chemical substance.
7. By-product: (See Substance Identification)
8. Co-product: (See Substance Identification)
9. Production Volume: The total amount of a chemical substance produced in the U.S. in a given year.
10. Amount by Site: The amount of a chemical substance produced or processed at a specific plant site in a given year.
11. Production Loss: The estimated amount of a chemical substance that is lost during normal production process. (See also Exposure)
12. Import Volume: The amount of a chemical substance imported into the U.S. in a given year.
13. Export Volume: The amount of a chemical substance exported from the U.S. in a given year.
14. Production Trend: The trend in production volume for a 10-year (or less) period.
15. Production Capacity by Site: (See Chemical Economics)
16. Sales Volume: Amount actually purchased by customer.

F. USE/DISPOSAL  
Sub-Categories

(Note: A categorizaion of use and disposal information should include data that are used in supporting estimation of exposure as well as chemical economic analysis. Use information covers both contained as well as dispersed uses.)

1. Function
2. Application
3. Additional use description (technical)
4. Additional use description (economic)
5. Mode of application
6. Use trend
7. Use amount
8. User location (See also Exposure and Production/Processing)
9. Use analog (technical)
10. Use analog (economic)
11. Method of disposal
12. Amount disposed



F. USE/DISPOSAL  
Definitions

1. Function: This describes "what, where and how" a chemical substance does in its prescribed use. This represents a general breakdown of use information.
2. Application: The end use application of a chemical substance. This is the manufacturing, service, or consumer activity in which the major function of a chemical substance is utilized. Application is therefore a specific breakdown of a major use type.
3. Additional Use Description (Technical): A detailed description of use based upon chemical structure, physical/chemical properties, and reactivity. This description highlights the technical aspects that make a particular substance suitable (or not suitable) for a particular use.
4. Additional Use Description (Economic): A detailed description of use based upon chemical marketing and other economic considerations. This description highlights the economic aspects of use.
5. Mode of Application: This describes how a chemical substance is applied in use. For example, spraying of paint.
6. Use Trend: The general trend and pattern for a use.
7. Use Amount: The amount of a chemical substance for a specific use category.
8. User Location: The name and address of a company which is a major user of a specific chemical substance. (See also Exposure: Geographic Distribution/Location Coordinates of Release and Production/Processing: Processor.)
9. Use Analog (Technical): A chemical substance that can perform the same function or application as another chemical substance, based on similarities of chemical structure, physical/chemical properties, and reactivities.
10. Use Analog (Economic): A chemical substance that can successfully substitute for another chemical substance in commerce. This definition also includes analogues for end use applications. These analogues are developed based on the price and availability of technical use analogues.

11. Method of Disposal: The method by which a chemical substance is discharged into the environment. Examples of disposal methods include incineration, open-burning, landfill, etc.
12. Amount Disposed: The amount of a chemical substance disposed by the various methods of disposal.

G. EXPOSURE  
Sub-Categories

(Note: Exposure covers such areas as release, fate, populations, monitoring as well as general location. Effects data are not included here. Headings in parentheses are included for easy understanding of the sub-categories; they are not intended for use as sub-categories.)

(Chemical Release and Control)

1. Production Technology (See Production/Processing)
2. Engineering Control Technology
3. Amounts/Rates/Characteristics of Releases
4. Geographic Distribution/Location Coordinates of Releases
5. Release Source Characteristics
6. Product Formulation and Characteristics
7. Function(s)/Application(s)/Mode of Application (See Use/Disposal)
8. Worker Activities
9. Personal Protective Equipments

(Environmental Fate)

10. Physical/Chemical Properties (See Physical/Chemical Properties)
11. Environmental Characteristics
12. Transport/Transformation Characteristics and Partitioning
13. Chemical Concentrations in Environmental Media

(Receptor Populations)

14. Geographic Distribution
15. Identity and Characteristics of Subpopulations
16. Behavioral/Demographic Characteristics
17. Non-human Populations

(Monitoring)

18. Source
19. Ambient
20. Personal
21. Tissue

(General Location)

22. Cartographic Data/Geographic Coding Files

(Route of Exposure)

23. Route of Exposure

G. EXPOSURE  
Proposed Definitions

(CHEMICAL RELEASE AND CONTROL)

1. Production Technology: (See Production/Processing)
2. Engineering Control Technology: This identifies the hardware, unit operations or equipment operating practices which limit the release of the chemical substances to the workplace or environment and describes any treatment of the contaminated media at the release or receptor site before it reaches the receptor. Treatment efficiencies are determined. Examples include POTW and industrial waste treatment used, disposal methods, potable water purification, and air purification systems in indoor ventilation.
3. Amounts/Rates/Characteristics of Releases: These are determined for any chemical release to workplace, environment, or consumer vicinity during the life cycle of the chemical, i.e., during its manufacture, processing, distribution, commercial or consumer use, and disposal. Amount of release indicates quantity. Rate of release indicates periodicity (e.g., batch ejection from an industrial outfall, or slow continuous leaching from disposal site) and exit volume/time. Characteristics of release include relevant physical/chemical properties of the waste stream, form of the chemical, mass, concentration, frequency and duration, etc. For example, a solid, liquid, gas, or particulate might be dispersed in an aerosol or smoke.
4. Geographic Distribution/Location Coordinates of Releases: These are also determined for release points during all phases of a chemical's life. Latitude/longitude coordinates of sources are the most useful data. Precise coordinates are usually only relevant to manufacturing sites, e.g., individual outfalls along a river reach. Another type of example would be the gross number or density of dry cleaning facilities in a city.
5. Release Source Characteristics: In general, this will identify the nature of the release source, e.g., an open air refinery, an enclosed plant, a disposal site, a truck or railroad car spill. This category also includes specific characteristics such as stack height, number of plant outfalls, and average capacity of transport vehicles.
6. Product Formulation and Characteristics: This describes products with regard to the chemical concentration in the product, the physical form of the product, relevant dispersion media specific to the product (such as solvents), and the chemical relationship of the chemical to the product

formulation (e.g., is the chemical bound in the product matrix?). Also, the performance characteristics of the product are discussed.

7. Function(s)/Application(s)/Mode of Application: (See Use/Disposal)
8. Worker Activities: Steps taken by workers in the workplace which can result in potential exposure.
9. Personal Protective Equipments: Equipments which reduce worker exposure to chemical substances released in the workplace.

(ENVIRONMENTAL FATE)

10. Physical/Chemical Properties: (See Physical/Chemical Properties)
11. Environmental Characteristics: These identify and characterize the medium that becomes contaminated, such as air, ground and surface water, or soil. This category would include meteorological data, such as wind speeds and rainfall, surface and groundwater characteristics, and soil types and their physical/chemical characteristics.
12. Transport/Transformation Characteristics and Partitioning: Partitioning refers to the relative distribution of a chemical among environmental media. Transport refers to the potential movement of the chemical from one media compartment to another. Transport parameters would include volatilization from surface water and soils and adsorption to soil and sediments. Transformation refers to a chemical's change in structure. The major processes that can effect transformation are photolysis, oxidation, hydrolysis, biotransformation as well as abiotic media (e.g., air and water). Bioconcentration (see Environmental Effects) is relevant to this category with regard to chemical concentration estimates in biotic media.

(RECEPTOR POPULATIONS)

14. Geographic Distribution: This describes "where" exposure will occur. Location and density of human populations are evaluated. In different types of assessments the distribution of residences in a particular city or county, or in U.S. urbanized areas in general, would be of interest.

15. Identity and Characteristics of Subpopulations: This describes "who" will be exposed, whether consumer, worker or general population. The potentially affected populations are identified, enumerated, and characterized with parameters such as their age, sex, and sensitivity to certain chemicals or exposure situations.
16. Behavioral/Demographic Characteristics: This describes "how" or to what extent the population is exposed. Examples of those data include consumption patterns of consumer population(s) and commuting patterns of the residential population(s). With regard to occupational exposure, the duration and frequency of activity that results in exposure, and use of protective equipment are relevant items.
17. Non-Human Populations: This category includes the "where, who, and how" for exposure to non-human populations as described for human populations above.

(MONITORING)

18. Source: This category includes data on release source and characteristics measured at point of actual release. Sources discharging to the air include point, line, and area sources. Sources discharging to water include point and non-point sources. Sources can be both fugitive in nature or from confined equipments.
19. Ambient: Point at which release is in media and can no longer be controlled.
20. Personal: Personal monitoring refers to the data collected by a portable sample collector carried by a volunteer. These data can provide an integrated picture of chemical exposure in all the microenvironments through which the volunteer passes.
21. Tissue: Tissue monitoring data include the amount of chemical substance in particular tissues or organs at a given time.

(GENERAL LOCATION DATA)

22. Cartographic Data/Geographic Coding Files: Cartographic data refer to computerized data that are digitized representations of maps. These are typically used in displaying other (thematic) data. Examples include county and state boundary files. Geographic coding files may be in hard copy or computerized and relate one type of geographic area coding to another, e.g., census tracts within ZIP code areas or cities within states.

(ROUTE OF EXPOSURE)

23. Route of Exposure: The mode by which human or the environment is exposed to a chemical substance. For example, route of human exposure may be dermal contact or inhalation, and route of environmental exposure may be air, water or land.

H. CHEMICAL ECONOMICS<sup>\*\*</sup>  
Sub-Categories

(Note: The data sub-categories include all those that are needed by OTS in performing economic analysis of chemical substances for purposes of implementing TSCA. From a data organization standpoint, many of these sub-categories are more appropriately listed under other data categories.)

1. Manufacturer (See Production/Processing)
2. Plant site (See Production/Processing)
3. Total annual sales
4. Annual chemical sales
5. Production capacity by site (See also Production/Processing)
6. Price
7. Price trend
8. Function (See Use/Disposal)
9. Application (See Use/Disposal)
10. Use trend (See Use/Disposal)
11. Use amount (See Use/Disposal)
12. Method of manufacture (See Substance Identification)
13. Production technology (See Production/Processing)
14. Sales by end uses
15. Employment by plant site (See also Exposure)
16. Production trend (See Production/Processing)
17. Production volume (See Production/Processing)
18. Production cost
19. Demand elasticity
20. Sales volume (See Production/Processing)

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<sup>\*\*</sup> Other sub-categories listed under Production/Processing and/or Use Disposal may be needed for chemical economics analysis. Please refer to those two categories.



H. CHEMICAL ECONOMICS  
Definitions

1. Manufacturers: (See Production/Processing)
2. Plant Site: (See Production; See also Exposure: Geographic Distribution/Location Coordinates of Releases.)
3. Total Annual Sales: The total annual sales of a company in terms of dollars for all products and services.
4. Annual Chemical Sales: The total annual sales of a company in terms of dollars for all chemical substances manufactured by that company.
5. Production Capacity by Site: The production capacity for a chemical substance within a plant site. (See also Production/Processing: Amount by Site.)
6. Price: The current sale price of a chemical substance.
7. Price Trend: The 10-year price trend of a chemical substance.
8. Function: (See Use/Disposal)
9. Application: (See Use/Disposal)
10. Use Trend: (See Use/Disposal)
11. Use Amount: (See Use/Disposal)
12. Method of Manufacture: (See Substance Identification)
13. Production Technology: (See Production/Processing)
14. Sales by End use: The amount of sales per use for a chemical substance.
15. Employment by Plant Site: The number of employees per plant site. This information is used to determine the number of employees that may be adversely affected by an EPA action. In many cases, the number of people outside a plant site (e.g., truck drivers) may also be needed. (See also Exposure)
16. Production Trend: (See Production/Processing)
17. Production Volume: (See Production/Processing)
18. Production Cost: The total cost for producing a chemical substance.

19. Demand Elasticity: The relationship between price and demand.
20. Sales Volume: (See Production/Processing)

## V. INFORMATION RESOURCES ATTRIBUTES MATRIX

This section presents the resources attributes of the major computerized data banks and data bases that can be used in support of the OTS functions and processes under TSCA. Manual resources are included in Section VII of the Notebook since they have few but significantly different attributes.

There are two types of resources attributes that are used to describe a computerized information resource, i.e., search attributes and system attributes. While search attributes pertain mainly to the searchability and retrieval features of the data, system attributes describe characteristics of the system including hardware and software used and access mode. The search and system attributes of online data bases outline for the user what features, information, and capabilities are available. This display will help to make the user aware of the variety of information resources available, decide which attributes can facilitate access and select the most appropriate resource(s) which can solve the information problems.

This section contains three parts. The first part is the matrix outline, listing resources attributes in a hierarchial format. Following the hierarchial listing is a matrix matching search and system attributes against computerized information resources. In this matrix, the attributes are listed on the horizontal axis in the same sequence as they appear in the hierarchial listing. The computerized information resources are placed on the vertical axis of the matrix and are divided into two main groups, i.e., bibliographic data bases and non-bibliographic data banks. Within each of these two groups, the systems are listed in alphabetical sequence. The major computerized models as discussed in Section VI are also included in the Matrix. In the matrix, the information resources are either indexed by a "X" symbol or by some other alpha or numeric notations. For explanations on the notations used in the matrix, consult the attributes definitions in this Section. The last part of this section is a listing of definitions (or sometimes scope notes) for the attributes.

For additional information on the information resources, the readers may consult the OTS Directory of Information Resources or the OTS Data Dictionary.

OTS Information Resources Attributes  
MATRIX Outline

I. Search Attributes

I.A. Chemical Searching

I.A.1. Substructure

I.A.1.a) Connection Table

I.A.1.b) Wiswesser Line Notation (WLN)

I.A.1.c) Key (Screen) Codes

I.A.1.d) Graphics (Searchable)

I.A.2. Chemical Reference Numbers

I.A.2.a) CASRN

I.A.2.b) Other

I.A.3. Name Match

I.A.3.a) Exact

I.A.3.b) Fragment

I.A.3.c) Non-Systematic (Synonym)

I.A.3.d) Systematic

I.B. Retrieval Features

I.B.1. Subject Searching

I.B.1.a) Free Text

I.B.1.b) Proximity Search

I.B.1.c) Index Terms

I.B.1.d) Thesaurus

I.B.2. Numeric/Alphanumeric Availability

I.B.2.a) Data Values

I.B.2.b) Data Values (Rangeable)

I.B.3. Bibliographic Information

I.B.3.a) Author

I.B.3.b) Title (Source Document)

I.B.3.c) Year of Publication

I.B.3.d) Title (Journal, Book)

I.B.3.e) Abstract

I.B.3.f) Language

I.B.3.g) Abbreviated/Coded Citation

I.B.4. Logical Searching

I.B.4.a) Field (Indirect) Search

I.B.4.b) Boolean Logic (Within Field)

I.B.4.c) Boolean Logic (Across Field)

I.C. Resource Characteristics

I.C.1. Display Features

I.C.1.a) Abbreviated

I.C.1.b) User Defined

I.C.1.c) Tables

I.C.1.d) Graphics

I.C.1.e) Offline

I.C.2. File Size and Use

I.C.2.a) No. Records

I.C.2.b) No. Chemicals

I.C.2.c) Frequency of Use

I.C.3. Data Base Characteristics

I.C.3.a) Update Cycle

I.C.3.b) Cost

I.C.3.c) Period of Coverage

I.C.4. Search Aids

I.C.4.a) Printed Source

I.C.4.b) Online Help

I.C.5. File/Content Characteristics

I.C.5.a) Unpublished

I.C.5.b) Ongoing research

I.C.5.c) Data Quality

I.C.5.d) International Sources

II. System Attributes

II.A. System Access

II.A.1. Source

II.A.2. Status

II.A.3. Interactive

II.A.4. Telecommunication

II.A.5. Restricted Access

II.B. Hardware

II.B.1. Computer Utilized

II.B.2. Computer Owner [1-EPA; 2-Contractor;  
3-Developer]

II.C. Software

II.C.1. Program Language [e.g., COBOL, PL/1, BASIC]

II.C.2. DBMS [e.g., System 2000, ADABAS]

II.C.3. Library Program [e.g., EASYTRIEVE,  
SAS, MARK IV]

II.C.4. Command Language [e.g., TSO]

II.D. Data Processing Features

II.D.1. Data Entry

II.D.2. Data Editing

II.D.3. Data Manipulation

II.E. System User Aids

II.E.1. System Documentation

II.E.2. Data Dictionary Defined

OTS Information Resource Attributes MATRIX  
Attribute Definitions

Standard dictionary definitions have been used or attributes have been described according to their use or as applied to OTS information activities. The definitions are listed in a hierarchial manner as presented in the matrix outline:

- I. Search Attributes: characteristics of the data base  
which denote content and accessibility options.
- I.A. Chemical Searching: search and retrieval options  
available to represent chemical substances or  
parts thereof which
- I.A.1. Substructure: a partial chemical structure represented by  
atoms and their bonding.
- I.A.1.a) Connection table - a method of representing  
chemical structure. Each atom in the  
structure is listed together with its attached  
atoms and bonds. Search on this type of data  
may be transparent to the user; but  
essentially does not use codes to indicate the  
presence of specific rings or fragments.
- I.A.1.b) WLN - Wiswesser Line Notation, a system of  
symbols (alphanumeric characters) designed to  
describe molecular structures in detail and  
permit computer searches.
- I.A.1.c) Key (Screen) Codes - standard codes (sometimes  
called "screen codes") which are used to  
retrieve specific substructures or functional  
groups. An example would be input of '48' to  
retrieve six-membered rings.
- I.A.1.d) Graphics (Searchable) - the full or partial  
structure of a chemical can be used to  
retrieve data.
- G - the structure can be generated for  
searching graphically.
- K - the structure can be generated for  
searching using strings of characters.



- I.A.2. Reference Numbers: any number used to uniquely identify a specific chemical or chemical class directly or indirectly.
- I.A.2.a) CAS Registry Number - a number assigned by Chemical Abstracts Services (CAS) as each substance is registered. Note: a check in this column indicates that the CAS Registry Number can be used to search for chemicals, not just displayed in a record.
- I.A.2.b) Other - any other alphanumeric term used to identify a chemical, company, standard, etc. and which refers directly or indirectly to a chemical or chemical class. Examples include NIOSH numbers (chemical), Standard Industrial Codes (company), and DOT label (standard).
- I.A.3. Name Match: the ability to retrieve a substance based on nomenclature.
- I.A.3.a) Exact - the name must be entered exactly as it appears in the database, including word order and punctuation.
- I.A.3.b) Fragment - substances can be retrieved based on partial names.
- I.A.3.c) Non-systematic (Synonym) - multiple names which may be available for a single substance. Such names may include trivial names, trade names, production names, or common names.
- I.A.3.d) Systematic - a chemical name assigned based on a specific naming scheme indicating the exact structure of a chemical. The two most widely used schemes are those designed by CAS and IUPAC.
- I.B. Retrieval Features: denotes the availability of textual and numeric information and the logical relationships available to access the information/data directly or serially.
- I.B.1. Subject Searching: concepts, topics and descriptions which can be specified in a search.

- I.B.1.a) Free Text - the data in the field is not taken from a controlled list of terms, but words are indexed as they are added.
- I.B.1.b) Proximity Search - the user may specify that certain words must appear adjacent to each other in the text, in the same sentence, in the same field, etc.
- I.B.1.c) Index Terms - a controlled vocabulary or terms used to describe the data in each field, which is available for searching.
- I.B.1.d) Thesaurus - list of controlled vocabulary terms, usually cross-referenced and often showing the relationship between terms, which is available to the user from the computer while using the search system or in hard copy.
- Coded: H = hard copy  
L = ONLINE
- I.B.2. Numeric/Alpha-numeric Availability: data is available in the record and can be searched and retrieved.
- I.B.2.a) Data values - indicates whether the exact content of a specific field can be used as a basis for searches. For example, if a database carries boiling points and compounds with a boiling point of 10°C can be retrieved, this attribute will qualify as searchable. Similarly, if a database carries toxicity data but compounds with e.g., a specific LD50 that cannot be retrieved, the numeric data is not searchable. If this column is checked, it indicates that at least some of the data reported is searchable or rangeable.
- I.B.2.b) Data (Rangeable) - data (as described above) can be searched by expressing a range of numeric values, rather than a specific value. For example, toxicities between 10 and 30 mg/kg or production volumes greater than 10,000 lbs/year. If this column is checked, it indicates that at least some data is range-searchable.

I.B.3. Bibliographic Information:

General information referring the user to the document from which the data was extracted (source document).

All bibliographic information columns are coded as follows:

P - this type of data may be displayed but cannot be used for searching.

S - this type of data can be used as the object of a search and/or displayed in retrieved records.

- I.B.3.a) Author - the author of the source document.
- I.B.3.b) Title - the title of the source document, including articles in journals.
- I.B.3.c) Year of publication - data on which the document was published.
- I.B.3.d) Journal - journal in which the source document appears.
- I.B.3.e) Abstract - summary of the content of a specific article.
- I.B.3.f) Abbreviated/coded citation - a truncated or less than full revision of the standard bibliographic reference, e.g., use of CODEN instead of journal title.
- I.B.4 Logic Searching: Operators or aids allowing manipulation of search terms to provide more specific comprehensive searches.
  - I.B.4.a) Field specific - capability to search selected specific fields (indirect search or serial search)
  - I.B.4.b) Boolean logic (within fields) - a method of logic developed by George Boole, an English mathematician, which uses logical operators - AND, OR, and NOT - to show relationships between sets or terms. In this case the sets or terms must involve the same field of data.

- I.B.4.c) Boolean logic (between fields) - logical operators can be used to link separate fields, such as toxicity and production.
- I.C. Resource Characteristics: Options for printing retrieved information and file-specific features relating to content, coverage, covering and cost.
- I.C.1. Display Features: Display features allow the user to examine search results.
- I.C.1.a) Abbreviated format - a portion of the record is shown, allowing the user to rapidly scan large files. This is preprogrammed, and varies in length.
- I.C.1.b) User defined - user can specify which fields are to be displayed from the full record.
- I.C.1.c) Tables - results can be displayed in a concise table, defined by the user.
- I.C.1.d) Graphics - capability to display structures, maps, statistical and other pictorial representations.
- Structure - chemical structures can be displayed after retrieval. This column is coded as follows:
- T - structure can only be displayed on the user's terminal
- O - structure can be displayed on the user's terminal or in hard copy offline.
- I.C.1.e) Offline - search results can be printed at the computer site, rather than on the user's terminal, and mailed to the user.
- I.C.2. File Size: Number of total unit records and number of chemicals included in the file.
- I.C.2a) No Records: A record is a unit of related information in a database. For example, a record is generally meant to include all the information stored for a particular document in a bibliographic system.

- I.C.2.b)  
No Chemicals:                      Number of unique chemicals, substances, formulations, generic classes, etc., in a database.
- I.C.3.      Data Base  
                 Characteristics:                      Information on currency, cost, and coverage.
- I.C.3.a)  
Update Cycle:                      Frequency of additions to the records in a database. This column is coded as follows:  
0 - closed file
- 1 - daily  
2 - weekly  
3 - biweekly/semimonthly  
4 - monthly  
5 - bimonthly  
6 - quarterly  
7 - semiannually  
8 - annually  
9 - irregular
- I.C.3.b) Cost:                      Cost per connect hour. This does not include subscript fees, print cost, or telecommunication fees.
- I.C.3.c) Coverage:                      Span of coverage.  
Curr = only latest information (e.g., last 3 months)
- I.C.4.      Search Aids:                      Tutorial help on searching the file; or description of file contents.
- I.C.4.a.) Printed  
Source:                      Data base, partial or complete, is available in hard copy.
- I.C.4.b) Online Help:                      Provides options for search and retrieval relative to a user's status with this interaction in a system.
- I.C.5.      File/Content  
                 Characteristics:                      Denotes publication type and quality of the data as described by the data base producer.
- I.C.5.a) Unpublished  
                 Data:                      Data which is not in the public domain, e.g., processing, communications, private files, etc.
- I.C.5.b) Ongoing  
                 Research:                      Database contains references to research which is in progress.

I.C.5.c) Data Quality:	Indicates whether the data has been evaluated by the database producer prior to incorporation, for accuracy, completeness, and quality. This column is coded as follows:
	0 - No evaluation prior to incorporation (data may be taken from referred journals).
	1 - Quality indicator available.
	2 - Peer evaluated.
I.C.5.d.) International Sources:	Data is taken from non-U.S. sources (may be in addition to U.S. sources).
II. System Attributes:	Characteristics and features of the hardware and software.
II.A. System Design Access:	Communication connections and availability of the data base to the end user.
II.A.1. Source:	Availability of the data base to the end user.
	C = commercial P = private
II.A.2. Status:	Denotes the current availability of a data base. D = developed U = under development
II.A.3. Interactive:	A system which allows the user to input instructions, receive a response, and then modify or manipulate the results.
II.A.4. Telecommunications:	The network which provided the link between the terminal and the host computer. This column is coded as follows:
	1 - International/National access. Via telecommunications network.
	2. - International access, no telecommunications network.
	3. - Local access, i.e., long distance call outside computer area.

4. - In-house access only, no telecommunications available.

- II.A.5. Restricted Access: The system is available to a limited user community, e.g., contains confidential data, is available only for "in-house" use, etc.
- II.B. Hardware: Denotes manufacturer name, series, level, model and owner of the equipment.
- II.B.1 Computer Utilized: Denotes specific hardware in which data base resides.
- VAX = VAX 11/780  
IBM = IBM  
UNI = Univac
- II.B.2 Computer Owner: Organization which owns or leases hardware.
- 1 - EPA  
2 - Contractor  
3 - developer of data base
- II.C. Software: Set of instructions (programs) or routines for handling input into the computer.
- II.C.1. Program Language: Defined set of Characters and rules used for writing a computer routine e.g., COBOL, PL/1, BASIC.
- II.C.2. DBMS: Denotes data base management system used e.g., System 2000, ADABAS.
- II.C.3. Library Program: Denotes use of a canned or standard software program e.g., EASYTRIEVE, SAS, Mark IV.
- II.C.4. Command Language: Provides direct interface with the central processing unit & determines data entry and editing facilities, submission and retrieval capabilities, and utility and data set manipulation functions e.g., TSO, ELHILL
- II.D. Data Processing Features: Denotes existence of facilities, and utilizes for handling data by the end-user.
- II.D.1 Data Entry: Capability exists to input data.
- II.D.2. Data Editing: Capability exists to add, delete, & modify data.

- II.D.3. Data Manipulation: Capability for statistical analysis and computation.
- II.E. System User Aids: Documentation for end user to facilitate interaction with the system.
- II.E.1. System Documentation: User manual available
- II.E.2. Data Dictionary Defined: Description of data element and its use within the organization that developed the data base.



## VI. OTS ANALYTICAL CAPABILITIES

In addition to drawing upon existing information in the form of data bases and manual resources, OTS functions and processes often require the development of new information. Much of this information is the result of applying a variety of analytical capabilities to existing data in order to draw conclusions useful in risk assessment. This section discusses these analytical capabilities which include computer models and estimation techniques and describes how they are used in support of OTS functions and processes.

OTS scientists utilize: (1) general statistical packages such as the Statistical Analysis System (SAS); (2) more specialized statistical analysis capabilities to perform complex univariate and multivariate analyses (e.g., cluster analyses using ARTHUR); (3) programs to generate molecular properties (descriptors) for Structure-Activity Relationship (SAR) analyses which are too time-consuming to compute manually (e.g., CHEMLAB); (4) physical/chemical property estimation programs such as CHEMEST derived from SAR research; (5) environmental fate and exposure models to predict environmental concentrations of chemicals and estimate population exposures; and (6) dose-response models which are used to describe risks, extrapolate risks from high to low doses, and to estimate health impacts of particular exposure levels and doses.

Mathematical models may be of many different forms, and include models based on statistically developed correlations such as nonlinear dose-response models, as well as complex mechanistic multimedia environmental fate models.

In the paragraphs that follow, three major types of analytical capabilities are discussed. These capabilities are:

- o Structure-Activity Relationship (SAR)
- o Fate and Exposure Modeling
- o Dose-Response Modeling

The discussion on SAR includes General Statistical Programs (e.g., SAS), Multivariate Data Analysis (e.g., ARTHUR), SAR Descriptor Generators (e.g., CHEMLAB), and Estimation Techniques (e.g., CHEMEST, CLOGP). Following each discussion, a table is included identifying the individual models or techniques that belong to each of the capabilities. Finally, there are two matrices matching the various classes of models and techniques against OTS functions and processes respectively. The purpose of these matrices is to indicate how these capabilities are used.

## Structure-Activity Relationships

Structure Activity Relationships (SAR) are often established through statistical methods to relate the presence of specific chemical structural features to a given biological activity or other expression of a chemical's nature, such as its physical/chemical properties. These properties/activities can also be correlated with one another as in the case of boiling point and vapor pressure, or octanol/water partition coefficient and bio-concentration factor. A wide range of statistical programs can be used to mathematically investigate and describe structure-activity relationships, depending on their complexity. For simple and multiple linear regressions, any one of a number of widely available statistical programs may be used. The most notable example of such programs commonly used within OTS is probably the Statistical Analysis System (SAS), resident on the NCC IBM and planned for implementation on the OTS VAX and IBM 4341 computers. SAS, in addition to its large variety of univariate, data management, and graphics procedures, also includes multivariate data analysis capabilities needed for more complex structure activity analyses. Another program newly available on the NIH/EPA Chemical Information System (CIS) entitled ARTHUR features a variety of methods for performing exploratory multivariate data analyses, including several clustering analysis techniques.

The CHEMLAB program on CIS provides a way of generating several molecular descriptors such as molecular volume and surface area which may be useful in SAR investigations. These descriptors are usually difficult and time-consuming to calculate and hence have not been widely used in quantitative SAR (QSAR) research except for drug design. CHEMLAB thus offers OTS researchers the capability to use a wider range of molecular properties in the development of QSARs.

Once these statistical relationships have been codified and incorporated into a procedure or computer program which allows scientists to readily calculate the value of one feature from the values or presence of one or more others, it is often referred to as an estimation technique.

Estimation techniques are thus the product of research into structure-activity relationships which allow a reasonably reliable quantitative estimate to be generated on a regular basis. While much work has been and is being performed in the SAR area, relatively few such analyses have resulted in the development of useful estimation techniques. These are mostly found in the area of physical/chemical property estimation, although some work in the environmental fate and ecological effects areas has also been useful in OTS risk analyses. In general, health effects SAR research has not yet generated many

useful quantitative relationships applicable in OTS work, although much significant work has been done in the area of drug design.

The OTS use of analytical capabilities relating to SAR involves both development and application areas. Estimation technique programs such as CLOGP and CHEMEST are applied in many of the chemical assessment activities of the office. A validation effort has been undertaken in FY 83 to assess the performance of the estimation techniques for classes of chemicals frequently encountered in PMN submissions. This work could also serve as a basis to extend existing estimation techniques to wider classes of chemicals and to develop new relationships for use in risk assessment.

Structure-Activity Relationship (SAR)  
Analytical Capabilities

SAR Development

General Statistical Programs (e.g., SAS)

Specialized Statistical Programs (e.g., ARTHUR)

Descriptor Generators (e.g., CHEMLAB)

SAR Application

CHEMEST (boiling point, vapor pressure, water solubility,  
Henry's Constant, volatilization from water half-  
life, activity coefficient, adsorption  
coefficient, bioconcentration factor)

CLOGP\* (log octanol water partition coefficient)

\*This program requires the input of chemical structural data  
using either the SFILES or SMILES entry programs.

## Fate and Exposure Modeling

OTS uses a variety of models to assess chemical fate and environmental or human exposure. These models predict the concentrations of chemicals in air, water and soil or a combination of environmental media. In a few cases, they also include programs to estimate the number of persons potentially exposed at specific levels. The models are used for screening-level applications as well as for detailed exposure analyses.

There is an ongoing effort to develop or acquire, implement and integrate models with data as part of the Graphical Exposure Modeling System (GEMS). This system, which also includes the CHEMEST and CLOGP property estimation program, is designed to give scientific users ready access to models, estimation techniques, data analysis, data management, and display capabilities. GEMS users are not required to be familiar with most of the computer-related aspects of running models; a subject-area knowledge plus a general familiarity with the program's features are usually sufficient to perform analyses. The program prompts users for English-language inputs and provides specific help information when necessary, thus allowing users to access data, run models or estimations and analyze results without using typical computer programming techniques.

The GEMS data bases are included in Section II. The estimation techniques and models available through GEMS are discussed in this section. A list of physical chemical properties which can be estimated using CHEMEST is included in the table entitled Structure-Activity Relationship: Analytical Capabilities. The table entitled "Fate and Exposure Models" lists the models available in GEMS by environmental media. In addition to the GEMS models, OTS has acquired a number of other models which also reside on the VAX 11/780 computer. These are much less frequently used than the first group, and hence have not yet been implemented in GEMS. They may be used for specific assessments as needed by creating special input data files. Because of this infrequent use, they are not discussed here in detail, with the exception of the Unified Transport Model-Toxics (UTM-TOX) which is planned for inclusion in GEMS in FY 84.

Fate and Exposure ModelsModels in GEMSAdditional Models Available\*Atmospheric

ATM80\*\*  
BOXMOD80\*\*  
PTDIS  
PTMAX

APRAC, CDM, CDMQC, CRSTER,  
HIWAY, PTMTP, PAL, VALLEY,  
RAM

Surface Water

EXAMS

PEST, RIVMOD, EXAMS2

Soil Water or Runoff

SESOIL

PRZM, ARM

Groundwater

AT123D

Multimedia

ENPART  
TOXSCREEN

UTM-TOX

\* These models have implemented on the VAX 11/780 and may be used outside of the GEMS environment.

\*\*These models outputs include population exposures.

### Dose-Response Modeling

Unlike fate/exposure models, which use, for the most part, deterministic simulations of environmental processes, dose-response models are typically stochastic representations of relationships between dose level and toxic effect(s). Ordinarily the "models" represent cumulative distribution functions of response conditional on dose. Several models currently in use presume tolerance distributions among individuals' responses. Others may functionally correspond to postulated biological mechanisms even though they have been developed totally from data description principles. Data from animal bioassay tests are usually input to the models, which use different statistical assumptions about the form of the relationship to estimate the probability a dose level is associated with a certain effect and/or how long it will be until the effect is manifested. To date, carcinogenicity is the effect which has been modeled most frequently in this manner.

The various computerized modeling programs are being unified by common input requirements and output variables. Interfaces with SAS graphics routines are being developed.

Dose-Response and Risk Estimation Models

Probit

MANTELAN

RISK 81

LOGIT

RISK 81

WEIBULL

RISK 81

WEIBULL 82

Multihit

MULTI80 G

RISK 81

One-Hit

ONE HIT MD

GLOBAL 82

MULTI 80 G

Multistage

GLOBAL 82

RANK 81

TIME-TO-OCCURRENCE

MRST

RANK 81



OTS FUNCTIONS/ANALYTICAL CAPABILITIES MATRIX\*

OTS Functions		Health Effects Analysis		Environmental Effects Analysis	Exposure Analysis	Risk Assessment
OTS Analytical Capability Classes	Chemical Analysis					
<hr/>						
<u>General Statistical Programs (e.g., SAS)</u>		X			X	
<u>Multivariate Data Analysis (ARTHUR)</u>		X			X	
<u>SAR Descriptor Generators (CHEMLAB)</u>		X		X		
<u>Estimation Techniques (CHEMEST, CLOGP)</u>	X			X	X	
<u>Fate/Exposure</u>					X	
<u>Atmospheric</u>					X	
Land					X	
Water					X	
Groundwater					X	
Multimedia					X	
<u>Dose-Response and</u>						
<u>Low-Dose Extrapolation</u>						
<u>Models</u>		X				X

\* Three OTS functions, i.e. Control Technology Analysis, Economic Analysis, and Regulatory Options Analysis do not use the analytical capabilities described herein. These three functions are not included in the matrix. Risk assessment, though not a function (see Section II), is included in the matrix.

# OTS PROCESSES/ANALYTICAL CAPABILITIES MATRIX

OTS Processes			
OTS Analytical Capabilities Classes	Chemical Testing	New Chemicals Review	Existing Chemicals Review
<u>General Statistical Programs (e.g., SAS)*</u>			X
<u>Multivariate Data Analysis (ARTHUR)*</u>			
<u>SAR Descriptor Generators (CHEMLAB)*</u>	X	X**	X
<u>Estimation Techniques (CHEMEST, CLOGP)</u>			
<u>Fate/Exposure Models</u>			
Atmospheric	X	X	X
Land	X	X	X
Water	X	X	X
Groundwater	X	X	X
Multimedia	X	X	X
<u>Dose-Response and Low-Dose Extrapolation Models</u>	X	X**	X

\* These programs are primarily used in research and in general data analysis not related to a specific assessment. SAS is also used to analyze monitoring data on existing chemicals, however.

\*\* For analogues of new chemicals.

VII. DATA CATEGORIES, DATA SUB-CATEGORIES/  
INFORMATION RESOURCE MATRIX

This section presents three sets of matrices which match respectively data categories and sub-categories (described in Section IV) against major information resources. While non-bibliographic computerized information resources are matched against data sub-categories, both the bibliographic data bases and manual resources are indexed by data categories only. It would have been technically infeasible to match bibliographic data bases and manual resources against data sub-categories.

The purpose of the matrices is to document the types of information (i.e. data categories or data sub-categories) available in the major information resources. By comparing these matrices against the data sub-categories/OTS functions matrices in the next section, information gaps may be easily seen.

The first set of matrices matches data sub-categories against computerized non-bibliographic data bases and computer models. This set of matrices establishes the relationship between information resources and data by indicating the specific types of data, i.e., data sub-categories that are available in these information resources. In using these matrices, the readers may want to consult simultaneously the resource attributes matrices in Section V in order to obtain a complete understanding about the availabilities as well as searchabilities of data.

The second set of matrices matches data categories against computerized bibliographic data bases. This establishes the availabilities of major types of data, i.e. data categories, in the bibliographic data bases. Again, the readers are urged to consult the resource attributes matrices on bibliographic data bases in Section V.

The third set of matrices in this section matches data categories against manual information resources. A matrix outline is included in this section. For each of these manual sources listed in the matrices, its major search attributes are included and indexed. Note that these attributes are few but are significantly different from those listed in Section V for the computerized information resources. Wherever a manual source is available at the OTS Technical Information Center, it is so indicated in the matrices.

When scanning the Matrix, the reader must use the "OTS Printed Resources Attributes Matrix Definitions" included in this section in order to decode the information presented.

The citation number (last column) on the matrix refers the reader to the full bibliographic citation in the "Author Index".

Also included in this chapter is the "Glossary of Abbreviations" which is useful in deciphering the linguistic shorthand associated with this and other chapters.

# OTS INFORMATION MATRIX—BIBLIOGRAPHIC DATABASES DATA CATEGORIES

SYSTEM TYPE/NAME	CHEMICAL ACCESS		OTS DATA CATEGORIES								
	NO. CHEMICALS	CAS RN	SUBSTANCE IDENTIFICATION	PHYSICAL-CHEMICAL PROPERTIES	HEALTH EFFECTS	ENVIRONMENTAL EFFECTS	PRODUCTION/PROCESSING	USE/DISPOSAL	EXPOSURE	ECONOMICS	REGULATIONS/CONTROL
<b>BIBLIOGRAPHIC DATABASES</b>											
<b>DIALOG DATABASES (CON'T.)</b>											
HARFAX INDUSTRY DATA SOURCES			X				X			X	
IRL LIFE SCIENCES COLLECTION			X		X	X					
ISMEC			X	X			X	X		X	
NTIS			X		X	X	X	X	X	X	X
OCEANIC ABSTRACTS			X			X			X		X
PAPERCHEM			X		X	X	X	X	X	X	X
POLLUTION ABSTRACTS			X	X	X	X		X	X		X
PTS F&S INDEXES			X				X	X	X	X	
PTS INTERNATIONAL FORECASTS			X				X			X	
PTS PROMT			X				X	X		X	
PTS U.S. FORECASTS			X				X			X	
SCISEARCH			X	X	X	X	X	X	X	X	X
SURFACE COATINGS ABSTRACTS			X		X	X	X	X	X	X	X
TEXTILE TECHNOLOGY DIGEST			X		X		X	X	X	X	X
TRADE AND INDUSTRY INDEX			X				X			X	X
WATER RESOURCES ABSTRACTS			X		X	X			X		X
<b>MEDLARS DATABASES</b>											
CANCERLIT	347K	X	X		X				X		
CANCERPROJ	21K	X	X		X				X		
MEDLINE	800K	X	X		X				X		
TOXLINE	570K	X	X		X	X			X		
<b>ORBIT DATABASES</b>											
BIOSIS			X		X	X	X	U	X	X	X
CA SEARCH	3M	X	X	X	X			U			
ENVIROLINE			X	X	X	X	X	X	X	X	X
FEDERAL REGISTER			X								X
NTIS			X		X	X	X	U	X	X	X
APIPAT			X				X	U			X
U.S. CLASS							X	U			X

## OTS INFORMATION MATRIX—BIBLIOGRAPHIC DATABASES DATA CATEGORIES

[illegible]

OTS PRINTED RESOURCES ATTRIBUTESMATRIX OUTLINE

- I. Chemical Access
  - A. No. (of) chemicals
  - B. CAS Registry Number (CAS RN)
- II. OTS Data Categories
  - A. Substance Identification
  - B. Physical-Chemical Properties
  - C. Health Effects
  - D. Environmental Effects
  - E. Production/Processing
  - F. Use/Disposal
  - G. Exposure
  - H. Economics
  - I. Regulations/Control
- III. Publication Location
  - A. Publication Type
  - B. Supplements
  - C. Frequency of Revision
  - D. Online Version
- IV. Shelf Locations
  - A. LC Call Number
- V. Author Index
  - A. Citation Number
- VI. Glossary of Abbreviations

OTS PRINTED RESOURCES ATTRIBUTES MATRIXDEFINITIONS

## I. Chemical Access:

denotes access to a limited number of chemicals or to specific chemical identification.

## I.A. No. (number of) chemicals:

denotes scope of coverage of chemical substances; an (\*) asterisk denotes an undetermined number of chemicals are covered.

## I.B. CAS RN:

denotes Chemical Abstract Service Registry Numbers are associated with the chemical nomenclature.

## II. OTS Data Categories:

general areas of chemical information requirements of OTS. (See Section IV of the notebook.)

## II.A. Substance Identification:

information is available to establish the identity of a chemical substance as defined by TSCA.

## II.B. Physical-Chemical Properties:

characteristics of substances related to reactivity.

## II.C. Health Effects:

contains human/animal toxicity data as well as biological and physiological effects of chemical substances.

## II.D. Environmental Effects:

contains data that OTS needs in evaluating the environmental effects of chemical substances.

## II.E. Production/Processing:

the processing of a chemical substance through the environment, includes source of emissions, amount produced, where and how a substance is produced.

## II.F. Use/Disposal:

contained and dispersed uses of chemical substances and disposal methods. U = use data only, D = disposal data only, X = both use and disposal data



## II.G. Exposure:

release, fate, populations, monitoring and geographic location of chemical and general substances.

## II.H. Economics:

production, distribution, consumption of chemical substances.

## II.I. Regulations/Control:

laws, standards, guidelines.

## III. Publication Information:

features related to the printed source.

## III.A. Publication Type:

- 1 - Handbook
- 2 - Monograph
- 3 - Encyclopedia
- 4 - Index
- 5 - Dictionary
- 6 - Other

## III.B. Supplements:

continuation of the printed resource

## III.C. Freq(uency) of Revision:

related to a time schedule followed for incorporating changes into the text.

- 1 - weekly
- 2 - monthly
- 3 - annually
- 4 - every 2-3 years
- 5 - every 4-5 years
- 6 - infrequent

## III.D. Online Version:

printed source in whole or part is computerized and available interactively.

## IV. Shelf Location:

Most resources are located in the OPTS Technical Information Center (TIC) E447, or EPA Headquarters Library M2404; other sources can be obtained on Interlibrary loan.

IV.A. LC Call Number:

Library of Congress call number is given to help locate the printed sources. The call number is interpreted as follows:

- 1 - a (✓) check after the call number indicates the book is in the TIC.
- 2 - an (\*) asterisk following the call number indicates the book is in the HQ Library.
- 3 - ( ) brackets around the call number indicates an inter-library loan is necessary.

V. Author Index:

Full bibliographic citation.

V.A. Citation Number:

Reference number which leads the user from the Handbooks/Printed Sources Matrix to the author index.

VI. Glossary of Abbreviations:

Definitions of abbreviations and acronyms appearing in the matrices.

## OTS INFORMATION RESOURCES MATRIX—HANDBOOKS/PRINTED SOURCES

TITLE OF PRINTED SOURCE	CHEMICAL ACCESS		OTS DATA CATEGORIES										PUBLICATION INFORMATION				SHELF LOCATION	AUTHOR INDEX
	NO. CHEMICALS	CAS RN	SUBSTANCE IDENTIFICATION	PHYSICAL-CHEMICAL PROPERTIES	HEALTH EFFECTS	ENVIRONMENTAL EFFECTS	PRODUCTION/PROCESSING	USE/DISPOSAL	EXPOSURE	ECONOMICS	REGULATIONS/CONTROL	PUBLICATION TYPE	SUPPLEMENTS	FREQ. OF REVISION	ONLINE VERSION	LC CALL NUMBER	CITATION NUMBER	
ACCIDENT PREVENTION MANUAL FOR INDUSTRIAL ...	*		X	X		X			X			1		6		[T55.83 1974]	317	
ACUTE TOXICTY IN THEORY AND PRACTICE ...	*		X		X				X			2		6		RA1270.P4877/	72	
ADSORPTION OF POLYCHLORINATED BIPHENYL ...	1		X	X		X			X			6		6			195	
ADVANCES IN FORENSIC AND CLINICAL ...	*				X			U	X			1		6		RA1211.C8*	114	
ADVANCES IN MODERN TOXICOLOGY, VOL. 1, PT. 1	*		X		X				X			1		6		RA1199048*	285	
ADVANCES IN MODERN TOXICOLOGY, VOL. 4	*		X		X			U	X			1		6		RL72.D47*	272	
ADVANCES IN MODERN TOXICOLOGY, VOL. 5	*		X	X	X		X	X	X		X	2		6		QH485.C5M87*	155	
ADVANCES IN NEUROTOXICOLOGY	~100		X		X				X			1		6		RC347.J65/	287	
ADVANCES IN PHARMACOLOGY AND ... II, VOL. V																	485	
ADVERSE EFFECTS OF ENVIRONMENTAL ... VOL. 2	*				X				X			2		6		RA1190837/	204	
AEROSOLS, AIRWAYS AND ASTHMA	*		X		X				X			1		6		[RC581.A33 1981]	429	
AGRICULTURAL CHEMICALS AND PESTICIDES ...	*		X	X	X	X					X	1		6	X		148	
AGRICULTURAL RUNOFF MANAGEMENT ...	*					X		U	X			6		6			125	
AIR POLLUTION																	464	
AIR POLLUTION, 3 ED: VOL. I	*		X		X	X		D	X		X	1		6		TD883.S83*	406	
AIR POLLUTION, 3 ED: VOL. II	*				X	X		D	X	X	X	1		6		TD883.S83*	408	
AIR POLLUTION, 3 ED: VOL. III	*							D	X		X	1		6		TD883.S83*	407	
AIR POLLUTION, 3 ED: VOL. IV	*						X	D	X		X	1		6		TD883.S83*	409	
AIR POLLUTION, 3 ED: VOL. V																TD883.S83*	410	
AIR POLLUTION FROM PESTICIDES AND AGRI ...	*		X		X	X	X	X	X	X	X	2		6		TD887.P46A35/	240	
THE AMPHETAMINES: TOXICITY AND ADDIC ...	*		X		X			X				2		6		[RA1242.A6K3]	221	
ANALYTICAL TOXICOLOGY METHODS MANUAL ...	N/A															[RA1221.A5]	400	
ANALYTICAL TOXICOLOGY METHODS MANUAL	*		X									1		6		[RA1221.A5 SUPPL.]	398	
ANIMALS IN TOXICOLOGY RESEARCH, 1ST ED. ...			X		X				X			2				[RA1199.A54 1982]	45	
AN ANNOTATED ACCESSION LIST OF DATA ...																	486	
AN ANNOTATED BIBLIOGRAPHY OF COMPILED ...	*											6		6		QC100.U67/	17	
ANNUAL REVIEW OF PHARM. AND TOXICOLOGY, VOL. 1	*		X	X	X	X			X			6		3		RM18.A83/	142	
ANNUAL REVIEW OF PHARM AND TOXICOLOGY, VOL. 16	*		X		X			U	X			6		3		RM18.A83/	143	
ANNUAL REVIEW OF PHARM. AND TOXICOLOGY, VOL. 17	*		X		X	X			X			6		3		RM18.A83/	144	
ANNUAL REVIEW OF PHARM. AND TOXICOLOGY, VOL. 18	*		X		X							6		3		RM18.A83/	167	
ANNUAL REVIEW OF PHARM. AND TOXICOLOGY, VOL. 19	*		X		X		X	U	X			6		3		RM18.A83/	168	
ANNUAL REVIEW OF PHARM. AND TOXICOLOGY, VOL. 20	*		X		X			U				6		3		RM18.A83/	169	
ANNUAL REVIEW OF PHARM. AND TOXICOLOGY, VOL. 21	*		X		X			U				6		3		RM18.A83/	170	
ANNUAL REVIEW OF PHARM. AND TOXICOLOGY, VOL. 22	*		X	X	X			U	X			6		3		RM18.A83/	171	
AQUATIC AND ENVIRONMENTAL QUALITY: PROBLEMS						X	X	D				1		6		[TD228.N37]	189	
AQUATIC TOXICOLOGY, VOL. I	*		X			X			X			1		6		[QH545.W3A85]	484	
AQUATIC TOXICOLOGY AND HAZARDOUS ASS ...	*		X	X		X			X			6		6		QH545.W3.A95/	69	
AQUATIC TOXICOLOGY AND HAZARDOUS ASS ...	*		X	X		X			X			6		6		QH545.W3.S95/	336	
AQUATIC TOXICOLOGY AND HAZARDOUS EVAL ...	*		X	X		X			X			6		6		QH545.W3.S95/	277	
AQUATIC TOXICOLOGY, PROCEEDING OF 2ND ANNUAL ...	*		X	X		X			X			6		6		QH545.W3S95/	269	
AQUATIC TOXICOLOGY, PROCEEDING OF 3RD ANNUAL ...	*		X	X		X			X			6		6		QH545.W3S95/	140	
AROMATIC HYDROCARBONS MANUFACTURE ...	*		X	X			X	U				1		6		QD341H958E17/	383	
ASSESSING TOXIC EFFECTS OF ENVIRONMENTAL ...	*				X				X			1		6		RA576.A2A87/	241	
ASSESSMENT OF AIRBORNE PARTICLES: FUNDAM ...	*				X				X		X	6		6		[QD549.R59]	290	
ASSESSMENT OF INDUSTRIAL HAZARDOUS ...	*							D	X			6		6			236	
ATMOSPHERIC CHEMISTRY MODELLING	*		X	X					X			6		2			84	
A BASIC TOXICITY CLASSIFICATION OF ...	*		X		X				X		X	1		6		[WN65016016]	208	
BEHAVIOR OF ORGANIC CHEMICALS IN THE ...	~700		X			X			X			1		6		TD427.67.W3*	364	
BEILSTEIN'S HANDBOOK OF ORGANIC CHEM ...	*		X	X								1	X			[GD251.B42B44]	49	

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	NO. CHEMICALS	CAS RN	SUBSTANCE IDENTIFICATION	PHYSICAL-CHEMICAL PROPERTIES	HEALTH EFFECTS	ENVIRONMENTAL EFFECTS	PRODUCTION/PROCESSING	USE/DISPOSAL	EXPOSURE	ECONOMICS	REGULATIONS/CONTROL	PUBLICATION TYPE	SUPPLEMENTS	FREQ. OF REVISION	ONLINE VERSION	LC CALL NUMBER	CITATION NUMBER	
BEILSTEIN'S HANDBOOK OF ORGANIC CHEM ...	*		X	X								1	X			[GD281.B42B46]	50	
BENZENE TOXICITY: A CRITICAL EVALUATION	1		X		X							2		7		[RA1242.B4B48]	237	
BIOCHEMICAL TOXICOLOGY OF ENVIRONMENTAL ...	*		X		X	X						1		6		RA1228.F67/	116	
BIOCHEMISTS' HANDBOOK	*		X	X		X						1		6		REFQD246.L6/	262	
BIOCONVERSION: FUEL FROM BIOMASS	4											6		6		[7784875]	369	
BIODEGRADATION AND DETOXIFICATION OF ...	*		X	X		X		X	X			6		6		QR66.B56/	86	
BIODEGRADATION OF PESTICIDES	61		X	X	X	X			X			6		6		[SB951.146.B54B56]	274	
BIODEGRADATION OF POLYMERS AND ...	*		X			X			X			2		6		QP617.B155/	377	
BIODEGRADATION TECHNIQUES FOR INDUSTRIAL ...	*		X				X	D	X			3				[TD897.5B56]	119	
BIODETERIORATION: 4TH INTL. SYMPOSIUM	*		X			X			X		X	6		6		[QH630.S167]	330	
BIODETERIORATION: 5TH INTL. SYMPOSIUM	*		X						X			1		6		[QH630.S167]	329	
BIODETERIORATION OF MATERIALS, VOL. I	*		X			X			X			6		6		[TA418.74J67]	480	
BIODETERIORATION OF MATERIALS, VOL. II	*		X			X			X			6		6		TA418.74J67*	481	
BIOLOGICAL ABSTRACTS	*		X	X	X	X			X		X	6		2	X	—	56	
BIOLOGICAL MONITORING FOR INDUSTRIAL ...	*		X		X				X			1		6		RB40.L66/	248	
BIOLOGICAL REACTIVE INTERMEDIATES ...	*		X	X	X							1		6		RA1191.B56*	218	
BULLETIN OF THERMODYNAMICS AND ...	*											6				[QD511.T462]	488	
BURGER'S MEDICINAL CHEM, 4TH ED; PTS. I, II, III	*		X	X				U				6		6		RS.403B6/	480	
CRC ATLAS OF SPECTRA DATA AND PHYSICAL ... 2ND ED	26,000		X	X								1		6		[QD291.C18]	162	
CRC HANDBOOK OF ANALYTICAL TOXICOLOGY	~1,338		X	X	X	X					X	1		6		RA1221.C52/	419	
CRC HANDBOOK OF CHEM. AND PHY. 82ND ED.	~20,000		X	X								1		3		QD65.H3/	483	
CRC HANDBOOK OF LABORATORY SAFETY, 2ND ED.	*		X		X				X			1		6		QD61.S88*	403	
CRC HANDBOOK SERIES IN NUTRITION AND FOOD ... VOL. I	*		X		X				X			1		6		[RC620.A1N67]	363	
CRC PERSISTENT PESTICIDES IN THE ENV ...	*				X	X						2		6		QM546.P4E3/	141	
CADMIUM TOXICITY	1				X	X			X			1		6		QV290.C128/	287	
CARCINOGENESIS AND MUTAGENESIS	*		X		X				X			2		6			284	
CARCINOGENESIS TESTING PROGRAM	273		X	X	X		X	U				2		6			304	
CARCINOGEN AND CHRONIC TOXIC HAZARD ...	*		X		X				X		X	2		6		[QP971.S3]	374	
CARDIAC TOXICOLOGY, VOL. I	*		X		X							2		6		RC582.C38/	36	
CARDIAC TOXICOLOGY, VOL. II	*		X		X							2		6		RC582.C38/	37	
CARDIAC TOXICOLOGY, VOL. III	*		X		X							2		6		RC582.C38	38	
THE CARE, HANDLING AND DISPOSAL OF ...	~520		X	X	X			X	X			2		6		[TP.149.B24]	186	
CASARETT AND DOULL'S TOXICOLOGY: THE ...	*		X		X	X		U	X		X	1		6		RA1211.C296	131	
CATALOG OF TERATOGENIC AGENTS, 2ND ED	~600		X		X						1	1		6		QM601.S63	378	
CELLULAR BIOLOGY AND TOXICITY ...	*		X		X			U				1		6		[RD78.3.C45]	152	
CHEM. SOURCE U.S.A.	*		X				X					4		3		[TP12.C44]	11	
CHEMICYCLOPEDIA	*		X	X			X	U		X	X	6		3		[TP12.C46]	3	
CHEMICAL ABSTRACTS	*		X	X	X	X	X	X	X	X	X	6		1	X		9	
CHEMICAL AND ENGINEERING NEWS ...	50		X				X	U		X		6	X	3			238	
CHEMICAL CARCINOGENS	*		X		X							2		6		RC266.BC48*	375	
CHEMICAL COMPOS. IN THE ATMO SPHERE	71,600		X	X								1		6		QC879.B673/	179	
CHEMICAL CONSTITUTIONS, INTERMEDIATE ...	*		X	X			X					2		5		TP910.S82/	106	
CHEMICAL ECONOMIC HANDBOOK	~1,386		X				X			X		1		6		HD9951.A.5.79/	386	
CHEMICAL ENGINEERS' HANDBOOK	*		X	X								1		6		TP151.C52	339	
CHEMICAL HAZARDS TO HUMAN REPRO ...	~25				X			U	X			6		6		QP251.C5	101	
CHEMICAL MARKETING REPORTER	*		X				X	U		X		6		6			372	
CHEMICAL MODELING IN AQUEOUS SYSTEMS	*		X	X		X			X			1		6		QD39.3.M3C48/	217	
CHEMICAL MUTAGENS	*	X	X		X			U				2		6		QH431.F57/	154	
CHEMICAL PROFILES	*		X				X	U		X		6		6			373	
CHEMICAL REFERENCE MANUAL, VOL. I	15K		X	X				D	X	X		6		6		[QD77M130]	266	

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CHEMICAL REGULATION REPORTER, CURRENT ...	*		X						X		X	6		1		[KF3958.A158A7]	28	
CHEMICAL REGULATION REPORTER, HAZARDOUS ...	*		X						X		X	1	X	6		[KF3958.A158A7]	23	
CHEMICAL REGULATION REPORTER, INDEX ...	*	X	X								X	4	X	6		[KF3958.A158A7]	27	
CHEMICAL REGULATION REPORTER, REF ...	*		X	X	X			U	X		X	1	X	6		[KF3958.A158A7]	25	
CHEMICAL REVIEWS	5,800		X	X								1		6			242	
CHEMICAL SAFETY DATA SHEETS	70		X	X	X			U	X		X	1		6		[RA1270.M29]	286	
CHEMICAL STRUCTURE AND PROPERTIES ...	16		X	X	X							6		6			159	
CHEMICAL SOURCE EUROPE	28,000		X				X					4		3		REFTP12.C617*	92	
CHEMICAL STUDIES ON BENCHMARK	*			X								6		6			93	
CHEMICAL TECHNOLOGY: AN ENCYCLOPEDIA ... IV	*		X	X			X	U		X		3		6		TP200.M35*	102	
CHEMICAL WASTE DISPOSAL AND ...								D				1		6			402	
CHEMICAL WEEK 1979 BUYER'S GUIDE ...	*		X	X			X	U		X		1	X	3		[TP12.C43]	278	
CHEMICAL ZOOLOGY, VOL. 1-11	*		X		X	X						1		6		QP514.F528/	156	
CHEMISTRY AND MODE OF ACTION ...	*		X		X	X		U	X			1		6			161	
CHLORINATED INSECTICIDES, VOL. II	*		X		X	X			X			1		6		S8952.C44876	71	
CIS INDEX TO PUBLICATION OF THE U.S. ...	*											1		6		T66.3.H3873	107	
CLINICAL TOXICOLOGY, 2ND ED	*		X	X	X							1		6		[RA1211.P6]	343	
CLINICAL TOXICOLOGY MANUAL	*		X		X		X	U	X			1		6		[RA1211.D393]	117	
CLINICAL TOXICOLOGY OF AGRICULTURAL ...	*		X	X	X	X		U	X		X	1		6		[RH1210.AHW33]	469	
CLINICAL TOXICOLOGY OF COMMERCIAL ...	~17,500	X	X	X	X			U				1	X	6	X	RA1211.G6/	175	
CLINICAL TOXICOLOGY OF DRUGS: PRIN ...	*		X		X	X		X	X			1		6		[RA1238.C54]	389	
COMPREHENSIVE INORGANIC CHEM, VOL. 1-5	*		X	X			X	U				6		6		REFQD161.2C84*	30	
COMPREHENSIVE ORGANIC CHEM, VOL. 1-6	~20,000		X	X								1		6		QD246.C86/	44	
COMPREHENSIVE ORGANOMETALLIC ... VOL. 1-3	*		X	X								1		6		[QD411.C86]	166	
CONCISE CHEMICAL AND TECH. DICTION ...	~52,000		X	X				U				6		6		QD6.B4/	51	
CONDENSED CHEMICAL DICTIONARY	~398,000		X	X	X			U	X		X	6		6		QD6.C5/	191	
CONTAMINANTS & SEDIMENTS, VOL. 1	*		X		X	X		D	X			2		6		TD195.D72C86/	33	
CONTAMINANTS & SEDIMENTS, VOL. 2	*		X	X	X	X			X			1		6		TD195.D72C86/	34	
COPPER IN BIOLOGY AND MEDICINE ...	1				X	X		U	X			2				[QP636.C983]	328	
CRITERIA FOR ORGANOCHLORINE PEST ...	20		X	X	X	X		U	X			1		6		RA1270.P4C74/	291	
CRITERIA FOR A RECOMMENDED ...	~100		X	X	X			X	X			2		6			306	
CRITICAL EVALUATION OF DATA IN ...																QC100.U.5753/	383	
CRITICAL MICELLE CONC. OF AQUEOUS ...	*		X	X								1		6		QC100.U67/	302	
A CRITICAL REVIEW OF RECENT LIT. ON ...	1		X	X		X			X			2		6		[SH.L77C83D88]	130	
CRITICAL STABILITY CONSTANTS, VOL. I	*		X	X								1	X	6		[QD.503M.37]	270	
CRITICAL STABILITY CONSTANTS, VOL. II	*		X	X								1	X	6		[QD.503M.37]	271	
A CRITIQUE OF ACCEPTED REG. AND ...	*		X		X				X		X	6	X				88	
CURRENT APPROACHES IN TOXICOLOGY	*		X		X							1		6		RA1211.C976*	41	
CURRENT CONCEPTS IN CUTANEOUS ...	*		X		X				X		X	1		6		[RL.31.C823]	134	
CURRENT INTELLIGENCE BULLETIN, 19-30	*		X		X	X		U	X		X	6		6		[QD.503.M.37]	311	
CUTANEOUS TOXICITY	*		X		X							6		6		RA1198.C86/	133	
DANGEROUS PLANTS, SNAKES, ARTHROPODS ...			X		X							1		6		[QL100.E44 1978]	146	
DANGEROUS PROPERTIES OF INDUSTRIAL ...	~16,000		X	X	X			U	X		X	1		6		T66.3.H383/	370	
DEGRADATION OF SYNTHETIC ORGANIC ...	87		X		X	X			X			6		6		QP617.B6D44*	314	
DERMATOTOXICOLOGY, 2ND ED.	*		X		X			U			X	2		6		[RL.72.D47 1983]	273	
THE DETECTION AND HAZARDS OF ...	*				X							6		6		TD172.M86	10	
DEVELOPMENTAL AND GENETIC ASPECTS ...	*		X		X	X			X			6		3		RA1198.E8*	137	
DEVELOPMENTAL TOXICOLOGY	*		X		X			U				2		6				
DEVELOPMENTS IN BIODEGRADATION OF ...	*		X	X		X			X			6		6		[QD.306.H6D.302]	462	

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DEVELOPMENTS IN TOXICOLOGY AND ...	*											8	8			RA1199.S96/	477
DICTIONARY OF ORGANIC COMPOUNDS ...	~1,300		X	X								5	X			QD251.D48/*	425
DIRECTORY OF CHEMICAL PRODUCERS ...	~10,000		X				X					6	X	8		TP12.D54/*	367
DISPOSITION OF TOXIC DRUGS AND ...	782		X		X			U	X			1		8		[RA122.B37 1982]	48
DISPOSITION OF TOXIC DRUGS AND ...	782		X		X			U	X			1		8		[RA122.B37 1982]	48
DISPOSITION OF TOXIC DRUGS AND ...	*		X		X			U	X			1		8		[RA1221.B37]	47
DISSOCIATION CONSTANTS OF INORGANIC ...	217		X	X								8				JK416.A3/	338
DISSOCIATION CONSTANTS OF ORGANIC ...	3,790		X	X								6	X			QD273.P35/	337
DOCUMENTATION OF THE THRESHOLD ...	*		X	X	X	X		U		X	X	1				RA1211.A6/	1
DRUG EFFECTS IN HOSPITALIZED ...	*		X		X			U				1		8		[RM282.D88]	298
DRUG INDUCED CLINICAL TOXICITY ...	*		X		X						X	2		8		[RA1238.D784]	282
EASTMAN ORGANIC CHEMICAL BULLETIN	*		X	X	X		X	X				6		2			139
ECOLOGICAL ASPECTS OF TOXICITY TESTING ...	*		X			X			X			8		8		QH918.D4E25/	54
ECOLOGICAL TOXICOLOGY RESEARCH: EFFECTS ...	~50		X	X					X			1		8		QH545.M45N37/	280
ECONOMIC ANALYSIS OF EFFLUENT ...	~100						X			X		8		8			20
EFFECTS AND DOSE RESPONSE RELATIONSHIPS ...	*		X		X			U				8		8		RA1231.M52E33*	321
EFFECTS OF CHRONIC EXPOSURE TO ...	*		X		X				X			1		8		[RA1270.P4E34 1983]	87
EMERGENCY HANDLING OF HAZARDOUS ...	*		X	X					X			1		8		[T55.3H3AAR]	415
ENCYCLOPEDIA OF CHEMISTRY	*		X	X								3		8		QD5.E58/	188
ENCYCLOPEDIA OF CHEMICAL TECHNOLOGY	*	X	X	X	X		X	U	X	X	X	3		8		TP9.E085/	183
ENCYCLOPEDIA OF ENVIRONMENTAL SCIENCE ...	*		X	X	X	X		X	X			3		8		TA170.E5*	340
ENCYCLOPEDIA OF OCCUPATIONAL ...	*		X	X	X		X	U	X			3		8		[RC983.J8]	211
ENCYCLOPEDIA OF POLYMER SCIENCE AND ...	*		X	X			X	U		X		3		8		TP156.P8E5/	268
ENERGY FROM BIOCONVERSION OF ...	*		X				X	D		X		8		8		TP782.D47/	118
ENVIRONMENT AND BIRTH DEFECTS	*		X		X							2		8		RD152.W5/	478
ENVIRONMENT REPORTER	*		X						X		X	6		1		KF3775.A6E48*	28
ENVIRONMENTAL AND OCCUPATIONAL ...	*		X	X	X			U	X		X	1		8		QM881.S63/	381
ENVIRONMENTAL CHEMISTRY	*		X						X			6		8		[QD31.2M38]	282
ENVIRONMENTAL ENGINEER'S HANDBOOK	*		X	X	X	X	X	X	X	X	X	1		8		TD145.E57*	251
ENVIRONMENTAL FATE AND ...	~12		X	X		X			X			8		8			257
ENVIRONMENTAL HAZARDS OF METALS: ...	*		X	X	X				X			2		8		RA1231.M52B8813	88
ENVIRONMENTAL HEALTH CRITERIA	*		X	X	X			X	X			2		8			467
ENVIRONMENTAL ISSUES REPORT 10	5					X						6		8		GF75.E88/	202
ENVIRONMENTAL LAW REPORTER	*										X	6		8			354
ENVIRONMENTAL POLLUTION AND TOXICOLOGY	*					X						2		8			352
ENVIRONMENTAL SCIENCE RESEARCH ...	*		X		X				X			6		8		RA1216.R58/	488
ENVIRONMENTAL TOXICOLOGY: PRINCIPLES ...	*		X		X	X			X			6		8		[RA1191.E58]	394
ENZYMATIC BASIS OF DETOXIFICATION, VOL. 1	*		X									2		8		QP601.E515/	212
ENZYMATIC BASIS OF DETOXIFICATION, VOL. 2	*		X	X	X							2		8		QP601.E515/	213
EPIDEMIOLOGY AND DETECTION OF ...	1		X		X	X		U	X		X	1		8		[RA1231.L4E84]	188
ESSAYS IN TOXICOLOGY, VOLS. 1-7	*		X		X							2		8		RA1190.E77/	193
ESSAYS IN TOXICOLOGY, VOL. 1	*		X		X	X		U	X			6		8		RA1190.E77/	57
ESSENTIALS OF TOXICOLOGY	0				X				X			1		8		RA1211.L8/	253
EVALUATION OF TOXICOLOGICAL DATA ...	*		X		X	X		U	X			6		8		RA1199.C64/	206
EXPERIMENTAL AND CLINICAL ...	*		X	X	X	X	X	U				3		8		RC347.E89/	397
FAO INVENTORY DATA ON ...	*					X						6		8		[SH1.F8716]	148
FAITH, KEYES AND CLARK'S INDUSTRIAL ...	140		X	X			X			X	X	1		8		TP200.F3/	255
FATE OF POLLUTANTS IN THE AIR ... PART 1	*								X			6		8		TD180.A38/	417

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FATE OF POLLUTANTS IN THE AIR ... PART 2	*		X		X	X			X			6	6			TD180.A38/	418
FATE OF SELECTED PESTICIDES IN THE ...	22				X	X			X			6	6				388
FENAROLI'S HANDBOOK OF FLAVOR ...	~200		X					U			X	1	6			TP450.F36*	182
FIFTEEN JAAR ZELFVERGIFTIGINGEN IN ...	*		X		X				X			6	6			ISBN 90 6203-089-0	428
FINAL TREATMENT: THE FILE ON DR. X	1				X							6	6			[RA1228.L53]	247
FINDING FUNGICITY FEASIBLE	*		X	X		X			X		X	6	2				260
FLUORINE AND DENTAL HEALTH: THE ...	1		X		X			U	X		X	6	6			[QP981.F55M8]	301
FORENSIC TOXICOLOGY	*		X		X	X			X			6	6			[RA1228.F67]	40
FORENSIC TOXICOLOGY: CONTROLLED ...	*		X		X							6	6			[HV8473.L76]	251
FORENSIC TOXICOLOGY FOR THE LAW ...	*		X		X							1	6			[RA1228.W64]	473
FORENSIC TOXICOLOGY: PROCEEDINGS ...	~350		X		X			U			X	1	6			[RA1228.J67]	327
FUNCTION TOXICITY OF ANESTHESIA	~40		X		X			U	X			2	6			[RA1270.A63876]	79
FURTHER STUDIES IN THE ASSESSMENT ...	*		X		X				X			6	X	6			90
GLOBAL CHEMICAL CYCLES AND THEIR ...	*		X			X			X			1	6			QES16.D25*	418
THE GOLDFISH AS A TEST ANIMAL ...	*		X		X				X			3	6			[QP941.P8]	345
GOOD LABORATORY PRACTICE: TOPICS ...	*								X			6	6			[RA1199.06 1979]	333
GOVERNMENT CONTRACTS GUIDE	*		X								X	3	6			[KF840.C6]	178
GUIDELINES FOR ANALYTICAL ...	*		X	X	X						X	1	6			RA1221.G84/	424
GUIDELINES FOR ENVIRONMENTAL ...	*		X	X		X			X			6	6			TX501.J47*	230
HANDBOOK FOR OBTAINING CHEMICAL USE ...	*																380
HANDBOOK OF ADHESIVES	*		X	X			X	U		X		1	6			TP988.S58*	388
HANDBOOK OF CHEMICAL PROPERTY ESTIMATION ...	*		X	X								1	6			[QD271.L95]	259
HANDBOOK OF EMERGENCY TOXICOLOGY	188		X	X	X			U				1	6			[RA1211.K3]	224
HANDBOOK OF EMERGENCY TOXICOLOGY: A GUIDE ...	*		X	X	X							1	6			[RA1211.K3]	225
HANDBOOK OF ENVIRONMENTAL CONTROL (CRC)	*		X	X	X	X	X	X	X		X	1	6			TD146.C2/	58
HANDBOOK OF ENVIRONMENTAL ... ORGANIC CHEMICALS	~1,000		X	X	X	X	X	X	X		X	1	6			TD196.073V47/	448
HANDBOOK OF EPOXY RESINS	*		X	X	X							1	6			[TP1180.E8L4]	239
HANDBOOK OF FINE CHEMICALS	~12,000		X	X	X		X	D		X	X	1	4				7
HANDBOOK OF IDENTIFIED CARCINOGENS AND ...	~800		X	X	X				X			1	6			RC288.B.C725/	383
HANDBOOK OF INDUSTRIAL TOXICOLOGY	*		X	X	X			U	X		X	1	6			RA1216.P55/	342
HANDBOOK OF INTERNATIONAL FOOD ... VOL. I	*					X					X	1	6			[RA1270.F6V47]	450
HANDBOOK OF INTERNATIONAL FOOD ... VOL. II	*		X		X			U	X		X	1	6			[RA1270.P4V47]	451
HANDBOOK OF OCULAR TOXICITY	*		X		X		X	U			X	1	6			[RE901.T87564]	390
HANDBOOK OF POISONING: DIAGNOSIS ...	*		X	X	X			U				1	6			RA1211.D77/	132
HANDBOOK OF REACTIVE CHEMICAL ...	~7,000		X	X								1	6			T55.3.H3373/	70
HANDBOOK OF SOLVENTS	*		X	X	X		X	U	X	X	X	1	6			TP247.5.S32*	371
HANDBOOK OF TABLES FOR ORGANIC COMPS ...	78,150		X	X								1	6			BKS QD291.R28.1987*	348
HANDBOOK OF TOXIC AND HAZARDOUS ...	~600		X	X	X			X	X		X	1	6			RA1193.S58/	387
HANDBOOK OF TOXICOLOGY, ACUTE, VOL. I	~2,383		X		X				X			1	6			[RA1211.H32]	391
HANDBOOK OF TOXICOLOGY, ANTIBIOTICS, VOL. II	340		X	X	X			U	X			1	6			RA1211.H32/	396
HANDBOOK OF TOXICOLOGY, INSECTICIDES, VOL. III	184		X	X	X	X		U	X			1	6			[RA1211.H32]	319
HANDBOOK OF TOXICOLOGY, FUNGICIDES, VOL. IV	196		X	X	X	X		U	X			1	6			[RA1211.H32]	125
HANDBOOK OF VAPOR PRESSURES AND HEATS ...	*		X	X								1	6			[QD305.H5W54]	474
HANDBOOK OF WATER SOLUBLE GUMS ...	*	X	X	X	X	X	X	U	X		X	2	6			TP978.H28/	115
THE HANSCH APPROACH	*		X	X	X	X			X			2	6			QD1.A356/	177
HAZARDOUS AND TOXIC EFFECTS OF ...	*		X		X				X		X	1	6			RA1229.S57/	385
HAZARDOUS CHEMICALS DATA	*		X	X	X				X		X	1	6			[T55.3.H398]	305
HAZARDOUS CHEMICALS DATA BOOK	~400		X	X	X	X	X		X		X	1	6			T55.3.H3H398/	487

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HAZARDOUS MATERIALS: EMERGENCY ...	43		X	X	X	X		D	X			1		8		[T55.3.H3455]	316	
HAZARDOUS MATERIALS GUIDE: SHIPPING ...	*		X								X	1		8		[KF3945.K44]	228	
HEALTH HAZARD EVALUATION SUMMARIES	*		X		X		X		X		X	8		8		RA1242.B.43W281*	312	
HERBICIDES: CHEMISTRY, DEGRADATION ... VOL. I	*		X	X	X	X		U				1		8		SB851.A.K4/	226	
HERBICIDES: CHEMISTRY, DEGRADATION ... VOL. II	*		X			X		U	X			8		8		SB851.A.K4*/	227	
HOW TO DISPOSE OF TOXIC SUBSTANCES ...	*						X	X		X	X	1				TD897.P88*/	348	
THE I/O-CHARACTERS TO DESCRIBE ...	7		X	X		X			X			8		8			275	
IMMUNOLOGIC CONSIDERATIONS ... VOL. I & II	*		X		X	X			X			1		8		QR188.35.J46/	378	
IMPORTS OF BENZENOID CHEMICALS ...	*		X				X	U		X		8		8		TP953.J4*	443	
INDEX HANDBOOKS OF OTOTOXIC ...	*		X		X			U	X			4		8		[RF285.083153]	482	
INDUSTRIAL AND ENVIRONMENTAL ...	~210				X							1		8	X	[RA1191.J53]	157	
INDUSTRIAL CONTROL EQUIPMENT ...	*		X	X	X	X		U	X	X		1		8		TD885.B86*	81	
INDUSTRIAL HYGIENE AND ... VOL. II	*		X	X	X			U	X			1		8			149	
INDUSTRIAL WASTE DISPOSAL	0							D	X		X	8		8		TD897.P87*	382	
INFORMATION RESOURCES IN TOXICOLOGY	*				X	X			X		X	8		8		[RA1193.A.W49]	489	
INTERNATIONAL ENCYCLOPEDIA OF ...	~50		X		X							1		8		[QP631.P48]	350	
INTERNATIONAL ENVIRONMENT REPORTER	*		X								X	8		2		[JD169.1573]	24	
INTERNATIONAL SYMPOSIUM ON ...	*				X							1		8		RA401.M15	358	
INTRODUCTION TO BIOCHEMICAL ...	*		X		X				X			1				RA1218.J55/	201	
INTRODUCTION TO ENVIRONMENTAL ...	*		X		X	X	X	X	X		X	8		8		QH545.A11575*	184	
INTRODUCTION TO FORENSIC TOXICOLOGY ...	*		X		X							8		8		[RA1228.J58]	111	
KINGZETT'S CHEMICAL ENCYCLOPEDIA	*		X	X			X	U				3		8		[QDS.K4 1988]	194	
KIRK-OTTMER ENCYCLOPEDIA, 2ND ED.	*		X	X	X		X	X	X	X	X	3	X	8		TP9.E885/	401	
KLINE GUIDE TO THE CHEMICAL ...	~300						X	U		X	X	1		8		HD9851.AK57	283	
KLINE GUIDE TO THE PLASTICS ...	*		X				X	U	X	X	X	1				HD9851.U82C48/	351	
KLINE GUIDE TO THE PULP & PAPER ...	*		X				X	U	X	X	X	1				HD9825.N82/	205	
LABOR. 29 CFR 1911.1 VOL. 29 PTS 911 ...	0										X	8		3		QD561.P45/	323	
LABOR. 29 CFR 1920.1 VOL. 29 PTS 120 ...	0										X	8		3		QD561.P45/	324	
LABORATORY MODEL ECOSYSTEM STUDIES ...	*		X	X		X			X			1		8			295	
LABORATORY WASTE DISPOSAL MANUAL ...	1,121		X	X								1		8		QD5.E58/	406	
LANGE'S HANDBOOK OF CHEMISTRY ...	4,000		X	X								1		1		QD85.LA/	121	
LEAD TOXICITY	1		X		X				X			2		8		RA123814L43*	379	
LIGNIN BIODEGRADATION & TRANSFER	1		X			X						1		1		[QK898.L5C7]	113	
LIGNIN BIODEGRADATION: MICROBIOLOGY ...	*		X	X		X						8				[T5933.L5L6]	233	
MANAGEMENT OF TOXIC SUBSTANCES ...	*		X		X	X			X			8		8		BKS QH545.AIM353/	108	
MAHNSVILLE CHEMICAL PRODUCTS ...	205		X	X	X		X	U	X	X		1		8			263	
MATERIALS HANDBOOK. AN ENCYCLOPEDIA ...	*		X	X								1		8		TA403.875/*	87	
MECHANISM OF TOXIC ACTION IN SOME ...	*		X		X				X			8		8		RA1190.E8/	89	
MECHANISMS OF ACTIONS OF NEUROTOXIC ...	~30		X		X	X		U	X			2		8		[RC347.M42]	347	
MECHANISMS OF TOXICITY AND ...	*		X		X				X			8		8		RM21.I58/	223	
MECHANISMS IN RESPIRATORY TOXICOLOGY	*		X		X							1		8		[RC732.M43 1982]	478	
MEMBRANE TOXICITY	*				X							8		8		[RA1199.R82]	297	
MERCK INDEX	~10,000	X	X	X	X							3		8		[R551.M4 1986]	292	
METABOLIC INHIBITORS: A COMP ...	*		X		X				X			1		8		QP801.A85H83/	186	
METABOLISM	*		X	X	X	X		X	X			1		8			8	
METABOLISM OF PESTICIDES	*		X		X	X						1		8		[SK381.A256 NO.127]	288	



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METABOLISM OF PESTICIDES: AN UPDATE	*		X		X	X						1		0		[SK381.A256 NO.184]	288
METABOLISM OF VOLATILE ANESTHETICS ...	*		X	X	X				X			1		0		[RD82.C84]	104
METAL TOXICITY IN MAMMALS. VOL. 1 & 2 ...	*				X			U	X			0		0		RA1221.M62L82*✓	258
METHODOLOGY FOR ANALYTICAL TOX ...	~51		X		X							1		0		RA1221.H36 1975*	420
METHODS FOR ECOLOGICAL TOXICITY ...						X						0		0		QH641.15T88M47*✓	185
METHODS IN TOXICOLOGY	0											0		0		RA1221.M45*✓	331
METHODS USED IN USSR FOR ...	*		X		X						X	0		0		[QK357.F72]	454
MIDDLE MOLECULES IN UREMIA ...	*		X	X	X							0	X	0		[RC915.S95 1980]	235
MIDWEST RES. INST. LOADING FUNCTIONS ...	*		X						X			1		0			279
MODEL ECOSYSTEM FOR THE EVALUATION	~20		X	X		X			X			0		0			280
MODEL ECOSYSTEM STUDIES OF THE ...	*		X			X		U	X			0		0			294
MODELING NONPOINT POLLUTION FROM ...	*								X		X	0		0			127
MODERN TRENDS IN TOXICOLOGY, VOL. 2	*		X		X	X			X			1		0			85
MOLECULAR BASIS OF BIOL. DEGRADATIVE ...	*				X							2		0		[QP609.P78M84]	52
MOLECULAR BASIS OF ENVIRON. TOXICITY	*		X		X	X						2		0		RA1191.M84✓	55
NATIONAL OCCUPATIONAL HAZARD ... VOL. II												1		0			308
NEPHROTOXIC MECHANISMS OF DRUGS ...	~100		X		X				X			0		0		[RC918.R4M46 1982]	344
NERVOUS SYSTEM TOXICOLOGY ...	*		X		X							0		0		[RC347.M47]	299
NEUROTOXICITY OF THE VISUAL SYSTEM	~20		X	X	X				X			1		0		[RE91.R83]	293
NEUROTOXICOLOGY	*		X		X			U				0		0		[RC346.M46]	360
NICKEL TOXICOLOGY	~1		X	X	X			U	X			0		0		[RA1231.M44157]	76
NITROGEN, PHOSPHORUS AND SULPHUR ...	*		X			X			X	X		3				[QH344.M57]	421
NON-AQUEOUS ELECTROLYTE HANDBOOK, VOL. I	210		X	X								1		0		QD580.J36✓	215
NON-AQUEOUS ELECTROLYTE HANDBOOK, VOL. II	310		X	X								1		0			216
NON-FLUORINATED PROPELLANTS AND ...	8		X	X	X			U	X			0		0		[RA1270.S6A84]	21
NON-POINT SOURCE MODEL: LOADING ...	*		X						X			1		0			437
NON-POINT SOURCE MODEL: MODELING NON ...	*								X		X	0		0			436
NON-POINT SOURCE MODEL: SIMULATION OF ...	*		X						X		X	1		0			439
NUTRITION AND THE BRAIN VOL. IV	*		X	X	X	X						0				[WLN08632.V.4.]	483
NUTRITIONAL TOXICOLOGY VOL. I	*		X	X	X	X		U	X			1		0		[RC622N894 1982]	190
NUTRITION STRESS AND TOXIC CHEMS ...	*			X					X			2		0		[RB151.V33]	445
OPD CHEMICAL BUYERS DIRECTORY 69 ED	14,744		X				X					0		3		TP12.06✓	322
OCCUPATIONAL DISEASES: A GUIDE	*		X	X	X			U	X		X	1		0		RC984.M37	310
OCCUPATIONAL EXPOSURE GUIDE	*		X		X				X		X	1		0		[KF3570.K45]	229
OCCUPATIONAL HEALTH GUIDELINES ...	*		X	X	X			X	X			1		0		TD55.3.H3N564✓	261
OCCUPATIONAL SAFETY & HEALTH REPORTER	*		X						X		X	0		1		[KF3570.A1025]	28
ON THE EVALUATION OF THE ... IARC	~600	X	X	X	X		X	U	X	X	X	2	X	0		RC268.57.I.57	209
ORGAN DIRECTED TOXICITY. CHEMICAL ...	*		X		X			U	X			0		0		RA1191.594 1981✓	74, 75
ORGANIC CHEMICAL PROCESS ENCYCLO ...	*		X					U				3		0		TP690.556 1968✓	381
PARENT COMPOUND HANDBOOK	*	X	X									1	X	4		QD281.R5P32✓	80
PARIKHS TEXTBOOK OF MEDICAL ...	*	X			X				X			2		0		RA1051.P34✓	335
PARTITION COEFFICIENT AND BIOACCUMULATION	34			X		X						0		0			94
PARTITION COEFFICIENTS AND THEIR USES	*		X	X								1		0			243
PARTITION COEFFICIENTS TO MEASURE ...	8		X	X		X			X			0		0			318
PATHOLOGY OF OXYGEN TOXICITY	1		X		X	X						1		0		[RA124.09834]	39
PATTY'S INDUSTRIAL HYGIENE & TOXICOL. I	*		X		X			U	X			1		0		RC987.P37. 1978✓	97
PATTY'S INDUSTRIAL HYGIENE & TOXICOL. IIA	*		X	X	X		X	U	X			1		0		RC987.P37 1978✓	98

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PATTY'S INDUSTRIAL HYGIENE & TOXICOL. HB	*		X	X	X		X	U	X			1		6		RC967.P37 1978/	98	
PATTY'S INDUSTRIAL HYGIENE & TOXICOL. HC	*		X	X	X		X	U	X			1		6		RC967.P37 1978/	109	
PATTY'S INDUSTRIAL HYGIENE & TOXICOL. HI	*											1		6		RC967.P37 1978/	110	
PERSPECTIVES IN TOXICOLOGY	*		X		X							1		6		QP631.P46/	53	
PESTICIDE CHEMIST & MODERN TOXICOLOGY	*				X						X	6		6		TP248.P47 P46/	42	
PESTICIDE TRANSPORT AND RUNOFF ...	*		X						X		X	6		6			112	
PESTICIDES ABSTRACTS	*		X		X	X		X	X		X	6	X	6	X		434	
PESTICIDES IN THE ENVIRONMENT, VOL. I PT I	*		X					U	X			6		6		SB951.W62*	470	
PESTICIDES IN THE ENVIRONMENT, VOL. II	*		X					U	X			6		6		SB951.W62*	471	
PESTICIDES IN THE ENVIRONMENT, VOL. III	*		X					U	X			6		6		SB951.W62*	472	
PHARMACOLOGICAL METHODS IN TOXICOLOGY	*		X		X				X			3		6		RA1238.P46*	487	
PHYSICAL AND THERMODYNAMIC PROPERTIES	722		X	X								2	X	6		QD306.A4.W39/	475	
A PHYSICAL CONCEPT OF SOIL-WATER ...	~20		X	X		X			X			6		6			96	
PHYSICAL PROPERTIES OF CHEMICAL I, II, III ...	~1,400		X	X								1		6		QD473.D73/	136	
PHYSICAL PROPERTIES OF MOLECULAR ...	*		X	X								1		6		[QD478.B62]	58	
PHYSICIANS' DESK REFERENCE ...	*		X	X	X		X	U	X		X	1	X	3		RS75.P5/	32	
PHYSICS AND CHEMISTRY OF ORGANIC ...	*		X	X								1		6		[QD906.F79]	158	
PHYSIOCHEMICAL PROPERTIES OF SOME ...	6		X	X	X	X			X			1		6			186	
POISONING: DIAGNOSIS AND TREATMENT	~7,100		X		X				X			1		6		RA1211.M613/	300	
POISONING: DIAGNOSIS AND TREATMENT	*				X			U			X	1		6			444	
POISONS — ANTIDOTES AND ANECDOTES	*				X			U			X	1		6		[RA1213.T65]	426	
POLLUTION DETECTION AND MONITORING ...	*				X	X						6		6		TD896.S57*	382	
POLYNUCLEAR AROMATIC HYDROCARBON ...	*		X	X	X				X			6		6		RC288.5.C36/	219	
POTENTIAL IND. CARCINOGENS & MUTA. VOL. 4	>178	X	X		X		X	U	X			1		6		RC288.6.F67*	163	
PREDICTING BIOLOGICAL EFFECTS AS A ...	25		X	X	X				X			1		6			13	
PREDICTING PESTICIDE RUNOFF FROM ...						X			X			6		6			31	
PREDICTION OF BIOCONCENTRATION ...	16		X	X		X			X			6		6			358	
PREDICTION OF CHRONIC TOXICITY ...	*		X	X	X	X			X			6		6		RA1190.E8/	138	
PREDICTIVE TOXICOMETRICS	*		X	X	X			U				1		2		RC143.B69	63	
PRELIMINARY ASSESSMENT OF SUSP ...	263		X		X				X			2		6		[RA692.A1U53]	436	
PRINCIPLES AND METHOD OF TOXICOLOGY	*											1		6		[RA1211.P74]	192	
PRINCIPLES AND PROCEDURES FOR EVAL ...												1		6		RA1199.37/	100	
PRINCIPLES OF BIOCHEMICAL TOXICOLOGY	*				X				X			2		6			427	
PRINCIPLES OF GENETIC TOXICOLOGY	*				X							1		6		QH465.C5878/	80	
A PRIORI PREDICTIVE METHODS OF ...	0											6		6		[TD462.C66 1977] EHA	234	
PRIORITY TOXIC POLLUTANTS: HEALTH ...	129		X	X	X	X		U	X		X	3		6		RA1193.P74/	386	
PROC. OF THE 1ST INTER. CONG. ON TOXICOL.	*		X		X	X			X		X	6		6		RA1191.J6/	341	
PROC. INHALATION, TOXICOL. & TECHNOLOGY SYM.	*		X		X				X			6		6		RA1270.A34154/	245	
PROC. OF THE INT'L COURSE ON THE ...	*											1		6		[RA1211.P74]	183	
PROGRAM AND ABSTRACTS SYMP. ON ...	*					X			X			6		6			173	
PROGRESS IN CHEMICAL TOXICOLOGY, 5 VOLS.	*		X		X			U	X			1		6		RA1221.P75*	413	
PROGRESS IN TOXICOLOGY, VOL. I	~5		X		X							1		6		RA1238.234	486	
PROGRESS IN TOXICOLOGY, VOL. II	0											1		6		RA1238.234	486	
PROTECTION OF ENVIRONMENT 40CFR 1.1, VOL. 40	*								X		X	6		3		QD561.P54	440	
PROTEIN DEFICIENCY AND PESTICIDE ...	~20		X		X				X			1		6		[RC627.P7889]	64	
THE PROPERTIES OF GASES & LIQUIDS ...	*		X	X								1		6		TP242.R4	357	
PULMONARY TOXICOLOGY OF RESPIRABLE ...	*		X	X	X				X			6		6		RC756.H3	389	
QUALITY CONTROL IN TOXICOLOGY	0										X	1		6		[RA1199.Q3]	332	
QUANTITATIVE TOXICOLOGY	*		X	X	X				X		X	2		6		BKS RA1229.Q3613	151	

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QUICK REFERENCE TO CLINICAL TOXICOLOGY	*		X	X	X			U	X			1		6		[RA1211.Q63]	187	
RADIOLOGY IN CLINICAL TOXICOLOGY	*		X		X			U	X			1		6		[RA1223.R33.A67]	14	
A RAPID METHOD FOR ESTIMATING LOG p...	~50			X								6		2			446	
REGISTRY OF TOXIC EFFECTS OF CHEMICAL ...	168,096	X	X	X	X				X		X	1		3	X	RA1221.U65/	313	
REPRODUCTIVE HAZARDS OF INDUSTRIAL ...	48		X		X			U	X		X	1		6			43	
RESEARCH PROGRAM ON HAZARD ...	88					X			X			6				PB 263 162*	348	
REVIEW OF THE ENVIRONMENTAL FATE ...	74		X	X	X	X	X		X			1		6			73	
REVIEWS IN BIOCHEMICAL ... VOL. I	*		X	X	X							1		3			197	
REVIEWS IN BIOCHEMICAL ... VOL. II	*		X	X	X							1		3			198	
REVIEWS IN BIOCHEMICAL ... VOL. III	*		X		X							1		6		[BKS RA1221.H6]	199	
REVIEWS IN BIOCHEMICAL ... VOL. IV	*		X	X	X							1		3			200	
ROOD'S CHEMISTRY OF CARBON CMPOS.	*		X	X								3		6		QD261.R62*	103	
THE ROLE OF TERRESTRIAL AND AQUATIC ...	*					X						2		6		[QX811.B7A36 NO.17]	12	
SAFETY EVALUATION OF CHEMICALS IN FOOD ...	38		X		X						X	1	X	6		Z7891.J57V47/	452	
SCIENTIFIC CONSIDERATIONS IN MONITORING ...	0											1		6		RA1199.S34/	180	
SECOND TOP 50 CHEMICAL COMPANIES ...	0						X			X		6	X	3		ISSN:0009-2347	414	
SELECTED CONSTANTS: OXIDATION-REDUCTION ...	~350		X	X								1	X	6		[QD63.D9C63]	91	
SELECTED VALUES OF CHEMICAL THERMODYNAMIC ...	*		X	X								1		6		QD155.5.U685/	468	
SELECTIVE TOXICITY AND RELATED TOPICS ...	*		X		X							6		6		RM262.A6 1973*	4	
SELECTIVE TOXICITY, THE PHYSICO-CHEMICAL ... 5TH ED.	*		X	X	X	X		U	X			1		6		RM262.A6 1973*	5	
SELECTIVE TOXICITY, THE PHYSICO-CHEMICAL ... 6TH ED.			X	X	X			U	X			1		6		[RM262.A6 1979]	6	
SIMULATION OF NUTRIENT LOADINGS IN ...	*		X						X			1		6			128	
SOLID WASTES: ORIGIN, COLLECTION, ...	*							D	X		X	1		6		BKS TD697.M38*	268	
SOLUBILITIES OF INORGANIC AND METAL-ORGANIC ... VOL. I	~100		X	X								1		6		QD68.L5*	249	
SOLUBILITIES OF INORGANIC AND METAL ... VOL. II	~100		X	X								1		6		QD68.L5*	250	
SOLUBILITIES OF INORGANIC AND ORGANIC ...	*		X	X								1		6		[QD643.N72 1963]	404	
SORPTION OF HYDROPHOBIC POLLUTANTS ON ...	10			X					X			6		6			222	
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SPECIFICATIONS FOR THE IDENTITY AND PURITY ...	~210		X		X				X			2		6			147	
STANDARD OPERATING PROCEDURES IN ...	*								X			1		6		BKS RA1199.57*	334	
STANDARD OPERATING PROCEDURES IN VITRO ...	*								X			1		6		ISBN:0-8391-4124-6	423	
STORAGE AND DISPOSAL OF DANGEROUS ...	*			X				D	X		X	6		2			463	
STRUCTURE-ACTIVITY CORRELATIONS ...	*		X	X	X	X						1		6		TD370.V3*	447	
STRUCTURE-ACTIVITY RELATIONSHIPS ...	14			X		X						6		6		TD370.V3/	448	
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A STUDY OF HAZARDOUS WASTE MATERIALS ... VOL. 2	13		X	X	X	X	X	X	X			6		6			61	
A STUDY OF HAZARDOUS WASTE MATERIALS ... VOL. 3	12		X	X	X	X	X	X	X	X		6		6			62	
A STUDY OF INDUSTRIAL DATA ON CANDIDATE ...	667		X		X		X	U	X	X		6		6		[TP9.58]	366	
SURFACTANT BIODEGRADATION	*		X			X			X			1		6		TP994.S96*	422	
SURVEY ANALYSIS AND SUPPLEMENTAL ...	7,000		X						X		X	1		6			309	
SURVEY MANUAL	~1,200		X								X	1		6	X		307	
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SURVEY OF CONTEMPORARY TOXICOLOGY ...	*		X	X	X	X		U	X			1		6		RA1211.S93~/	431	
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SYNTHETIC ORGANIC CHEMICALS	*		X				X			X		1		3		[HD9999.D9U6]	442	

## OTS INFORMATION RESOURCES MATRIX—HANDBOOKS/PRINTED SOURCES

TITLE OF PRINTED SOURCE	CHEMICAL ACCESS		OTS DATA CATEGORIES										PUBLICATION INFORMATION				SHELF LOCATION	AUTHOR INDEX
	NO. CHEMICALS	CAS RN	SUBSTANCE IDENTIFICATION	PHYSICAL-CHEMICAL PROPERTIES	HEALTH EFFECTS	ENVIRONMENTAL EFFECTS	PRODUCTION/PROCESSING	USE/DISPOSAL	EXPOSURE	ECONOMICS	REGULATIONS/CONTROL	PUBLICATION TYPE	SUPPLEMENTS	FREQ. OF REVISION	ONLINE VERSION	LC CALL NUMBER	CITATION NUMBER	
TLVS THRESHOLD LIMIT VALUES FOR ...	~900		X	X	X			U	X		X	1	X	3		[RC963.3A64]	2	
THERMOCHEMISTRY OF ORGANIC AND ...	*		X	X								1		8		QD511.C88*	109	
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TOXICITY OF CHEMICALS AND PULPING ...	*					X			X			8		8		[SH177W64L68]	254	
TOXICITY OF HEAVY METALS ... PT. 1	~25				X	X			X			8		8		RA1231.M62T89✓	328	
TOXICITY OF HEAVY METALS ... PT. 2	~50				X	X			X		X	8		8		RA1231.M62T89✓	78	
TOXICITY OF INDUSTRIAL METALS	45		X	X	X			U	X			1		8		[RA1231.M6287]	325	
TOXICITY OF PLUTONIUM, AMERICIUM ...	3		X	X	X			U	X			2		8		[RA1231.R55M46]	320	
TOXICITY OF PURE FOODS	*		X		X			U				1		8		[RA1258.888]	65	
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TOXICOLOGICAL AND PATHOLOGICAL STUDIES ...	*		X	X	X				X			2		8		[RA1228.G87]	178	
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TOXICOLOGY: MECHANISMS ... VOL. 2	*		X		X				X			1		8		RA1211.573*	412	
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## Glossary of Abbreviations

ACS:	American Chemical Society
AD:	Assessment Division
ADCR:	Automated Document Control Register System
AEROS:	Aerometric and Emission Reporting System
AGRICOLA:	Agricultural Online Access
AIS:	Section 8(a) Asbestos Information System
APILIT:	Index to American Petroleum Institute Abstracts of Refining Literature
APIPAT:	Index to American Petroleum Institute Patents
APTIC:	Air Pollution Technical Information Center
AQUATOX:	Columbia National Fisheries Research Laboratory Data
AQUIRE:	Aquatic Toxicity Data File
ARM:	Agricultural Runoff Model-Version II
ASFA:	Aquatic Sciences and Fisheries Abstracts
ASI:	American Statistical Index
ASTM:	American Society for Testing and Materials
ATM:	Atmospheric Transport Model
BBIP:	BRS-Books in Print
BEHAVIORTOX:	Behavioral Effects Data File
BETS:	Basic Extramural Tracking System
BHRA FLUID ENGINEERING:	British Hydromechanics Research Association
BIOL:	Biological Sciences Information Service
BIOSIS:	Biological Sciences Information Service
BMDPS:	Bio-Medical Statistical Package
BPS:	Budget Planning System
BRS:	Bibliographic Retrieval Services
CA-CON:	Chemical Abstracts Condensates
CA SEARCH:	Chemical Abstracts Service Search
CAB ABSTRACTS:	Commonwealth Agricultural Bureaux Abstracts
CAB:	Commonwealth Agricultural Bureaux Abstracts
CANCERLIT:	Cancer Literature Information Online



CANCERPROJ:	Cancer Literature of Ongoing Research Projects
CAS:	Chemical Abstracts Services
CBI:	Confidential Business Information
CBDS:	Carcinogenesis Bioassay Data Systems
CCAS:	Central Chemical Assessment File
CCD:	Chemical Control Division
CCS:	Chemical Collection System
CDI:	Comprehensive Dissertation Index
CEB:	Chemical Engineering Branch
CECATS:	CHIB Existing Chemical Tracking System
CEER:	Consumer and Environmental Exposure Report
CFB:	Chemical Fate Branch
CFR:	Code of Federal Regulations
CHEM:	Chemical Abstracts Service Search
CHEMABS:	Chemical Abstracts Service Search
CHEMDEX:	Chemical Index Database
CHEMFATE:	Environmental Fate Database
CHEMLAB:	Chemical Modeling Laboratories
CHEMLINE:	Chemical Dictionary Online
CHEMNAME:	Chemical Abstracts Chemical Name Dictionary
CHEMSEARCH:	
CHEMSIS:	Chemical Dictionary for Singly Indexed Substances
CHIB:	Chemical Hazard Identification Branch
CHIP:	Chemical Hazard Information Profile
CHRIS:	Chemical Hazard Response Information System
CICIS:	Chemicals in Commerce Information System
CIN:	Chemical Industry Notes
CIDS:	Chemical Information and Data System (U.S. Army)
CIRB:	Chemical Information Reporting Branch
CIS:	Chemical Information System
CLAIMS/CLASS:	Index to U.S. Patent Office's Classification Codes

CLEAR:	EPA Data Base and Environmental Model Index
CLOGP:	A Program for Estimating log P
COMPENDEX:	Computerized Engineering Index
CPSC:	Consumer Product Safety Commission
CRB:	Chemical Regulation Branch
CRC:	The Chemical Rubber Company
CREB:	Chemical Review and Evaluation Branch
CRGS:	Chemical Regulations and Guidelines System
CRIS/USDA:	Current Research Information System
CSIN:	Chemical Substances Information Network
CSR/TSR:	Chemical Status Report or TSCA Status Report
CTCP:	Clinical Toxicology of Commercial Products
D&B:	Dun & Bradstreet
DARC:	Description Acquisition Recovery and Design
DDB:	Design and Development Branch
DDS:	Data Dictionary System
DMI:	Dun's Market Identifiers
DOE:	Department of Energy
DOE-EDB:	Department of Energy - Energy Data Base
DOT:	Department of Transportation
DTS:	Document Tracking System
DWRC:	Denver Wildlife Research Center
Dermal:	OTS Dermal Absorption Database
EAB:	Exposure Assessment Branch
EB:	Epidemiology Branch
EDNOHS:	Exposure Dictionary for National Occupational Hazards Survey
EDS:	Environmental Data Index - NOAA
EEB:	Environmental Effects Branch
EED:	Exposure Evaluation Division
EIS:	Economic Information Systems
EMIC:	Environmental Mutagen Information Center
ENDEX:	Environmental Data Index - NOAA
EN PART:	Environmental Partitioning Model

ENVIROLINE:	Environmental Abstracts Online
EPA:	Environmental Protection Agency
EPACASR:	EPA Chemical Activity Status Report
ERL:	Environmental Research Laboratory
ETD:	Economics and Technology Division
ETIC:	Environmental Teratogen Information Center
EXAMS:	Exposure Analysis Modeling System
EMBASE:	Excerpta Medica
FAO:	Food and Agricultural Organization
FDA:	Food and Drug Administration
FEDREG:	Federal Register Abstracts
FIND/SVP:	
FISH REPRODUCTIVE:	Fish Reproductive Toxicity Data File
FLUIDEX:	British Hydromechanics Research Association
FMIS:	Facilities Management Information System
FRSS:	Federal Register Search Service
FSB:	Full Studies Branch
FYI SUBMISSIONS:	For Your Information Submissions
GEMS:	Graphical Exposure Modeling Systems
GENE-TOX:	Mutagenicity Data File
GIS:	Global Indexing System
GLOBAL 79:	A Fortran Program to Extrapolate Dichotomous Animal Carcinogenicity to Low Doses
GRB:	General Regulations Branch
HANES II:	Health and Nutrition Survey
HERD:	Health and Environmental Review
HHS:	Health and Human Services
HWDMs:	Hazardous Waste Data Management System
IAEA:	International Atomic Energy Agency
IAO:	Industry Assistance Office
IARC:	International Agency for Research on Cancer
IRL:	Information Retrieval Ltd.
IRRS/CTS:	Inventory Reporting Regulation System/Correspondence Tracking System
ICB:	Industrial Chemistry Branch

ICRS:	Index Chemicals Registry System
IFD:	Industrial Facilities Discharge
IMSL:	International Mathematical and Statistical Library
ISHOW:	Information System for Hazardous Organics in Water
ISMEC:	Information Service in Mechanical Engineering
ISSB:	Information Support Services Branch
ITC PROFILES:	Interagency Testing Committee Hazard Information Profiles
ITC REVIEWS:	Interagency Testing Committee Hazard Information Reviews
ITC TRACKING SYSTEM:	Interagency Testing Committee Tracking System
ITI:	The International Technical Information Institute
IUPAC:	International Union of Pure and Applied Chemistry
IUPHAR:	International Union of Pharmacology
MANTELAN:	Mantel-Bryan Low-Dose Extrapolation Model
MEDLARS:	Medical Literature Analyses and Retrieval System
MEDLINE:	Medlars Online
METADEX:	Metals Abstracts/Alloys Index
MOB:	Management Operations Branch
MPTEA:	Multiple Point Gaussian Dispersion Algorithm with Optional Terrain Adjustment
MRST:	Statistical Methodology for Toxicological Research
MSD:	Management Support Branch
MSSS:	Mass Spectral Search System
MULTILOG 80:	A Computer Program for the Risk Assessment of Toxic Substances
NBS:	National Bureau of Standard
NCI:	National Cancer Institute
NFPA:	National Fire Protection Association

NHMS:	National Human Adipose Tissue Survey (Program)
NIOSH:	National Institute for Occupational Safety and Health
NIOSHTIC:	National Institute for Occupational Safety and Health Technical Information Center
NLM:	National Library of Medicine
NOHS:	National Occupational Hazard Survey
NPDES:	National Pollutant Discharge Elimination System
NRB:	Notice Review Branch
NTIS:	National Technical Information Service Bibliographic Data File
NWDS:	National Water Data System
OAQPS:	Office of Air Quality Planning and Standards
OB:	Oncology Branch
OCABS:	Oceanic Abstracts
OCLC:	Online Computer Library Center
ODW:	Drinking Water File
OHM-TADS:	Oil and Hazardous Materials Technical Assistance Data System
ONE HIT MD:	One-Hit Low-Dose Extrapolation Model
OPD:	Oils, Pigments and Drugs
OPP:	Office of Pesticide Programs
ORBIT:	Online Retrieval of Bibliographic Information, Timeshared
ORNL:	Oak Ridge National Laboratory
OSHA:	Occupational Safety and Health Administration
OTS:	Office of Toxic Substances
PAL:	Point, Area, Line Source Algorithm
PAPERCHEM:	Paper Chemistry Abstracts
PASCAL:	Programme Applique a la Selection et a la Compilation Automatiques de la Litterature
PERS:	Personnel System
PHYTOTOX/UTAB:	Phytotoxicity and Plant Uptake and Metabolism

PMN DATA:	Data Submitted Collected and Generated during PMN Assessment
PMN:	Premanufacturing Notification
POLLUTION:	Pollution Abstracts
PPDB:	Policy and Program Development Branch
PPS:	Project Performance System
PRE-CHIP:	Pre-Chemical Hazard Identification Profile
PREFER:	Preferred Chemical Name
PROMT:	Predicasts Overviews of Marketing and Technology
PTS:	Predicasts Terminal Systems
RANK TIME:	A Fortran Program for Risk Assessment Using Dose-Response Data Time-to-Occurrence
RANN:	Research Applied to National Need
RAPRA ABSTRACTS:	Rubber and Plastics Research Association Abstracts
RIB:	Regulatory Impacts Branch
RTECS:	Registry of Toxic Effects of Chemical Substances
RTP:	Research Triangle Park
RTS:	Request Tracking System
SANSS:	Structure and Nomenclature Search Service
SAS/ETS:	SAS/Econometrics and Time-Series Library
SAT:	Structure Activity Team
SCI:	Scisearch
SDB:	Systems Development Branch
SESOIL:	Seasonal Soil Model
SOB:	Systems Operation Branch
SPHERE:	Scientific Parameters in Health and the Environment-Retrieval and Estimation
SPSS:	Statistical Package for the Social Sciences
SRI:	Stanford Research Institute
STAR:	Stability Tubular Array
SWEMS:	Soil and Water Environmental Monitoring System
SYMN:	Synonyms of Chemical Names

TAS RTP:	SDB Request Tracking
TDB:	Toxicology Data Bank
TDIS:	Technical Data Indexing System
TEB:	Toxic Effects Branch
TED:	Toxics Economics Database
TERATOX:	Teratology Data File
TERRE-TOX:	Published Terrestrial Toxicity Data File
TICIRC:	Technical Information Center Circulation Control
TLV:	Threshold Limit Values
TME DATA:	Data Submitted, Collected and Generated During Test Market Exemption Assessment
TOX-TIPS:	Toxicology Testing in Progress
TOXLINE:	Toxicology Information Online
TRDB:	Test Rules Development Branch
TSCA:	Toxic Substances Control Act
TSCAPP:	Toxic Substances Control Act Plant and Production Search System
TSI:	Test Study Inventory
TSSMS:	Time-Sharing Service Management System
ULRI:	Ulrich's International Periodicals Directory and Irregular Serials and Annuals
US CLASS:	U.S. Patent Master Classification File
USDA:	United States Department of Agriculture
USITC:	United States International Trade Commission
USPA/USP77/USP 70:	U.S. Patent Copies
UTM-TOX:	Unified Transport Model-Toxics
VAX:	An EPA Owned Computer Modelling System
UVCB:	Unidentified or Variable Composition, Complex Reaction Product, or Biological Chemicals
WATERDROP:	Water Distribution Register of Organic Pollutants
WHO:	World Health Organization
WNPI:	World Patent Index
WPIL:	World Patent Index Latest

VIII. DATA SUB-CATEGORIES/OTS FUNCTIONS MATRIX

This section is comprised of a series of matrices matching data sub-categories (as described in Section IV of the Notebook) against major OTS functions (as described in Section II of the Notebook). The purpose of these matrices is to establish a relationship between data sub-categories and OTS functions, showing the types of information needed in support of each of the functions. By comparing these matrices against the Data Sub-categories/Information Resources Matrix (See Section VII of the Notebook), major information gaps can be easily identified.

No attempt is made to match data sub-categories against OTS sub-functions. Such a matrix would be too complex to construct and may be misleading.

In general, the matrices highlight the following points:

1. Certain types of data are exclusively used in support of certain specific functions. These are:

<u>Data Category</u>	<u>OTS Function</u>
Chemical economics	Economics analysis
Health effects	Health effects analysis
Environmental effects	Environmental effects analysis
Exposure	Exposure analysis
Regulations/Controls	Regulatory options analysis

2. Other types of data are widely used to support more than one function. They are:

<u>Data Category</u>	<u>OTS Function</u>
Physical/Chemical properties	Chemical analysis Control technology analysis Exposure analysis Health effects analysis Environmental effects analysis
Production/Processing	Chemical analysis Control technology analysis Exposure analysis Economic analysis
Use/Disposal	Chemical analysis Control technology analysis Exposure analysis Economic analysis



3. Substance identification data appear to be widely used for supporting a number of the functions. This is not totally unexpected since OTS' mission is the investigation of chemical substances. Therefore, every function is chemically oriented and the substance in question has to be properly identified. However, it is believed that substance identification data are mainly used in support of the chemical analysis function, and that the other functions rely more on the results of chemical analysis for identifying the substances. The matrix, in this case, does not distinguish between gathering information directly from information resources and obtaining information from a product generated by a function that uses the information directly.

A total of nine matrices are presented, with each matrix matching a data category against the OTS functions. The sub-categories of a category are listed on the horizontal axis, and the functions are on the vertical axis of each matrix.

Each matrix shows what specific data sub-categories within a certain data category are used in support of the OTS functions. As discussed in Section IV of this Notebook, certain sub-categories may belong to more than one data category and cross-references are used to denote this relationship. In the aforementioned matrices, the cross-referenced sub-categories are included in all of the pertinent matrices. For example, "Method of Manufacture" appears in both the "Substance Identification vs. OTS Functions Matrix" as well as the "Production/Processing vs. OTS Functions Matrix." It is hoped that the handling of cross-referenced sub-categories in this manner will make each matrix more complete and will allow the users to visualize immediately, without going into another matrix, the relationship between a data category and the functions.

As described in Section II of this Notebook, Regulatory Options Analysis mainly integrates products from other functions and has no specific information requirements except for data pertaining to regulations and controls. For this reason, information requirements for Regulatory Options Analysis are indicated only in the "Regulations and Controls vs. OTS Functions Matrix."

## IX. DATA REQUIREMENTS FOR OTS PROCESSES

In Section III of this Notebook, the three major OTS processes, i.e., New Chemicals Review, Existing Chemicals Review, and Chemical Testing, are discussed. Associated with each of the three processes in Section III are the major information resources specifically designed or used in support of that process. These information resources are mostly indexing or tracking systems and do not include the traditional bibliographic or non-bibliographic scientific and technical information systems listed in Section V of this Notebook. This section defines data requirements for the three OTS processes.

For the OTS functions (see Section II), information requirements are identified in terms of data categories and sub-categories (see Section IV). Furthermore, the computerized scientific and technical bibliographic and non-bibliographic information systems (see Section V) and manual sources (see Section VII) containing pertinent data are presented. The data requirements for the functions are indexed in matrices (see Section VIII). Therefore, a direct relationship has been established among OTS functions, data categories and sub-categories, and information resources in terms of computerized and manual scientific and technical systems. In general, an OTS function is data specific, i.e., a function requires a specific category of data. The data are usually available in specific information systems.

The operation of OTS processes obviously needs support from a variety of scientific and technical systems and sources that are not included in Section III of this Notebook. However, unlike a function, a process is not data specific. This is because organizationally a process is largely supported by almost all functions. While different functions require different data categories, all data categories are required for a process since all functions are involved. Therefore, as far as scientific and technical data are concerned, the information requirements for the three processes are essentially identical. Nevertheless, each process may prescribe a slightly different responding time and depth of data coverage, based on the specific time constraints of that particular process. Additionally, each process has different requirements in terms of specific indexing or tracking systems, as discussed in Section III.

Instead of presenting a matrix matching a process against specific data categories or sub-categories, as in the case of the functions (see Section VIII), this section attempts to define data requirements for the processes in a different manner. If such a matrix were developed, almost all columns would be checked for all three processes.

- 
- (a) A quick search of a few major data bases on the PMN chemical.  
(b) A more comprehensive search of additional data bases and manual

Existing Chemicals Review Process

<u>Milestones</u>	<u>Data Categories</u>
1. Entry Review	
a. Step 1: substances not previously evaluated under TSCA	Substance identification Health effects Environmental effects Production/processing Use/disposal Regulations/control
b. Step 2: substances previously evaluated under TSCA (From CHIP or Section 4 Chemical Testing)	Health effects* Environmental effects* Exposure*
2. Problem Characterization	Physical/chemical properties
3. Information Gathering & Risk Analysis	Health effects Environmental effects Production/processing Use/disposal Exposure Chemical economics (Market profile & substitutes) Regulations/control (handling and labeling)
4. Risk Reduction Analysis	Chemical economics
5. Risk Management	Information obtained from above activities

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\*Information requirements for CHIP. Literature search is limited to secondary sources. For information requirements on Chemical Testing, see the table entitled Chemical Testing Process: Test Rules Development.

Chemical Testing Process  
Test Rules Development

<u>Milestones</u>	<u>Data Categories</u>
1. Obtain data from ITC Report	Substance identification Production/processing Use/disposal Exposure
2. Obtain unpublished health & safety studies from industry (Section 8(d) submissions)	Health effects Exposure Regulations/control
3. Literature search for Testing Needs Analysis (also from Section 8(a) Level A submissions)	Substance identification Physical/chemical properties Health effects Environmental effects Production/processing Use/disposal Exposure Regulations/control
4. Preliminary Economic Analysis	Production/processing Chemical economics
5. Preliminary Exposure Analysis	Health effects Environmental effects Production/processing Use/disposal Exposure
6. Preliminary Testing Needs Analysis	Information obtained from above activities
7. Support Document	Same as 6
8. Economics Analysis Document	Information from 5

## X. CONCLUSION

The foregoing sections of this Notebook have identified information requirements for the OTS functions and processes as well as pertinent information resources and analytical capabilities that are currently available. Wherever feasible, matrices have been developed to highlight the relationship among information requirements, information resources and analytical capabilities, and OTS functions and processes. Furthermore, the resources attributes matrices facilitate both user awareness of the wide variety of information resources available and proper selection of the most appropriate resource(s) to satisfy an information requirement.

This section presents some analyses of the major findings in the foregoing sections of this Notebook. Major conclusions of these analyses are summarized as follows:

1. There are seven major functions and three processes within OTS, and each of these functions or processes has certain information requirements. In general, the information requirements for a process is much broader than those for a function. This can be explained by the simple fact that all functions are involved in supporting a process by performing technical and scientific reviews and analyses for that process. Scientific and technical data are therefore needed directly in support of these functions which in turn support the processes.
2. OTS has diversified information needs, based on the data categories and sub-categories that have been identified. Although all data categories and sub-categories are needed by OTS, the relative value of each data category or sub-category to the successful implementation of TSCA is, however, difficult to determine.
3. In general, functions are data specific. This means that instead of requiring all types of data, a function usually needs one or a few specific categories of data, as discussed in Section VIII of this Notebook. For example, health effects analysis requires essentially health effects data, and exposure analysis needs data on exposure, physical chemical properties, production/processing, and use/disposal of chemical substances.
4. Certain data categories are each exclusively used in support of one function while some other categories are used by more than one function. For example, chemical economics data are used exclusively in support of economic analysis while use information is needed for exposure analysis, economic analysis, chemical analysis, as well as control technology analysis.
5. Processes are not data specific. In general, a process requires all kinds of scientific and technical information. Therefore, unlike the functions, information requirements are almost identical for the three OTS processes. Each process,

1. The first of these is the fact that the *Journal* is a very important source of information for the public. It is a source of information that is not only accurate but also timely. It is a source of information that is not only accurate but also timely.

1. 1940年12月，国民党政府颁布《战时新闻纸杂志图书检查办法》，规定所有出版物的内容必须经过审查，不得含有危害国家利益、破坏社会秩序、煽动叛乱等言论。

[illegible]

2000

1. The first step in the process of the investigation is the identification of the problem. This is done by the investigator who is responsible for the study. The next step is to collect data. This is done by the investigator who is responsible for the study. The next step is to analyze the data. This is done by the investigator who is responsible for the study. The next step is to interpret the data. This is done by the investigator who is responsible for the study. The next step is to draw conclusions. This is done by the investigator who is responsible for the study. The next step is to report the results. This is done by the investigator who is responsible for the study. The next step is to discuss the results. This is done by the investigator who is responsible for the study. The next step is to conclude the study. This is done by the investigator who is responsible for the study.

1. The first step in the process is to identify the problem or issue that needs to be addressed. This involves gathering information and understanding the context of the problem.

2. Once the problem is identified, the next step is to define the objectives and goals of the project. This helps to clarify what needs to be achieved and provides a clear direction for the team.

3. The third step is to develop a plan or strategy to address the problem. This involves breaking down the problem into smaller, manageable tasks and determining the resources needed to complete them.

4. The fourth step is to implement the plan. This involves putting the strategy into action and monitoring progress to ensure that the project is on track.

5. The final step is to evaluate the results of the project. This involves assessing the outcomes against the objectives and goals and identifying any areas for improvement.

The following information was obtained from the records of the  
 Bureau of Prisons, Department of Justice, Washington, D.C.  
 and the Federal Bureau of Investigation, Department of Justice,  
 Washington, D.C.

however, may prescribe a slightly different responding time and different depth of the information coverage.

6. In addition to scientific and technical information, the processes also require systems to track process management decisions or to index submission data. As a result, several tracking or indexing systems have been specifically developed to support the processes. Examples of these systems include the TDIS, PMN Tracking System, CECATS, 8(a) Level A Information System, etc. Functions, on the other hand, use exclusively scientific and technical information.

7. For each of the three processes, major milestones and products are identified. In general, the preparation of these products requires the support of a number of the OTS functions and, therefore, a number of the data categories. In some cases, a product may be data specific, i.e. it requires a specific category of data. In any case, the same categories of data may be needed for different products for a particular process, as evidenced in Section IX of this Notebook. This may be explained by one of the following:

- o The two different products requiring similar information may pertain to different chemicals, e.g., PMN subject chemicals and PMN analogs.
- o Although the information requirements are similar in terms of data categories, the depth of coverage may be quite different. For example, one product may require only a quick search of a few major computer data bases, while another product needs a more comprehensive search including manual sources.
- o Different products may be prepared at relatively the same period of time. Similar information is needed simultaneously in preparing these products. The time constraints do not allow these products to be prepared consecutively, so that the output from one product would become the input for the next product.

8. The analytical capabilities developed by OTS are used to support all three processes and essentially three functions, i.e. health effects analysis, environmental effects analysis, and exposure analysis. These analytical capabilities are used to supplement the existing computerized and manual resources as a source of information support for TSCA. Specifically, where certain types of critical data are lacking, OTS uses the analytical capabilities to develop data based on estimation or modeling techniques. Examples include the use of estimation techniques for generating physical/chemical properties, fate and exposure modeling techniques for assessing chemical fate and environmental or human exposure, and dose-response modeling techniques for estimating relationships between dose level and toxic effects.





9. The existing computerized bibliographic and non-bibliographic data bases alone cannot fully satisfy OTS information needs. These data bases are being supplemented by manual resources, expert opinions, and data development via rule-making or estimation techniques. Specifically, OTS relies on estimation techniques to develop many of the sub-categories for physical/chemical properties, and on computer models for certain kinds of exposure data. Furthermore, OTS uses manual and unpublished resources and depends on expert opinions for certain sub-categories of data on economics, production, processing, use and disposal of chemical substances. Health and environmental effects data in general appear to be more readily available in the computer data bases, with the exception of end-point and testing data.

10. There are approximately 200 computerized and 500 manual information resources which have been identified as pertinent sources for supporting the OTS functions and processes. A series of resource attributes matrices are developed to evaluate and document the usefulness of these information resources. However, the quality of either the data or the data bases cannot be determined. Each of these information resources contains certain information that is needed to support TSCA. Therefore, it will be counter-productive to compare or rank these information resources in terms of their relative usefulness or contribution to TSCA. The successful implementation of TSCA requires many different categories of data that are available from a wide variety of information resources, i.e., bibliographic data bases, non-bibliographic data bases, manual sources, unpublished data, expert opinion, etc.

11. The bibliographic data bases (e.g. Toxline, Medline) usually provide the users with abstracts and bibliographic information, while the non-bibliographic data bases (e.g. RTECS, SPHERE) contain end-point data or data in an extracted format. OTS needs to use both types of data bases, since they contain different data and serve different purposes. Different search techniques must be used to search the two different types of data bases. It appears that end-point data can be more readily used if only a preliminary review of a chemical is conducted. Abstracts and bibliographic data will be more useful for more in-depth reviews of chemicals.

12. OTS does not seem to rely heavily on peer-reviewed data. In fact, most of the scientists interviewed indicated that they prefer to conduct their own analyses and draw their own conclusions. However, in using the data bases, they would prefer to have data with certain types of quality indicators.

13. OTS must more actively and effectively utilize existing unpublished data. Currently, there does not seem to be a formal mechanism for identifying and acquiring unpublished data, especially those from other agencies.

THE FOLLOWING IS A SUMMARY OF THE INFORMATION RECEIVED FROM THE  
OFFICE OF THE ATTORNEY GENERAL, NEW YORK, ON THE SUBJECT OF THE

RECORDS OF THE NEW YORK STATE DEPARTMENT OF CORRECTIONS, RELATIVE TO  
THE CASE OF THE PRISONER KNOWN AS "JOHN DOE".

IT IS STATED THAT THE PRISONER WAS RECEIVED INTO THE  
STATE PRISON ON JANUARY 1, 1900, AND WAS HELD IN THE  
PRISON UNTIL JANUARY 1, 1901, WHEN HE WAS RELEASED ON  
BOND. HE WAS THEN HELD IN THE PRISON AGAIN ON JANUARY 1, 1902,  
AND WAS RELEASED ON BOND ON JANUARY 1, 1903.

THE PRISONER WAS HELD IN THE PRISON AGAIN ON JANUARY 1, 1904,  
AND WAS RELEASED ON BOND ON JANUARY 1, 1905. HE WAS THEN HELD  
IN THE PRISON AGAIN ON JANUARY 1, 1906, AND WAS RELEASED ON  
BOND ON JANUARY 1, 1907. HE WAS THEN HELD IN THE PRISON AGAIN  
ON JANUARY 1, 1908, AND WAS RELEASED ON BOND ON JANUARY 1, 1909.

HE WAS THEN HELD IN THE PRISON AGAIN ON JANUARY 1, 1910,  
AND WAS RELEASED ON BOND ON JANUARY 1, 1911.

HE WAS THEN HELD IN THE PRISON AGAIN ON JANUARY 1, 1912,  
AND WAS RELEASED ON BOND ON JANUARY 1, 1913.

HE WAS THEN HELD IN THE PRISON AGAIN ON JANUARY 1, 1914,  
AND WAS RELEASED ON BOND ON JANUARY 1, 1915.

HE WAS THEN HELD IN THE PRISON AGAIN ON JANUARY 1, 1916,  
AND WAS RELEASED ON BOND ON JANUARY 1, 1917.

HE WAS THEN HELD IN THE PRISON AGAIN ON JANUARY 1, 1918,  
AND WAS RELEASED ON BOND ON JANUARY 1, 1919.

HE WAS THEN HELD IN THE PRISON AGAIN ON JANUARY 1, 1920,  
AND WAS RELEASED ON BOND ON JANUARY 1, 1921. HE WAS THEN HELD  
IN THE PRISON AGAIN ON JANUARY 1, 1922, AND WAS RELEASED ON  
BOND ON JANUARY 1, 1923. HE WAS THEN HELD IN THE PRISON AGAIN  
ON JANUARY 1, 1924, AND WAS RELEASED ON BOND ON JANUARY 1, 1925.

14. In matching the data categories and sub-categories against information resources the following trends and data gaps are observed:

- o All data categories are covered to some extent by the bibliographic and non-bibliographic data bases, and manual resources.
- o The technical aspects of chemical information (i.e., Substance Identification, Physical-Chemical Properties, Health Effects, and Environmental Effects) appear to be adequately covered by the identified sources, with the exception of end-point and testing data.
- o The technological and economic aspects of chemical information (i.e., Production/Processing, Use/Disposal, Exposure, and Chemical Economics) need additional sources. In many cases, expert opinions are being used.
- o The legal aspects (i.e., Regulations/Control), with the exception of the Consumer Affairs sub-category, are covered but could use some additional sources.
- o Of the 19 sub-categories for Chemical Economics, 7 sub-categories (37%) have no source for data.
- o Of the 16 sub-categories for Production/Processing, 4 sub-categories (25%) have no information source.
- o For Use/Disposal category, 7 of the 12 sub-categories (58%) have no source for data.
- o Of the 23 sub-categories for Exposure, 4 subcategories (17%) have no source for data.
- o In the Health Effects Category, no information sources are found for the Epidemiology sub-category, an unexpected finding.

15. The TSCA Chemical Substances Inventory, in spite of the apparent obsolescence of some of its data, is still the most complete single source for production volume and manufacturing plant site data. If more current data are needed, OTS must obtain the data through rule-making.

U.S. Environmental Protection Agency  
GLNPO Library Collection (PL-12J)  
77 West Jackson Boulevard,  
Chicago, IL 60604-3590

U.S. Environmental Protection Agency  
Region 5,  
77 West Jackson Boulevard, 12th Floor  
Chicago, IL 60604-3590