How to Find Chemical Information

A Guide for Practicing Chamists, machers, and Students

HOW TO FIND CHEMICAL INFORMATION

A Guide for Practicing Chemists, Teachers, and Students

ROBERT E. MAIZELL

Olin Corporation Research Center New Haven, CT.

A WILEY-INTERSCIENCE PUBLICATION

JOHN WILEY & SONS New York • Chichester Brisbane • Toronto

Copyright © 1979 by John Wiley & Sons, Inc.

All rights reserved. Published simultaneously in Canada.

Reproduction or translation of any part of this work beyond that permitted by Sections 107 or 108 of the 1976 United States Copyright Act without the permission of the copyright owner is unlawful. Requests for permission or further information should be addressed to the Permissions Department, John Wiley & Sons, Inc.

Library of Congress Cataloging in Publication Data Maizell, Robert Edward, 1924-

How to find chemical information.

"A Wiley-Interscience book."
Includes index.

1. Chemical literature. I. Title.

QD8.5.M34 540'.7 78-23222 ISBN 0-471-56531-8

Printed in the United States of America

10 9 8 7 6 5 4

PREFACE

One of the basic premises on which this book is written is that of change. Just as chemistry and chemical engineering change, so do the sources of information chemists and engineers use. New and improved information tools are constantly being introduced, and, concurrently, older tools become less valuable, become obsolete, or are discontinued. Accordingly, this book presents the most important and enduring of the classical tools of chemical information; the more significant newer tools; and, most importantly, the underlying methods, principles, and keys the chemist and engineer need to cope with the constantly changing array of chemical information sources and tools.

There are reasons why rapid, sometimes dramatic, change is an integral part of the chemical information scene. One is the advances and improvements made possible by computerized information handling and processing techniques. Another is the sharp escalation in publishing costs. This, when coupled with the vast amount of chemical information, has caused the demise of some older standard sources, significant changes in other tools, and numerous recent innovative attempts to provide improved approaches.

Because this book emphasizes the more enduring principles that lead to the most effective use of chemical information, the coverage of sources, methods, and tools is selective. And because most chemists and engineers are employed at some time in industry, emphasis is on approaches to meet practical needs. The equally important needs and interests of chemists and engineers in academic work (both teachers and students), and in government or independent research and development work, are also emphasized.

VIII PREFACE

Whenever possible, comments are made on the pros and cons of the major sources. These comments should aid the reader in his evaluation of other sources. Additionally, estimates as to future outlook and developments are given as

appropriate.

As applied to the needs of chemists in research and development and others in similar functions, this work is written in a climate reflecting the changing emphasis in programs and expenditures, which now stress: (1) the toxicological and other safety aspects, including pollution abatement and control; (2) improvement of existing products and processes; (3) the development of new products, which in many cases are built on existing strengths rather than new departures; and (4) an increasingly close relationship with the marketing function.

Information science students, teachers, and practitioners with special interest in chemistry and chemical engineering

or of seddenings no in alcedique in . To no still tests to the sed and alcedening the control test periods and in the control test of the control

will also find material of value in this volume.

ROBERT E. MAIZELL

spenymen been deal with as a world tree.

New Haven, Connecticut November 1978

ACKNOWLEDGEMENTS

I am grateful to my colleagues at Olin Corporation for providing outstanding and timely insights into their specialties as well as the broad overview. Words of special thanks go to Mr. R. H. Bachman, Mr. W. M. Clarke, Dr. L. A. Krause, and Mr. D. D. Palm.

Dr. Russell J. Rowlett, Jr., Editor, Chemical Abstracts Service, contributed importantly to review of the chapter on Chemical Abstracts. In so doing, he also helped provide an appropriate total perspective and indirectly fine-tuned my writing emphasis and style. Mrs. Helen Lawlor, Institute for Scientific Information, was most helpful in developing a review of the innovative activities of her organization. Several managers at the United States Patent Office aided in sharpening my views on the role of patents as an information source for chemists. Dr. Brian Gore, Derwent Publications, Ltd., London, England, and Dr. Phillip Pollick, Chemical Abstracts Service, also contributed insight on patents. Dr. David R. Lide and Dr. Howard White, United States National Bureau of Standards, strengthened more fully the discussion of physical properties and related data and provided invaluable material, parts of which are briefly excerpted.

All material of a copyright nature is used here with permission of the copyright owners, to whom the author expresses his appreciation. These include the following:

Figures 5, 9, 10, 11, 14, 16, and 18 are reprinted from *Chemical Abstracts*. Material reproduced from *Chemical Abstracts* is copyrighted by the American Chemical Society and is reproduced with permission. No further copying is permitted.

Figure 6, reprinted with permission of Smithsonian Science Information Exchange, Inc., Washington, D.C.

Figure 17, reprinted from Gmelins Handbuch der Anorganischen Chemie, Springer-Verlag, Heidelberg. With permission.

Material beginning on page 73, with thanks to the Institute for Scientific Information (ISI), 325 Chestnut Street, Philadelphia, Pennsylvania. Other material from ISI as referred to elsewhere in this book also used with permission of ISI, including Figures 2, 3, 7, and 12 as well as appropriate textual material.

Page 108, © Verlag Chemie GmbH, Ullmanns Encyklopaedie der Technischen Chemie, published by Verlag Chemie Weinheim, New York. Volumes 1-6 Thematic Section General Principles and Methodology.

Page 109, reprinted from J. J. McKetta, Encyclopedia of Chemical Processing and Design, Volume descriptive material, Marcel Dekker, Inc., New York, New York.

Material beginning on page 112, with thanks to Beilsteins Handbuch der Organischen Chemie, Springer-Verlag, Heidelberg. With permission.

Material beginning on page 116, with thanks to Gmelins Handbuch der Anorganischen Chemie, Springer-Verlag, Heidelberg. With permission.

Page 136 and subsequent paragraphs on Derwent, with thanks to Derwent Publications Ltd., London, England.

Material beginning on page 195, with thanks to Dr. Bruno J. Zwolinski, Executive Director, Thermodynamics Research Center, A&M Research Foundation, P.O. Box 130, College Station, Texas 77843.

Material beginning on page 196, with thanks to Dr. Y. S. Touloukian, Director CINDAS, Purdue University, West Lafayette, Indiana.

Excerpts, pages 198-199 with permission of American Chemical Society, Washington, D.C.

Material beginning on page 225 and other material relating to Chemical Data Services, Stamford Street, London, England, used with thanks and permission.

Material beginning on page 221, 231, with thanks to John

C. Dean, SRI International, Menlo Park, California.

Excerpts beginning on page 232 copyright 1976 by Chem

Systems, Inc. With permission.

I am indebted to members of the John Wiley staff who helped importantly in the shaping of the manuscript and production of the book. These include Georgia Chuhay Smith, Editor; Frances Tindall, Editorial Supervisor; and Shirley Thomas, Production Supervisor.

R.E.M.

SOME CAVEATS

The terms chemist, chemical engineer, and engineer are meant to be used and understood as similar or related in most parts of this book. In most places the chemist is used as the term of choice, primarily to save space and reading time. Somewhat similar reasoning applies to the use of he as the arbitrarily preferred term over she; both terms are implied in every case.

This book represents the views and opinions of the author; it does not necessarily reflect those of his organization.

Although the material presented is aimed primarily at the United States audience, the author sincerely hopes that readers in other countries will find this volume helpful in their work and studies.

FIGURES

1 The Current Awareness Triangle / 16

2 Selected ASCATOPICS® / 22-23

3 Example of ASCATOPICS® Output / 24-25

- 4 Macroprofiles available from the United Kingdom Chemical Information Service / 26
- 5 Typical SDI Output Based on Chemical Abstracts / 28
- 6 Notice of Research Project, Smithsonian Science Information Exchange / 34

7 Example of Request-A-Print® / 39

- 8 Locations of Libraries that have Copies of United States Patents Arranged in Numerical Order / 42
- 9 Development of CA Collective Indexes / 54

10 CA Index Growth / 63

- 11 Chemical Abstracts Section Groupings / 66-67
- 12 Permuterm Index to Science Citation Index / 77
- 13 Some Tools of Chemical Interest Searchable On-Line / 82

14 Example of On-Line Search of CA / 83-86

- 15 Examples of Term Variations Used in On-Line Searching / 92
- 16 Information Centers that Provide Services Based on Files Licensed from Chemical Abstracts Service and (in Many Cases) from Other Sources / 95-99
- 17 Gmelin System of Elements and Compounds / 117-118
- 18 CA Patent Coverage / 144-145

CONTENTS

Chapter	1 — Some Basic Concepts The Surrogate Concept in Literature Use The Administrator and Information / 3	/ 2
Chapter	2 — Information Flow and Communi-	
	cation Patterns in Chemistry	5
Chapter	3 — Search Strategy	9
Chapter	4 — Keeping-Up-To-Date—Current	
	Awareness Programs	13
	Reading Clubs / 15	-
	Personal Plan of Action / 15	
	Base of the Triangle / 16	
	Middle Part of the Triangle / 17	
	Apex of the Triangle / 20	
	Meetings / 29	
	Getting Copies of Meeting Papers / 30	
	Research in Progress; Dissertations / 32	
	5 — How To Get Access to Articles,	
	Books, Patents, and Other Documen	ts
	Quickly and Efficiently	37
	Help Available From Chemistry	
	Librarians / 40	
	Patents / 41	
	Translations / 43	
	Other Options and Future Outlook / 47	

49

71

Chapter 6 — The Chemical Abstracts Service

Coverage / 50

Abstract and Index Content / 50

Speed of Coverage and

Indexing / 51

CA Indexes / 52

CA Nomenclature / 55

Parent Compound Handbook / 58

Registry Handbook-

Common Names / 59

Use of Subdivisions / 60

Size / 62

Complexity / 62

Patent Coverage / 63

Reviews / 64

Chemical Marketing and Business

Information / 64

Dissertations / 65

Coverage of Documents from

the Soviet Union / 65

Availability of Materials Covered by CA / 65

Mistakes / 68

Cost / 68

Future / 69

Chapter 7 — Other Abstracting and Indexing Services

Institute for Scientific Information / 73 Services Published Outside

the United States / 76

Services Intended Primarily for

Nonchemists / 78

Chapter	8 — Computer-Based On-Line and	
V (8) 1 1 10	Off-Line Information Retrieval	
	Systems and Services	79
	Why Use On-Line Service / 79	
	Some Characteristics of One-Line	
	Searching / 80	
	Sources of Interest to Chemists that	
	are Searchable On-Line / 81	
	On-Line Output / 82	
	Use of On-Line Services / 82	
	Costs / 88	
	Search Strategy On-Line / 89	
enter Side	Information Centers / 92	in in the
	Information "Brokers" / 94	#12 F12 200
	Patent Sanchary 192	
Chapter	9 — Reviews	101
	Conferming and State Land	
Chapter	10 - Encyclopedias and Other Major	
C.I.I.P.	Reference Books	105
	Encyclopedias—Introductory	
	Remarks / 106	
	Specific Encyclopedias / 107	
	Kirk-Othmer / 107	
	Ullmanns Encyklopaedie der	10000
	Technischen Chemie / 108	
	McKetta / 109	
	Mark / 110	
	Which Encyclopedia to Use / 110	
	The Handbuch Concept / 111	
	Organic Chemistry—Some Important	
	Reference Works / 112	
	Beilsteins Handbuch der	
	Organischen Chemie / 112	

Some Other Important Organic
Chemistry Reference Works / 113
Inorganic Chemistry—Some Important
Reference Works / 116
Gmelins Handbuch der
Anorganischen Chemie / 116
Mellor / 119
Some Other Important Inorganic
Chemistry Reference Works / 120
Keeping Up With and Identifying
Books / 120

Chapter 11 — Patents

123

Why Patents are Important / 123 Patent Structure / 124 The Role of Patents in Idea Generation and Creativity / 125 Patents as Information Tools / 127 Patents versus Journals and Books; Quick-Issue Patents / 128 Official Government Sources of Patent Information / 131 **Obtaining Information About** United States Patents / 132 Derwent Patent Information Services / 136 Derwent Central Patents Index / 136 Derwent World Patents Index (WPI) and World Patents Abstracts (WPA) / 139 On-Line Access to Derwent W-PI/CPI / 140

Efficient Use of Derwent / 141

Advantages and Disadvantages of Derwent / 141 Coverage of Patents by Chemical Abstracts / 143 IFI/Plenum Data Co. Patent Services / 146 IFI Comprehensive Database to United States Chemical Patents / 147 Uniterm Index to United States Chemical Patents / 147 The IFI Assignee Index to United States Patents / 148 Claims / 148 International Patent Alerting Service / 149 Some Advantages and Disadvantages of IFI/Plenum Services / 149 Other Sources of Patent Information / 150 Patent Equivalents or Families / 151

Chapter 12 — Safety and Related Topics

Future Outlook / 152

Other Remarks on Patents / 154

157

Locating Pertinent Safety Data / 159
Books and Related Information
Sources / 162
On-Line Sources / 166
Government Regulations and Related / 168
Professional Societies and Other
Associations / 170
Chemical Abstracts and Other Abstracting
and Indexing Services / 173

Toxicity to Aquatic Organisms / 178 Biodegradability / 179 Water Quality Data / 180 Examples of Key Journals / 181 Newsletters / 181 Other / 181

Chapter 13 — Locating and Using Physical Property and Related Data

183

Sources of Data / 184 Recording Property Data / 185 National Standard Reference Data System / 185

Data Centers and Projects / 189 Thermodynamics Research Center / 195

Center for Information and Numerical Data Analysis and Synthesis / 196

Committee on Data for Science and Technology / 197

> Journal of Chemical and Engineering Data and Other Journals / 198

Trade Literature / 199

Bulletin of Chemical Thermodynamics / 200

Handbooks / 200

International Critical Tables / 203

Examples of Other Reference Sources / 203

Evaluating Data from Conflicting or Unevaluative Sources / 208

Determining or Estimating Properties / 210

CONTENTS xxi Chapter 14 — Chemical Marketing and **Business Information Sources** 213 Using Marketing Data / 213 Information About Manufacturers / 214 Buyer's Guides and Related Tools / 215 International Buyer's Guides / 218 More General Guides / 219 Other Sources for Locating Chemicals / 219 Prices / 220 General Chemical Business Information / 220 Chemical Economics Handbook / 221 Multiclient Studies / 222 Product Data / 224 Other Sources and Tools / 225 Other Remarks / 227 Chapter 15 — Process Information 229 Specialized Services / 230 References 234 Appendix 243

251

Index