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INDUSTRIAL ORGANIC CHEMICALS IN PERSPECTIVE

PART I: RAW MATERIALS AND MANUFACTURE

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FOREWORD

The American Chemical Society study, *Chemistry in the Economy* (Washington, DC, 1973), was carried out by a committee that it was my privilege to chair jointly with my good friend, Dr. Max Tischler. In the course of the study we became acutely aware that the science and technology of chemistry directly and indirectly interact with every phase of everyday living—the food we eat, the clothes we wear, our health, welfare, housing, transportation, and national security. In addition, the study indicated that about 70% of all chemists and chemical engineers in the United States work in industry. It is surprising therefore to find the science and technology of chemistry in industry to be largely unexplored in modern curricula in our colleges and universities.

Based on that study, the American Chemical Society has recommended that more industrial courses be included in both the undergraduate and graduate chemical curricula. We are very pleased, accordingly, to have two volumes that bring the real world of industrial organic chemistry and technology into the classroom. *Industrial Organic Chemicals in Perspective* is based on courses that Dr. Wittcoff organized at the University of Minnesota and Dr. Reuben has been presenting at the University of Surrey and the Polytechnic of the South Bank in London, England. Both of the authors have extensive industrial background and experience.

It is especially fascinating to observe how these volumes trace the flow of organic chemicals through industry. For example, the petroleum refinery provides only a few basic starting materials. From these, through complex and sophisticated chemistry, much of it based on homogeneous and heterogeneous catalysis, there result billions of pounds of numerous products that give rise to a vast and important technology to which a large portion of this book is devoted.

This textbook should provide the basis for much needed courses in industrial organic chemistry in colleges and universities. Such courses will endow students entering the chemical and allied industries with a level of knowledge and understanding of its application that could materially shorten, and in some instances even eliminate, the painful and unproductive induction period that all too often is the lot of the scientist entering industry.

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PREFACE

All of a sudden the organic chemicals industry is middle-aged. Gone are the heady days of the 1950s with new products and processes evolving so fast that improvement of existing processes seemed hardly worthwhile. Gone, too, are the exciting 1960s when every ethylene cracker had twice the capacity of the last one, and it really looked as if the trees might grow to the sky.

Instead, the growth rate has slackened. US natural gas supplies are diminishing. The price of oil has shot up, and "doom boom" proponents point to the rapid depletion of irreplaceable natural resources and speculate on the catastrophe their exhaustion will create. Environmental pressures have caused the chemical industry to take a hard look at its safety procedures and safeguards for workers with toxic chemicals.

The organic chemicals industry has become a large industry playing a large part in the economy. It has matured, and maturity brings the ability to see things in perspective. These two volumes are just such a perspective, presenting a picture of the organic chemical industry in terms of both chemistry and technology. Chemistry may be defined as the creation of molecules; technology as the application of those molecules to the creation of goods and services.

Of course we have written in detail about the petrochemicals industry—it is the dominant side of the industry—but we have also looked at other raw materials that are commonly used and that might be used more if oil or natural gas were not available. We have emphasized the versatility of industrial organic chemistry and tried to outline an alternative technology to which we could turn if the necessity arose.

We appreciate the problems of describing industrial organic chemistry. Tens of thousands of organic chemicals are manufactured. Processes are legion; information on them is frequently confidential or buried obscurely

in patents. Small wonder that the average organic chemistry textbook is content to pass lightly over industrial processes.

It is possible to simplify the picture, however, by a study of where industrial organic chemicals come from and what they are used for. Of the 250 billion pounds of chemicals produced annually in the United States, 85 billion pounds are produced from 25 billion pounds of ethylene. Seventy percent of US organic chemicals are based on ethylene, propylene, and benzene. If we add to these three starting materials the C_4 olefins, toluene, xylenes, and methane and recognize that small but important groups of chemicals are derived from coal, fats and oils, and carbohydrates, then the question of where chemicals come from becomes more straightforward.

A study of the uses of organic chemicals, that is, of their technology, is similarly simplified by the realization that over 40% of them find their way into the polymer production and processing industries. There are, of course, many other industries that use chemicals. Their diversity makes organization more difficult, and we have tried to give a broad overall picture together with a study in depth of selected cases.

Furthermore, we have tried to look at organic chemicals not only from the point of view of the producer who is manufacturing a specific chemical entity but also from the point of view of the consumer who is buying not a chemical as such but a property that he requires. We discuss many of the materials downstream of the organic chemicals industry—elastomers, fibers, plastics, adhesives, surface coatings, solvents, plasticizers, lubricating oils, surfactants, drugs, food chemicals, dyes and pigments, and agrochemicals—and have considered why their manufacturers buy organic chemicals and how they use them. We think these two volumes are unique among textbooks in dealing with the problems of formulating chemicals into saleable mixtures.

Finally, we have tried to place the US and world organic chemicals industries in their contexts in US and world economies at the beginning of the last quarter of the twentieth century.

These volumes are suitable for anyone who wishes to gain a perspective on the organic chemicals industry and are intended as a textbook for chemistry and chemical engineering graduate students and for undergraduates who have completed a course in organic chemistry. Part I will be useful for a one-quarter or one semester course. Part II provides a textbook for a second quarter or semester and is a useful reference for a shorter course.

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H.A.W
B.G.R.

CONTENTS

CONTENTS FOR PART TWO

Chapter 0
HOW TO USE "INDUSTRIAL ORGANIC CHEMICALS IN PERSPECTIVE" PARTS I AND II

0.1 STRUCTURE AND LAYOUT

Part I starts with an overview of the chemical industry and its place in the national economy (Chapter 1). It continues with a discussion basic to the chemistry of industrial organic chemicals. Where do organic chemicals come from? Chapter 2 deals with petroleum sources and Chapter 3 with sources other than petroleum. Chapter 4 describes how polymers are made, and Chapter 5 describes aspects of catalysis that are basic to modern chemistry. In Chapter 6 we speculate about the future of the chemical industry and the role of the chemist in it.

Part II describes the technology of the industry—how chemicals are used. Chapter 1 considers the various industries that buy chemicals and how those chemicals are chosen. Polymers are a major outlet for chemicals. Thus Chapters 2 to 6 cover the uses of polymers in plastics, fibers, elastomers, surface coatings, and adhesives. Chapters 7 to 14 deal with some of the industries using chemicals that are not mainly polymers, notably surface active agents, drugs, solvents, lubricating oils, plasticizers, agrochemicals, dyes and pigments, and food chemicals.

Each chapter is numbered, and these chapters are divided and sub-

divided. For example Chapter 3 deals with sources of chemicals other than natural gas and petroleum; Section 3.3 covers carbohydrates, and Section 3.3.2 refers to starch in particular. All cross-references—and we have provided them profusely—refer to the numbered subsections and indicate in which volume these occur. A reference "see note" directs the reader to the notes and references section at the end of each chapter, and the note is found under the decimal heading in which the reference occurs.

0.2 STANDARD INDUSTRIAL CLASSIFICATION

We define all industries and branches of industry according to the US Standard Industrial Classification (SIC), which appears on the Standard Industrial Classification Manual: 1972 available from the US Government Printing Office, Washington, DC 20402. The classification divides the economy into broad sectors, such as the manufacturing industry, which are then subdivided further. Thus the manufacturing industry is split into 20 two-digit major groups such as SIC 28, chemicals. These are subdivided into industry groups such as SIC 282, plastics and synthetic fibers, and a fourth digit defines a specific industry such as SIC 2823, cellulosic man-made fibers. The industries associated with the Chemical and Allied Products Industries are shown in Table 1.2.

The definition of the chemical industry in countries other than the United States differs in detail from that given above, and those wishing to tackle official statistics should beware of such pitfalls.

0.3 UNITS AND NOMENCLATURE

The widespread introduction of the SI (Système International) system of units based on the meter, the kilogram, and the second has worsened the chaos among the units used by the chemical industry. Three kinds of ton are in common use—the short ton (2000 lb), the metric ton or tonne (1000 kg or 2204.5 lb), and the long ton (2240 lb). US statistics tend to be given in millions of pounds which are unambiguous, and we have followed this example apart from occasional references to tons. For the most part we try to quote figures in the units actually used by industry (e.g., petroleum is measured in barrels, benzene in gallons, and toluene in pounds). Conversions into the SI or other well-known scientific units are included when necessary. A table of conversion factors is given on the end papers.

Similarly, in naming chemicals we tend to use the names conventional in industry rather than the more academic nomenclature of the International Union of Pure and Applied Chemistry (IUPAC). Thus we write hydrogen, not dihydrogen; ethylene, acetylene, and acetic acid, not ethene, ethyne, and ethanoic acid. We will refer to the compound $C_6H_5CH(CH_3)_2$ as cumene, the name by which it is bought and sold, rather than by the more informative names of isopropylbenzene, 2-phenylpropane, or (1-methylethyl)benzene. Similarly, the word ethanal would be likely to be misread as ethanol in industry where the compound would still be known as acetaldehyde. So important is trivial nomenclature that the pharmaceutical industry could not operate without it. We apologize to those who are unacquainted with the trivial names, but we feel that this best serves our aim of introducing the student to chemical industry practice.

0.4 GENERAL BIBLIOGRAPHY

In many ways the greatest service a book like this can provide is to introduce the student to the industrial chemical literature. We follow each chapter with an annotated bibliography that lists some of the standard literature on the subject of the chapter, cites the sources of much of our own information, and adds occasional notes to matters discussed in the chapter.

Certain books are of general interest and are discussed below. When referred to later in the book, they are cited in an abbreviated form. For example, *The Chemical Economy*, by B. G. Reuben and M. L. Burstall, Longman, London, 1974, is referred to as *The Chemical Economy*.

In our bibliographies we largely confine ourselves to material published after 1970. References to earlier works may be found in *The Chemical Economy*, *Kirk-Othmer*, and other encyclopedias (see below) and in the bibliography, *Literature of Chemical Technology*, J. F. Smith, Ed. Advances in Chemistry Series No. 78, American Chemical society, Washington, DC 1968.

0.4.1 ENCYCLOPEDIAS

The most important single work of reference is Kirk-Othmer's *Encyclopedia of Chemical Technology*, 22 volumes plus one supplementary volume, 2nd ed., Interscience, New York, 1962–1971. It provides comprehensive and well-referenced coverage of almost every aspect of industrial chemistry. The earlier volumes are inevitably dated, but seven volumes