Ellis Horwood series in chemical science

COMPUTER AIDS TO CHEMISTRY

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and

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ELLIS HORWOOD LIMITED
Publishers · Chichester

Halsted Press: a division of
JOHN WILEY & SONS
New York · Chichester · Brisbane · Toronto

First published in 1986 by
ELLIS HORWOOD LIMITED
Market Cross House, Cooper Street, Chichester, West Sussex, PO19 1EB, England

The publisher's colophon is reproduced from James Gillison's drawing of the ancient Market Cross, Chichester.

Distributors:
Australia and New Zealand:
Jacaranda-Wiley Ltd., Jacaranda Press,
JOHN WILEY & SONS INC.
GPO Box 859, Brisbane, Queensland 4001, Australia
Canada:
JOHN WILEY & SONS CANADA LIMITED
22 Worcester Road, Rexdale, Ontario, Canada
Europe and Africa:
JOHN WILEY & SONS LIMITED
Baffins Lane, Chichester, West Sussex, England
North and South America and the rest of the world:
Halsted Press: a division of
JOHN WILEY & SONS
605 Third Avenue, New York, NY 10158, USA

British Library Cataloguing in Publication Data
Computer aids to chemistry —
(Ellis Horwood series in chemical science)
1. Chemistry — Data processing
I. Vernin, G II Chanon, M
542'.8 QD39 3 E46

Library of Congress Card No. 86-10452

ISBN 0-85312-774-3 (Ellis Horwood Limited)
ISBN 0-470-20338-2 (Halsted Press)

Phototypeset in Times by Ellis Horwood Limited
Printed in Great Britain by The Camelot Press, Southampton

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Foreword

The development over the past twenty years of big computers has accelerated calculations in many fields—quantum chemistry, molecular mechanics, computer-assisted chemical synthesis are only some typical examples. A new surge in the contribution made by computers to progress in chemistry is the result of more recent commercialization of the high-performance personal computers (PCs). Thanks to its relatively low price and easy availability, such equipment has become commonplace in most chemistry laboratories throughout the world. The purpose of this book is to show chemists, with the aid of judiciously selected examples, how such recently developed and easily available techniques can be of invaluable assistance.

The eight chapters deal with such varied topics as organic synthesis, chemical education, chemical kinetics, analysis of chemical data, crystallography, structural analysis through data banks, and chemical information. Although far from exhaustive, this list is quite representative of the types of aid that microcomputers can offer to chemists. The presentation of the mathematical basis of these computational methods is reasonably condensed, allowing the average chemist to understand their development and applications. The contributors are experimental chemists applying computational methods to their own fields of research or teaching which is at least one reason why this text is so naturally assimilable.

This excellent book fills a gap in chemical education and will without doubt be of valuable help to a large population of chemists in research, teaching and industry. I am quite confident it will do just this.

Marseille. France
May 1986

Jacques V. Metzger

Introduction

Chemistry is an evergreen subject. This is so because chemistry has roots in conceptual fields which range from quantum mechanics to the molecular organization of life, and because chemistry deals with such a wide variety of problems in diverse fields, such as analytical, synthetic, physical, and industrial, living as well as inanimate matter, solid state as well as solution and gas phase systems, and from the simplest molecules to the most complex structures. Consequently, advances in nearly any area of scientific endeavor has an effect on chemistry, and vice versa.

One of the more recent revolutions to affect the field of chemistry is the advancement of spectroscopic techniques such that they have become ubiquitous in the everyday life of the chemist. Although far from over, this spectroscopic revolution is already undergoing its own revolution as a consequence of a new advance affecting the lives of all chemists. The new advance is, of course, the effect of the computer sciences on chemistry, made possible by the commercial availability of computers with ever-increasing capabilities and steadily-decreasing prices. Thirty years ago, computers were already known and used, but perhaps 90% or more of the chemists then working functioned quite well without them. However, this is no longer the case; within the next twenty years, quite the opposite will no doubt hold true.

The goal of this book is to show why the swing to computer aids to chemistry is occurring as well as examples of how. Since we accept the multifaceted nature of the field of chemistry, we have selected some representative, yet quite different, facets which exemplify the changes computers have made in the activity of chemists.

Of the eight chapters, three (Chapters IV, V, and VI) treat typical quantitative data. They have been written so as to be understandable to any chemist willing to understand how a computer makes such fundamental tools as X-ray Crystallography, Kinetics, and Data Analysis/Experimental Design easier to use. Chemists often complain of being inundated by information from all directions and thus being unable to keep abreast of current topics either in general or specific areas of chemistry. Three chapters, one devoted to information access (Chapter VIII) and two treating the specific areas of spectrometry databases (Chapter VII) and synthetic organic chemistry (Chapter I) bring good news in these areas. The computer can ease the burden of keeping abreast of the wave of chemical information not only by efficient information management, but also in the 'pretreatment' of information for a given chemical speciality.

Finally, each of us is familiar with our own process of learning chemistry, both as a student and throughout our careers. Two chapters describe how computers are affecting this aspect of our lives as chemists. Chapter II summarizes some of the exciting uses of computers as complements to the teaching and learning of chemistry. Chapter III deals more specifically with computer graphics and its effects far beyond activities concerned only with teaching. Chemistry has often been the battlefield and proving ground for mathematical models of all sorts. It was often fashionable to denigrate the chemist's intuition (which is somewhat impressionistic) in favor of the precision of mathematicians. The cross-fertilization of these approaches was strongly inhibited, since even though the chemists had an idea of the phenomena they had extracted from their laboratory experiments, they often felt unable to understand the mathematics involved in the elaboration of various models. With modern computer graphics this situation changes, since every mathematical model can be transformed into something tangible and observable. Thus, the problem of communication is solved, and the chemist can say to the mathematician, 'Although I do not fully understand the mathematics involved, your model does (or does not) fit my knowledge and understanding of my experiments, in such and such respects'.

Early in his history (actually in *pre*-history), Man realized that tools, adapted to specific tasks, extended the usefulness and efficiency of his own hands and fingers. Now, at the close of the twentieth century and on the verge of the twenty-first, it becomes apparent that a tool is now being introduced to extend the usefulness and efficiency of Man's own *brain*. This is a fantastic advance, and chemists should not attempt to avoid it. However, a good tool in awkward and inexperienced hands does a poor job. Thus, although each chapter attempts to show what computers have brought to a subject, we also try to illustrate in which ways the human brain must direct and decide, drawing comparisons between the abilities of man and the computer as often as possible.

This book is illustrative rather than exhaustive, as the extent of the topic precludes even an attempt at exhaustivity. One still may ask, 'Why no chapters dealing with quantum chemistry, infrared and n.m.r. databases, drug design, instrumentation interfacing, robotics, etc.?' Our only answer is the