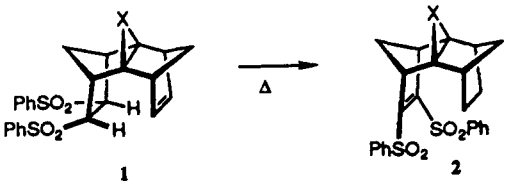
Patrick Murray for the analysis of **4c**. We also thank Dr. T. Rathmann of the FMC Corporation for a gift of *sec*-BuLi. We are grateful for support of this research by the National Science Foundation and the National Institutes of Health.

Supplementary Material Available: Experimental details, enantiomeric purity assays, and spectral data for compounds **1**, **4a–e**, **5**, and **6** (14 pages). Ordering information is given on any current masthead page.

Additions and Corrections

Intramolecular Reaction Rate Is Not Determined Exclusively by the Distance Separating Reaction Centers. The Kinetic Consequences of Modulated Ground State Strain on Dyotropic Hydrogen Migration in Systems of Very Similar Geometric Disposition [*J. Am. Chem. Soc.* **1991**, *113*, 7761–7762]. LEO A. PAQUETTE,* GEORGE A. O'DOHERTY, and ROBIN D. ROGERS

Page 7761: Structure **2** was depicted with a double bond that is not present. The correct reaction is given below:



1 **2**

Book Reviews *

Chemical Information Systems—Beyond the Structure Diagram. Edited by David Bawden (Pfizer Central Research) and Elenor M. Mitchell (Cambridge Crystal Data Centre). Ellis Horwood: Chichester. 1990. 178 pp. $58.00. ISBN 0-13-126582-2.

This is a thin (172 pages plus an index) book that aims to cover a very broad area for chemists in the information field. It developed from a Chemical Structure Association meeting in Durham, England, in 1989. The book contains 10 chapters, an introduction, and a good 6-page subject index, but no author index. The book is divided into five sections, with 1–4 chapters in each section. The sections (with the respective number of chapters in parentheses after the title) are the following: Overview (1), Three-Dimensional Structure Handling (4), Reactions and Synthesis (2), Property Prediction and Analysis (3), and Integrated Systems (1).

The book starts off with an introduction from the editors explaining that the book is designed to cover two areas which are "beyond the structure diagram". These are computation chemistry and access to a wider array of chemical data.

Chapter 1, by S. Ward, describes the management point of view of chemical information for the pharmaceutical industry. It is well-written by an experienced person in the field. The next chapter, by J. Barnard and colleagues, describes activities in the area of representing stereochemistry in two-dimensional structure representations. As the authors point out in the first sentence of this chapter, "this paper is out of place in this book".

Chapter 3 is a presentation of a commercial software system, MACCS-3D, by the company that developed the system. Chapter 4, by P. Willett and his research group at Sheffield, is an excellent introduction to structure (graph) matching techniques of 3-D structures. This probably is the best chapter in the book.

The chapter on the Cambridge Crystal database is primarily a historical presentation of the activities of this center. It also describes the evolution of their software which is used to search the database. As much better software is available from other sources, I found the value of this chapter is for someone who wishes to create their own 3-D database.

The next two chapters are about reactions and synthesis. The first describes a commercial reaction database system, ORAC. As it is one of the few papers published by this company, it merits reading. The second chapter in this section is a good overview of the many synthesis planning programs by F. Loftus, a researcher at ICI Pharmaceutical.

The property prediction and analysis section starts off with a chapter on a new software language, GLOBAL, which the eight authors from Proteus Biotechnology have developed. They then go on to explain how this polymorphic programming environment is a useful tool for many scientific activities of the company. No actual applications are given to chemistry.

The next chapter by D. Rouvray, the longest in the book, describes the use of topological indices for property prediction, with both a historical description and some recent work by the author. This is followed by a chapter by M. Johnson of The Upjohn company, on similarity-based moths for predicting chemical and biological properties. This is a good, but short, discussion of the topic.

The book concludes with a chapter on the progress being made toward integrated chemical information systems by D. Bawden, one of the editors of this book. The chapter contains some very general comments on the subject and describes, very briefly, what is being done at Pfizer in this area.

Overall I found this a useful but somewhat limited book. As the bulk of the chapters are written by people in the UK, it is difficult to expect a wide variety and in-depth coverage of the many opportunities offered by today's computer systems, software, and databases.

Stephen R. Heller, *USDA, ARS*

*Unsigned book reviews are by the Book Review Editor.