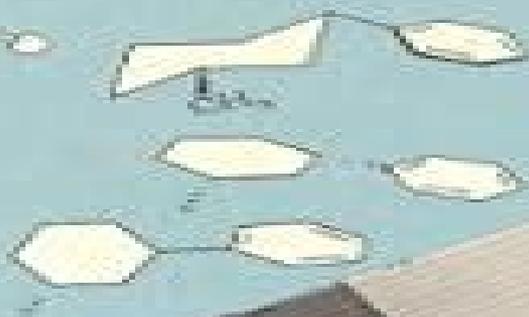


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Chemical Structures Wendy A. Warr, 2012-12-06 This book constitutes the Proceedings of the conference Chemical Structures The International Language of Chemistry which was held at Leeuwenhorst Congress Centre Noordwijkerhout in the Netherlands between May 31 and June 4 1987 The conference was jointly sponsored by the Chemical Structure Association the American Chemical Society Division of Chemical Information and the Chemical Information Groups of the Royal Society of Chemistry and the German Chemical Society The purpose of the conference was to bring together experts and an international professional audience to discuss and to further basic and applied research and development in the processing storage retrieval and use of chemical structures to focus international attention on the importance of chemical information and the vital research being carried out in chemical information science and to foster co operation among major chemical information organisations in North America and Europe Subjects covered included integrated in house databases substructure searching methodology spectral databanks new technologies microcomputers CD ROM parallel processing and expert systems and chemical reactions The keynote address was given by Mike Lynch of the University of Sheffield In this the opening chapter of the book Mike discusses progress made in chemical information science in the last fifteen years and describes his own approach to research In a plenary session Myra Williams of Merck Sharp and Dohme considered future trends from the point of view of the information manager and strategic planner in industry She emphasises the need for integration open architecture and a uniform user interface

Chemical Structures 2 Wendy A. Warr, 2012-12-06 This book constitutes the Proceedings of the second conference in the series Chemical Structures The International Language of Chemistry which was held at Leeuwenhorst Congress Centre Noordwijkerhout in the Netherlands between June 3 and June 7 1990 The conference was jointly sponsored by the Chemical Structure Association the American Chemical Society Division of Chemical Information the Royal Netherlands Chemical Society and the Chemical Information Groups of the Royal Society of Chemistry and the German Chemical Society The purpose of the conference was to bring together experts and an international professional audience to discuss and to further basic and applied research and development in the processing storage retrieval and use of chemical structures to focus international attention on the importance of chemical information and the vital research being carried out in chemical information science and to foster co operation among major chemical information organisations throughout the world Subjects covered included structure property correlations spectral database

systems chemical nomenclature generic structures stereochemistry substructure search systems connection table formats ring perception information integration three dimensional substructure searching similarity searching and systems for handling chemical reaction information All the papers were peer reviewed or given by invited speakers Many internationally recognised teams in the field of chemical structure handling are represented in the chapters of this book *Computer Graphics and Chemical Structures* Stanley V. Kasperek,1990-01-29 Describes computer systems for storage and retrieval of chemical structures and the numeric and textual data associated with them The first section covers the CAS ONLINE Registry File including the system s historical background design development and operation and its techniques for building graphic and generic structures searching techniques and options for displaying retrieved records Included are numerous examples for creating structures in addition to real computer sessions for search and retrieval Parts 2 3 and 4 describe in detail the Molecular Design Limited Systems CHEMBASE MACCS II REACCS and CHEMTALK which have become standard for chemical information systems in industry and academia **Graphics for Chemical Structures** Wendy A.

Warr,American Chemical Society. Division of Chemical Information,1987 **Chemical Structure Information Systems** Wendy A. Warr,1989 With the advent of computer graphics the proliferation of PCs and the development of user friendly software the average chemist can now build chemical databases search structures and substructures and generate chemical reports However these many systems and databases cannot be linked in a seamless manner This book addresses this concern in 12 chapters written by people from diverse backgrounds from software developers to information specialists Some of the specific topics covered include the need for flexibility in file formats to enable free exchange of chemical data the interrelated forces that restrict compatibility the attributes of a standard interface chemical structure browsing the use of a host language interface PC to mainframe communication programs and the standard molecular data format as an integration tool

Computerized Metallurgical Databases J. R. Cuthill,N. A. Gokcen,J. E. Morral,1988 **Biomedical Index to**

PHS-supported Research ,1990 Computer-Aided Molecular Design Charles H. Reynolds,American Chemical Society. Division of Computers in Chemistry,American Chemical Society. Division of Agrochemicals,American Chemical Society. Meeting,1995-07-27 Developed from a symposium sponsored by the Division of Computers in Chemistry and the Division of Agrochemicals at the 207th National Meeting of the American Chemical Society San Diego California March 13 17 1994

Molecular Design A.L. Horvath,1992-01-17 This book is a systematic presentation of the methods that have been developed for the interpretation of molecular modeling to the design of new chemicals The main feature of the compilation is the co ordination of the various scientific disciplines required for the generation of new compounds The five chapters deal with such areas as structure and properties of organic compounds relationships between structure and properties and models for structure generation The subject is covered in sufficient depth to provide readers with the necessary background to understand the modeling techniques The book will be of value to chemists in industries involved in the manufacture of

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