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Computer Graphics and Chemical Structures: Data Base Management Systems

Kasperek, Stanley V.

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Computer Graphics And Chemical Structures Database Management Systems

Daniela Niemeyer



Computer Graphics And Chemical Structures Database Management Systems:

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 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

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