

COMPUTER ASSISTED ANALYTICAL SPECTROSCOPY

1982-1983

John H. Johnson

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Computer Assisted Analytical Spectroscopy

Steven D. Brown



Computer Assisted Analytical Spectroscopy:

Computer-Assisted Analytical Spectroscopy Steven D. Brown, 1996-08-06 Based on presentations at the Fifth Symposium of Computer Enhanced Analytical Spectroscopy 1994 Computer Assisted Analytical Spectroscopy is essentially divided into two parts The first focuses on innovations associated with modern analytical measurements brought about through the use of computer methods in spectroscopy Enhancements to vibrational fluorescence and mass spectroscopy are discussed The main emphasis of the second part is placed on novel methods for dealing with problems arising in computer assisted analysis of spectroscopic data Throughout practical applications of the techniques presented are described **Computer-Enhanced Analytical Spectroscopy Volume 4** Charles L. Wilkins, 1994-01-31 The current volume covers research advances in nuclear magnetic resonance mass spectrometry and optical spectroscopy with emphasis on computer assisted interpretation methodologies **Computer-Enhanced Analytical Spectroscopy** Henk Meuzelaar, Thomas L. Isenhour, 2013-03-08 June 1986 brought together some of the world's leaders in computer enhanced analytical spectroscopy at Snowbird Utah for what the attendees decided to call The First Hidden Peak Symposium With the remarkable advances in both computer hardware and software it is interesting to observe that while many computational aspects of spectroscopic analysis have become routine some of the more fundamental problems remain unsolved The group that assembled included many of those who started trying to interpret chemical spectroscopy when computers were ponderous slow and not very accessible as well as newcomers who never knew the day that spectrometers were delivered without attached computers The synergism was excellent Many new ideas as well as this volume resulted from interactions among the participants The conclusion was that progress would be made on more fundamental problems now that hardware software and mathematics were coming together on a more sophisticated level The feeling was that the level of sophistication is now adequate and that it is only a matter of time before automated spectral interpretation surpasses all but the most advanced human experts

Computer-Enhanced Analytical Spectroscopy Volume 4 Henk L. C. Meuzelaar, Thomas L. Isenhour, 1993 Carbon 13 nuclear magnetic resonance spectrum simulation New approaches to computer aided NMR interpretation and structure prediction Multivariate data analysis of 2D NMR matrices Deconvolution and quantitative enhancement of multidimensional spectra Automatic analysis and simulation of mass spectra Multivariate analysis of time resolved pyrolysis mass spectral data Extracting qualitative and quantitative information from infrared emission spectral data Confirmation of detected species using Kovats indices and very low resolution spectrometry correlation analysis The synergy of computational chemistry and spectroscopy in understanding molecular structure and dynamics at interfaces Enhancement of chemical information through computer assisted examination of spectral variations Resolving unmodeled components from UV visible spectra with adaptive filtering Artificial intelligence and neural networks applied to ion mobility spectrometry Reviews in Computational Chemistry, Volume 17 Kenny B. Lipkowitz, Donald B. Boyd, 2003-04-24 Computational chemistry is increasingly used in most

areas of molecular science including organic inorganic medicinal biological physical and analytical chemistry Researchers in these fields who do molecular modelling need to understand and stay current with recent developments This volume like those prior to it features chapters by experts in various fields of computational chemistry Two chapters focus on molecular docking one of which relates to drug discovery and cheminformatics and the other to proteomics In addition this volume contains tutorials on spin orbit coupling and cellular automata modeling as well as an extensive bibliography of computational chemistry books

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Pharmaceutical Applications of Computer-aided Methods in Analytical Spectroscopy and Liquid Chromatography A. A. Fasanmade, 1985 Conference on Computers in Activation Analysis and Gamma-Ray Spectroscopy, May 1-4, 1978, Mayaguez, Puerto Rico ,1978 *The Cumulative Book Index* ,1997 A world list of books in the English language Energy Research Abstracts ,1977 Semiannual with semiannual and annual indexes References to all scientific and technical literature coming from DOE its laboratories energy centers and contractors Includes all works deriving from DOE other related government sponsored information and foreign nonnuclear information Arranged under 39 categories e g Biomedical sciences basic studies Biomedical sciences applied studies Health and safety and Fusion energy Entry gives bibliographical information and abstract Corporate author subject report number indexes Atlas of polymer and plastics analysis: Kunststoffe, Fasern, Kautschuk, Harze, Ausgangs- und Hilfsstoffe, Abbauprodukte Dieter O. Hummel, 1988

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web membership is open to anyone with a commercial interest in bioenergy our members include land and forestry owners wood processors feedstock suppliers fuel and energy suppliers equipment supplies manufacturers consultants contractors energy researchers educators regulators and investors