

Mass Spectra Of Geochemicals Petrochemicals And Biomarkers Specdata

Karl Pfleger, Hans H. Maurer, Armin A. Weber

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Handbook of GC/MS Hans-Joachim Hübschmann, 2008-11-21 This is the first comprehensive reference work for GC MS now in its second edition It offers broad coverage from sample preparation to the evaluation of MS Data including library searches Fundamentals techniques and applications are described A large part of the book is devoted to numerous examples for GC MS applications in environmental food pharmaceutical and clinical analysis These proven examples come from the daily practice of various laboratories. The book also features a glossary of terms and a substance index that helps the reader to find information for his particular analytical problem The author presents in a consistent and clear style his experience from numerous user workshops which he has organized This is a thoroughly revised and updated English edition based on an edition which was highly successful in Germany Wiley / NBS Registry of Mass Spectral Data, 7 Volume Set Fred W. McLafferty, Douglas B. Stauffer, 1989-02-08 Mass spectrometry is used extensively to identify unknown chemicals in almost all areas of chemistry biochemistry medical chemistry and the environmental sciences This massive work has been compiled and written by two acknowledged leaders in their field McLafferty and Stauffer are the authors of two previous books on mass spectral data and of various database versions of the data but the present 7 volume work Registry of Mass Spectral Data 2nd Edition is by far the most complete and up to date collection of mass spectra available in book form In it are presented the Mass Spectral and GC Data of Drugs, Poisons, Pesticides, Pollutants and registry spectra for 108 173 compounds Their Metabolites Karl Pfleger, Hans H. Maurer, Armin A. Weber, 2000-06-22 Announcing a new volume of Pfleger Maurer Weber Mass Spectral and GC Data of Drugs Poisons Pesticides Pollutants and Their Metabolites Unmatched in scope quality and reliability this collection is the result of a unique effort Part 4 of this famous reference work contains 2000 new mass spectra more than 6300 in Part 1 4 data of nearly all the new drugs relevant to clinical and forensic toxicology doping control food chemistry etc nearly complete coverage of trimethylsilylated perfluoroacylated perfluoroalkylated and methylated compounds data revision of already published volumes in this second edition updated sections on sample preparation and GC MS methods tables covering all the data of Parts 1 4 with directions as to page and volume on in which the data can be found as well as the appropriate entry numbers of the electronic versions tables listed by names and categories The complete set of Part 1 4 now comprises more than 6300 mass spectra and reaches far beyond the needs of clinical and forensic toxicologists The inclusion of pesticides and pollutants makes this data collection invaluable for environmental chemists occupational toxicologists and food analysts too The data of the supplement volume will also be provided as an up grade of the computer libraries PMW TOX3 by producers of mass spectrometers e g Hewlett Packard Finnigan MAT CE Automass Shimadzu and Mass Spectrometry in Environmental Sciences O. Hutzinger, F.W. Karasek, S. Safe, 2013-11-11 During the past Varian ten years a variety of methods involving mass spectrom etry have been developed for the analysis of environmentally important compounds Much has been accomplished in that period to solve some of the important problems in the field

Growth of this methodology and its accomplishments has reached the point where an individual scientist can no longer have an in depth knowledge of all the areas involved We have attempted to provide this in depth picture to those scientists con cerned by having the important topics treated by experts in the subject matter In order to provide all the relevant material in one volume we begin with the general topics which provide the basic background material necessary to understand the techniques discussed in the in depth topics These general chapters are kept brief containing only the essentials needed by the working scientist to deal with the practical applications References in these chapters are chosen to permit a more complete study of each chapter The concept for this book was developed during the activities of two of the editors under a NATO travel grant These editors gratefully acknowledge this support which made the initial planning of this book possible The editors would like to thank the individual authors of each chap ter for their cooperation and generously giving of their time for this project HDBK OF MASS SPECTRA OF ENVIRONMENTAL CONTAMINANTS R. A. Hites, 1985-09-10 Handbook of Mass Spectra of Environmental Contaminants Second Edition is a collection of the electron impact mass spectra of 533 commonly encountered environmental pollutants The compounds were selected from an analysis of several U S Environmental Protection Agency and World Health Organization databases All data have been reviewed by a panel of experienced mass spectrometrists To help identify unknown compounds all spectra have been indexed by common chemical name CAS registry number exact molecular weight and intense peaks Completely revised and expanded the Handbook of Mass Spectra of Environmental Contaminants Second Edition provides information essential to environmental laboratory specialists world wide This handbook is a collection of the electron impact mass spectra of 533 commonly encountered environmental pollutants selected from U S Environmental Protection Agency and World Health Organization databases

Interpretation of Mass Spectra of Organic Compounds Mynard C. Hamming, Norman G. Foster, 1972 Interpretation of Mass Spectra of Organic Compounds Mass Spectra Hans H. Maurer, Karl Pfleger, Armin A. Weber, 2007 Mass Spectra and Isotopes Francis William Aston, 1960 Mass Spectrometry of Priority Pollutants Brian Middleditch, 2012-12-06 When the list of organic priority pollutants was first published many mass spec troscopists went scrambling to their reference books GC MS was mandated for the analysis of 114 compounds yet the spectra of many of them if they had been recorded at all were scattered throughout the literature Moreover it soon became apparent that even if a sufficient number of instruments could be made available to undertake the task of monitoring 114 substances in the effluents of 21 categories of industry the personnel could not be trained to perform the analyses and interpret the results The solution to this problem has been the development of highly automated mass spectrometers which can be operated by personnel without the traditional research training This book is for the new breed of mass spectroscopist who is not interested in the esoteric details of mass spectral fragmentation but who merely wishes to identify specific pollutants in effluents Our inclusion of comprehensive lists of synonyms and bibliographic data should make the book of even greater value to the

reader who is not too familiar with the idiosyncrasies of chemical nomenclature and the scientific literature The experienced mass spectroscopist should also benefit from having all of the data collected together in one volume This is a book to be used rather than deposited in a library distant from the laboratory we would hope that it will fmd a place on top of every mass spectrometer used for the analysis of priority pollutants Wiley Registry of Tandem Mass Spectral Data, Ms4id Herbert M. Oberacher, 2011-03-14 High Resolution LC MSMS Library The Wiley Registry of Tandem Mass Spectral Data MS for ID contains 10 000 positive and negative mode spectra of over 1200 compounds of interest for forensics toxicology and pathology Areas covered include Illicit drugs Pharmaceutical compounds Pesticides Other small bioorganic molecules Each compound has been carefully measured by the Oberacher team at Institute of Legal Medicine Innsbruck Medical University in a series of controlled conditions to enable accurate reliable and reproducible search results in a variety of settings The Wiley Registry of Tandem Mass Spectral Data MS for ID comes bundled with one of the most accurate search algorithms developed for LC MSMS and is also made available in formats compatible with current LC MSMS software systems Mass Spectra of Organic Compounds ,1977 Mass Spectra of Organic Compounds Bruce H. Kennett, 1977 GC Data of Drugs, Poisons, Pesticides, Pollutants and Their Metabolites Karl Pfleger, Hans H. Maurer, Armin Weber, 1992

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Molecular Geochemistry Applied to Petroleum Systems (North Slope, Alaska) and Environmental (oil Spills) Studies Ye Wang, 2009 A petroleum system can be classified only as speculative or hypothetical by geological and or geophysical inference Geochemical correlation is needed for a petroleum system to be termed known To better define the petroleum systems on the North Slope of Alaska the oil cracking mixing and correlation studies were accomplished by biomarkers and diamondoids in Chapter One of this dissertation Biomarkers are complex molecular fossils derived from biochemicals particularly lipids in once living organisms Biomarkers can provide information on the age source rock lithology the organic matter in the source rock environmental conditions during its deposition and burial the thermal maturity experienced by rock and oil and the degree of oil biodegradation Because biomarkers can be measured in both oils and source rock extracts the distributions of biomarkers can be used to correlate oil and oil or oil and source rock Diamondoids are small thermally stable cage like hydrocarbons in petroleum Due to high thermal stability diamondoids resist oil cracking and become more concentrated while biomarkers crack and decrease in concentration Therefore the extent of oil cracking can be investigated by comparing both diamondoid and biomarker concentrations Furthermore mixtures of high and low maturity oil can be identified when concentrations of both biomarkers and diamondoids are high The compound specific isotope analysis of

diamondoids CSIAD analyses were used to correlate the high maturity components while biomarkers especially those providing information on the age of the source rock were used to correlate the lower maturity components Forty one crude oil samples from the North Slope of Alaska have variable diamondoid and biomarker concentrations which indicate different extents of oil cracking Some of the samples are mixtures of high and low maturity components because they contain high concentrations of both diamondoids and biomarkers The North Slope oils in this study were grouped according to their related source rock formations into Triassic Shublik Formation Jurassic Kingak Shale Lower Cretaceous pebble shale and Hue GRZ and Tertiary Canning Formation Two Lisburne designated oils were determined to be generated from Shublik source rock in this study Four oil samples collected from wells located to the North of the Barrow Arch show unique biomarker characteristics but biomarker parameters indicate that they were generated from a clay rich equivalent of the calcareous Shublik Formation from North of the Barrow Arch Molecular geochemistry was also applied to environmental studies e q oil spills in the open ocean Petroleum enters the ocean from both natural oil seeps and oil spills every year The fate of spilled oil in the ocean and the biodegradation rate of oil were investigated through molecular geochemistry including biomarkers and nonbiomarkers In Chapter Two oil biodegradation in the open ocean was simulated in the laboratory Chemostats were newly invented and fabricated to incorporate features that could simulate open ocean conditions for refreshing water agitation temperature and other factors Oil compositional changes were observed by gas chromatography coupled with flame ionization detection GC FID Gas Chromatography coupled with mass spectrometry GC MS helped to detect changes in the biomarkers and polycyclic aromatic hydrocarbons PAHs in the oil The work in Chapter Two summarized the various factors influencing biodegradation of oil after it was spilled into the marine environment Significant factors controlling oil compositional changes include 1 air flow 2 oil amount 3 stirring rate 4 bacterial compositions in the seawater itself 5 temperature and 6 nutrients Some other factors such as seawater flow rate and water washing of the oil do not exhibit important effects on oil biodegradation rates The mean halftimes of selected hydrocarbon compounds in the oil were estimated by equations derived from the measured compositional changes Phylogenetic and qPCR studies helped to identify which bacteria in the seawater play important roles in the biodegradation of oil components n alkanes isoprenoids and the UCM Some genera of microorganisms were more effective in degrading different fractions of oil **Mass Spectra**

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