

# Interpretation Of Mass Spectra Of Organic Compounds

## Interpreting Spectra of Organic Molecules

Understanding Mass Spectra: A Basic Approach, Second Edition combines coverage of the principles underlying mass spectral analysis with clear guidelines on how to apply them in a laboratory setting. Completely revised from the first edition, an updated and unified approach to mass spectral interpretation emphasizes the application of basic principles from undergraduate organic, analytical, and physical chemistry courses. A detailed overview of theory and instrumentation, this useful guide contains step-by-step descriptions of interpretative strategies and convenient lists and tables detailing the information needed to solve unknowns. Other features include real-world case studies and examples, skill-building problems with clearly explained answers, and easy-to-follow explanations of the important mathematical derivations.

## Interpretation of Mass Spectra of Organic Compounds

Interpretation of Mass Spectra of Organic Compounds outlines the basic instrumentation, sample handling techniques, and procedures used in the interpretation of mass spectra of organic compounds. The fundamental concepts of ionization, fragmentation, and rearrangement of ions as found in mass spectra are covered in some detail, along with the rectangular array and interpretation maps. Computerization of mass spectral data is also discussed. This book consists of nine chapters and begins with a historical overview of mass spectrometry and a discussion on some important developments in the field, along with a summary of interpretation objectives and methods. The following chapters focus on instruments, ion sources, and detectors; recording of the mass spectrum and the instrumental and sample variables affecting the mass spectrum; sample introduction systems; and fragmentation reactions. Correlations as applied to interpretations are also considered, with emphasis on applications of the branching rule as well as beta-bond and alpha-bond cleavages. Example interpretations, calculations, data-processing procedures, and computer programs are included. This monograph is intended for organic chemists, biochemists, mass spectroscopists, technicians, managers, and others concerned with the whys and wherefores of mass spectrometry.

## Organic Mass Spectrometry in Art and Archaeology

Advances in Mass Spectrometry, Volume 2 documents the proceedings of a conference on mass spectrometry held in Oxford in September 1961. This compilation is categorized into six major topics — mass spectrometry in research; mass spectrometry of inorganic compounds; instruments and techniques; theory and correlation of mass spectra; mass spectra and analysis; and ionization and dissociation. Under these major topics, parts of the papers discussed include field ionization mass spectroscopy; initial kinetic energy discrimination effects in crossed-field ion sources; mass spectrometric study of CaO and Ta; and spark source mass spectrometry as an analytical technique. The book also covers discussions on initial energy of hydrocarbon fragment ions; determination of the structure of alkaloids by mass spectrometry; and application of a time-of-flight mass spectrometer to the examination of ion-molecule interactions. This volume is a useful reference to students and researchers conducting work on mass spectrometry.

## Understanding Mass Spectra

An Introduction to Spectroscopic Methods for the Identification of Organic Compounds, Volume 2 covers the theoretical aspects and some applications of certain spectroscopic methods for organic compound identification. This book is composed of 10 chapters, and begins with an introduction to the structure determination from mass spectra. The subsequent chapter presents some mass spectrometry seminar problems and answers. This presentation is followed by discussions on the problems concerning the application of UV spectroscopy and electron spin resonance spectroscopy. Other chapters deal with some advances and development in NMR spectroscopy and the elucidation of structural formula of organic compounds by a combination of spectral methods. The final chapter surveys seminar problems and answers in the identification of organic compounds using NMR, IR, UV and mass spectroscopy. This book will prove useful to organic and analytical chemists.

## Organic Trace Analysis

Practical Organic Mass Spectrometry Second Edition A Guide for Chemical and Biochemical Analysis J. R. Chapman Kratos Analytical Instruments, Manchester, UK This volume provides a comprehensive survey of current techniques for the use of mass spectrometry in organic chemical and biochemical analysis. Every aspect of modern instrumentation and technique is discussed. The new edition retains the effective division of material applied in the author's previous volume-theory, practical requirements and applications. However, it has been thoroughly revised and extended to include all recent advances in mass spectrometry, and is complete with extensive

references. This is essentially a book for the practising mass spectroscopist which will appeal to both biochemists and organic chemists. Some familiarity with basic principles is assumed but the author has employed a style which makes this volume suitable for beginners and more advanced students alike. The present volume will be particularly valuable to anyone who wishes to evaluate and compare alternative techniques. Main Contents-Instrumentation; Sample Introduction; Chemical Ionization (Ion-Molecule Reactions); Negative Ion Chemical Ionization; The Ionization of Labile Materials (Part I); The Ionization of Labile Materials (Part II); Tandem Mass Spectrometry (The Dissociation of Ions); Quantitative Analysis.

## **Organic Spectroscopy Workbook**

Although numerical data are, in principle, universal, the compilations presented in this book are extensively annotated and interleaved with text. This translation of the second German edition has been prepared to facilitate the use of this work, with all its valuable detail, by the large community of English-speaking scientists. Translation has also provided an opportunity to correct and revise the text, and to update the nomenclature. Fortunately, spectroscopic data and their relationship with structure do not change much with time so one can predict that this book will, for a long period of time, continue to be very useful to organic chemists involved in the identification of organic compounds or the elucidation of their structure. Klaus Biemann Cambridge, MA, April 1983 Preface to the First German Edition Making use of the information provided by various spectroscopic techniques has become a matter of routine for the analytically oriented organic chemist. Those who have graduated recently received extensive training in these techniques as part of the curriculum while their older colleagues learned to use these methods by necessity. One can, therefore, assume that chemists are well versed in the proper choice of the methods suitable for the solution of a particular problem and to translate the experimental data into structural information.

## **Interpretation of Mass Spectra of Organic Compounds**

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## **Structural Identification of Organic Compounds with Spectroscopic Techniques**

Provides a comprehensive description of mass spectrometry basics, applications, and perspectives. Mass spectrometry is a modern analytical technique, allowing for fast and ultrasensitive detection and identification of chemical species. It can serve for analysis of narcotics, counterfeit medicines, components of explosives, but also in clinical

chemistry, forensic research and anti-doping analysis, for identification of clinically relevant molecules as biomarkers of various diseases. This book describes everything readers need to know about mass spectrometry—from the instrumentation to the theory and applications. It looks at all aspects of mass spectrometry, including inorganic, organic, forensic, and biological MS (paying special attention to various methodologies and data interpretation). It also contains a list of key terms for easier and faster understanding of the material by newcomers to the subject and test questions to assist lecturers. Knowing how crucial it is for young researchers to fully understand both the power of mass spectrometry and the importance of other complementary methodologies, *Mass Spectrometry: An Applied Approach* teaches that it should be used in conjunction with other techniques such as NMR, pharmacological tests, structural identification, molecular biology, in order to reveal the true function(s) of the identified molecule. Provides a description of mass spectrometry basics, applications and perspectives of the technique Oriented to a broad audience with limited or basic knowledge in mass spectrometry instrumentation, theory, and its applications in order to enhance their competence in this field Covers all aspects of mass spectrometry, including inorganic, organic, forensic, and biological MS with special attention to application of various methodologies and data interpretation Includes a list of key terms, and test questions, for easier and faster understanding of the material *Mass Spectrometry: An Applied Approach* is highly recommended for advanced students, young scientists, and anyone involved in a field that utilizes the technique.

## **Interpretation of Mass Spectra**

This succinct compilation of essential reference data for the interpretation of NMR, IR, UV/Vis, and mass spectra also provides a hands-on guide for interpreting experimental spectral data and elucidating the structure of the respective compounds behind them. This fourth edition of the highly successful and concise textbook contains about 20% new data.

## **Mass Spectrometry**

Clearly structured, easy to read and optimal to understand, this extensive compendium fills the gap between textbooks devoted to either spectra interpretation or basic physical principles. The original Chinese editions have already sold over 18,500 copies, and the material is taken from the latest literature from around the world, plus technical information provided by the manufacturers of spectroscopic instruments. Alongside basic methods, Professor Ning presents up-to-date developments in NMR, MS, IR and Raman spectroscopy, such as pulsed-field gradient technique, LC-NMR, and DOSY. He stresses the application of spectroscopic methods, interpreting them in great detail and depth since most of the selected spectra may be applied to practical work, as well as

summarizing the rules for their interpretation. He also incorporates his original ideas, including a comparison of the common points in different spectroscopic techniques. This monograph features a unique structure, a typical example being the discussion of 2D NMR starting from pulse sequence units, which construct various pulse sequences for related 2D NMR. A complete chapter deals with the determination of configurations and conformations of organic compounds and even biological molecules from the viewpoint of spectroscopic methodologies, while one whole section is dedicated to the interpretation of mass spectra produced by soft ionization techniques. The principles of mass analyzers, especially the ion trap, are discussed in great depth, together with a concise summary of the MS fragmentation and rearrangement of common compounds, allowing readers to easily predict related mass spectrometric reactions. All the three kinds of library retrieval of mass spectra are presented in detail, together with recent developments in molecular vibration spectroscopy. The whole is rounded off with several appendices, including a subject index for rapid reference. With a foreword by the Nobel prizewinner, Richard R. Ernst.

## **Tables of Spectral Data for Structure Determination of Organic Compounds**

First published over 40 years ago, this was the first text on the identification of organic compounds using spectroscopy. This text is now considered to be a classic. This text presents a unified approach to the structure determination of organic compounds based largely on mass spectrometry, infrared (IR) spectroscopy, and multinuclear and multidimensional nuclear magnetic resonance (NMR) spectroscopy. The key strength of this text is the extensive set of practice and real-data problems (in Chapters 7 and 8). Even professional chemists use these spectra as reference data. Spectrometric Identification of Organic Compounds is written by and for organic chemists, and emphasizes the synergistic effect resulting from the interplay of the spectra. This book is characterized by its problem-solving approach with extensive reference charts and tables. The 8th edition of this text maintains its student-friendly writing style - wording throughout has been updated for consistency and to be more reflective of modern usage and methods. Chapter 3 on proton NMR spectroscopy has been overhauled and updated. Also, new information on polymers and phosphorus functional groups has been added to Chapter 2 on IR spectroscopy.

## **Interpretation of Mass Spectra**

Structural Analysis of Organic Compounds covers some practical analytical aspects of organic structural analysis by combined application of spectroscopic methods. This book is composed of three parts encompassing 35 chapters that specifically describe

infrared-, ultraviolet-, proton and carbon-13 nuclear magnetic resonance and mass spectroscopy. Considerable chapters discuss the problems intended to cover a wide variety of chemical structure and spectroscopic argument, thereby exemplifying interpretations and comment on specific practical aspects of the problem solving procedure. The remaining chapters provide short supplementing research concerning various aspects of structural analysis. This book will prove useful to organic and analytical chemists.

## **Introduction to Mass Spectrometry of Organic Compounds**

Practical Organic Mass Spectrometry

## **Structure Determination of Organic Compounds**

Spectroscopy is used in physical and analytical chemistry for the identification of substances through the spectrum emitted from or absorbed by them. The derivation of structural information from spectroscopic data is now an integral part of many courses in chemistry and related subjects at most universities. This workbook: Features exercises to help develop the student's understanding of how structures are determined from spectra and to promote the student's own interpretation of different spectra. Covers a large range of spectroscopic data, including mass spectrometry, infrared and  $^1\text{H}$  and  $^{13}\text{C}$  nuclear magnetic resonance, typically used in the routine analysis of small-sized organic molecules. Presents in full-color, in a workbook-friendly format the spectra for interpretation with explanations and analyses on the facing page. Related to the workbook the authors have an online resource of the problems featured in the workbook, available at: <http://spectros.unice.fr/> By using the print edition alongside the online spectra, students will be able to enhance their understanding of the interpretation of multiple spectra.

## **Interpretation of Mass Spectra of Organic Compounds**

This book is a logical, step-by-step guide to identification of organic compounds by mass spectrometry. The book is organized into chapters covering the major types of organic compounds, including alcohols, acids and esters, aldehydes and ketones, ethers, hydrocarbons, halogenated compounds, amines and amides, and sulfur-containing compounds. In each chapter, the mechanisms of the major fragmentation pathways are discussed, with reference to several simple sample compounds. By teaching the user to recognize typical fragmentations, the book removes the need to search databases, often limited, of electronic spectra. Key features of the book include:

- \* 200 representative spectra of common organic compounds
- \* Functional group

approach to mass spectra interpretation \* Appendix of 'unknown' spectra with step-by-step guide to identification This book is a must for anyone who needs to identify organic molecules by mass spectrometry but does not need to know the detailed workings of a mass spectrometer.

## Interpretation of Mass Spectra

Originally published in 1962, this was the first book to explore teh identification of organic compounds using spectroscopy. It provides a thorough introduction to the three areas of spectrometry most widely used in spectrometric identification: mass spectrometry, infrared spectrometry, and nuclear magnetic resonance spectrometry. A how-to, hands-on teaching manual with considerably expanded NMR coverage--NMR spectra can now be intrepreted in exquisite detail. This book: Uses a problem-solving approach with extensive reference charts and tables. Offers an extensive set of real-data problems offers a challenge to the practicing chemist

## Mass Spectrometry of Organic Compounds

While modern techniques of nuclear magnetic resonance and mass spectrometry changed the ways of data acquisition and greatly extended the capabilities of these methods, the basic parameters, such as chemical shifts, coupling constants, and fragmentation pathways remain the same. This explains the ongoing success of the earlier editions of this book. However, since the amount of available data has considerably increased over the years, we decided to prepare an entirely new manuscript. It follows the same basic concepts, i. e. , it provides a representative, albeit limited set of reference data for the interpretation of  $^{13}\text{C}$  NMR,  $^1\text{H}$  NMR, IR, mass, and UV Nis spectra. On the other hand, the book has undergone a number of changes. The amount of reference data has been doubled at least (especially for MS and IR) and the order and selection of data for the various spectroscopic methods is now arranged strictly in the same way. In addition, the the enclosed compact disc contains programs for estimating NMR chemical shifts and generating isomers based on structural information. Unfortunately, our teachers and colleagues, Prof. Wilhelm Simon and Prof. Thomas Clerc are no longer among us, and Prof. Joseph Seibl has retired years ago. Their contributions to developing the concept and the earlier editions of this work cannot be overemphasized. We also thank numerous colleagues who helped us in many different ways to complete the manuscript. We are particularly indebted to Dr.

## Mass Spectrometry

This book is a well-established guide to the interpretation of the mass, ultraviolet,

infrared and nuclear magnetic resonance spectra of organic compounds. It is designed for students of organic chemistry taking a course in the application of these techniques to structure determination. The text also remains useful as a source of data for organic chemists to keep on their desks throughout their career. In the seventh edition, substantial portions of the text have been revised reflecting knowledge gained during the author's teaching experience over the last seven years. The chapter on NMR has been divided into two separate chapters covering the 1D and 2D experiments. The discussion is also expanded to include accounts of the physics at a relatively simple level, following the development of the magnetization vectors as each pulse sequence is introduced. The emphasis on the uses of NMR spectroscopy in structure determination is retained. Worked examples and problem sets are included on a chapter level to allow students to practise their skills by determining the chemical structures of unknown compounds.

## Interpretation of Mass Spectra of Organic Compounds

Provides comprehensive coverage of the interpretation of LC–MS–MS mass spectra of 1300 drugs and pesticides Provides a general discussion on the fragmentation of even-electron ions (protonated and deprotonated molecules) in both positive-ion and negative-ion modes This is the reference book for the interpretation of MS–MS mass spectra of small organic molecules Covers related therapeutic classes of compounds such as drugs for cardiovascular diseases, psychotropic compounds, drugs of abuse and designer drugs, antimicrobials, among many others Covers general fragmentation rule as well as specific fragmentation pathways for many chemical functional groups Gives an introduction to MS technology, mass spectral terminology, information contained in mass spectra, and to the identification strategies used for different types of unknowns

## Mass Spectrometry

Completely revised and updated, this text provides an easy-to-read guide to the concept of mass spectrometry and demonstrates its potential and limitations. Written by internationally recognised experts and utilising "real life" examples of analyses and applications, the book presents real cases of qualitative and quantitative applications of mass spectrometry. Unlike other mass spectrometry texts, this comprehensive reference provides systematic descriptions of the various types of mass analysers and ionisation, along with corresponding strategies for interpretation of data. The book concludes with a comprehensive 3000 references. This multi-disciplined text covers the fundamentals as well as recent advance in this topic, providing need-to-know information for researchers in many disciplines including pharmaceutical, environmental and biomedical analysis who are utilizing mass spectrometry

## Structure Determination of Organic Compounds

A unique advanced textbook on spectroscopy. This interactive tutorial presents text, software and data in a state-of-the-art introduction to the interpretation of  $^{13}\text{C}$ - and  $^1\text{H}$ -nuclear magnetic resonance, infrared, mass and UV/VIS spectra. Designed as a hands-on guide, the newcomer or student learns not only by reading but by experimenting, using the powerful software tools and data provided on the accompanying CD-ROM. The software, based on the outstanding SpecTool product, enables you to learn how to interpret molecular spectra correctly, rapidly and easily. Moreover, you can check your progress by working through the examples embedded in this self-study course that demonstrate how to identify an organic compound and to elucidate its structure. All the material and software presented are the essence of the two authors' longstanding teaching experience.

## Interpretation of MS-MS Mass Spectra of Drugs and Pesticides

With contributions from noted experts from Europe and North America, Mass Spectrometry Instrumentation, Interpretation, and Applications serves as a forum to introduce students to the whole world of mass spectrometry and to the many different perspectives that each scientific field brings to its use. The book emphasizes the use of this important analytical technique in many different fields, including applications for organic and inorganic chemistry, forensic science, biotechnology, and many other areas. After describing the history of mass spectrometry, the book moves on to discuss instrumentation, theory, and basic applications.

## Instrumentation for Trace Organic Monitoring

Mass spectrometry has played an integral part in the study of organic molecular structures for more than 50 years, offering significant information from small amounts of sample. The mass spectrum produced by electron impact ionization presents a pattern of peaks that can often give definitive structural information about an unknown compound. Introd

## Interpretation Of Mass Spectra

Interpretation of Mass Spectra, say the authors, "aims at correlating ion dissociation mechanisms on a much broader scale, with emphasis on basic attributes such as ionization energies, proton affinities, and bond dissociation energies". They stress that the most important part of learning how to interpret unknown mass spectra is to practise doing it. "Prof. McLafferty's text has become a classic for classroom or self study

concerned with interpreting mass spectra in order to discern molecular structures or identities of compounds.\" International Journal of Mass Spectrometry

## **Structural Analysis of Organic Compounds by Combined Application of Spectroscopic Methods**

Seit über 50 Jahren gehört die Massenspektrometrie zu den wichtigsten analytischen Methoden. Neben einem technologiehistorischen Überblick konzentriert sich dieser Band auf die Analytik von Metallen und Elementen. Beschrieben werden Anwendungen aus der Meteorologie, Kerntechnik, Astrochemie, Geowissenschaft und Umwelttechnik. Dabei wird auf zahlreiche spezielle Verfahren eingegangen, u.a. auf die Sektorfeld- und die Sekundärionen-MS, auf induktiv gekoppelte Plasmen und beschleunigergestützte MS. Erläutert werden auch Isotopenverfahren zur Altersbestimmung von Proben.

## **Spectra Interpretation of Organic Compounds**

It is estimated that there are about 10 million organic chemicals known, and about 100,000 new organic compounds are produced each year. Some of these new chemicals are made in the laboratory and some are isolated from natural products. The structural determination of these compounds is the job of the chemist. There are several instrumental techniques used to determine the structures of organic compounds. These include NMR, UV/visible, infrared spectroscopy, mass spectrometry, and X-ray crystallography. Of all the instrumental techniques listed, infrared spectroscopy and mass spectrometry are the two most popular techniques, mainly because they tend to be less expensive and give us the most structural information. This book is an introductory text designed to acquaint undergraduate and graduate students with the basic theory and interpretative techniques of mass spectrometry. Much of the material in this text has been used over a period of several years for teaching courses in materials characterization and chemical analysis. It presents the mass spectra of the major classes of organic compounds and correlates the fragmentation pattern of each spectrum with the structural features of the compound it represents. This has been done for hydrocarbons, organic acids, ketones, aldehydes, esters, anhydrides, phenols, amines, and amides. The text discusses the origin of the fragments, techniques, innovations, and applications in mass spectrometry. It is interspersed with many illustrations, examples, an adequate but not overwhelming bibliography, and problems for students. It will serve as a lecture text for a one-semester course in mass spectrometry or can be used to teach the mass spectra portion of a broader course in material characterization and chemical analysis.

## An Introduction to Spectroscopic Methods for the Identification of Organic Compounds

Instrumentation for Trace Organic Monitoring provides comprehensive coverage of instrumental analysis techniques for trace organic analytes in environmental analysis. Sampling/sample preparation is discussed, in addition to mass spectrometry techniques, including GC-MS, HRMS, LCMS, APIMS, and MS-MS. This important book also covers new chromatography techniques, supercritical fluid, solid-phase extraction, and ion mobility spectrometry, which is a new ultra-sensitive technique. Difficult problems, such as dioxin/furan analysis, organometallic speciation, atmospheric organic vapors, water analysis, and flyash toxicity testing are addressed.

## A Beginner's Guide to Mass Spectral Interpretation

This introduction to organic spectroscopic analysis aims to provide the reader with a basic understanding of how nuclear magnetic resonance (NMR), infrared (IR) and ultraviolet-visible (UV-Vis) spectroscopy, and mass spectrometry (MS) give rise to spectra, and how these spectra can be used to determine the structure of organic molecules. The text aims to lead the reader to an appreciation of the information available from each form of spectroscopy and an ability to use spectroscopic information in the identification of organic compounds. Aimed at undergraduate students, Organic Spectroscopic Analysis is a unique textbook containing large numbers of spectra, problems and marginal notes, specifically chosen to highlight the points being discussed. Ideal for the needs of undergraduate chemistry students, Tutorial Chemistry Texts is a major series consisting of short, single topic or modular texts concentrating on the fundamental areas of chemistry taught in undergraduate science courses. Each book provides a concise account of the basic principles underlying a given subject, embodying an independent-learning philosophy and including worked examples.

## Mass Spectrometry

Although there are a number of books in this field, most of them lack an introduction of comprehensive analysis of MS and IR spectra, and others do not provide up-to-date information like tandem MS. This book fills the gap. The merit of this book is that the author will not only introduce knowledge for analyzing nuclear magnetic resonance spectra including  $^1\text{H}$  spectra (Chapter 1),  $^{13}\text{C}$  spectra (Chapter 2) and 2D NMR spectra (Chapter 3), he also arms readers systematically with knowledge of Mass spectra (including EI MS spectra and MS spectra by using soft ionizations) (Chapter 4) and IR spectra (Chapter 5). In each chapter the author presents very practical application skills by providing various challenging examples. The last chapter (Chapter 6) provides the strategy, skills and methods on how to identify an unknown compound through a

combination of spectra. Based on nearly 40 years researching and teaching experience, the author also proposes some original and creative ideas, which are very practical for spectral interpretation.

## **Applications of Inorganic Mass Spectrometry**

\"Organic Trace Analysis\" presents the basics of trace analysis, from sample preparation to the measurement: Students are introduced to statistical evaluation, quality control technologies, sampling and preparation of organic traces, as well as to enrichment and separation of samples. Spectroscopic techniques as chromatography, capillary electrophoresis, mass spectrometry, and receptor-based bioanalysis are presented in detail.

## **Introduction to Mass Spectrometry**

Offers an overview of the analysis of art and archaeological materials using techniques based on mass spectrometry. Illustrates basic principles, procedures and applications of mass spectrometric techniques. Fills a gap in the field of application on destructive methods in the analysis of museum objects. Edited by a world-wide respected specialists with extensive experience of the GC/MS analysis of art objects. Such a handbook has been long-awaited by scientists, restorers and other experts in the analysis of art objects.

## **Organic Spectroscopic Analysis**

This textbook provides an introduction to the types of spectroscopy commonly used to determine the structure of organic molecules. Strategies for interpreting spectra are emphasized and the reader is encouraged to develop a systematic approach to elucidating molecular structure from the types of spectroscopic data routinely obtained in the laboratory.

## **Interpretation of Organic Spectra**

Mass spectrometry is an analytical technique that can be used for the structural characterization and quantification of a wide range of molecules. The technique is extensively used by chemists for the analysis of small and volatile organic compounds. Mass spectrometry has long been an important technique for the identification of materials ranging from pure compounds to complex mixtures. Mass spectrometry can be used to determine molecular weight of compounds or using different ionization conditions, can provide more structural details through the analysis of fragmentation patterns. This level of detail can be attained for pure compounds and some mixtures.

Mass spectrometry can also be combined with separation techniques such as gas chromatography or liquid chromatography to allow more complex mixtures to be examined. These hyphenated techniques provide a range of options for the characterization of complex materials.

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