

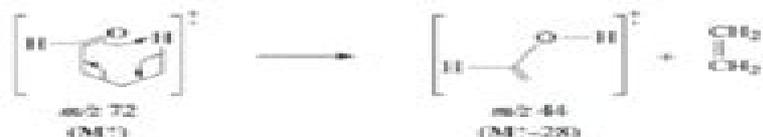
# Mass Spectrometry: PART 2

## some solved problems

### Question 1

- A compound with molecular formula  $C_4H_8O$  has a strong IR adsorption at  $1730\text{ cm}^{-1}$ . Its mass spectrum includes key peaks at  $m/z$  44 (the base peak) and  $m/z$  29. Propose a structure and write fragmentation equations showing how these peaks are formed.

Answer: the compound is butanal. The peak at  $m/z$  44 arises from a McLafferty rearrangement (see next slide for an example). This rearrangement happens to carbonyl compounds that have a hydrogen on their alpha carbon.



The peak at  $m/z$  29 arises from a fragmentation producing an acylium ion.



✧ Ketones

● McLafferty rearrangement



# Mass Spectroscopy Problems And Solutions

**Lei Shi**



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Concise Organic Spectroscopy Problems with solutions Basavarajaiah S M, 2022-11-25 This book Concise Organic Spectroscopy Problems with solutions illustrates the determination of structures of organic compounds by spectroscopic methods which are generally incorporated in the syllabi of Indian universities for undergraduate and postgraduate courses It covers the introductory part of all the spectroscopy techniques with questions and answers It also describes structure elucidation of organic compounds by spectra like UV IR NMR and mass spectral data This book is advantageous for students of UG PG and research students

**The Organic Chemistry Problem Solver** Research and Education Association, 1998 Principal classes of organic compounds are covered Topics include nomenclature preparation synthesis and reactions characterization tests and spectroscopy

**Organic Spectroscopy** William Kemp, 2017-03-01 This latest edition of the highly successful text Organic Spectroscopy continues to keep both student and researcher informed of the most recent developments in the various fields of spectroscopy New features of the third edition include 100 new student exercises worked examples and problem exercises An expanded chapter on nuclear magnetic resonance Details of the latest developments in Fourier transform instrumentation

**Study Guide & Solutions Manual to Accompany Organic Chemistry, Third Edition** G. Marc Loudon, Joseph G. Stowell, 1995

The Mass Spectra of Organic Molecules John Herbert Beynon, R. A. Saunders, Albert Edward Williams, 1968

**Nuclear Science Abstracts**, 1966

**Mass Spectrometry: Techniques and Applications** George W. A. Milne, 1971

**Encyclopedia of Spectroscopy** Heinz-Helmut Perkampus, 1995-03-07 Covers spectroscopic principles methods and applications ranging from atomic to molecular spectroscopy Many entries on instrumentations will help in trouble shooting spectrometers

The Encyclopedia of Mass Spectrometry Michael L. Gross, Richard Caprioli, 2006-12-21 Volume 6 Ionization Methods captures the story of molecular ionization and its phenomenal evolution that makes mass spectrometry the powerful method it is today Chapters 1 and 2 cover fundamentals and various issues that are common to all ionization e.g accurate mass isotope clusters and derivatization Chapters 3-9 acknowledge that some ionization methods are appropriate for gas phase molecules and others for molecules that are in the solid or liquid states Chapters 3-6 cover gas phase molecules dividing the subject into 1 ionization of gas phase molecules by particles e.g EI 2 ionization by photons 3 ionization by ion molecule and molecule molecule reactions e.g APCI and DART and ionization in Strong electric fields i.e Electrohydrodynamic and Field Ionization Desorption Ionization in a Strong Electric Field illustrates the transition to ionization of molecules in the solid or liquid states covered in Chapters 7-9 1 spray methods for ionization e.g electrospray 2 desorption ionization by particle bombardment e.g FAB and 3 desorption by photons e.g MALDI Electrospray and MALDI also lead to applications in biophysical chemistry the theme of Chapter 10 Chapter 11 reconsiders ionization from the view of choosing an ionization method The range of subjects is from ionization of organic and biomolecules to the study of microorganisms

**Notes, Problems and Laboratory Exercises in Mechanics,**

**Sound, Light, Thermo-mechanics and Hydraulics** Halsey Dunwoody, 1917     *Relevant Problems for Chemical Principles*  
Ian S. Butler, Arthur E. Grosser, 1984     *New Scientist*, 1974     **Spectroscopy** Edward Charles Cyril Baly, 1927

**Organic Structural Spectroscopy** Joseph B. Lambert, 1998 Appropriate for courses in organic spectroscopy or organic spectroscopic techniques in senior undergraduate and graduate programs This text authoritatively covers currently used techniques for determining the structure of organic and biological compounds ideal for any practicing or future organic or biochemist The fundamentals of all four principal spectroscopic methods are covered in depth each by an experienced author who is a practicing expert in that area The material is easy to grasp beginning at the most elementary level and progressing to the level required for organic research Highlights include the most thorough and current treatment of NMR available ample problem material and two new chapters devoted to multiple pulse and two dimensional methods     Bell Laboratories

Talks and Papers Bell Telephone Laboratories. Libraries and Information Systems Center, 1977     **Current Chemical Papers** Chemical Society (Great Britain), 1964 A classified world list of new papers in pure chemistry     **Chromatography and Mass Spectrometry in Biomedical Sciences, 2** Alberto Frigerio, 1983     **Optics and Spectroscopy**, 1960

Proceedings of the ... ASMS Conference on Mass Spectrometry and Allied Topics, 1990     **Advances in Mass Spectrometry** P. G. Kistemaker, N. M. M. Nibbering, 1992 These proceedings containing the texts of the invited lectures cover all aspects of mass spectrometry including theory fundamental studies applications and instrumentation Emphasis is placed on recent developments A complete listing of the posters is included

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