



Designing Exercises to Determine the Structural Formula of Organic Compounds Based on the Experimental Data

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Abstract This paper introduces the way to design exercises to determine the structural formula of organic compounds based on the experimental data. They are structure, physical properties, typical chemical properties, synthesis methods and application. From that the authors have built the scheme to design exercises. On that basis, the authors compiled some exercises which are used for teaching and learning organic chemistry in university and high school.

Keywords: *designing exercise, structural formula, organic compound, experimental data, teaching and learning organic chemistry, mechanisms of reactions*

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1. Introduction

Designing exercises is essential in teaching chemistry, an indispensable activity of chemistry teacher at the universities and high schools. Organic chemistry exercises have more interesting contents, special exercises for identified structural formula of organic compounds will require students to have a basic knowledge of organic chemistry such as stereochemistry, reaction mechanisms or organic synthesis, etc [1].

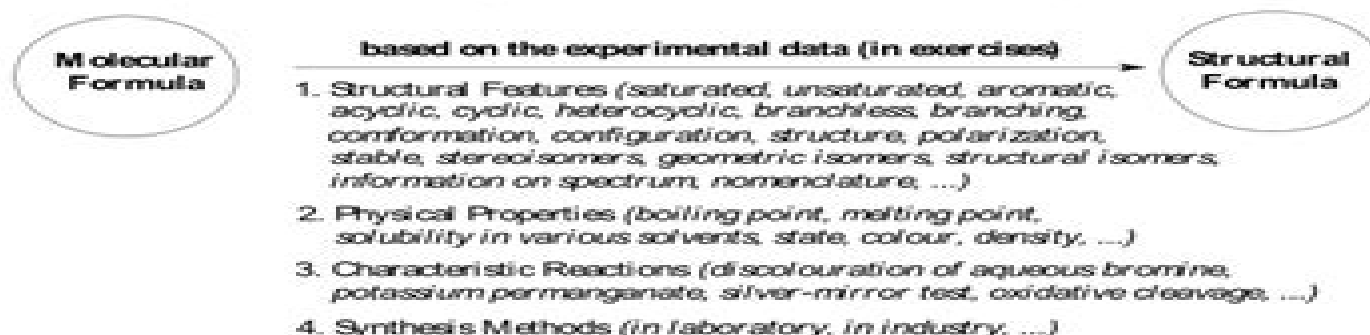
Exploiting the experimental data to determine the structure of organic compounds are important skills to help students practice on scientific research in the university. Solving this exercises will help students to

form experimental thinking in teaching of chemistry and research of organic chemistry.

2. Method – Desining Exercises

In order to determine the structural formula of organic compounds must first identify the components of qualitative and quantitative elements present in organic compounds, mean that molecular formula. Since it is based on experimental data on the molecular structure, chemical and physical properties of organic compounds and synthetic methods, we can argue to determine correctly structural formula of the organic compounds [2].

General scheme to design exercises as shown below.



Spectral Exercises In Structural Determinatin Of Organic Compounds

Ensheng Dong



Spectral Exercises In Structural Determination Of Organic Compounds:

Spectral Exercises in Structural Determination of Organic Compounds Robert H. Shapiro, 1969 For undergraduate students *Structure Determination of Organic Compounds* Ernő Pretsch, Philippe Bühlmann, Christian Affolter, 2000 Table

Combination tables ¹³C NMR spectroscopy ¹H NMR spectroscopy IR spectroscopy Mass spectrometry UV Vis spectroscopy

Structure Determination By Spectroscopic Methods Raul SanMartin, Maria Teresa Herrero, 2020-11-26 The authors travel with the reader through the challenging maze of structure determination showing how to distinguish between valuable and deceiving data from IR NMR and MS spectra extracting structural conclusions and putting all the pieces together to solve the structure elucidation puzzle Indeed human reasoning is key to combining the information contained in those bands signals and peaks by a rationale that enables the makeup of a chemical structure A number of increasingly more complex problems will act as trip segments and in addition to the spectra themselves each chapter is supplemented with figures and tables that decipher the above data and serve as maps for the journey *Organic Spectroscopy Workbook* Tom Forrest, Jean-Pierre Rabine, Michel Rouillard, 2011-07-08 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 ¹H and ¹³C 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://spectro.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 Structure Elucidation by Modern NMR H.

Duddeck, W. Dietrich, 2012-12-06 For several years we have been organizing seminars and workshops on the application of modern one and two dimensional NMR methods at the faculty of chemistry in the Ruhr University Bochum FRG and elsewhere addressing researchers and graduate students who work in the field of organic and natural products chemistry In 1987 we wrote a workbook *Strukturaufklärung mit moderner NMR Spektroskopie* Steinkopff Darmstadt FRG 1988 in German language based on our experience in these courses Many of the exercises described therein have been used in such courses and some of them have been shaped by the participants to a great extent The response of readers and discussions with colleagues from many countries encouraged us to produce an English translation in order to make the book accessible to a wider audience Moreover the content has been increased from 20 exercise examples in the German to 23 in the English version This book could not have been written in the present form without the help of a number of colleagues and therefore

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Challenges in Molecular Structure Determination Manfred Reichenbächer, Jürgen Popp, 2012-03-22 Taking a problem based approach the authors provide a practice oriented and systematic introduction to both organic and inorganic structure determination by spectroscopic methods This includes mass spectrometry vibrational spectroscopies UV VIS spectroscopy and NMR as well as applying combinations of these methods The authors show how to elucidate chemical structures with a minimal number of spectroscopic techniques Readers can train their skills by more than 400 problems with varying degree of sophistication Interactive Powerpoint Charts are available as Extra Materials to support self study

Instrumental Methods of Chemical Analysis V. K. Ahluwalia, 2023-07-24 This textbook describes the theory underlying each instrumental procedure and applications of all instrumental methods It comprehensively covers the instrumental methods of chemical analysis chromatography thermal methods of chemical analysis electrochemical methods and instrumental methods of analysis of inorganic compounds These include thermogravimetric analysis differential thermal analysis thermometric titrations and some miscellaneous thermal methods like derivative thermogravimetric analysis thermobarography differential scanning calorimetry thermomechanical analysis and electric thermal analysis flame photometry fluorimetry and phosphorimetry nephelometric and turbidimetric techniques refractory and interferometry and X ray methods Each chapter consists a set of problems to aid self learning This textbook is highly useful for graduate and postgraduate students on chemistry and its allied fields It can also be used as a quick reference material by professionals working in the various fields of chemistry and material science

Structure Determination of Organic Compounds Ernő Pretsch, Philippe Bühlmann, Martin Badertscher, 2009-04-05 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

Organic Spectroscopic Structure Determination Douglass F. Taber, 2007 Organic Spectroscopic Structure Determination is a sophomore level book with emphasis on structure problem solving It consists of four sections that attempt to engage the imagination of the student Taber has arranged the material in such a way that the students can work the problems and learn the procedures on their own minimizing the time taken in lecture The first section contains three chapters of instruction on the methods of organic spectroscopy The second contains fifty problems with just data sets of spectroscopic data The third section is comprised of fifty problems that show starting materials and reaction conditions with spectroscopic data for the product The final section includes tables of spectroscopic data

Organic Structures from Spectra L. D. Field, S. Sternhell, John R. Kalman, 2011-09-07 Organic Structures from Spectra Fourth Edition consists of a carefully selected set of over 300 structural problems involving the use of all the major spectroscopic techniques The problems are graded to develop and consolidate the

student's understanding of Organic Spectroscopy with the accompanying text outlining the basic theoretical aspects of major spectroscopic techniques at a level sufficient to tackle the problems. Specific changes for the new edition will include a significantly expanded section on 2D NMR spectroscopy focusing on COSY, NOESY and CH Correlation. Incorporating new material into some tables to provide extra characteristic data for various classes of compounds. Additional basic information on how to solve spectroscopic problems. Providing new problems within the area of 10 2D NMR spectroscopy. More problems at the simpler end of the range. As with previous editions, this book combines basic theory, practical advice and sensible approaches to solving spectra problems. It will therefore continue to prove invaluable to students studying organic spectroscopy across a range of disciplines.

Organic Structures from Spectra L. D. Field, S. Sternhell, J. R. Kalman, 2013-02-18. The derivation of structural information from spectroscopic data is now an integral part of organic chemistry courses at all Universities. A critical part of any such course is a suitable set of problems to develop the student's understanding of how structures are determined from spectra. *Organic Structures from Spectra* Fifth Edition is a carefully chosen set of more than 280 structural problems employing the major modern spectroscopic techniques: a selection of 27 problems using 2D NMR spectroscopy, more than 20 problems specifically dealing with the interpretation of spin-spin coupling in proton NMR spectra and 8 problems based on the quantitative analysis of mixtures using proton and carbon NMR spectroscopy. All of the problems are graded to develop and consolidate the student's understanding of organic spectroscopy. The accompanying text is descriptive and only explains the underlying theory at a level which is sufficient to tackle the problems. The text includes condensed tables of characteristic spectral properties covering the frequently encountered functional groups. The examples themselves have been selected to include all important common structural features found in organic compounds and to emphasise connectivity arguments. Many of the compounds were synthesised specifically for this purpose. There are many more easy problems to build confidence and demonstrate basic principles than in other collections. The fifth edition of this popular textbook includes more than 250 new spectra and more than 25 completely new problems, now incorporates an expanded suite of new problems dealing with the analysis of 2D NMR spectra. COSY, CH Correlation spectroscopy, HMBC, NOESY and TOCSY has been expanded and updated to reflect the new developments in NMR and to retire older techniques that are no longer in common use. Provides a set of problems dealing specifically with the quantitative analysis of mixtures using NMR spectroscopy. Features proton NMR spectra obtained at 200, 400 and 600 MHz and ¹³C NMR spectra include DEPT experiments as well as proton coupled experiments. Contains 6 problems in the style of the experimental section of a research paper and two examples of fully worked solutions. *Organic Structures from Spectra* Fifth Edition will prove invaluable for students of Chemistry, Pharmacy and Biochemistry taking a first course in Organic Chemistry.

Contents: Preface, Introduction, Ultraviolet Spectroscopy, Infrared Spectroscopy, Mass Spectrometry, Nuclear Magnetic Resonance Spectroscopy, 2D NMR Problems, Index, Reviews from earlier editions. Your book is becoming one of the go-to books

for teaching structure determination here in the States Great work I would definitely state that this book is the most useful aid to basic organic spectroscopy teaching in existence and I would strongly recommend every instructor in this area to use it either as a source of examples or as a class textbook Magnetic Resonance in Chemistry Over the past year I have trained many students using problems in your book they initially find it as a task But after doing 3 4 problems with all their brains activities working out the rest of the problems become a mania They get addicted to the problem solving and every time they solve a problem by themselves their confident level also increases I am teaching the fundamentals of Molecular Spectroscopy and your books represent excellent sources of spectroscopic problems for students

Organic Structural Analysis Joseph B. Lambert, 1976

Problems Of Instrumental Analytical Chemistry: A Hands-on Guide (Second Edition) Jose Manuel Andrade Garda, Alatzne Carlosena-zubieta, Marcos Gestal-pose, Maria Paz Gomez-carracedo, Miguel A Maestro-saavedra, Maria Del Carmen Prieto-blanco, Rosa Maria Soto-ferreiro, Javier Teran-baamonde, 2025-07-02

The complex field of analytical chemistry requires knowledge and application of the fundamental principles of numerical calculation Problems of Instrumental Analytical Chemistry provides support and guidance to help students develop these numerical strategies to generate information from experimental results in an efficient and reliable way The book contains exercises that provide standard protocols for the most common calculations in the daily work of a laboratory Also included are easy to follow diagrams to facilitate understanding and avoid common errors making this textbook perfect as a hands on accompaniment to in class learning The subjects covered follow a course in analytical chemistry from the initial basics of data analysis to applications of mass UV VIS infrared and atomic spectrometry and chromatography concluding with an overview of nuclear magnetic resonance and electrochemistry Intended as a self training tool for undergraduates in chemistry analytical chemistry and related subjects this book is also useful as a reference for scientists looking to brush up on their knowledge of instrumental techniques in laboratories This second edition builds upon the first with new and updated content as well as QR codes distributed throughout directing readers to dedicated materials and websites hosting additional information examples and models

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Structural Analysis of Organic Compounds by Combined Application of Spectroscopic Methods J.T. Clerc, E. Pretsch, J. Seibl, 2012-12-02

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

NMR-Spectroscopy: Modern Spectral Analysis Ursula Weber, Herbert

Thiele,2008-11-21 The state of the art in NMR spectral analysis This interactive tutorial provides readers with a comprehensive range of software tools and techniques as well as the necessary theoretical knowledge required to analyze their spectra and obtain the correct NMR parameters Modern Spectral Analysis provides expert guidance by presenting efficient strategies to extract NMR parameters from measured spectra A database of selected spectra and modern powerful WIN NMR software designed by Bruker are provided on the enclosed CD ROM The programs provided are 1 D WIN NMR WIN DAISY WIN DR and WIN DYNAMICS and direct data exchange between all these programs is possible Readers are shown how they can obtain maximum structural information from their 1 D NMR spectra with time saving computer assistance Practical problems that can occur and their solutions are discussed at length using clear easy to follow examples Both homo and heteronuclear and first and second order spin systems are demonstrated Moreover relaxation analysis nuclear Overhauser effects and magnetic site exchange are all covered in this hands on guide to NMR spectral analysis

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Spectrometric Identification of Organic Compounds Robert M. Silverstein,Francis X. Webster,David J. Kiemle,David L. Bryce,2014-09-29 First published over 40 years ago this was the first text on the identification of organic compounds using spectroscopy This text presents a unified approach to the structure determination of organic compounds based largely on mass spectrometry infrared IR spectroscopy as well as 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 spectra This text is characterized by its problem solving approach with numerous practice problems and extensive reference charts and tables

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An Introduction to Spectroscopic Methods for the Identification of Organic Compounds F. Scheinmann,2013-10-22 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

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Table of Contents Spectral Exercises In Structural Determinatin Of Organic Compounds

1. Understanding the eBook Spectral Exercises In Structural Determinatin Of Organic Compounds
 - The Rise of Digital Reading Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Advantages of eBooks Over Traditional Books
2. Identifying Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Spectral Exercises In Structural Determinatin Of Organic Compounds
 - User-Friendly Interface
4. Exploring eBook Recommendations from Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Personalized Recommendations

- Spectral Exercises In Structural Determinatin Of Organic Compounds User Reviews and Ratings
- Spectral Exercises In Structural Determinatin Of Organic Compounds and Bestseller Lists
- 5. Accessing Spectral Exercises In Structural Determinatin Of Organic Compounds Free and Paid eBooks
 - Spectral Exercises In Structural Determinatin Of Organic Compounds Public Domain eBooks
 - Spectral Exercises In Structural Determinatin Of Organic Compounds eBook Subscription Services
 - Spectral Exercises In Structural Determinatin Of Organic Compounds Budget-Friendly Options
- 6. Navigating Spectral Exercises In Structural Determinatin Of Organic Compounds eBook Formats
 - ePub, PDF, MOBI, and More
 - Spectral Exercises In Structural Determinatin Of Organic Compounds Compatibility with Devices
 - Spectral Exercises In Structural Determinatin Of Organic Compounds Enhanced eBook Features
- 7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Highlighting and Note-Taking Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Interactive Elements Spectral Exercises In Structural Determinatin Of Organic Compounds
- 8. Staying Engaged with Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Spectral Exercises In Structural Determinatin Of Organic Compounds
- 9. Balancing eBooks and Physical Books Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Spectral Exercises In Structural Determinatin Of Organic Compounds
- 10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
- 11. Cultivating a Reading Routine Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Setting Reading Goals Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Spectral Exercises In Structural Determinatin Of Organic Compounds
 - Fact-Checking eBook Content of Spectral Exercises In Structural Determinatin Of Organic Compounds

- Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
- 14. Embracing eBook Trends
 - Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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