

# Theoretical Investigation of Some Contact Lens Materials' Geometric, Electronic, and Spectroscopic Properties

Sinem Sipahioglu Kara<sup>1</sup>, Nergin Gunay<sup>2</sup>

<sup>1</sup>Bilecik Seyh Edebali University, Vocational School of Health Services, Department of Medical Services and Techniques, Bilecik Seyh Edebali University, 11210 Bilecik/Türkiye  
Email: sinem.sipahioglu@fat@bilecik.edu.tr

<sup>2</sup>Beykent University, Faculty of Health Sciences, Audiometry Department, Beykent University, 34500 Istanbul/Türkiye  
Email: nergin.gunay@fat@beykent.edu.tr

**Abstract:** *The goal of this study is to provide a detailed summary of the quantum physical calculations used to theoretically investigate the geometric, electrical, and spectroscopic characteristics of particular molecular structures that are employed as lens materials. An assessment of the typical behaviors displayed by the considered structures will be undertaken by contrasting the mathematical results with the experimental research reported in the literature. The crystallographic geometries of the molecular structures were used as a starting point for the optimization process. Using the 6-311++G(d,p) and LanL2DZ basis sets and the HF and DFT/B3LYP techniques, stable molecular structures were discovered in the ground state. Quantum chemical calculations, geometry, normal modes, and HOMO-LUMO energy vacancies of the molecule are displayed by GaussView 6[1] using Gaussian 16[2] software. All calculations were performed in the gas phase. The <sup>1</sup>H and <sup>13</sup>C NMR isotropic shifts based on the optimized structure in the gas phase were calculated by the GIAO, CSGT, and IGAIM methods.*

**Keywords:** contact lens, methyl methacrylate, 2-hydroxyethyl methacrylate, HF, and DFT

## 1. Introduction

Contact lenses are medical devices that are placed on the cornea and fixed refractive errors in the eyes. The history of the contact lens has a long and complex history. Ideas about contact lenses can be traced back to the 16th century. The first work on contact lenses was suggested as an idea by Leonardo da Vinci in 1508. Studies are still being conducted today to develop contact lenses[3]. The materials used to obtain the contact lens have reached an advanced level in their chemistry as well as their intraocular performance.

When contact lens wear, it touches the cornea, for this reason, it negatively impacts on cornea's healthy. There are important points for cornea health. These are high oxygen transmission, good tear film wetting for comfort and vision, superior material strength, and adequate water permeability to maintain lens movement[4]. Contact lenses depend on many parameters such as wettability, oxygen permeability, water content, mechanical properties, and thickness from a materials science perspective[5].

The first material used in the production of contact lenses was glass, followed by the development of materials science, the first used polymer type was Methyl Methacrylate (MMA)[6]. MMA is used to obtain hard and soft contact lenses. It was especially used because it had acceptable surface wettability, inexpensiveness, excellent durability, inflexibility, and a well-known nature of its structure. The only disadvantage is the lack of oxygen delivery to the conjunctiva and cornea [7]. Today, contact lenses made of MMA occupy modest on the market due to this disadvantage [5].

2-Hydroxyethyl Methacrylate (HEMA) is the first soft contact lens material. HEMA, which has hydrophilic for the property, is an important motive to prefer contact lens material. Its water content is about 38%. In order to have more than 38% water content, contact lenses must have other hydrophilic monomers in structure, that is to say, they are not made of 100% HEMA. The contact lenses, which contain HEMA, are extremely easy to use but they have some disadvantages like easy contamination, fragility, difficulty in using low minus prescriptions, bacterial adhesion, and low Dk. Nowadays HEMA-containing contact lenses are doped with various monomers by producing companies, in this way they aim to eliminate the disadvantages. It is used to increase the water content of HEMA-containing copolymer contact lenses above 38% [4].

In the past, many raw materials have been used in the production of contact lenses. In this study, we will examine two of the most striking of these. MMA is the first polymer used in the manufacture of contact lenses and is therefore important. HEMA is important because it is the most used polymer in contact lens production today. These two molecules' structures will investigate the geometric, electronic, and spectroscopic properties (IR, NMR, and Raman) by theoretical survey, and then quantum physics calculations will be made. These results will be compared with the experimental results in the literature.

## 2. Material and Calculation Methods

In this investigation, a very extensive program called Gaussian 16[2] package program, which has various theory and fundamental set options and incorporates molecular mechanics, quasi-experimental, and *ab initio* approaches,

# Spectroscopic Group Theoretical Method

**RD Boyd**



## **Spectroscopic Group Theoretical Method:**

## The Enigmatic Realm of **Spectroscopic Group Theoretical Method**: Unleashing the Language is Inner Magic

In a fast-paced digital era where connections and knowledge intertwine, the enigmatic realm of language reveals its inherent magic. Its capacity to stir emotions, ignite contemplation, and catalyze profound transformations is nothing lacking extraordinary. Within the captivating pages of **Spectroscopic Group Theoretical Method** a literary masterpiece penned by a renowned author, readers attempt a transformative journey, unlocking the secrets and untapped potential embedded within each word. In this evaluation, we shall explore the book's core themes, assess its distinct writing style, and delve into its lasting affect the hearts and minds of those that partake in its reading experience.

[https://ftp.thebrandexperience.com/data/virtual-library/index.jsp/the\\_golden\\_dawn\\_the\\_inner\\_teachings.pdf](https://ftp.thebrandexperience.com/data/virtual-library/index.jsp/the_golden_dawn_the_inner_teachings.pdf)

### **Table of Contents Spectroscopic Group Theoretical Method**

1. Understanding the eBook Spectroscopic Group Theoretical Method
  - The Rise of Digital Reading Spectroscopic Group Theoretical Method
  - Advantages of eBooks Over Traditional Books
2. Identifying Spectroscopic Group Theoretical Method
  - 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 Spectroscopic Group Theoretical Method
  - User-Friendly Interface
4. Exploring eBook Recommendations from Spectroscopic Group Theoretical Method
  - Personalized Recommendations
  - Spectroscopic Group Theoretical Method User Reviews and Ratings
  - Spectroscopic Group Theoretical Method and Bestseller Lists

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

### **Spectroscopic Group Theoretical Method Introduction**

In this digital age, the convenience of accessing information at our fingertips has become a necessity. Whether its research papers, eBooks, or user manuals, PDF files have become the preferred format for sharing and reading documents. However, the cost associated with purchasing PDF files can sometimes be a barrier for many individuals and organizations. Thankfully, there are numerous websites and platforms that allow users to download free PDF files legally. In this article, we will explore some of the best platforms to download free PDFs. One of the most popular platforms to download free PDF files is Project Gutenberg. This online library offers over 60,000 free eBooks that are in the public domain. From classic literature to historical documents, Project Gutenberg provides a wide range of PDF files that can be downloaded and enjoyed on various devices. The website is user-friendly and allows users to search for specific titles or browse through different categories. Another reliable platform for downloading Spectroscopic Group Theoretical Method free PDF files is Open Library. With its vast collection of over 1 million eBooks, Open Library has something for every reader. The website offers a seamless experience by providing options to borrow or download PDF files. Users simply need to create a free account to access this treasure trove of knowledge. Open Library also allows users to contribute by uploading and sharing their own PDF files, making it a collaborative platform for book enthusiasts. For those interested in academic resources, there are websites dedicated to providing free PDFs of research papers and scientific articles. One such website is Academia.edu, which allows researchers and scholars to share their work with a global audience. Users can download PDF files of research papers, theses, and dissertations covering a wide range of subjects. Academia.edu also provides a platform for discussions and networking within the academic community. When it comes to downloading Spectroscopic Group Theoretical Method free PDF files of magazines, brochures, and catalogs, Issuu is a popular choice. This digital publishing platform hosts a vast collection of publications from around the world. Users can search for specific titles or explore various categories and genres. Issuu offers a seamless reading experience with its user-friendly interface and allows users to download PDF files for offline reading. Apart from dedicated platforms, search engines also play a crucial role in finding free PDF files. Google, for instance, has an advanced search feature that allows users to filter results by file type. By specifying the file type as "PDF," users can find websites that offer free PDF downloads on a specific topic. While downloading Spectroscopic Group

Theoretical Method free PDF files is convenient, its important to note that copyright laws must be respected. Always ensure that the PDF files you download are legally available for free. Many authors and publishers voluntarily provide free PDF versions of their work, but its essential to be cautious and verify the authenticity of the source before downloading Spectroscopic Group Theoretical Method. In conclusion, the internet offers numerous platforms and websites that allow users to download free PDF files legally. Whether its classic literature, research papers, or magazines, there is something for everyone. The platforms mentioned in this article, such as Project Gutenberg, Open Library, Academia.edu, and Issuu, provide access to a vast collection of PDF files. However, users should always be cautious and verify the legality of the source before downloading Spectroscopic Group Theoretical Method any PDF files. With these platforms, the world of PDF downloads is just a click away.

### **FAQs About Spectroscopic Group Theoretical Method Books**

How do I know which eBook platform is the best for me? Finding the best eBook platform depends on your reading preferences and device compatibility. Research different platforms, read user reviews, and explore their features before making a choice. Are free eBooks of good quality? Yes, many reputable platforms offer high-quality free eBooks, including classics and public domain works. However, make sure to verify the source to ensure the eBook credibility. Can I read eBooks without an eReader? Absolutely! Most eBook platforms offer webbased readers or mobile apps that allow you to read eBooks on your computer, tablet, or smartphone. How do I avoid digital eye strain while reading eBooks? To prevent digital eye strain, take regular breaks, adjust the font size and background color, and ensure proper lighting while reading eBooks. What the advantage of interactive eBooks? Interactive eBooks incorporate multimedia elements, quizzes, and activities, enhancing the reader engagement and providing a more immersive learning experience. Spectroscopic Group Theoretical Method is one of the best book in our library for free trial. We provide copy of Spectroscopic Group Theoretical Method in digital format, so the resources that you find are reliable. There are also many Ebooks of related with Spectroscopic Group Theoretical Method. Where to download Spectroscopic Group Theoretical Method online for free? Are you looking for Spectroscopic Group Theoretical Method PDF? This is definitely going to save you time and cash in something you should think about. If you trying to find then search around for online. Without a doubt there are numerous these available and many of them have the freedom. However without doubt you receive whatever you purchase. An alternate way to get ideas is always to check another Spectroscopic Group Theoretical Method. This method for see exactly what may be included and adopt these ideas to your book. This site will almost certainly help you save time and effort, money and stress. If you are looking for free books then you really should consider finding to assist you try this. Several of Spectroscopic Group

Theoretical Method are for sale to free while some are payable. If you arent sure if the books you would like to download works with for usage along with your computer, it is possible to download free trials. The free guides make it easy for someone to free access online library for download books to your device. You can get free download on free trial for lots of books categories. Our library is the biggest of these that have literally hundreds of thousands of different products categories represented. You will also see that there are specific sites catered to different product types or categories, brands or niches related with Spectroscopic Group Theoretical Method. So depending on what exactly you are searching, you will be able to choose e books to suit your own need. Need to access completely for Campbell Biology Seventh Edition book? Access Ebook without any digging. And by having access to our ebook online or by storing it on your computer, you have convenient answers with Spectroscopic Group Theoretical Method To get started finding Spectroscopic Group Theoretical Method, you are right to find our website which has a comprehensive collection of books online. Our library is the biggest of these that have literally hundreds of thousands of different products represented. You will also see that there are specific sites catered to different categories or niches related with Spectroscopic Group Theoretical Method So depending on what exactly you are searching, you will be able to choose ebook to suit your own need. Thank you for reading Spectroscopic Group Theoretical Method. Maybe you have knowledge that, people have search numerous times for their favorite readings like this Spectroscopic Group Theoretical Method, but end up in harmful downloads. Rather than reading a good book with a cup of coffee in the afternoon, instead they juggled with some harmful bugs inside their laptop. Spectroscopic Group Theoretical Method is available in our book collection an online access to it is set as public so you can download it instantly. Our digital library spans in multiple locations, allowing you to get the most less latency time to download any of our books like this one. Merely said, Spectroscopic Group Theoretical Method is universally compatible with any devices to read.

### **Find Spectroscopic Group Theoretical Method :**

**the golden dawn the inner teachings**

**the gift of life the right to life a workshop on abortion**

the good and the bad only in america the route from nigeria to

the giles alleghany and jackson virginia artillery

**the german empire.**

**the glory of the nightingales**

the gigantic joke

the gilbert and sullivan companion

**the gem of lordsburg the lordsburg hotel college building 18871927**

**the ghosts at manor house**

the godowsky collection vol. 3 - paperback

the gentleman from san francisco and other stories

**the gold companion the az of mining marketing trading and technology**

~~the gnome from nome~~

*the gold of the pharaohs*

### **Spectroscopic Group Theoretical Method :**

Barron's SAT Math Workbook by Leff M.S., Lawrence This workbook's fifth edition has been updated to reflect questions and question types appearing on the most recent tests. Hundreds of math questions in ... SAT Math Workbook (Barron's Test Prep) ... Barron's SAT Math Workbook provides realistic questions for all math topics on the SAT. This edition features: Hundreds of revised math questions with ... SAT Math Workbook (Barron's Test Prep) Barron's SAT Math Workbook provides realistic questions for all math topics on the SAT. This edition features: Hundreds of revised math questions with ... Barron's SAT Math Workbook, 5th Edition Synopsis: This workbook's fifth edition has been updated to reflect questions and question types appearing on the most recent tests. ... Here is intensive ... Barron's SAT Math Workbook, 5th Edition Aug 1, 2012 — This workbook's fifth edition has been updated to reflect questions and question types appearing on the most recent tests. Hundreds of math ... Barron's SAT Math Workbook, 5th Edition Barron's SAT Math Workbook, 5th Edition. Barron's SAT Math Workbook - Leff M.S., Lawrence This workbook's fifth edition has been updated to reflect questions and question types appearing on the most recent tests. Hundreds of math questions in ... Barron's SAT Math Workbook, 5th Edition by Lawrence Leff ... Barron's SAT Math Workbook, 5th Edition by Lawrence Leff M.S. (2012,...#5003 ; Condition. Very Good ; Quantity. 1 available ; Item Number. 281926239561 ; ISBN. Barron's SAT Math Workbook book by Lawrence S. Leff This workbook's fifth edition has been updated to reflect questions and question types appearing on the most recent tests. Hundreds of math questions in ... Barron's SAT Math Workbook, 5th Edition by Lawrence Leff ... Home Wonder Book Barron's SAT Math Workbook, 5th Edition ; Stock Photo · Cover May Be Different ; Or just \$4.66 ; About This Item. Barron's Educational Series. Used ... 25.2 Nuclear Transformations Flashcards Study with Quizlet and memorize flashcards containing terms like Band of stability, Positron, Half-life and more. Nuclear Chemistry Chapter 25 (25.2, 25.3, 25.4) Worksheet ... Pearson Chemistry; Nuclear Chemistry Chapter 25 (25.2, 25.3, 25.4) Worksheet Answers. ... Chapter 25.2-Nuclear Transformations vocabulary and key concepts. 9 ... Nuclear Chemistry 2. The three types of nuclear radiation are radiation, radiation, and radiation. 25.2 Nuclear Transformations. 25.2 Nuclear Transformations Carbon-14 emits beta radiation and decays with a half-life ( $t_{1/2}$ ) of 5730 years. Assume you start with a mass of 2.00 10<sup>12</sup> g of carbon-14. a. How long is ... ECON101 - Ch.25 Section Review

Answers For the electronic transition from  $n = 3$  to  $n = 5$  in the hydrogen atom. a) Calculate the energy. b) Calculate the wavelength (in nm).

Chapter 25 Nuclear Chemistry 25.2 Nuclear Transformations Sep 5, 2017 — Nuclear Chemistry Targets: 1.I CAN Utilize appropriate scientific vocabulary to explain scientific concepts. 2.I CAN Distinguish between fission ... Matter and Change • Chapter 25 When a radioactive nucleus gives off a gamma ray, its atomic number increases by. 12. The three types of radiation were first identified by Ernest Rutherford. Nuclear Chemistry - Lake Central High School Jul 12, 2015 — What is the change in atomic number after the alpha decay? It decreases by 2. b. ... answer the following questions.

**Nuclear** ... 25.2 Nuclear Transformations | Lecture notes Chemistry These nuclei decay by turning a neutron into a proton to emit a beta particle (an electron) from the nucleus. This process is known as beta emission. It ... 60 s - 1 min SECTION 25.2 NUCLEAR TRANSFORMATIONS. 1. Write a nuclear equation for the following radioactive processes. a. alpha decay of francium-208  $^{208}\text{Fr} \rightarrow$  b ...

Anesthesiology Board Review Pearls of Wisdom 3/E Maximize your anesthesiology exam score! This powerful, results-oriented study guide delivers everything you need to improve your knowledge, confidence, and ... Anesthesiology Board Review Pearls of Wisdom 3/E Jul 17, 2012 — Print bound version of the complete text. Table of contents. ACID BASE, FLUIDS AND ELECTROLYTES AIRWAY AND INTUBATION Anesthesiology Board Review Pearls of Wisdom 3/E ... Anesthesiology Board Review Pearls of Wisdom 3/E (Pearls of Wisdom Medicine) by Ranasinghe, Sudharma Published by McGraw-Hill/Appleton & Lange 3rd (third) ... Anesthesiology Board Review Pearls of Wisdom 3/E By ... Aug 7, 2012 — This powerful, results-oriented study guide delivers everything you need to improve your knowledge, confidence, and recall. Featuring a rigorous ... Anesthesiology Board Review Pearls of Wisdom 3/E This powerful, results-oriented study guide delivers everything you need to improve your knowledge, confidence, and recall. Featuring a rigorous quick-hit Q&A ... Anesthesiology Board Review Pearls of Wisdom 3/E Maximize your anesthesiology exam score! This powerful, results-oriented study guide delivers everything you need to improve your knowledge, confidence, ... Anesthesiology Board Review Pearls of Wisdom 3/E This powerful, results-oriented study guide delivers everything you need to improve your knowledge, confidence, and recall. Featuring a rigorous quick-hit Q&A ...

Anesthesiology Board Review Pearls of Wisdom 3/E ISBN: 9780071761451 - 3rd Edition - Paperback - McGraw Hill / Medical - 2012 - Condition: new - In Never used condition - Anesthesiology Board Review Pearls ... Anesthesiology Board Review Pearls of Wisdom 3/E ... Aug 7, 2012 — Featuring a rigorous quick-hit Q&A format consisting of short clinical questions with brief answers, this is truly your most effective weapon ... Anesthesiology Board Review Pearls of Wisdom 3rd edition Anesthesiology Board Review Pearls of Wisdom 3rd Edition is written by Sudharma Ranasinghe; Kerri M. Wahl; Eric Harris; David J. Lubarsky and published by ...