

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

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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 ¹H and ¹³C 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,

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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
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 - Spectroscopic Group Theoretical Method Compatibility with Devices
 - Spectroscopic Group Theoretical Method Enhanced eBook Features
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 - 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

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