

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,

Spectroscopic Group Theoretical Method

Felix Bloch



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Spectroscopic and Group Theoretical Methods in Physics Felix Bloch, 1968 **Group Theory, Spectroscopy and Diffraction Methods** Mr. Rohit Manglik, 2024-03-24 EduGorilla Publication is a trusted name in the education sector committed to empowering learners with high quality study materials and resources Specializing in competitive exams and academic support EduGorilla provides comprehensive and well structured content tailored to meet the needs of students across various streams and levels *Group Theory in Chemistry and Spectroscopy* Boris S. Tsukerblat, 2006-08-18 This handbook on group theory is geared toward chemists and experimental physicists who use spectroscopy and require knowledge of the electronic structures of the materials they investigate Accessible to undergraduate students it takes an elementary approach to many of the key concepts Rather than the deductive method common to books on mathematics and theoretical physics the present volume introduces fundamental concepts with simple examples relating them to specific chemical and physical problems The text is centered on detailed analysis of examples Since neither chemists nor spectroscopists require theorem proofs very few appear here Instead the focus remains on the principal conclusions their meaning and their use In keeping with the text's practical bias the main results of group theory are presented in all sections as procedures making possible their systematic and step by step application Each chapter contains problems that develop practical skill and provide a valuable supplement to the text *Group Theoretical Methods in Physics* M. A. Markov, A. E. Shabad, 1985 *Crystal Symmetry, Lattice Vibrations, And Optical Spectroscopy Of Solids: A Group Theoretical Approach* Baldassare Di Bartolo, Richard C Powell, 2014-05-21 This book provides a comprehensive treatment of the two fundamental aspects of a solid that determine its physical properties lattice structure and atomic vibrations phonons The elements of group theory are extensively developed and used as a tool to show how the symmetry of a solid and the vibrations of the atoms in the solid lead to the physical properties of the material The uses of different types of spectroscopy techniques that elucidate the lattice structure of a solid and the normal vibrational modes of the atoms in the solid are described The interaction of light with solids optical spectroscopy is described in detail including how lattice symmetry and phonons affect the spectral properties and how spectral properties provide information about the material's symmetry and normal modes of lattice vibrations The effects of point defects doping on the lattice symmetry and atomic vibrations and thus the spectral properties are discussed and used to show how material symmetry and lattice vibrations are critical in determining the properties of solid state lasers *Spectroscopic Methods in Mineralogy* A. Beran, E. Libowitzky, 2004 **Recent Advances in Group Theory and Their Application to Spectroscopy** John C. Donini, 2012-12-06 The last few years have seen a resurgence in the applications of group theory to the problems posed by various characteristics of transition metals and lanthanides In particular with the commercial availability of more sophisticated experimental techniques such as Magnetic Circular Dichroism MCD Electron Paramagnetic Resonance EPR or ESR and Single Crystal Polarised Spectra

experimental data of a much more sophisticated and selective nature than the old stand by absorption spectra and magnetic susceptibility has become available This new wealth of high quality experimental data thus presents challenges of interpretation and organization of the data which the new developments in group theory strive to meet The wealth and quality of this new data makes the nuances and differences implicit in the traditional strong and weak field approach testable Thus these approaches can be tested more fully and new formalisms can be meaningfully tested by comparison to experiment Hence the characteristic implicit in the strong and weak field approaches are revealed by studies into their formal structures as exemplified by Drs E Konig S Kremer and S Piepho Similarly works proceed apace on the knotty problem of correlation and generalization of these properties through approaches such as those of Drs P H Butler J C Donini and M Kibler On a similar vein the deep structure of group representation and correlations of representation of various groups is explored by the afore mentioned and by Drs Fritzer Patera and Sharp

THEORETICAL SPECTROSCOPY S. MOHAN, 2019-06-07

Molecular Spectroscopy deals with absorption emission and scattering by molecules and it is used to determine the structure of the molecules Infrared spectroscopy played a vital role in the characterization of materials until Raman Spectroscopy was discovered Raman and Krishnan jointly discovered scattering spectroscopy which was named after Sir C V Raman Subsequently he was awarded Nobel Prize for his valuable discovery After 1930 spectroscopic scenario changed in materials characterization Combining group theory infrared spectroscopy and Raman spectroscopy the structure of molecules were established The discovery of laser gave a big boost to spectroscopy and first renaissance was seen in Raman spectroscopy Then laser Raman spectroscopy became popular and was widely used not only by physicists but also by material scientists chemists pharmacologists geologists etc Around 1986 the emergence of Fourier transform spectroscopy gave rise to new instrumentations such as Fourier transform infrared spectroscopy and Fourier transform Raman spectroscopy Fourier transform Raman spectroscopy is free from fluorescence and hence it is possible to record spectra of grease and rhodamine 6G very precisely In 1960s theoretical spectroscopy which was developed by Wilson Jr et al was widely studied to evaluate potential constants vibrational frequencies mean amplitudes Coriolis coupling constants centrifugal distortion constants inertia defects shrinkage effects and thermodynamic properties of various molecules Even today this classical method has several problems in providing the solution for secular equations due to mathematical inability

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