

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

M. A. Markov, A. E. Shabad



Spectroscopic Group Theoretical Method:

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

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 aforementioned and by Drs Fritzer Patera and Sharp

Infrared Spectroscopy of Symmetric and Spherical Spindles for Space Observation 1 Pierre-Richard Dahoo, Azzedine Lakhli, 2021-04-23 This book is dedicated to the description and application of various different theoretical

models to identify the near and mid infrared spectra of symmetric and spherical top molecules in their gaseous form. Theoretical models based on the use of group theory are applied to rigid and non rigid molecules characterized by the phenomenon of tunneling and large amplitude motions. The calculation of vibration rotation energy levels and the analysis of infrared transitions are applied to molecules of ammonia NH_3 and methane CH_4 . The applications show how interactions at the molecular scale modify the near and mid infrared spectra of isolated molecules under the influence of the pressure of a nano cage, the substitution site of a rare gas matrix, clathrate, fullerene or zeolite or a surface and allow us to identify the characteristics of the perturbing environment. This book provides valuable support for teachers and researchers but is also intended for engineering students, working research engineers and Masters and doctorate students.

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.

Group Theoretical Methods in Physics M. A. Markov, A. E. Shabad, 1985. *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 inertial defects shrinkage effects and thermodynamic properties of various molecules Eventoday this classical method has several problems in providing the solution for secular equations due to mathematical inability Spectroscopic Methods in Mineralogy A. Beran, E. Libowitzky, 2004 **Vibrational Spectroscopy** D. N. Sathyanarayana, 2015-07

Vibrational Spectroscopy Provides In A Very Readable Fashion A Comprehensive Account Of The Fundamental Principles Of Infrared And Raman Spectroscopy For Structural Applications To Inorganic Organic And Coordination Compounds Theoretical Analyses Of The Spectra By Normal Coordinate Treatment Factor Group Analysis And Molecular Mechanics Are Delineated The Book Features Coverage From First Principles To Recent Advances Relatively Self Contained Chapters Experimental Aspects Step By Step Treatment Of Molecular Symmetry And Group Theory Recent Developments Such As Non Linear Raman Effects Comprehensive Treatment Of Rotation Spectroscopy Band Intensities Spectra Of Crystals End Of Chapter Exercises Suitable For Students And Researchers Interested In The Field Of Vibrational Spectroscopy No Prior Knowledge Of Concepts Specific To Vibrational Spectroscopy Is Necessary Mathematical Background Such As Matrices And Vectors Are Provided *Spectroscopic Methods in Mineralogy and Geology* Frank C. Hawthorne, 2018-12-17 Volume 18 of Reviews in Mineralogy provides a general introduction to the use of spectroscopic techniques in Earth Sciences It gives an Introduction To Spectroscopic Methods and covers Symmetry Group Theory And Quantum Mechanics Spectrum Fitting Methods Infrared And Raman Spectroscopy Inelastic Neutron Scattering Vibrational Spectroscopy Of Hydrous Components Optical Spectroscopy Mossbauer Spectroscopy MAS NMR Spectroscopy Of Minerals And Glasses NMR Spectroscopy And Dynamic Processes In Mineralogy And Geochemistry X Ray Absorption Spectroscopy Applications In Mineralogy and Geochemistry Electron Paramagnetic Resonance Auger Electron And X Ray Photoelectron Spectroscopies and Luminescence X Ray Emission and New Spectroscopies The authors of this volume presented a short course entitled Spectroscopic Methods in Mineralogy and Geology May 13 15 1988 in Hunt Valley Maryland Bibliography on the Analyses of Optical Atomic Spectra Charlotte Emma Moore, 1969 Bibliography on the Analyses of Optical Atomic Spectra: 57La-71 Lu; 89Ac-99 Es Charlotte Emma Moore, 1968 **The Theory of Atomic Structure and Spectra** Robert D. Cowan, 2023-11-15 Both the interpretation of atomic spectra and the application of atomic spectroscopy to current problems in astrophysics laser physics and thermonuclear plasmas require a thorough knowledge of the Slater Condon theory of atomic structure and spectra This book gathers together aspects of the theory that are widely scattered in the literature and augments them to produce a coherent set of closed form equations suitable both for computer calculations on cases of arbitrary complexity and for hand calculations for very simple cases Both the interpretation of atomic spectra and the application of atomic spectroscopy to current problems in astrophysics laser physics and thermonuclear plasmas require a thorough knowledge of the Slater Condon theory of atomic structure and spectra Th Operator Techniques in Atomic Spectroscopy Brian R. Judd, 2014-07-14

In the 1920s when quantum mechanics was in its infancy chemists and solid state physicists had little choice but to manipulate unwieldy equations to determine the properties of even the simplest molecules. When mathematicians turned their attention to the equations of quantum mechanics they discovered that these could be expressed in terms of group theory and from group theory it was a short step to operator methods. This important development lay largely dormant until this book was originally published in 1963. In this pathbreaking publication Brian Judd made the operator techniques of mathematicians comprehensible to physicists and chemists. He extended the existing methods so that they could handle heavier more complex molecules and calculate their energy levels and from there it was another short step to the mathematical analysis of spectra. This book provides a first class introduction to continuous groups for physicists and chemists. Although first written from the perspective of atomic spectroscopy its major topics and methods will appeal to anyone who has an interest in understanding particle theories of nuclear physics. Originally published in 1998 The Princeton Legacy Library uses the latest print on demand technology to again make available previously out of print books from the distinguished backlist of Princeton University Press. These editions preserve the original texts of these important books while presenting them in durable paperback and hardcover editions. The goal of the Princeton Legacy Library is to vastly increase access to the rich scholarly heritage found in the thousands of books published by Princeton University Press since its founding in 1905.

Handbook of High-resolution Spectroscopy Martin Quack, Frederic Merkt, 2011-09-26 The field of High Resolution Spectroscopy has been considerably extended and even redefined in some areas. Combining the knowledge of spectroscopy laser technology chemical computation and experiments *Handbook of High Resolution Spectroscopy* provides a comprehensive survey of the whole field as it presents itself today with emphasis on the recent developments. This essential handbook for advanced research students graduate students and researchers takes a systematic approach through the range of wavelengths and includes the latest advances in experiment and theory that will help and guide future applications. The first comprehensive survey in high resolution molecular spectroscopy for over 15 years. Brings together the knowledge of spectroscopy laser technology chemical computation and experiments. Brings the reader up to date with the many advances that have been made in recent times. Takes the reader through the range of wavelengths covering all possible techniques such as Microwave Spectroscopy Infrared Spectroscopy Raman Spectroscopy VIS UV and VUV. Combines theoretical computational and experimental aspects. Has numerous applications in a wide range of scientific domains. Edited by two leaders in this field. Provides an overview of rotational vibration electronic and photoelectron spectroscopy. Volume 1 Introduction Fundamentals of Molecular Spectroscopy Volume 2 High Resolution Molecular Spectroscopy Methods and Results Volume 3 Special Methods Applications.

Symmetry (Group Theory) and Mathematical Treatment in Chemistry Takashiro Akitsu, 2018-07-18 The aim of this book *Symmetry Group Theory and Mathematical Treatment in Chemistry* is to be a graduate school level text about introducing recent research examples associated with symmetry group theory and

mathematical treatment in inorganic or organic chemistry physical chemistry or chemical physics and theoretical chemistry Chapters contained can be classified into mini review tutorial review or original research chapters of mathematical treatment in chemistry with brief explanation of related mathematical theories Keywords are symmetry group theory crystallography solid state topology molecular structure electronic state quantum chemistry theoretical chemistry and DFT calculations

Applications of Theoretical Methods in Vibrational Spectroscopy Shoichi Yamaguchi, 2025-10-02 This book provides unique introduction for experimentalists to theoretically calculate vibrational IR Raman SFG spectra of molecules in liquid and solid phases Vibrational spectroscopy is the most popular and valuable tool for scientists to obtain physicochemical insight into complex molecular systems Although standard softwares of quantum chemistry calculations routinely provide predictions of spectra this book describes dynamic aspects and spectroscopic accuracy enough to compare our experimental data directly to computations that lack in the softwares The quantum classical mixed approach presented in this book allows researchers including graduate students of chemistry and physics to extract microscopic information of structure and dynamics from their vibrational spectroscopic experimental data with no help from theoreticians Progress in Atomic Spectroscopy W. Hanle, 2013-11-11 H J BEYER AND H KLEINPOPPEN During the preparation of Parts A and B of Progress in Atomic Spectroscopy a few years ago it soon became obvious that a comprehensive review and description of this field of modern atomic physics could not be achieved within the limitations of a two volume book While it was possible to include a large variety of spectroscopic methods inevitably some fields had to be cut short or left out altogether Other fields have developed so rapidly that they demand full cover in an additional volume One of the major problems already encountered during the preparation of the first volumes was to keep track of new developments and approaches which result in spectroscopic data We have to look far beyond the area of traditional atomic spectroscopy since methods of atomic and ion collision physics nuclear physics and even particle physics all make important contributions to our knowledge of the static and dynamical state of atoms and ions and thereby greatly add to the continuing fascination of a field of research which has given us so much fundamental knowledge since the middle of the last century In this volume we have tried to strike a balance between contributions belonging to the more established fields of atomic structure and spectroscopy and those fields where atomic spectroscopy overlaps with other areas Nuclear Science Abstracts , 1976

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