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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 ^{1}H and ^{13}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, was employed. The Gaussian 16 is the latest in the series of Gaussian electronic structure programs used by chemists, chemical engineers, biochemists, physicists, and other scientists all over the world. The models can be applied to both stable species and substances that are difficult or impossible to observe experimentally due to their nature (such as toxicity, flammability, radioactivity, short-lived intermediates, and transition structures).

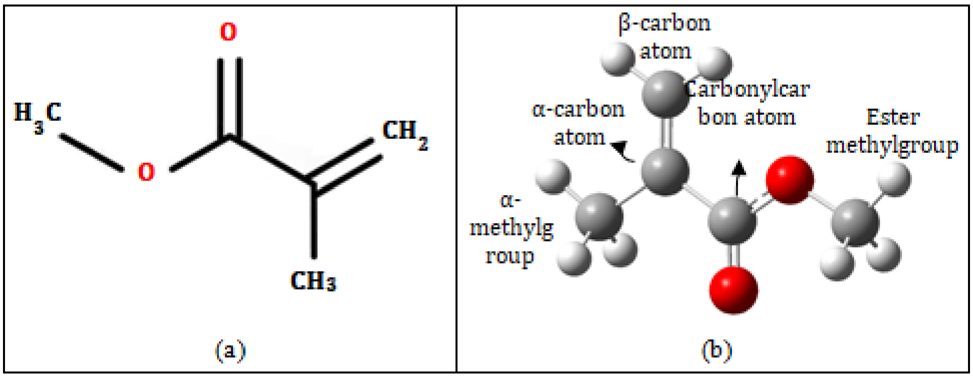
The energies of atoms and molecules may be computed, geometric optimizations can be made, and vibration frequencies, force constants, and dipole moments that depend on energy can also be calculated using the Gaussian 16 [2]program, which is based on the fundamental equations of quantum physics. The program may search for minimums, transition states, and reaction pathways while navigating the potential energy surface. It can also assess the stability of the wave function. Numerous other atomic and molecular properties, including IR and Raman spectra, thermochemical properties, bond and reaction energies, molecular orbitals, atomic charges, multipolar moments, NMR and magnetic susceptibility vibrational intensities, electron affinity and ionization energies, polarizability and hyperpolarizability, electrostatic potential, electron density, etc., can also be calculated using this program. Calculations can be done for each of these properties in the gas phase, in solutions, and in crystal structures. An atom or molecule's excited or ground state can be employed in computations.

The GaussView software is a graphical user interface that is a part of the Gaussian package programs and allows users to graphically describe a molecule's properties, make adjustments to these values, and begin calculations by entering input data [1].GaussView 6 [1] was used to draw the approximate three-dimensional geometries, which were then used as input data in the Gaussian 16 [2] package program to perform the calculations.With the help of this program, we can view molecules, rotate, move, and alter them. We can also visually inspect the outcomes of calculations made for a molecule investigated by the Gaussian program. These findings include optimal molecular structures, molecular orbitals, electrostatic potential surfaces, atomic charges, IR, Raman, NMR, VCD spectra, and normal mode animations depending on the vibration frequencies.

3. Results

3.1. Molecular structure calculations of MM molecule

The MMA molecule, with the chemical formula $C_5H_8O_2$, has a density of 1.21 g/cc and a molecular weight of 100.1 g/mol [8]. Figure 1.(a) depicts a representative representation of the MMA structure, while Figure 1.(b) depicts the optimized molecular geometry at HF/6-311++G(d,p) in the gas phase.



(a)
(b)

Figure 1: (a) a typical illustration, and **(b)** theoretical (obtained using the HF/6-311++G(d,p) method) molecular structure of the MMA molecule.

Table 1 displays the unscaled theoretical geometry parameters of the aforementioned molecule as well as experimental bond length data. Bond lengths are given in angstrom, bond angles and plane angles in degrees. It was observed that the values of bond lengths, bond angles, and dihedral angles calculated by HF and B3LYP methods were found to be reasonably close to each other. The MMA molecule has two conformations: the O = C – C = C angle structure, where the angle (1) is 180° when the CH_2 group is in the trans position to the oxygen, and (2) it is 0° when the CH_2 group is in the cis position to the oxygen.

Table 1: Calculated bond angles (°) and dihedral angles (°), as well as experimental and theoretical bond lengths (Å) of MMA molecule.

Parameters	Experimental	Theoretical			
Bond Lengths (Å)	[9]	UHF 6-311++G(d,p)	UHF LanL2DZ	UB3LYP 6-311++G(d,p)	UB3LYP LanL2DZ
$C = CH_2$	1.53	1.32211	1.33491	1.33641	1.35298
$C – CH_3$	1.53	1.50551	1.51074	1.50427	1.51384
C – C	1.52	1.49650	1.49272	1.49532	1.49888
C – O	1.36	1.32148	1.34917	1.35061	1.38562
C = O	1.22	1.18698	1.22228	1.21117	1.24632
$O – CH_3$	1.45	1.41556	1.45133	1.43775	1.47274
	R^2	**0.6837**	**0.6346**	**0.6647**	**0.6062**
Bond Angles (°)					

O = C – O	-	122.98597	121.85962	122.87665	122.06677
C – O – CH_3	-	117.28800	119.69260	115.86374	116.67873
O = C – C	-	122.84552	125.40838	123.45637	126.26540
C(O) – C = C	-	120.84839	117.50343	121.19610	117.23317
O – C – C	-	114.16850	112.73200	113.66698	111.66783
C = C – CH_3	-	124.07109	124.35660	123.83020	124.06567
C(O) – C – CH_3	-	115.08052	118.13997	114.97370	118.70116
Dihedral Angles (°)					
O = C – O – CH_3	-	0.01781	–0.01377	0.00178	–0.00638
C – C – O – CH_3	-	179.98235	–179.99054	179.99786	179.99070
O – C – C = C	-	0.01860	179.98845	0.00156	–179.98876
O – C – C – CH_3	-	–179.98216	–0.01202	–179.99843	0.01088
O = C – C = C	-	179.98319	0.01266	179.99762	0.00817
O = C – C – CH_3	-	–0.01757	–179.98780	–0.00238	–179.99219

3.2. Vibration frequency calculations of MMA molecule

Experimental research on the MMA molecule's vibration spectrum in the 4000-500 cm^{-1} middle infrared range has already been done [10]. In this investigation, calculations were performed theoretically in the same region using the HF and B3LYP methods in order to compare with the experimental data. Understanding the vibration spectrum and chemical properties depends on these computations. Since quantum mechanical calculations offer the electronic structure of the molecule using quantum mechanical laws and take into account the Schrödinger equation solution, we used quantum physical calculations to determine the vibrational frequencies and modes of molecules. Figure 2 displays the MMA molecule's theoretical (in the UHF/6-311++G(d,p) model) and experimental (FTIR) IR spectra.

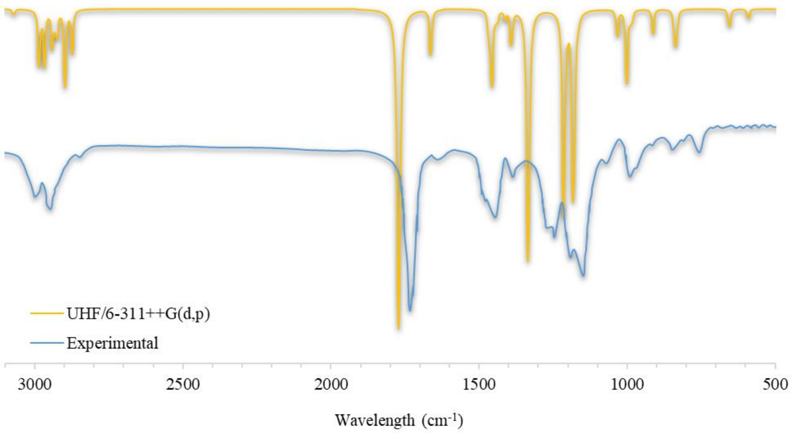


Figure 2: The MMA molecule's experimental [10] and calculated IR spectra

3.3. ^{13}C and ^{1}H chemical shift calculations of MMA molecule

Three alternative approach models -GIAO, CSGT, and IGAIM- were used to determine NMR shift values in accordance with the TMS reference material. Table 2 lists the experimental data and resulting chemical shift values. In order to make the compatibility of the theoretical approaches with the experimental data clear, the values for the linear correlation coefficients (R^2) are also provided at the bottom of the tables. As a result, there is often good agreement between the experimental and theoretical results.

Whereas the ^{13}C and ^{1}H NMR chemical shift values of the molecule were computed in the ranges of 172.9–21.5 ppm and 6.89–2.14 ppm, respectively, the experimental data were obtained in the ranges of 167.9–18.4 ppm and 6.10–1.95 ppm, respectively (Table 2).

Table 2: The MMA molecule's experimental [11]and theoretical (with basis set 6-311++G(d,p)) ^{13}C and ^{1}H isotropic NMR chemical shifts (in ppm units according to TMS).

	Experimental	**Theoretical (6-311++G(d,p))**					
Atom	**[11]**	GIAO		IGAIM		CSGT	
^{13}C		**HF**	**B3LYP**	**HF**	**B3LYP**	**HF**	**B3LYP**
C (= O)	167.92	172.9948	172.3715	172.7262	171.5558	172.7216	171.5541
C (= CH_2)	136.48	146.5760	146.0980	146.8771	146.0979	146.8777	146.1015
C (CH_2)	125.42	137.0123	129.9373	136.7879	129.6250	136.8109	129.6503
C (– O)	51.81	52.6723	52.7459	53.8172	53.1843	53.8355	53.2060
C (CH_3)	18.36	23.7050	20.6272	24.9552	21.4578	24.9750	21.4807
	R^2	**0.9967**	**0.9985**	**0.9968**	**0.9982**	**0.9968**	**0.9982**
^{1}H							
H (CH_2)	6.098	6.6271	6.3470	6.8833	6.5727	6.8872	6.5764
H (CH_2)	5.554	6.0869	5.7633	6.6694	6.3317	6.6730	6.3352

H (CH_3 – O)	3.752	3.7601	3.7069	4.3483	4.3269	4.3496	4.3284
H (CH_3 – O)	3.752	3.7597	3.7069	4.3480	4.3268	4.3494	4.3284
H (CH_3 – O)	3.752	3.6307	3.4901	4.1871	4.0252	4.1883	4.0265
H (CH_3)	1.946	2.2041	2.0536	2.8149	2.6639	2.8162	2.6652
H (CH_3)	1.946	2.2040	2.0536	2.8148	2.6639	2.8162	2.6652
H (CH_3)	1.946	1.7974	1.5130	2.4583	2.1378	2.4584	2.1381
	R^2	**0.9844**	**0.9864**	**0.9835**	**0.9836**	**0.9834**	**0.9835**

3.4. HOMO - LUMO energy analysis of MMA molecule

Intramolecular interactions are characterized by frontier molecular orbitals (FMOs) in molecular orbital theory. The electron distribution of the boundary orbitals, as well as the symmetry and energy of the orbitals, all play key roles in determining a molecule's reaction capacity and attributes in chemical reactions. The interaction of boundary orbitals determines the interaction of molecules with each other in reactions. Strong interactions occur between one of the molecules' highest occupied molecular orbitals (Highest Occupied Molecular Orbital, HOMO) and the other's lowest unoccupied molecular orbital (LUMO). The chemical stability of a molecule is defined as the difference between HOMO and LUMO energy levels. The chemical stability of a molecule is defined as the difference between HOMO and LUMO energy levels. The stronger the contact between the reactants and the reaction, the closer the symmetry and energy levels of the border orbitals in interacting molecules (the lower the ΔE energy difference).

Figure 3 depicts contour plots of gas phase FMOs from HOMO-1 to LUMO+1 to help comprehend the binding strategy and facilitate discussion of molecular transitions. The positive and negative charge distributions are represented by the red and green colors, respectively. HOMO refers to the charge density localized on the methylene group in MMA.

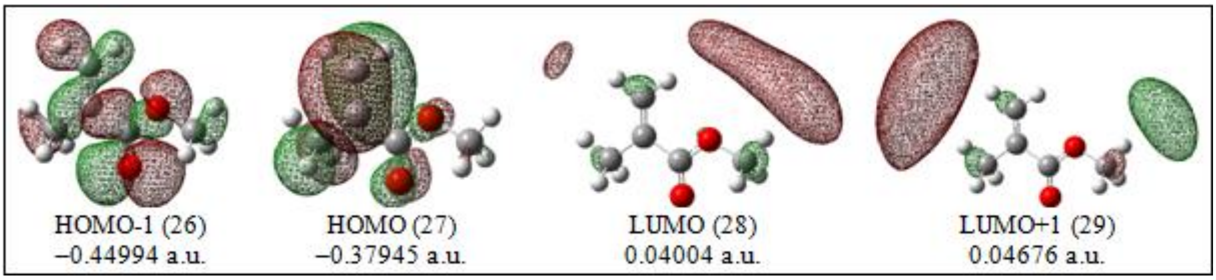


Figure 3: HOMO, LUMO, HOMO-1, LUMO+1 energy levels (in a.u.) for the MMA molecule determined with the HF method using the 6-311++G(d,p) basis set

The outermost orbital, HOMO, which contains electrons, is important in determining the electron-donating affinity to the neighboring orbital, whereas the innermost orbital, LUMO, which contains free sites to accept electrons, is important in determining the electron-accepting affinity. At the HF/6-311++G(d,p) level, the HOMO energy value is –10.325 eV and the LUMO energy value is 1.090 eV.

As determined by the HF approach utilizing the 6-311++G(d,p) base set, the values for the electronic structural parameters (ionization potential, electron affinity, electronegativity, chemical hardness and softness, and electrophilic) are shown in Table 3. Since there is a significant energy difference between HOMO and LUMO, molecules have stable structures.

Table 3: FMOs and physical-chemical characteristics (in eV) for the MMA molecule as calculated using (HF/6-311++G (d, p)).

Property	Expression	Value (eV)
HOMO energy	E_{HOMO}	–10.325
LUMO energy	E_{LUMO}	1.090
HOMO-LUMO energy gap	ΔE	–11.415
Ionization potential	$IP = E_{\mathrm{cation}} - E_{neutral}$	8.819
Electron affinity	$EA = E_{\mathrm{neutral}} - E_{\mathrm{anion}}$	–1.075
Electronegativity	$\chi = (IP + EA)/2$	3.872
Chemical potential	$\mu = -\chi = -(IP + EA)/2$	–3.872
Chemical hardness	$\eta = (IP - EA)/2$	4.947
Chemical softness	$S = 1/\eta$	0.202
Electrophilic (in terms of chemical potential and hardness)	$\omega = \mu^2/2\eta$	1.515

3.5. Molecular structure calculations of HEMA molecule

The HEMA molecule, with the chemical formula $C_6H_{10}O_3$, has a density of 1.079 g/cm^3 and a molecular weight of 130.141 g/mol [12]. Figure 4. (a) depicts a representative representation of the HEMA structure, and Figure 4. (b) depicts the optimized molecular geometry HF/6-311++G(d,p) level in the gas phase.

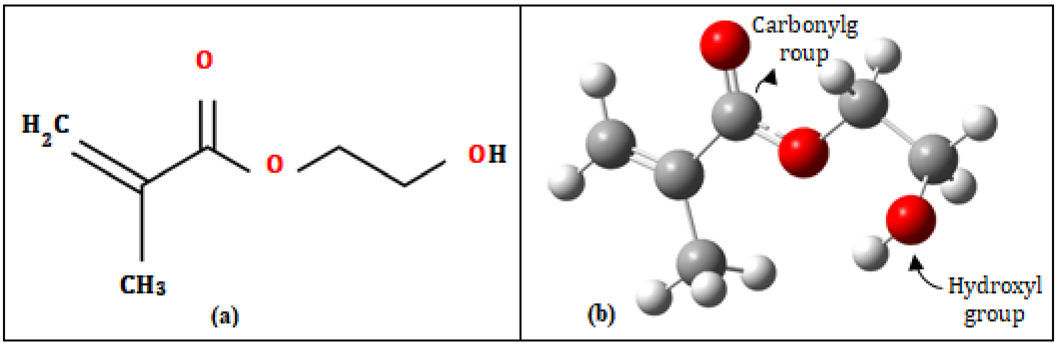


Figure 4: (a) a typical illustration, and **(b)** theoretical (obtained using the HF/6-311++G(d,p) method) molecular structures of the HEMA molecule.

HEMA molecule contains a carbonyl (C = O) and a hydroxyl (O – H) group[13]. The O – H group acts as both a proton donor and proton acceptor, while the C = O group acts only as a proton acceptor [14, 15]. Table4 shows the theoretical values of bond lengths, bond angles in degrees, and plane angles in angstrom units of the aforementioned molecule. It was observed that the values of bond lengths, bond angles, and dihedral angles calculated by the HF and B3LYP methods were found to be reasonably close to each other.

Table 4: Calculated bond lengths (Å), bond angles (°) and dihedral angles (°) for the HEMA molecule

Parameters	**UHF**		**UB3LYP**	
Bond Lengths (Å)	**6-311++G(d,p)**	**LanL2DZ**	**6-311++G(d,p)**	**LanL2DZ**
C = CH_2	1.32167	1.33498	1.33591	1.35304
C – CH_3	1.50714	1.51077	1.50584	1.51412
C – C(= 0)	1.49975	1.49183	1.49887	1.49807
C(O) – C(O)	1.51095	1.51562	1.51446	1.52327
C (= 0)– O	1.32504	1.35323	1.35624	1.38903
C = O	1.18503	1.22088	1.20821	1.24507
O – CH_2	1.42400	1.46064	1.44795	1.48449
O(H) – CH_2	1.39731	1.43293	1.42119	1.45742
Bond Angles (°)				
O = C – O	122.83252	121.59239	122.69244	121.82940
O = C – C	124.96353	125.44193	125.66185	126.24779
O – C(O) – C	112.20360	112.96528	111.64523	111.92227
C – C – CH_3	123.83688	124.23925	123.62820	123.93674
C(O) – C – CH_2	117.04323	117.42000	117.04841	117.15083
C(O) – C – CH_3	119.11988	118.34073	119.32338	118.91238
C – O – CH_2	117.84144	120.01234	116.39917	117.11230
O – C – C(OH)	107.13197	106.03595	106.92013	105.87319
O(H) – C – C	112.62337	111.78020	112.85186	112.03301
Dihedral Angles (°)				
O = C – C – CH_2	0.73334	0.51435	0.47924	0.46805
O = C – C – CH_3	–179.24397	–179.42800	–179.49442	–179.45620
O – C – C – CH_2	–179.05704	–179.25466	–179.27370	–179.26746
O – C – C – CH_3	0.96565	0.80298	0.75264	0.80830
O = C – O – C	0.74696	0.85284	0.65706	0.84167
C – O – C – C(OH)	–178.64195	–176.62837	–177.08372	–174.96775
C – C – O – C	–179.45748	–179.36809	–179.58145	–179.40939
O – C – C – O	–63.61535	–63.69868	–64.10841	–64.20167

3.6. Analysis of the HEMA molecule's vibrational modes

Raman spectroscopy uses inelastic scattering to generate the vibrational spectrum of sample molecules. The intensity of the scattered radiation is measured in this type of spectroscopic analysis as a function of the frequency shift of the incident radiation. The intensity of the Raman peaks is related to the concentration of the analyte [16].Figure 5 compares the band range of 3500-500 cm^{-1} in experimental[17] and computational Raman spectra of the HEMA molecule.

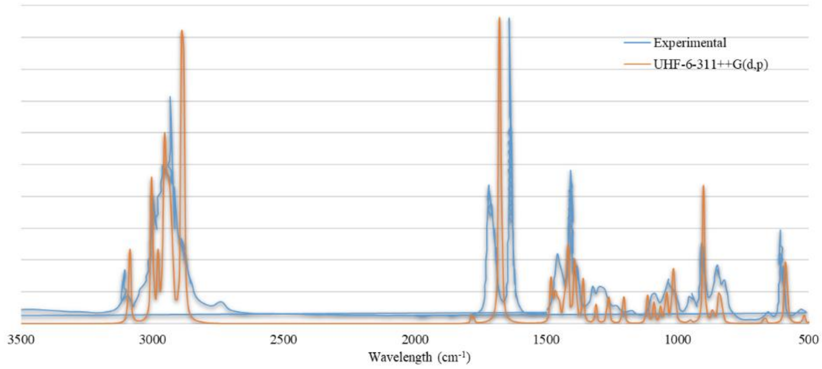


Figure 5: The HEMA molecule's experimental [10] and calculated Raman spectra.

The HEMA molecule is a molecule consisting of N=19 atoms. When the translational and rotational movements along the coordinate axes are subtracted, 51 fundamental vibrations will be obtained according to the (3N–6) relation. These vibrations' types of symmetry, as well as which ones will be visible in IR spectroscopy and which ones in Raman spectroscopy, can be determined using X-rays and group theory.

In this section, the frequencies of the molecule have been marked, and the marked bands have been carefully examined by considering the reference number [18]. All of the vibrational frequencies of the optimized molecules were scaled with fit factors of 0.909 in the HF method and 0.967 in the B3LYP method for the 6-311++G(d,p) set. The outcomes of the theoretical and experimental studies were compared. In accordance with the assignments of the IR absorption bands in the HEMA spectra, as previously reported by Morita, S., *et al*., a large spectral shape change of around 3700-3200 cm^{-1} was observed in the O–H stretching region, while only weak variations were detected in the other spectral regions [18].

In this study, five characteristic O–H stretch bands at 3640, 3624, 3519, 3431, and 3354 cm^{-1} and two C=O stretch bands at 1725 and 1709 cm^{-1} were identified. Two overlapping bands at 3640 and 3624 cm^{-1} were assigned to free OH. The reason for the cleavage of free OH was assumed to be the presence of rotational isomers. Since the vibration frequency of the band at 3431 cm^{-1} is approximately twice that of the free C = O at 1724 cm^{-1}, the band at 3431 cm^{-1} is assigned to the C = O stretch [18].

The molecular imaging program GaussView 6 was used to mark the calculated movements [1]. The values of 3797 cm^{-1} determined by the HF method and 3701 cm^{-1} determined by the B3LYP method using the 6-311++G(d,p) basis set of the O–H strain mode are quite close to the experimentally observed values of 3640-3624 cm^{-1}. It was found that in vibration markings, the asymmetric stress values for CH_2 and CH_3 were higher than the symmetric stress values. The C = O bond strain mode of the HEMA molecule was observed at 1725 cm^{-1} in the previous study[18]. In this study, this ligament strain mode was obtained as 1780 cm^{-1} (HF) and 1715 cm^{-1} (B3LYP).

3.7. Electrostatic potential energy map of the HEMA molecule

The charge distributions of molecules are displayed on the molecular electrostatic potential (MEP) map or surface, making them maps that let us see regions with variable loads. They enable us to identify charge-dependent characteristics and interactions between molecules, as well as the dimensions and shapes of molecules. The surface of electron density is depicted in color on the MEP map. The red areas on the map represent the parts of the molecules that repel the electrons of the other molecules. The red regions have the lowest potential energy and indicate the region with electronegative potentials. The blue parts of the molecule, which have the highest potential energy value and are positively charged, are those that strongly attract outer electrons.

By imaging the electrostatic potential map of the molecules, the regions where electrophile and nucleophile reactions will occur in the molecule are predicted and provide important information about intramolecular hydrogen bond formation. Positive regions are related to nucleophile reactions, while negative regions are related to electrophile attacks. Such research is helpful, for instance, in drug design studies where the interaction between a molecule and the enzyme's active components is examined [19].Obtained the MEP map, using the 6-311++G(d,p) basis set for the HEMA molecule is shown in Figure 6. In the neutral molecule, the red regions represent electron-rich regions, the blue regions represent electron-poor regions.

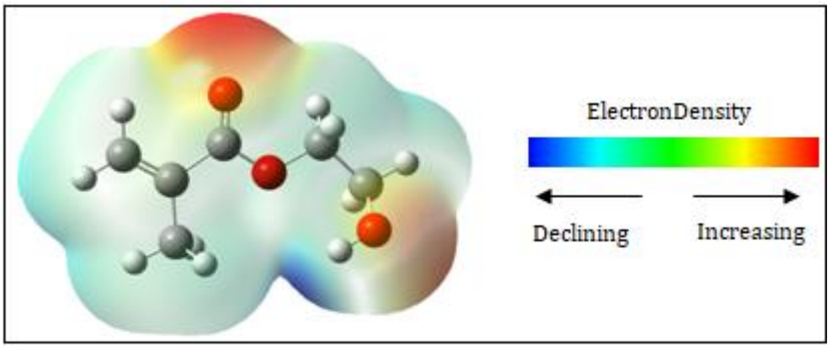


Figure 6: MEP map of the HEMA molecule obtained by the HF/6-311++G(d,p) method

The carbonyl group region has the largest density of electrons, whereas the –OH group region has the lowest density of electrons.

4. Conclusions

In this paper, the geometry and electronic structure of the title compounds (MMA and HEMA) were investigated at both the *ab initio* HF and the B3LYP levels. Theoretical results at the HF and DFT levels of theory with the 6-311++G(d,p) and LanL2DZ basis sets are provided. The optimized geometric parameters, vibrational frequencies, and ^{1}H and ^{13}CNMR chemical shift values of MMA molecule are calculated and compared with experimental values. The NMR data were calculated using the GIAO, CSGT, and IGAIM methods. Additionally, the molecular frontier orbital energies and electronic structural parameters of HEMA molecule in the ground state have been determined. Geometric parameters, harmonic vibrational wave numbers, and the molecular electrostatic potential map of HEMA molecule have been computed.

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