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Research Article

The substituent group activity in the anion of cholinium carboxylate ionic liquids on thermo-physical, chemical reactivity, and biological properties: A DFT study

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ABSTRACT

The thermo-physical, chemical reactivity and biological interaction of cholinium cation Ionic Liquids (ILs) were investigated as theoretical by density functional theory (DFT). Some thermo-physical parameters such as free energy, entropy, dipole moment, binding energy, nuclear energy, electronics energy, the heat of formation were computed. The chemical reactivity of molecule like highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), HOMO-LUMO gap, ionization potential, electronegativity, hardness, softness and electron affinity were calculated. Properties like charge density, surface area grid, volume, LogP, polarizability, refractivity, and molecular mass were calculated using the quantitative structure activity relationship (QSAR). The cholinium benzoate (IL01), cholinium-2-nitro-benzoate (IL02), cholinium-2-methylbenzoate (IL03), cholinium -2-hydroxy benzoate (IL04), cholinium -2-chlorobenzoate (IL05), and cholinium -2-flurobenzoate (IL06) were taken for study. With adding of substituent groups to the anion, the chemical stabilit increased, and chemical reactivity decreased in the order of -H > -CH3 > -OH > -Cl > F- > $-NO_2$ groups. The physical properties and biological activity are observed to be changed irregularly for different substituent groups.

Keywords: Choline, ionic liquids, HOMO-LUMO, QSAR, vibrational spectroscopy.

Kolinum karboksilat iyonik sıvıların anyonundaki sübstitüe grubun thermo-fiziksel, kimyasal reaktivite ve biyolojik özellikler üzerine aktivitesi: Bir DFT çalışması

ÖZ

Cholinium katyon iyonik sıvılar (ILs) 'nin termo-fiziksel, kimyasal reaktivitesi ve biyolojik etkileşimi yoğunluk fonksiyonel teorisi (DFT) ile teorik olarak araştırılmıştır. Serbest enerji, entropi, dipol momenti, bağlayıcı enerji, nükleer enerji, elektronik enerji, oluşum ısısı gibi bazı termo-fiziksel parametreler hesaplanmıştır. En yüksek işgal edilen moleküler orbital (HOMO), en düşük boş moleküler orbital (LUMO), HOMO-LUMO boşluğu, iyonlaşma potansiyeli, elektronegatiflik, sertlik, yumuşaklık ve elektron afinitesi gibi molekülün kimyasal reaktivitesi hesaplanmıştır. Yük yoğunluğu, yüzey alanı ızgarası, hacim, LogP, polarizasyon, kırılma ve moleküler kütle gibi özellikler, nicel yapı aktivite ilişkisi (QSAR) kullanılarak hesaplanmıştır. Cholinium benzoat (IL01), cholinium-2-nitro-benzoat (IL02), cholinium-2-metilbenzoat (IL03), cholinium -2-hidroksi benzoat (IL04), cholinium-2-klorobenzoat (IL05) ve cholinium-2-flurobenzoat (IL06) çalışma için alındı. Anyona sübstitüe gruplarının eklenmesi ile kimyasal kararlılık arttı ve kimyasal reaktivite -H > -CH3 > -OH > -Cl > F- > $-N0_2$ sırasına göre azaldı. Fiziksel özellikler ve biyolojik aktivite farklı sübstitüe gruplar için düzensiz olarak değiştiği gözlendi.

Anahtar Kelimeler: Kolin, iyonik sıvılar, HOMO-LUMO, QSAR, titreşimsel spektroskopi.

1. INTRODUCTION

Ionic Liquids (ILs) is defined as liquid salts or melted salts at room temperature.[1] Several types of ILs are documented last twenty years. The most important and fascination to ILs for their vast applications belong to almost all areas of chemistry, chemical engineering, material science, and pharmaceutical industry. Due to tunable physical, and chemical properties like almost null vapor pressure, low volatility, low toxicity, high thermal

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stability, and biodegradability, they have become green solvents for industrial uses.[2] Nowadays, the ammonium, imadozolium, pyridium, phosphonium, and thiazolium etc are the most common ILs using for various purposes. The last decades, the high rising voice of scientists and researchers for ILs is going to the pharmaceutical active ingredients and microbial activity with sustainable methods.[3] Among them, ammonium, cholinium, and phosphonium cation based ILs are highly considerable cation to obtain the microbial activity and drug discovery. On the other hand, some ammonium carboxylate and cholinium carboxylate have established the biological activity against both of bacterial and fungal micro pathogens,[4-7] even some cholinium and phosphonium ILs were found the anticancer potential.[8]

In general, the choline is considered as the natural molecule and mostly used as nutrient for animal especially in poultry farm. For this reason, the choline is effortlessly found in synthetic or natural form.[9] In our study, the choline was taken to design the new cholinium based carboxylate ILs in view of theoretical investigation using a computational approach. The second point is noted that the carboxylate was selected as anion with cholinium cation for their biodegradable properties. As there were vast publications and documents on cholinium cation based ILs during last ten years particularly in experimental fields such as synthesis, antimicrobial, catalysis, application in chemical process and organic synthesis, there are well poor data for theoretical investigation. For this point, the cholinium carboxylate ILs were chosen for the development of thermophysical properties, chemical reactivity, and biological activity.[10-12] The computational approach is the best tool to explain the theoretical study of molecules. The estimation of HOMO and LUMO of molecules belongs to the region of electrophilic and electrophonic area. Our previous work for different investigation and prediction of ionic liquids and complex of metallic crystal[13,14] shows that the HOMO, LUMO values vary from -9.00 to -7.00, and also the values used to calculate the chemical reactivity indices vary from -2.00 to 0.50.[14-17] The second addressing documents for thermophysical and physical properties which contribute a theoretical profile for their applications were documented using the computational tools.[18] Finally, the biological activity was evaluated by the quantitative structural activity relationship (QSAR) which includes the surface area, volume, refractivity, polarizibitily, logP, and molecular weight. The logP expresses the toxicity and non toxicity having value of positive and negative. Herein, because the all molecules were designed regarding new bioactive on basis of cholinium cation,[19-20] they have no scope to compare with experimental study or data. Due to have the lacking of experimental profile of predicted ILs, this study represents a theoretical profile using computational approaches only.[21] The most beneficial of the study is safe the money including conducting cost of chemicals in laboratory and consumption of time in the laboratory. It provides the theoretical prediction of the examined molecule to safe use in any area.

2. COMPUTIONAL METHOD

To create the spatial chemical structure of each calculated molecule, the two-dimensional structure of the molecule shall be built step-by-step by drawing. Then hydrogen atoms are automatically added from building option and chemical structure is converted into a 3D structure. The first step in getting the main characteristic parameters of molecules is to optimize the molecular structure to obtain a configuration characterized by minimum free energy. In sitting the DFT was fixed via 6G-31G*, and B3LYP.[22] For this calculation, model build was done at first, then fixed the 6G-31G*, total charge zero, spin multiplicity one, UHF, convergence limit is 1e-006. The cut off is fixed 1e-006 with core Hamialtaian calculation and done geometry optimization to record the data of free energy, entropy, dipole moment, binding energy, nuclear energy, electronics energy, the heat of formation, the HOMO, LUMO, 3D mapped structure of electrostatic potential. The QSAR properties were also calculated.

3. RESULTS AND DISCUSSION

3.1 Optimized structure

A representation of the molecular structure optimized which contains the values of the reactivity indices is called the reactive molecular diagram. The optimized structures of molecules are represented in Figure 1. All of the ILs (IL01 to IL06) belongs to the class asymmetry, and non-planar and they have more than one element of symmetry and the plane of the molecule.

3.2. HOMO and LUMO

The possible electronic transition is explained by HOMO and LUMO indicating the electrophilic and nucleophilic attraction region in the molecule. They are highlighted in Figure 2, where the green color is a positive value and blue color is a negative value. The region of HOMO was found on the cation area, and LUMO on the anion area. The HOMO can be found of all molecules in near of -7.00 to 9.00 surrounding in cation. On the other hand, the LUMO was addressed in full of anion having -0.2 to 2.0. The magnitudes of HOMO and LUMO are introduced in Table 1 for zero energy level.

3.3. Chemical reactivity

The energy difference between HOMO and LUMO orbital is called an energy gap which is an important parameter that determines the stability of the structures

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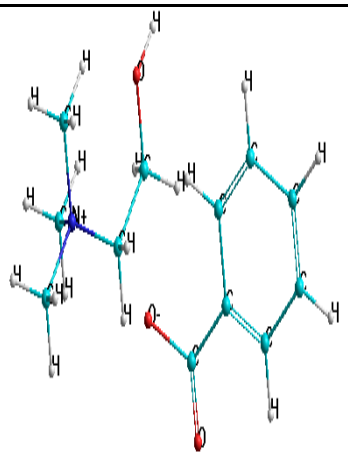
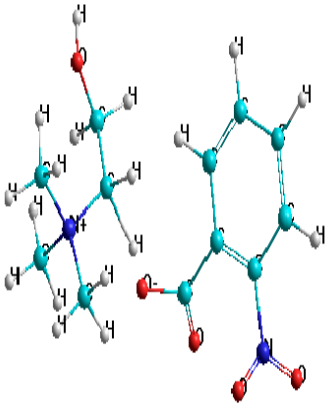
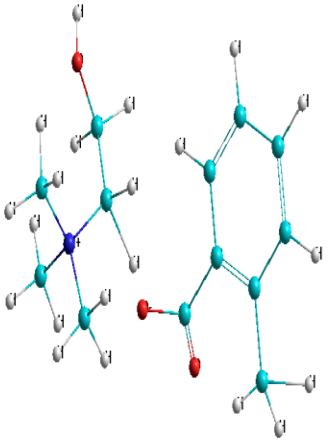
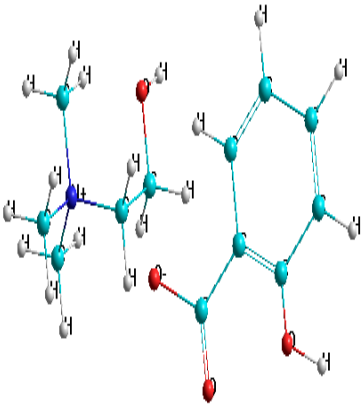
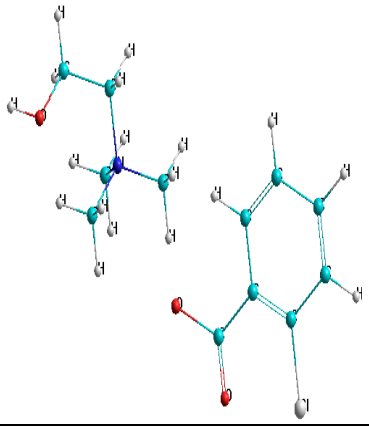
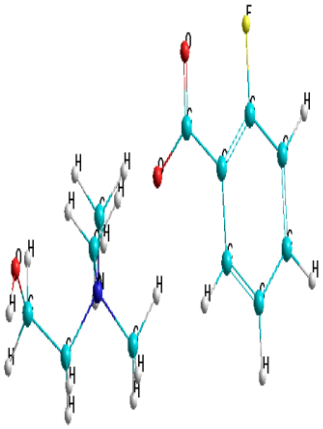
IL01, Cholinium benzoate	IL02, Cholinium 2-nitro-benzoate	IL03,Cholinium-2-methyl-benzoate
		
IL04, Cholinium 2-hydroxy-benzoate	IL05, Cholinium 2-chloro-benzoate	IL06, Cholinium 2-fluro-benzoate
		

Figure 1. Optimized structure in a cylinder shape, Color: Red is oxygen, cyan is carbon, white is hydrogen, nitrogen is blue, chlorine is white in large size.

and chemical reactivity. The shorter LUMO-HOMO gap is considered to provide the high reactivity (Table 1). In addition, according to Koopmans' theorem the energy gap, ΔE, defined as the difference between HOMO and LUMO energy,[18] it is reperesented by Eq. (1).

$$\Delta E = (E_{LUMO} - E_{HOMO}) \approx IP - EA \quad (1)$$

The ionization potential (I) and electron affinity (A) can be estimated from the HOMO and LUMO energy values using Equations (1) and (2).

$$I = -E_{HOMO} \quad (2)$$

$$A = -E_{LUMO} \quad (3)$$

The HOMO and LUMO energies are used for the determination of global reactivity descriptors. It is important that Electrophilicity (ω), the chemical potential (μ), Electronegativity (χ), hardness (η) and softness (S) are calculated from Equations (4-8) , and they are listed in Table 1.

$$(\mu) = -\frac{I+A}{2} \quad (4)$$

$$(\eta) = \frac{I-A}{2} \quad (5)$$

$$(S) = \frac{1}{\eta} \quad (6)$$

$$(\chi) = \frac{I+A}{2} \quad (7)$$

$$(\omega) = \frac{\mu^2}{2\eta} \quad (8)$$

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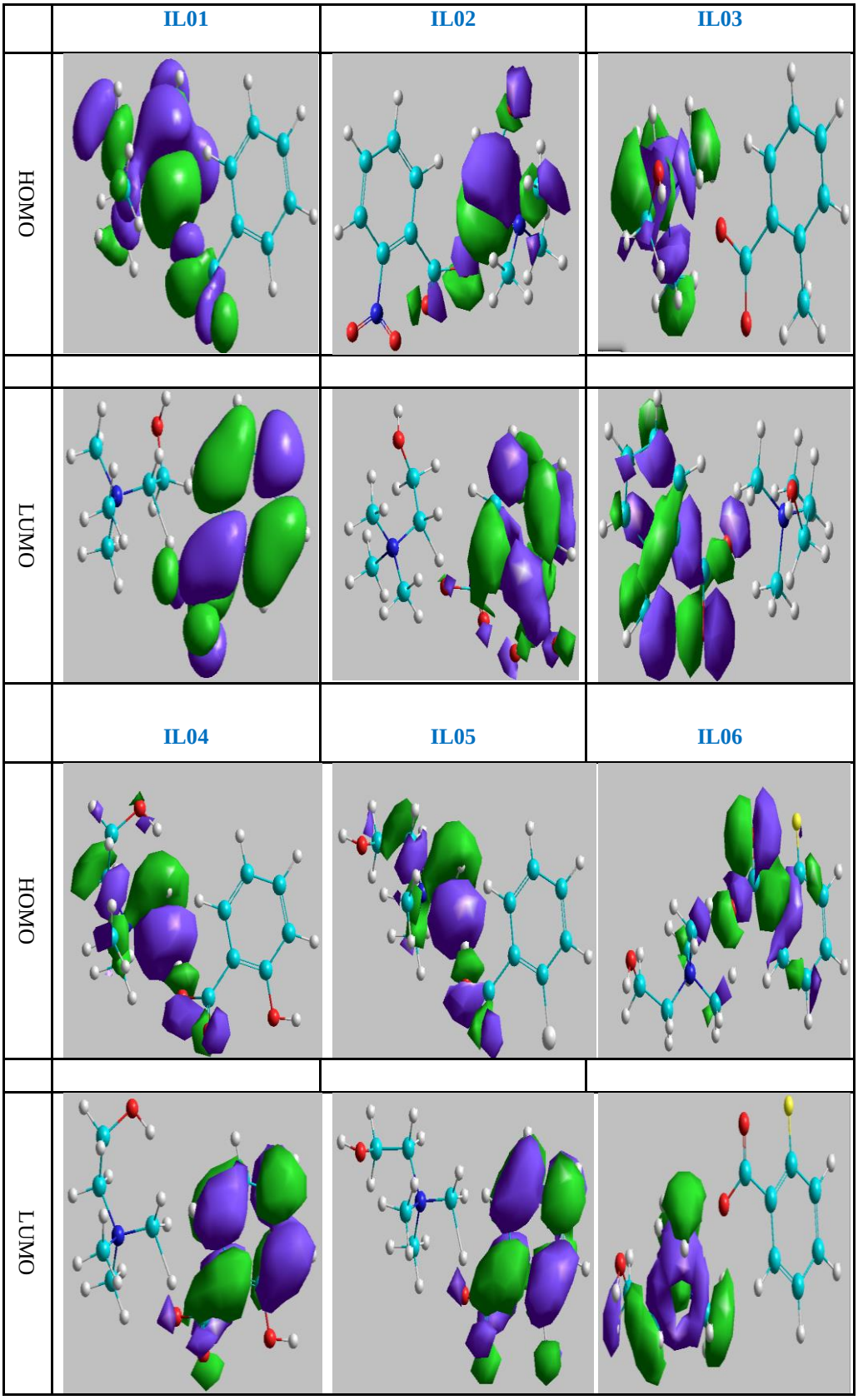

Figure 2. HOMO, LUMO orbitals.

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Table 1. Data for LUMO- HOMO gap, ionization potential, and electron affinity

	IL01	IL02	IL03	IL04	IL05	IL06
HOMO, eV	-7.0353	-9.2864	-7.3580	-9.1795	-8.2770	-8.6962
LUMO, eV	-2.1986	-1.6350	-1.4058	-1.5770	-0.6715	-0.1868
ΔE, eV	4.8367	7.6496	5.9522	7.6025	7.6055	8.5100
Ionization potential (I), eV	7.0353	9.2864	7.3580	9.1795	8.2770	8.6962
Electron affinity (A), eV	2.1986	1.6350	1.4058	1.5770	0.6715	0.1868
Hardness (η)	2.4183	3.8257	2.9761	3.8012	3.8027	4.255
Softness (S)	0.4135	0.2613	0.3360	0.2630	0.2629	0.2350
Electrophilicity (ω)	4.0719	3.8972	3.2258	3.8047	2.6321	2.3113
Chemical potential (μ)	-4.6169	-5.4607	-4.3819	-5.3782	-4.4742	-4.4350
Electronegativity (χ)	4.6169	5.4607	4.3819	5.3782	4.4742	4.4350

Table 2. Thermochemical properties

Properties	IL01	IL02	IL03	IL04	IL05	IL06
Total energy (kcal mol^{-1})	-63530.50	-80368.10	-67003.00	-70316.80	-60113.70	-73371.5
Free energy (kcal mol^{-1})	-63530.50	-80368.10	-67003.00	-70316.80	-60113.70	-73371.5
RMS gradient (kcal mol^{-1})	8.51	1.56	1.81	1.92	2.81	0.0119
Binding energy (kcal mol^{-1})	-3369.24	-3528.57	-3673.75	-3483.02	-3120.46	-3422.2
Heat of formation (kcal mol^{-1})	-36.94	-16.26	-66.36	-91.17	-63.26	-123.07
Electronic energy	-395312.1	-489865.0	-449066.7	-425083.1	-369498.6	-453058.2
Nuclear energy	331781.64	409497.11	382063.77	354766.36	309385.00	379686.01

As seen from Table 1, fluorine atom shows the highest activity on hardness while each group shows activity and the opposite trends are found for softness and electrophilicity. The nitro and methyl groups show the highest chemical potential and electronegativity while all substituent groups show this activity.

3.4. Vibration spectrum

The vibration spectra of cholinium based ILs confirmed the presence of carboxylate (-COO-) from the symmetric and asymmetric stretching peak at ~1770 cm^{-1} to ~1550 cm^{-1}, respectively, with the former being overlapped by N-H vibrations. The broad absorption around ~3335-3441 cm^{-1} can be assigned the presence of -OH groups. The aromatic ring is assigned the presence of C=C bond stretching of two values at ~1540 to ~1600 cm^{-1} and ~1460 cm^{-1}. Then the C-O bond has also confirmed the peak of 1260-1000 cm^{-1} in the carbonate salts. The board peak of 2400 cm^{-1} to 2700 cm^{-1} indicates the cholinium ion shown in Figure 3.

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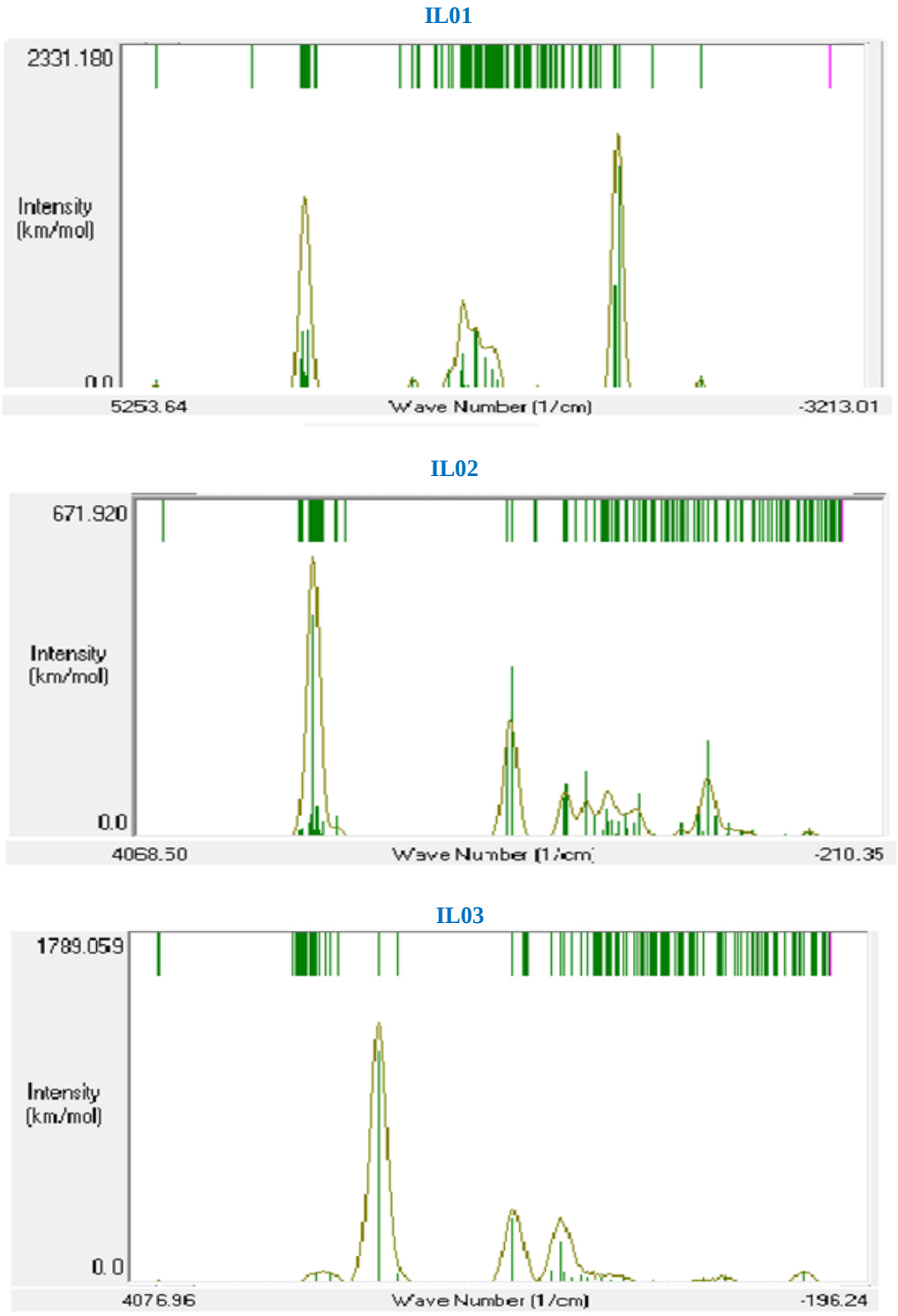

Figure 3. Vibration spectrum of IL01, IL02, IL03.

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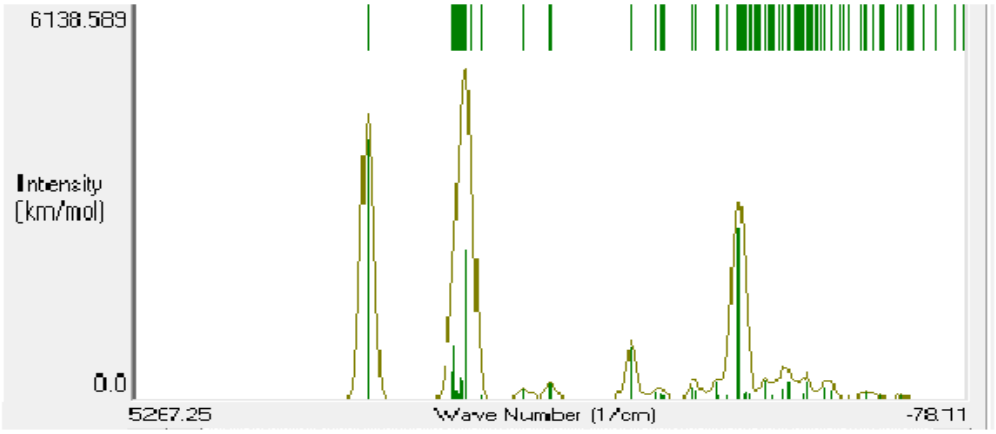
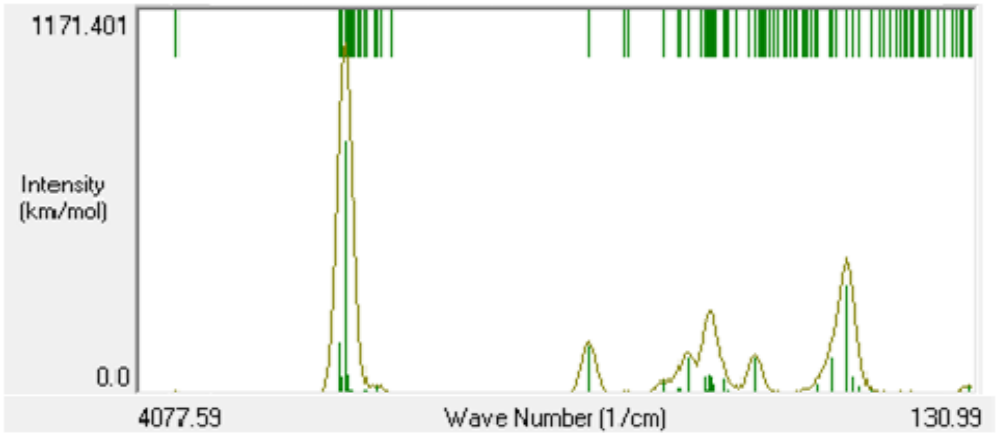
IL04



IL05



IL06

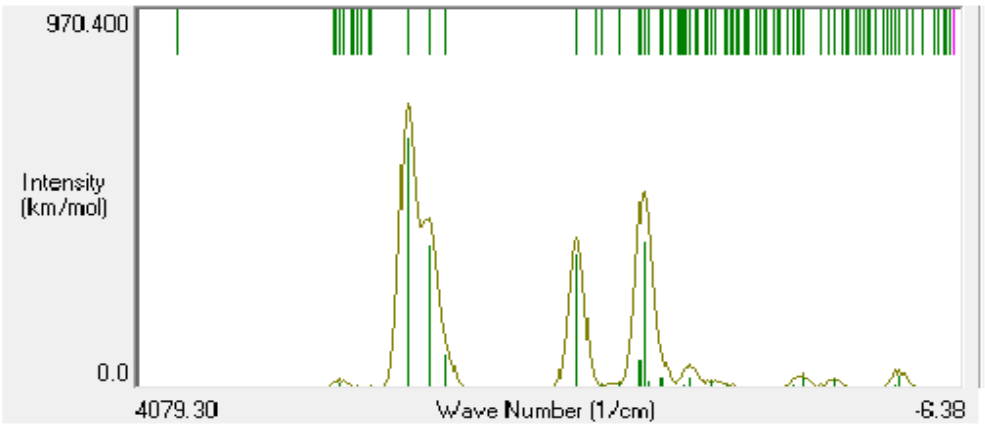


Figure 3. (continued) Vibration spectrum of IL04, IL05 and IL06.

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3.5. Thermophysical properties

In order to correlate the molecular structure or properties derived from a molecular structure with a particular chemical or biochemical activity, this method is widely used in pharmaceutical chemistry in the environment and in the search for certain properties. The molecule with minimum binding energy will have the maximum binding affinity and having the maximum binding affinity, indicating as the best molecule for drug leads molecules targeting computationally. From Table 2, it is seen that all ILs have minimum binding energy and the values are very close.

4. BIOLOGICAL ACTIVITIES OF OPTIMIZED MOLECULES

4.1. Distribution electrostatic potential

Electrostatic potential maps or electrostatic potential energy maps, or molecular electrical potential surfaces demonstrate the charge distributions of molecules three dimensionally, which show variably charged regions of a molecule, and molecular interactions with one another.

According to the mechanism of antimicrobial activity and antimicrobial agents of bioactive molecules, the positive charge end of molecules is responsible for damage the plasma membrane of pathogens. To kill pathogens, the region of molecules was used in the positive charge area of the molecule. In this case, the most important factors are explained that the higher surface area having a positive charge is considered as the high antimicrobial activity. In Figure 4, the blue color is the highest charge distribution indicator, and red color as the lowest charge distribution. It can be said that the highest charge distribution occurs in LI05, then IL01, IL03, and IL06, and as lowest in IL02, IL04.

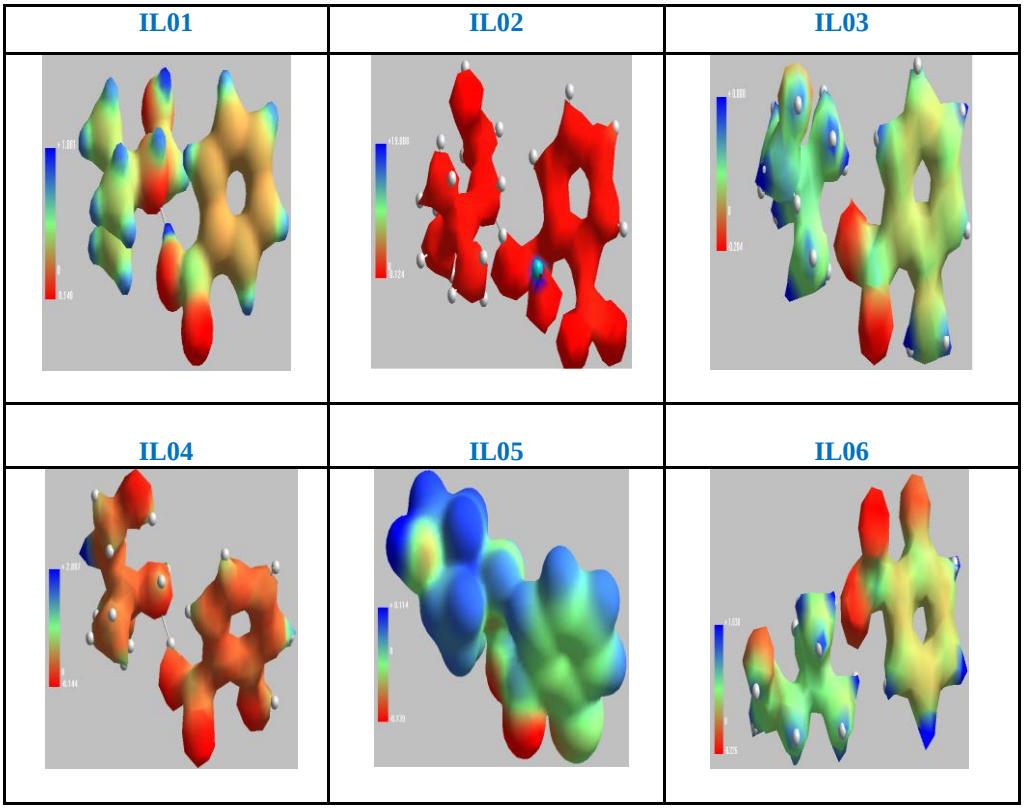

Figure 4. 3D electrostatic potential energy difference of two levels.

Here, E1= Electrostatic potential energy in positive value, E2= Electrostatic potential energy in negative value**,** and ΔE = Electrostatic potential energy difference of two level.

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Table 3. Data of electrostatic potential energy difference of two levels

	IL01	IL02	IL03	IL04	IL05	IL06
E1	+1.633	+2.1790	+1.424	+1.473	+2.729	+1.038
E2	-0.262	-0.088	-0.266	-0.385	-0.725	-0.226
ΔE = E2-E1	-1.895	-2.0291	-1.690	-1.858	-3.454	+1.264

Table 4. Data of QSAR

	IL01	IL02	IL03	IL04	IL05	IL06
Partial charge (e)	0.00	0.00	0.00	0.00	0.00	0.00
Surface Area(grid), Å^2	460.15	549.25	470.40	496.51	473.31	455.22
Volume, Å^3	754.74	887.12	779.81	826.54	781.46	740.50
Log P	5.06	-1.89	2.74	2.56	4.28	1.83
Refractivity, Å^3	63.96	68.75	68.17	65.06	68.28	64.04
Polarizability, Å^3	23.90	25.74	25.73	24.53	25.28	23.81
Mass (amu)	225.29	270.29	239.31	241.29	259.73	243.31

Table 5. Correlation in case of substituent groups in anions

	Pi, π		**Refractivity, (MR)**		**Surface Area, (SA)**	
Pi, π		Biological activity		Biological activity	SA	Biological activity
H	0.0	--	0.0	--	0.0	--
F-	+3.23	more	-0.08	more	4.93	more
Cl-	-0.78	Less	4.28	Less	13.16	more
-CH_3	-2.32	Less	4.21	Less	10.25	more
-OH	-2.50	Less	1.1	Less	36.36	More
-NO_2	+6.95	more	4.79	more	89.1	more

4.2. Biological study by QSAR

When the biological activity of a molecule is mentioned, its surface area is considered an important parameter. Greater charged surface area of a molecule can be able to kill more pathogens. The charged distribution from electrostatic potential completely depends on the surface area. The greater positive charged surface area means a higher biological activity.[23]

On the other hand, a negative value of logP refers to the hydrophilicity, and a positive value of LogP indicates the hydrophobicity that plays an important role in biochemical interactions and bioactivity. Hydrophobic drugs tend to be more toxic, because they are kept generally longer and have a wider distribution in the body. Also, they are somewhat less selective in their binding to molecules and finally are often extensively metabolized. Therefore ideal distribution coefficient for a drug is usually intermediate (not too hydrophobic or too hydrophilic). From the data inTable 4, the IL02 has -1.89 value that indicates lower hydrophobicity, and other are positive values having hydrophilicity as 1.83, 2.56, 2.74, 4.28 and 5.06 of IL06, IL04, IL03, IL05, and IL01, respectively. The bond dipole moment is the idea of an

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electric dipole moment to measure the polarity of a chemical bond within a molecule. In view of pharmaceutical industries, the dipole moment was a parameter for the drug by which a drug is to be used open or close packet. If any drug has a dipole moment, it can be able to absorb the ultraviolet light and have a possibility of properties. The five optimized ILs show zero dipole moment so that it can be used without any protection from UV or sunlight.

4.3. Correlation in case of substituent groups in anions

The value of Pi (π), MR, and can be calculated as the following equation from Table 4. π, MR, SA = LogP of cholinium benzoate –LogP of cholinium benzoate derivative. From Table 5, it was accounted for the correlation on basis of their different substituent groups in cation, while the F^- and NO_2 show the highest biological activity.

5. CONCLUSIONS

As the cholinium cation is bioactive molecules, some benzoate anions have attached to form new theoretical ILs and use thed computational tools to predict their activity using DFT method. It is summarized that the result optimized molecules of cholinium based ILs like cholinium benzoate, cholinium-2-nitro-benzoate, cholinium -2-methylbenzoate, cholinium -2-hydroxy benzoate, cholinium -2-chlorobenzoate, and cholinium -2-flurobenzoate were recorded. To make a comparative study among all for the physical properties, chemical reactivity and biological activity, a computational method was used. From the LogP value, it can be said that all ILs are hydrophobic, trending to bioactive. There are five substituent groups in anion as benzene ring at which the nitro group has more active in biological properties.

Conflict of interests

Authors declare that there is no a conflict of interest with any person, institute, company, etc.

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