Jurnal Ilmu Fisika (JIF)
Vol. 13, No. 2, September 2021, pp. 80–91
ISSN: 1979-4657 (Print); 2614-7386 (Online)
https://doi.org/10.25077/jif.13.2.80-91.2021

Jurnal Ilmu Fisika
Open Access

Effect of Citric Acid on Electrochemical Properties of Liquid Electrolytes

Nur Farah Izzati Mohd Noor[1], Saiyidah Nafisah Saidin[1], Nur Hani Ra'il[1], Nadhratun Naiim Mobarak[1]

[1] Department of Chemical Sciences, Faculty of Science and Technology, Universiti Kebangsaan Malaysia, 43600 Bangi, Selangor Darul Ehsan, Malaysia

Article Info

Article History:

Received: April 02, 2021
Revised: May 03, 2021
Accepted: May 14, 2021

Keywords:

liquid electrolyte
citric acid
lithium nitrate
ionic conductivity
density functional theory (DFT)

Corresponding Author:

Nadhratun Naiim Mobarak
Email: nadhratunnaiim@ukm.edu.my

ABSTRACT

Effect of citric acid as plasticizer on the electrochemical properties of liquid electrolyte has been studied. Liquid electrolyte was prepared by dissolving citric acid in 1% acetic acid with presence of lithium nitrate salt. Liquid electrolyte is characterized using a conductivity meter to measure the ionic conductivity value. Computer simulation of Density Functional Theory (DFT) with B3LYP/6-31G ++ (d, p) basic set was performed to identify the dominant functional group of citric acid when interact with lithium salt. Increasing the weight of citric acid has increased the ionic conductivity up to 44.89 mS/cm with an optimum weight of 4 g, while the ionic conductivity increases up to 43.00 mS/cm when the percentage of lithium nitrate salt increases up to 30%. The ionic conductivity increases as the salt percentage increases due the interaction between salt and functional group of citric acid. Based on computer simulation of DFT, the dominant functional group in citric acid that interact with lithium salt are carboxylic acid group which is located in the middle of the citric acid chain causing lithium ions to be more likely interact with citric acid.

1. INTRODUCTION

Solid polymer electrolytes have the potential to be used in electrochemical cell applications such as rechargeable batteries, fuel cells, and dye-sensitized solar cells. However, having a lower ionic conductivity in polymer electrolytes has proven that it often becomes a limiting factor for its use to be applied in electrochemical cells. Several factors have been identified to have influenced the ionic conductivity for polymer electrolytes such as the dissociation ability of the salt, the crystallinity behaviors of a substance, and the interaction between the salt and the active site on the host polymer (Arya & Sharma 2017; Aziz et al. 2018; Khan & Shakoor 2015; Long et al. 2016). In order to improve the ionic conductivity of polymer electrolytes, plasticizers such as ethylene carbonate (EC), propylene carbonate (PC), dimethyl carbonate (DMC), and polyethylene glycol (PEG) have been used as alternatives to increase the ionic conductivity (Walker Jr. & Solomon 1993; Hirankumar & Mehta 2014; Kobayashi et al. 2021).

According to Pradhan et al. (2008), the ionic conductivity of polymer electrolytes had been improved in the presence of plasticizers. They reported that when PEG is used, the amorphous area increases, the surface roughness and texture of the crystal decreases, and the movement of the chain segments becomes easier. The findings of this study also showed that the ionic conductivity of the polymer electrolyte increased from 8.9×10^{-8} Scm^{-1} to 2.2×10^{-6} Scm^{-1} when 50% concentration of PEG was used in the polymer electrolyte. They also reported that as higher concentrations of the plasticizer used, the salt dissociation and ion movement in polymer electrolyte became higher thus resulting in an increased value of ionic conductivity.

In this study, the potential of citric acid as a plasticizer has been studied due to the functional groups in its structure that consist of three carboxyl group and one hydroxyl group compared to ethylene carbonate and propylene carbonate. Both of these functional groups are able to act as an active site to promote salt dissociation and interactions with lithium salts to occur. However, citric acid has a large number of functional groups on its structure. Therefore, computer simulations through density function theory (DFT) method of citric acid were used to identify the dominant functional group to interact with lithium salt.

2. METHOD

2.1 Materials

Citric acid (Sigma Aldrich, ≥ 99.5%), Acetic acid (Sigma Aldrich, ≥ 99.5%) and Lithium Nitrate (Sigma Aldrich, 99.9% trace metal basis).

2.2 Preparation of liquid electrolyte

2.2.1 Effect of citric acid weight on liquid electrolyte

Citric acid with different weight (1 – 4 g) were dissolved in 1% acetic acid with 30% lithium nitrate salt separately and continuously stirred for 24 hours.

2.2.2 Effect of lithium nitrate percentage on liquid electrolyte

The optimum weight of citric acid achieved after ionic conductivity analysis was dissolved in acetic acid solution with various lithium nitrate percentages (5 – 30%) and stirred separately for 24 hours until the solution completely dissolved.

2.3 Characterization method

2.3.1 Ionic conductivity

The ionic conductivity of the solution was measured using Mettler Toledo conductivity meter at room temperature, 25 °C.

2.3.2 Computer simulation using Density Functional Theory (DFT)

The density functional theory (B3LYP) method with 6-31G ++ (d, p) basic set were used to optimize the molecular structure of citric acid and to study the structural changes that may occur upon interaction with lithium nitrate salt using GaussView software 5 and Gaussian 09.

3. RESULTS AND DISCUSSION

3.1 Ionic conductivity

The ionic conductivity of liquid electrolyte at a different weight of citric acid with constant salt percentage (30%) were shown in Figure 1. It can be observed that the ionic conductivity increased as the weight of citric acid was increased. The high ionic conductivity for citric acid is 44.83 mS/cm for 3.5 g citric acid. The increase of ionic conductivity with the increasing weight of citric acid was due to the availability of active sites in the citric acid as it contains three carboxyl group and one hydroxyl group which capable to act as a donor of electrons and also as an active site for the interaction with lithium-ion as well as promotion of salt dissociation. According to Mobarak et al. (2012), as we increase the active site in the electrolyte system, it is expected to provide more sites for cations to interact thus resulting in higher ionic conductivity value. Moreover, the highest ionic conductivity was achieved at a weight of 3.5 g of citric acid which was 44.83 mS/cm. This is because, the values of ionic conductivity at the weight of 3.5 g and 4.0 g citric acid statistically indistinct, which are 44.83 and 44.90 mS/cm respectively. The small difference between these two values indicates that the concentration of citric acid in the system becomes increasingly saturated as the weight of citric acid increases from 3.5 g to 4.0 g.

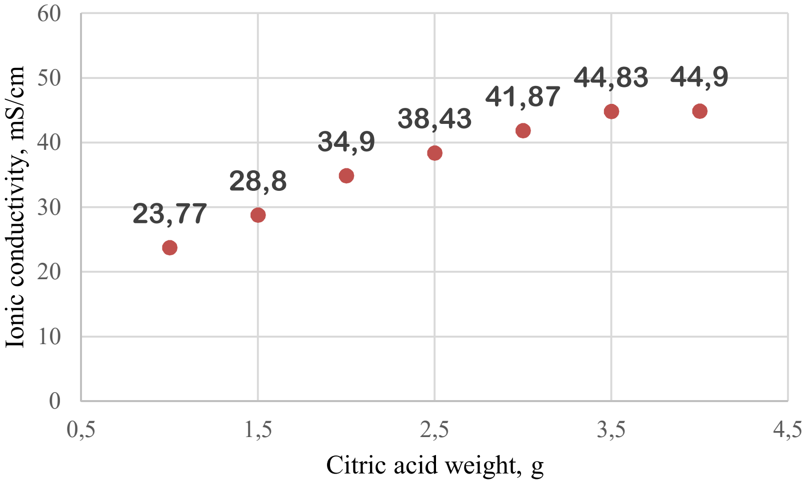


Figure 1. Ionic conductivity at room temperature for citric acid at different weight percentage.

The effect of lithium nitrate percentage on ionic conductivity was shown in Figure 2. It was observed that the ionic conductivity increased as the percentage of lithium nitrate salt increased. The highest ionic conductivity recorded was at 43.0 mS/cm for 30% salt percentage. Based on the Figure 2, shown that lithium nitrate salt directly affects ionic conductivity. This is because when lithium nitrate dissolved in acetic acid, it will dissociate into two charge conditions which are Li^+ and NO_3^-. The dissociation of the salt has also been speeded up by the presence of citric acid. It causes the amount of Li^+ that acts as charge carriers to increase and moves into the liquid electrolyte system. When the salt concentration increases, the number of available charge carriers increases. As a result, the conductivity increases. Overall, it can be concluded that both lithium nitrate salts percentage and citric acid weight do affect the ionic conductivity of the liquid electrolyte system.

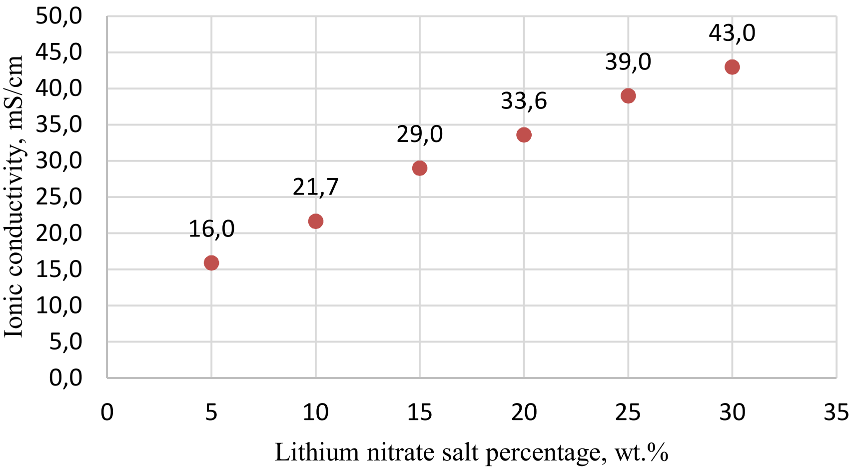
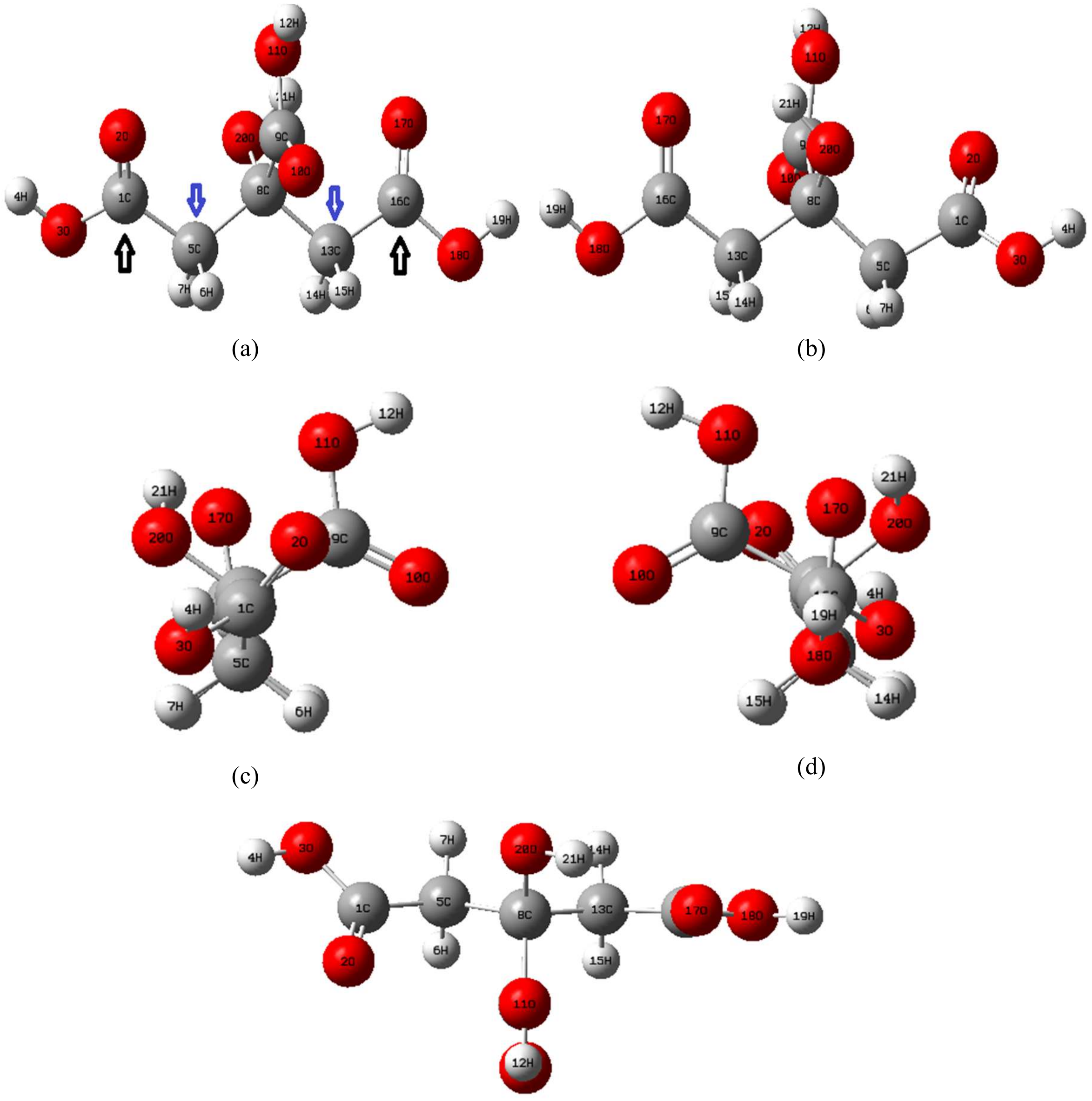


Figure 2. Ionic conductivity at room temperature for different percentage of lithium nitrate salt.

3.2 Computer simulation using Density Functional Theory (DFT)

3.2.1 Optimization geometry

Theoretically, the molecular formula for citric acid is $C_6H_8O_7$ where it contains three carboxyl functional groups and one hydroxyl group. Figure 3 showed the optimized structure of citric acid. It can be observed from the top view that carbon atoms (C5) and carbon atoms (C13), as well as carbon atoms (C1) and carbon atoms (C16), are in a position that is parallel to each other. Beside that O2 and O3 atoms are antiparallel with long chains of citric acid, O17 and O18. Also the hydrogen atoms (H19) are in a symmetrical position with a long chain of citric acid. Table 1 shows the optimal parameters for the bond lengths atoms in citric acid.



(a) (b)

(c) (d)

(e)

Figure 3. The optimum structure of the citric acid (a) from the foreground, (b) from the back, (c) from the left, (d) from the right and (e) from the top is performed using the DFT method on the basic set of 6- 31G ++ (d, p).

The bond lengths listed in Table 1 indicate that the bond between carbon and oxygen at double bonds (C1 = O2, C9 = C10, and C16 = O17) is shorter than the bond at a single oxygen atom (C1-O3, C9-O11, and C16-O18). According to Housecroft and Sharpe (2012), carbon atoms of double bonds with oxygen atoms form bonds shorter and closer to each other because the double bond is stronger than a single bond. They also say that the double bond required a lot of energy to be held. The oxygen atoms from the carbonyl group has isolated electrons and the π bond shows more electron-rich and more electronegative than oxygen atoms in the hydroxyl group (Bond Energies, 2020).

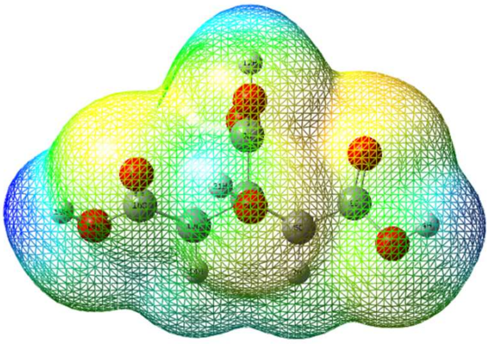
Table 1 Optimal structural parameters such as bond length (Å) for citric acid were performed using DFT method on 6-31G ++ (d, p) basic set.

DFT/B3LYP 6-31G ++ (d, p)	
Parameter	Bond length (Å)
C1 – C5	1.54
C1 – O2	1.26
C1 – O3	1.43
C5 – C8	1.54
C5 – H6	1.07
C5 – H7	1.07
C8 – C9	1.54
C8 – C13	1.54
C8 – O20	1.43
C9 – O10	1.26
C9 – O11	1.43
C13 – C16	1.54
C13 – H14	1.07
C13 – H15	1.07
C16 – O17	1.26
C16 – O18	1.43
O3 – H4	0.96
O11 – H12	0.96
O18 – H19	0.96
O20 – H21	0.96

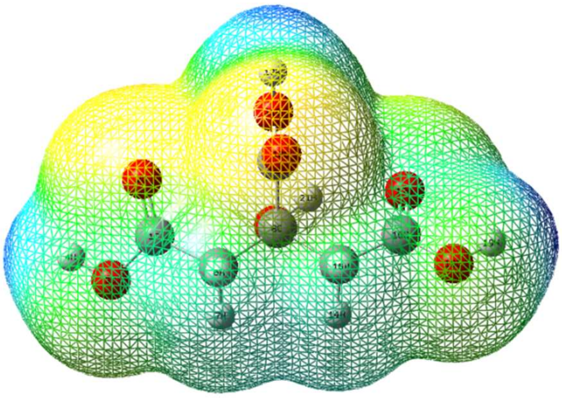
3.2.2 Molecular electrostatic potential (MEP)

The electrostatic potential of a molecule is the projection of charge distribution in a molecule of three dimensions by using color code. It is also strongly related to density electrons and useful in identifying electrophilic and nucleophilic attack sites in a molecule. Each atom or presence of active sites in a molecular structure has varying electron densities. The result for differences electrostatic potential value are represented by color code around it. The electrostatic potential increases in sequence of red < orange < yellow < green < blue where red represent most negative areas, green for most positive areas and blue refers to neutral areas (Joshi and Chaudhary, 2013; Karimzadeh et al., 2021).

Based on Figure 4, the red and orange molecular electrostatic potentials representing negative regions indicate high electron accumulation density while blue molecular electrostatic potentials represent positive regions and it indicates lower electron accumulation density for citric acid molecules.



(a)



(b)

Figure 4. Molecular electrostatic potential of citric acid (a) in the foreground and (b) in the back is performed using the DFT method on the basic set of 6-31G ++ (d, p).

Based on the observations of the molecular electrostatic potential of citric acid in Figure 4, it shows that the three oxygen atoms (O2 O10 and O17 atoms) that are double bonded to carbon atoms surrounded by orange color code (negative regions). In addition, three oxygen atoms (O3, O11 and O18) that are single bonds with hydrogen atoms surrounded by green code (less negative or positive area) while a single oxygen atom (O20) that are single bonds with hydroxyl group were surrounded by orange color code (negative code). Code blue (positive area) can only be seen surrounded the carbon atoms and hydrogen atoms which indicates that the negative charges are more likely to circulate the oxygen atom at the hydroxyl groups and the double bonded of carbonyl group. Murray and Politzer (2011) state that most atoms with high electronegativity such as N, O, F and S atoms are assisted by the presence of isolated electrons and π electrons in unsaturated molecules. They also stated that this area is a negative electrostatic potential which is more likely to draw protons against it. The area that exhibits negative electrostatic potential and high electronegativity are capable of providing an active site for ongoing interactions (Akman, 2017). Therefore, it is clearly shown that the oxygen sites in the carboxyl group and hydroxyl groups show the high electronegativity properties are capable of providing an active site for interaction to occur with lithium ions.

3.2.3 Mulliken charge analysis

Mulliken charge analysis plays an important role in the application of chemical quantum computation to molecular system and is also related to the nature of molecular vibration (Sangeetha et al., 2013). They also stated that the Mulliken charge had an impact on polar moments, the electronic structure and solubility of molecule. Figure 5 showed the charge distribution of the atoms in citric acid structure by using B3LYP/631G++ (d, p) method, while Table 2 shows the value of Mulliken charge of each oxygen atom in citric acid. Figure 5 shows that there are positive charge on carbon and hydrogen atoms, while the negative charge is on the oxygen atom.

Based on Table 2, the Mulliken charge value for O2 atoms is the highest (-0.44e) and shows the highest electronegativity properties in citric acid. The Mulliken charge value for O17 atom are closer to O2 atoms which is -0.43e compared to other oxygen atoms. Both O2 and O17 atoms are double bonded atoms with carbon in the carbonyl group. This negative value shows that these oxygen atoms are assisted by the presence of π electrons and isolated electrons. However, the Mulliken charge value for O10 atom which is also double bonded with carbon in the carboxyl group showed the lowest value of -0.36e although the O10 atomic environment shows the orange color code in the electrostatic potential of the molecule in Figure 5. This shows that the O10 atom is the least electronegativity oxygen atoms to attract lithium ions instead of the other oxygen atoms. This is probably because it is influenced by the environment around the O10 atoms and the structure of the carbonyl group that located at the center of a long chain of citric acid. Where it lies between the oxygen atoms from the two carbonyl groups at the end of the carbon chain that is causing rival from the others.

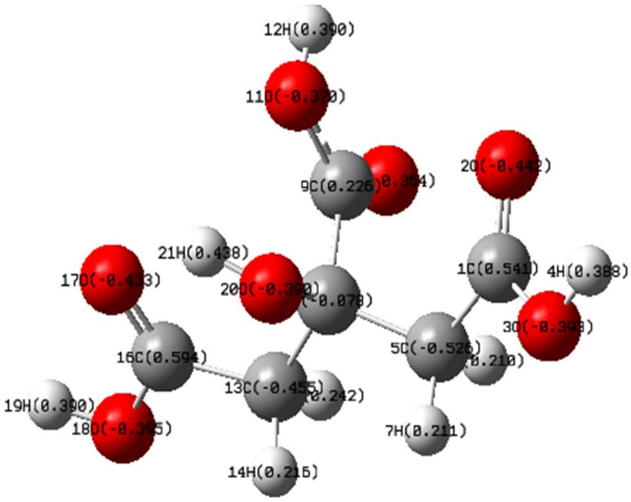


Figure 5. Mulliken charge distribution for citric acid made using the DFT method on the basic set of 6-31G ++ (d, p).

Table 2 Mulliken charge atomic distribution of citric acid made using DFT method on 6-31G ++ (d, p) basic set.

DFT/B3LYP 6-31G ++ (d, p)	
Atoms	Mulliken charge
O2	-0.44
O3	-0.39
O10	-0.36
O11	-0.37
O17	-0.43
O18	-0.40
O20	-0.39

3.2.4 Interaction between citric acid and lithium ion

In this study, the interaction between citric acid and lithium ion was performed to identify the dominant functional group in citric acid that will interact with lithium ions. This interaction was done by placing lithium ions (Li22) close to every oxygen atom in citric acid. Figure 6 shows the structure of citric acid that has been optimized and interact with lithium ions using B3LYP/631G++ (d, p) method.

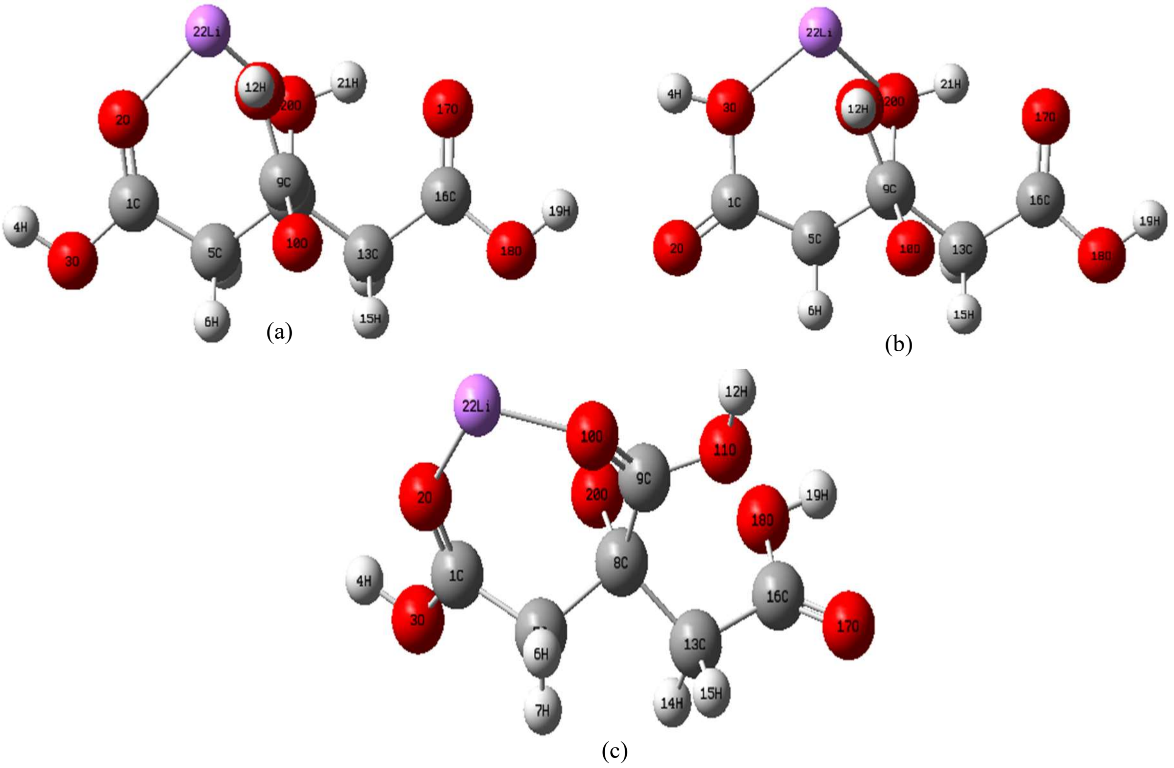
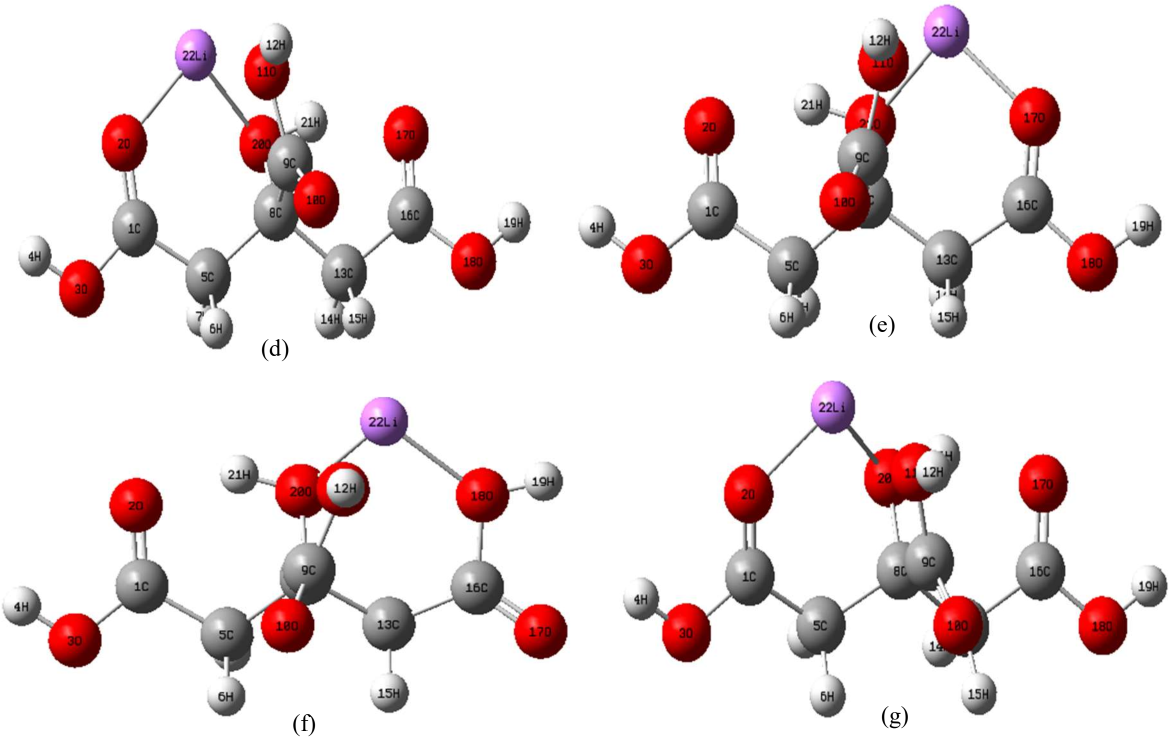


Figure 6. Optimal structure of citric acid that interact with lithium ion, (a) O2-Li-O20, (b) O3-Li-O20, (c) O10-Li-O2.



(d) (e) (f) (g)

Figure 6. (continued) (d) O2-Li-O20, (e) O17-Li-O20, (f) O18-Li-O20 and (g) O20-Li-O2.

The interaction between citric acid and lithium ions can be analyzed by using information obtained from DFT method. Among them, the information on the bond length between lithium ions and the oxygen atoms in citric acid are shown in Figure 3. Meanwhile, Table 4 shows the information on relative energy or the bonding energy between citric acid and lithium ion that can be obtained by some calculation for each oxygen atom namely O2, O3, O10, O11, O17, O18 and O20.

Table 3 The bond lengths of oxygen atoms in citric acid with lithium ions were performed using DFT method on 6-31G ++ (d, p) basic set.

DFT/B3LYP 6-31G ++ (d, p)		
Structure	Bond length (Å)	
O2-Li-O20	O2-Li = 1.86	Li-O20 = 1.93
O3-Li-O20	O3-Li = 1.94	Li-O20 = 1.89
O10-Li-O2	O10-Li = 1.84	Li-O2 = 1.88
O11-Li	-	
O17-Li-O20	O17-Li = 1.88	Li-O20 = 1.93
O18-Li-O20	O18-Li = 1.94	Li-O20 = 1.89
O20-Li-O2	O20-Li = 1.93	Li-O2 = 1.88

Based on Figure 6, it showed that lithium ions are more likely to interact and bonded together with two oxygen atoms at the same time. Each position of the lithium ion that interact with the oxygen atom can be observed where the interactions that occur between carbonyl groups in the middle of the long chain and at the end of the long chain of citric acid. This study can be proven by a study conducted by Abdullah and Ang (2018). In their study, the interaction between citric acid and Ba^{2+}, Y^{3+}, Zr^{4+} ions was performed and studied using B3LYP/6-31G*. They reported that the potentially negative area is between the middle and at one end of the chain of citric acid molecules.

However, it is also found that interaction and bonding between lithium ions and O11 atom in citric acid do not occur. In fact, the final result of the structure simply shows the interaction between O2 and O20 atoms, although the lithium-ion is placed close to the O11 atoms. O11 atom is an oxygen atom that is single-bonded with carbon in the carboxyl group where this carboxyl group is located in the middle of a long chain of citric acid. Therefore, there is no information obtained for the relative energy and bond length between O11 atoms and lithium ions. This is because the Mulliken charge for O11 is relatively low (-0.37e) compared to other oxygen atoms. Besides, the atomic position for O11 that located at the center and between two carboxyl groups that contain O2 and O17. Both atoms have a high Mulliken charge causing competition between the oxygen atoms to interact with lithium ions.

Besides that, lithium-ion is placed near the O10 atom, the lithium-ion is more interested in interacting with O10 and O2 atom compared to O20 as O20 does not interact with O10. This is because the potentially negative electrostatic areas are among the middle carboxyl groups and one of the carboxyl groups at the end of the citric acid chain. Next, when the lithium-ion is placed near the O2 atom, the interaction between lithium-ion and O2 will occur. This is because the position of the atom O2 in the carboxyl group is at the end of the chain is in an inconsistent state and slightly diagonal towards the middle of the carboxyl group. The Mulliken charge of O2 was also high (-044e). This will cause the lithium ions to be more interactive with O2 and O17 atoms instead of O20 and O17 that relatively at a distant position.

Besides O2, the interaction of lithium ions and O20 will also occur. O20 in this hydroxyl group is at the center of the citric acid chain and shows a potentially negative area that is orange in the electrostatic molecules map in Figure 4. However, the bond length between O2 atoms and lithium-ion is shorter compared to O20. This is due to the electron density and the Mulliken charge on O2 is higher than O20. The interaction between lithium-ion and O17 atom in the carboxyl group at the end of the citric acid chain has also occurred with O20. However, the bond length between lithium-ion and O17 is shorter due to the Mulliken charge value of O17 that is higher than O20. Besides, the O3 and O18 atoms is single bonded with carbon in the carboxyl group at the end of the citric acid chain can also show the interaction between lithium-ion and O20. Although the Mulliken charge value of O20 is lower than O3 and O18, the bond between the lithium-ion and O20 atom are shorter. This is because the O20 atom is negative electrostatic potential is more likely to induce the pull of lithium ions towards the atom compared to the less negative green region of O3 and O18 atom.

Table 4 showed that the binding energy between citric acid at O2, O17, O20 atoms, and lithium ions are more negative (-3.09 eV) compared to other oxygen atoms. According to Abdullah and Ang (2018), the more negative the energy binding between citric acid and lithium-ion, the complex will be stable resulting in stronger interaction. This shows the interaction structure between lithium ions and citric acid in O2, O17 and O20 is the structural interaction that is more stable and stronger compared to other oxygen atoms.

Overall, the analysis of the interaction between lithium ions and citric acid shows that O20 atom in hydroxyl groups being the most dominant functional group in the citric acid structure to interact with lithium-ion. After all the information obtained from DFT methods such as bond length, molecular electrostatic potential, Mulliken charge, and energy binding between citric acid structure and lithium ions was analyzed, this research proves that the dominant functional group does not depend solely based on the information above in analyzing the interaction between citric acid and lithium-ion, but also depends on the geometry and position of the atoms in citric acid.

Table 4 Calculation for relative energy when citric acid interact with lithium ions at each oxygen site at O2, O3, O10, O11, O17, O18 and O20.

DFT/B3LYP 6-31G ++ (d, p)				
Structure	Energy (a.u)	Energy (eV)	Total energy (eV)	Relative energy (eV)
Citric acid	-760.12	-20683.90		
Lithium ion	-7.28	-198.22	-20882.12	0.00
O2-Li-O20	-767.52	20885.21	-20885.21	-3.09
O3-Li-O20	-767.50	-20884.72	-20884.72	-2.60
O10-Li-O2	-767.50	-20884.79	-20884.79	-2.67
O11-Li	-	-	-	-
O17-Li-O20	-767.52	-20885.21	-20885.21	-3.09
O18-Li-O20	-767.50	-20884.72	-20884.72	-2.60
O20-Li-O2	-767.52	-20885.21	-20885.21	-3.09

4. CONCLUSION

The preparation of liquid electrolytes based on citric acid-lithium salts has been successfully conducted at the various citric acid weight and percentages of lithium nitrate. The highest ionic conductivity value obtained was 44.83 mS/cm at 3.5 g of citric acid. While the ionic conductivity of different lithium salt concentrations showed that the ionic conductivity increased as the lithium salt concentration increased. The highest ion conductivity value acquire was 43.00 mS/cm at 30% salt concentration. DFT analysis through computer simulation showed the interaction between citric acid and lithium due to the negative electrostatic potential. Analysis of the interaction between citric acid and lithium showed that the O20 atom in the hydroxyl functional group was the dominant group in citric acid.

ACKNOWLEDGEMENT

This research was supported financially by the grants GUP-2018-036. We gratefully thank you, our colleagues from Faculty Science and Technology who provided insight and expertise that greatly assisted the research. We also would like to thank Prof. Madya Dr. Ku Halim Ku Bulat from Universiti Malaysia Terengganu that has been providing the Gaussian software.

REFERENCES

Abdullah, N.A.F. & Ang, L.S. (2018). Binding sites of deprotonated citric acid and ethylenediaminetetraacetic acid in the chelation with Ba^{2+}, Y^{3+} and Zr^{4+} and their electronic properties: A density functional theory study. *Acta Chimica Slovenia,* 65(1): 231-238. DOI: 10.17344/ACSI.2017.3890

Akman, F. (2017). Prediction of Chemical Reactivity of Cellulose and Chitosan Based on Density Functional Theory. *Cellulose Chemistry and Technology,* 51: 253–262.

Arya, A. & Sharma, A.L. (2017). Polymer electrolytes for lithium ion batteries: a critical study. *Ionics,* 23, 497–540. DOI: 10.1007/s11581-016-1908-6

Aziz, S.B., Woo, T.J., Kadir, M.F.Z. & Ahmed, H.M. (2018). A conceptual review on polymer electrolytes and ion transport models, *Journal of Science: Advanced Materials and Devices*, 3(1), 1-17. DOI: 10.1016/j.jsamd.2018.01.002

Bond Energies. (2020). Retrieved 4 May 2021. https://chem.libretexts.org/@go/page/1981.

Housecroft, C.E. & Sharpe, A.G. (2012). *Inorganic Chemistry,* 4th Ed. London: Pearson.

Joshi, B. & Chaudhary, P. (2013). Molecular Structure, Mesp, Homo-Lumo And Vibrational Analysis Of B-Asarone Using Density Functional Theory. *Kathmandu University Journal of Science, Engineering and Technology,* 9(2): 1–14. DOI: 10.3126/sw.v14i14.34978

Karimzadeh, S., Safei, B. & Jen, T.C (2021). Theoretical investigation of adsorption mechanism of doxorubicin anticancer drug on the pristine and functionalized single-walled carbon nanotube surface as a drug delivery vehicle: A DFT study. *Journal of Molecular Liquids*. 322: 114890, 1-22. DOI: 10.1016/j.molliq.2020.114890

Khan, M.S. & Shakoor, A. (2015). Ionic conductance, Thermal and Morphological Behavior of PEO-Graphene Oxide-Salts Composites. *Journal of Chemistry*, 3: 1-6, DOI: 10.1155/2015/695930

Kobayashi, K., Pagot, G., Vezzu, K., Bertasi, F., Di Noto, V. & Tominaga, Y. (2021). Effect of plasticizer on the ion-conductive and dielectric behavior of poly(ethylene carbonate)-based Li electrolytes. *Polymer Journal*, 53, 149-155. DOI: 10.1038/s41428-020-00397-4

Long, L., Wang, S., Xiao, M. & Meng, Y. (2016). Polymer electrolytes for lithium polymer batteries. *Journal of Materials Chemistry A,* 4: 10038-10069. DOI: 10.1039/C6TA02621D

Mobarak, N.N., Ramli, N., Ahmad, A. & Rahman, M.Y.A. (2019). Chemical interaction and conductivity of carboxymethyl *k*-carrageenan based green polymer electrolyte. *Solid State Ionics*, 224: 51-57. DOI: 10.1016/j.ssi.2012.07.010

Murray, J.S. & Politzer, P. (2011). The electrostatic potential: An overview. *Wiley Interdisciplinary Reviews: Computational Molecular Science,* 1(2): 153–163. DOI: 10.1002/wcms.19

Pradhan, D.K., Choudhary, R.N.P. & Samantaray, B. K. (2008). Studies of dielectric relaxation and AC conductivity behavior of plasticized polymer nanocomposite electrolytes. *International Journal of Electrochemical Science,* 3(5): 597–608.

Sangeetha, V., Govindarajan, M., Kanagathara, N., Marchewka, M.K., Drozd, M. & Anbalagan, G. (2013). Vibrational, DFT, and thermal analysis of 2,4,6-triamino-1,3,5-triazin-1-ium 3-(prop-2-enoyloxy) propanoate acrylic acid monosolvate monohydrate. *Journal of Molecular Structure,* 1054–1055: 307–320. DOI: 10.1016/j.molstruc.2013.10.005