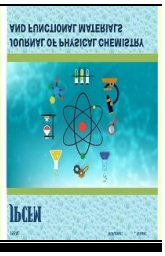
Journal of Physical Chemistry and Functional Materials

Home Page of Journal: https://dergipark.org.tr/jphcfum



Chemical Structural and Vibrational Analysis of Potassium Acetate: A Density Function Theory Study

[a,*] Ibrahim Nazem Qader, [b]Srwa Hashim Mohammed Al-Nabawi , [c]Ahmad Mohammad, [d]Yousif Hussein Azeez, [e]Riyadh Saeed Agid, [a]Henar Sleman Hassan

[a] *University of Raparin, College of Science, Department of Physics, Sulaimanyah, Iraq*
[b] *University of Garmian, College of education, Department of Chemistry, Kalar, Iraq*
[c] *Department of Physics, Faculty of Science, Firat University, 23119 Elazig, Turkey*
[d] *University of Halabja, College of Science, Department of Physics, Halabja, Iraq*
[d] *University of Salahaddin-Erbil, College of Science, Department of Physics, Arbil, Iraq*

Revised: 18-June-2019, **Accepted**: 08-July-2019
ISSN: 2651-3080

ABSTRACT

Potassium acetate ($C_2H_3KO_2$) is an essential macromineral for the human body and it is been used in many areas due to its stellar properties. In this study, $C_2H_3KO_2$ was optimized by applying the density functional theory (DFT) using Gaussian program. The highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (LUMO) were plotted. Also, based on the obtained results, the band gap energy was calculated. In addition, the obtained FTIR was compared with its corresponding experimental result. Besides, ultraviolet to visible spectroscopy for the ($C_2H_3KO_2$) molecule was illustrated. Other theoretical calculations were made and results were plausible when compared with experimental data.

ARTICLE INFO

Keywords:

Potassium Acetate
Density function theory (DFT)
Molecular orbitals

1. Introduction

Material science is one of active subjects among research field, which has a plenty different branches such as functional materials [1-6], nano materials [7, 8], and molecular dynamics [9, 10]. Since, understanding about molecular characteristic is an important issue for lots of researcher, so this field of study is growing among chemists, physicists, and material scientists, quickly. Potassium acetate acid derivation is the potassium salt of the acidic acid, and its chemical formula (CH_3COOK) [11]. It is produced through the response between a potassium base, for example, potassium hydroxide or potassium carbonate with acidic acid. It is a substantial of macromineral with numerous physiological abilities and is basic for nerve conduction, heart, skeletal and smooth muscle constriction, energy generation, nucleic acid synthesis as well as mainlining the blood pressure and normal renal function [12]. It can be taken as a healthful supplement with antihypertensive impacts and counteractive action impacts against hypokalemia.

Potassium acetate is in the form of powder white monoclinic crystalline- resembles salt and has an average molar mass of 98.14 grams per mole [13]. Potassium acetate is an important material due to its physical and chemical characteristic, which makes it to be used in many areas, e.g. in medicine it is utilized for treating diabetic ketoacidosis because it is able to break down into bicarbonate and help to balance the acidic state. It is also used in mixtures applied for tissue preservation, fixation, and mummification [14]. In addition, potassium acetate can be used to replenish electrolytes, for the restoration of water-electrolyte balance, as well as a urinary and systemic alkalizer, which can be administered orally or by intravenous infusion. And it also maintains intracellular tonicity. Energy band gap between Higher Occupied Molecular Orbital (HOMO), and Lower Unoccupied Molecular Orbital (LOMO) and UV spectrum can be found by using density function theory [15].

Previously, M. GASGNIER and A. PETIT have studied the effect of microwave and heating treatments on the properties of crystallographic of potassium acetate powder.

* Corresponding author:
E-mail (*i.nazm@yahoo.com*)

These studies showed that either microwave treatments at low power (60 watts) or heating at the low temperature can be used to obtain potassium powder with a lower water content [16]. Both Hatibuara and Barry observed through previous findings that the crystallographic properties of potassium acetate were obtained by two processes; the first was the temperature between (297 K) and the melting point (583 K), whereby three phases can be classified such that monoclinic III (297 K), monoclinic II (348 K), and orthorhombic I (428 K) [17]. The second is the transitions that can be specified by differential scanning calorimeter, or Raman investigations [18].

2. Materials and procedure

2.1. Theoretical methods

All atomic calculations and simulations were made using Gaussian 09W software [19]. The atomic configuration for potassium acetate molecule consists of one potassium atom, two oxygen, two carbon, and three hydrogen atoms. The types of chemical bonds between atoms are due to their number of electron in the valence band. In this case, since, almost all of outer electrons participated in molecular bonds, then it is electrically neutral. The theoretical distance between atoms was optimized using the Density Function Theory (DFT) technique, along with B3LYP. The 3–21G basis set and singlet spin estimation were performed and the optimized molecule was used for the rest calculations. To find the UV-VIS spectrum and all related vibrational modes, harmonic vibrational frequency calculation in standard temperature and pressure (STP) were carried out. Since, all output modes had positive values, so the results imply the effectiveness of the chosen technique.

2.2. Theoretical methods

A thin disc was produced by grinding 1 mg of the potassium acetate (CH3COOK) with 100-250 mg of potassium bromide powder using a mortar and pestle. The very fine powder is then put into a circular die, and placed under a mechanical pressure of 1–7 × 108 Nm-2 (15 000–100 000 pounds per square inch) under vacuum chamber. The sample was kept for six min under a constant pressure. Thus, the obtained disc is utilized for recording the spectrum. It is noticeable that a very fine powder must be produced, otherwise the radiation will simply reflect from the surface of the particles. There are some other related parameters and conditions, including 3000-3600 humidly H-bond stretching, 2935-2655 aliphatic C-H, 1656-1568 C= O, 1411 C- aliphatic, 649 C-H, 1051-1024 C-O.

3. Results and discussions

After running Gaussian program, the optimized geometry obtained as shown in Figure 1. In the tile of the molecule, there is a carbon (1C) that bonds with three hydrogen atoms (2H, 3H, and 4H) and the second carbon atom (6C). The angle between bonds in 1C atom is 120°. The second carbon has a single bond with potassium (8K) and a double bond with two oxygen atoms (5O and 7O).

New orbitals appear in molecules which are different from atomic orbitals. The energy difference between Highest Occupied Molecular Orbital (HOMO) to Lowest Unoccupied Molecular Orbital (LUMO) depicts the type and nature of the molecule. The geometry and its energy correspondence are shown in Figure 2. The obtained energy gap is equal to 3.669 eV, which is calculated by subtracting HOMO and LUMO energy levels.

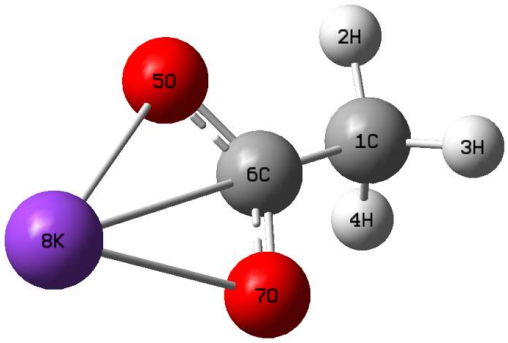


Figure 1. The schematic representation of potassium acetate. Atoms are labels according to their correspondence geometry.

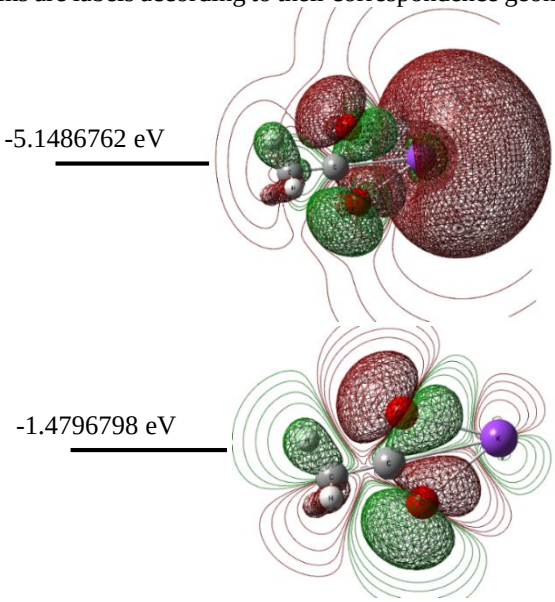


Figure 2: Boundary molecular orbitals and energy levels for HOMO and LUMO orbitals of $C_2H_3KO_2$.

One of the best methods for analyzing and detecting constituents in a specific molecule is FTIR spectroscopy. The infra-red radiation can pass through the sample, and some of that radiation may absorbs by the sample and the rest can passes through it, which is called transmitted radiation.

The theoretical and experimental results of Fourier-Transform Infrared Spectroscopy (FTIR) spectrum is correlated, and shown in Figure 3. The most peaks positions of the theoretical spectrum have a good prediction with its experimental data, however, there are some differences between transmittance rates. In the experimental result, there are two band represent water; a wide band which centered

around 3370 cm^{-1}, and a narrow band, which is centered around 1570 cm^{-1}. Since, water content is not assumed in the theoretical calculation, so there is no a noticeable band.

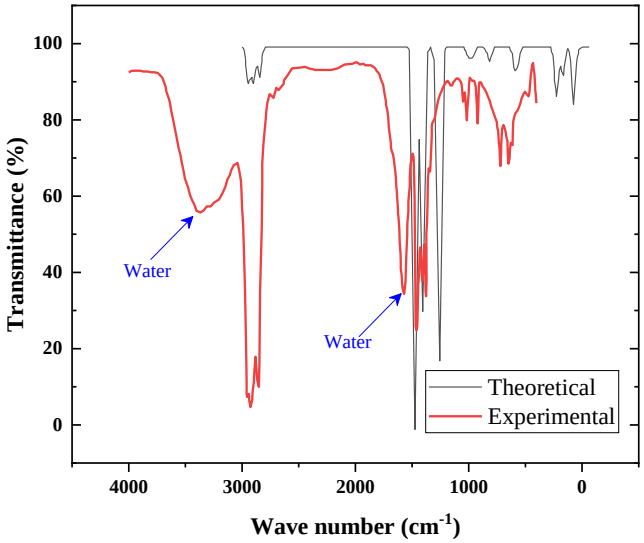


Figure 3. The correlation between theoretical (blue) and experimental (red) FTIR transmittance spectrum of potassium acetate.

4. Conclusion

In this study some physical properties of potassium acetate ($C_2H_3KO_2$) has been investigated. The molecule was made by using Gaussian program and then a quantum mechanical-based model has been utilized to obtain molecular orbital for HOMO and LUMO energy level. Some parameters like FTIR and UV spectrum has been found by Density Function Theory (DFT) technique. To conclude some important outcomes of this study is as follows:

- The model could successfully visualize the boundary orbitals of the molecule.
- The orientation of atoms in the molecule and the different vibrational modes has been found such that potassium atom is located in head of the molecule with a concentrated LUMO orbital.
- The energy gap between HOMO and LUMO was found as 3.669 eV.
- The theoretical FTIR spectrum could successfully confirm experimental result.

Acknowledgments

The authors would like to thanks Prof. Dr. Niyazi BULUT for his scientific help.

REFERENCES

[1] Z.-l. Wang, Z.C. Kang, Functional and smart materials: structural evolution and structure analysis, Springer Science & Business Media, 2012.

[2] I.N. Qader, M. Kök, F. Dağdelen, Effect of heat treatment on thermodynamics parameters, crystal and microstructure of (Cu-Al-Ni-Hf) shape memory alloy, Physica B: Condensed Matter, 553 (2019) 1-5.

[3] F. Dagdelen, M. Aldalawi, M. Kok, I. Qader, Influence of Ni addition and heat treatment on phase transformation temperatures and microstructures of a ternary CuAlCr alloy, The European Physical Journal Plus, 134 (2019) 66.

[4] M. Kök, H.S.A. Zardawi, I.N. Qader, M.S. Kanca, The effects of cobalt elements addition on Ti2Ni phases, thermodynamics parameters, crystal structure and transformation temperature of NiTi shape memory alloys, The European Physical Journal Plus, 134 (2019) 197.

[5] F. Dagdelen, M. Kok, I. Qader, Effects of Ta Content on Thermodynamic Properties and Transformation Temperatures of Shape Memory NiTi Alloy, Metals and Materials International, (2019) 1-8.

[6] E. Ercan, F. Dagdelen, I. Qader, Effect of tantalum contents on transformation temperatures, thermal behaviors and microstructure of CuAlTa HTSMAs, Journal of Thermal Analysis and Calorimetry, (2019) 1-8.

[7] D.M. Rowe, Thermoelectrics handbook: macro to nano, CRC press, 2018.

[8] I.N. Qader, M. Omar, Carrier concentration effect and other structure-related parameters on lattice thermal conductivity of Si nanowires, Bulletin of Materials Science, 40 (2017) 599-607.

[9] B. Leimkuhler, C. Matthews, Molecular Dynamics, Springer, 2016.

[10] M.H. Kebiroglu, C. Orek, N. Bulut, O. Kaygili, S. Keser, T. Ates, Temperature dependent structural and vibrational properties of hydroxyapatite: A theoretical and experimental study, Ceramics International, 43 (2017) 15899-15904.

[11] A. Hybl, R.E. Rundle, D.E. Williams, The Crystal and Molecular Structure of the Cyclohexaamylose-Potassium Acetate Complex1, Journal of the American Chemical Society, 87 (1965) 2779-2788.

[12] G. Bram, A. Loupy, M. Majdoub, E. Gutierrez, E. Ruiz-Hitzsky, Alkylation of potassium acetate in “dry media” thermal activation in commercial microwave ovens, Tetrahedron, 46 (1990) 5167-5176.

[13] R.E. Miller, E.R. Stadtman, Glutamate synthase from Escherichia coli an iron-sulfide flavoprotein, Journal of Biological Chemistry, 247 (1972) 7407-7419.

[14] D. Ulmer, Fixation: The key to good tissue preservation, J Int Soc Plastination, 8 (1994) 7-10.

[15] P.N. Dyer, R.S. Edayathumangalam, C.L. White, Y. Bao, S. Chakravarthy, U.M. Muthurajan, K. Luger, Reconstitution of nucleosome core particles from recombinant histones and DNA, in: Methods in enzymology, Elsevier, 2003, pp. 23-44.

[16] M. Gasgnier, A. Petit, Effects of microwave and heating treatments on the crystallographic properties of a potassium acetate powder, Journal of materials science, 29 (1994) 6479-6484.

[17] P. Ferloni, M. Sanesi, P. Franzosini, Phase Transitions in the Alkali C1—n. C4 Alkanoates, Zeitschrift für Naturforschung A, 30 (1975) 1447-1457.

[18] T. Jenkins, P. O'Brien, A thermal and Raman investigation of the phase transitions above room temperature in anhydrous potassium acetate, Journal of Physics and Chemistry of Solids, 44 (1983) 565-568.

[19] M. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. Petersson, Gaussian 09, revision D. 01, in, Gaussian, Inc., Wallingford CT, 2009.