Synthesis, Structure, Elastic, Electric and Charge Storage Capacity of Li₆O₆ Crystals

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Abstract: The Li₆O₆ is synthesized by employing a simple procedure and studying the single-crystal structure. The prepared sample belongs to a monoclinic crystal system with a P2₁/n space group, and the cell parameters a = 8.485(3) Å, b = 10.237(3) Å, c = 11.946(4) Å, β = 96.208°, and Z = 4. Characterization studies of this material indicate a weak energy storage density. Further, the elastic constants and other physical parameters are computed using dynamic molecular study and compared with Li-O-based compounds to understand the compound better. The dielectric constant, conductivity, and dielectric loss were determined as a function of ac frequency and varying temperature, and the results were analyzed.

Keywords: Li₆O₆; crystal structure; energy storage density; elastic constants; Li-ion battery; ELATE; dielectric constant.

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1. Introduction

Lithium-ion batteries have become a better choice for today's modern technological fields such as electric vehicles, power tools, portable electronics due to their long life, environmentally friendly properties, low cost, etc. [1-4]. Li-ion battery was discovered by Akira Yoshino in 1985, and it has played an important role in the lives of people around the world after its initiation in the market [5]. Since then, a lot of improvement in the efficiency of Li-O-based batteries has been reported in the literature [6-8]. Improvement of storage capacity and shelf life of the Li-O-based batteries have been studied extensively using physical and chemical approaches [9-11]. An insight into the kinetics operating the battery operation leading to battery capacity retention in Carbon nanotube-based Li-ion batteries has been reported recently [12]. The density functional theoretical approach was also used to simulate good performing energy storage materials [13]. The diffusion path and rate characteristics of Li-O-based compounds have been investigated experimentally and using the DFT approach [14]. Nanostructured Li-O-based material with excess Li has been studied to understand the impact on electrochemical performance [15]. Kim has extensively studied the electrochemical properties of sulfide-based Li-O compounds to understand the electrochemical properties [16]. Based on the change in the UV-Vis spectrum, the changes in the aggregation of Li-O have been reported [17]. Nanocomposite-based Li-O compounds indicated improvement in
electrochemical properties [18]. Crystallographic defects in the Li-ion diffusion path in several materials were simulated using the DFT method has been reported [19]. Crystal structure and properties of Prismatic Li$_6$O$_6$ core in Lithium phenolates show interesting results [20].

In this article, the synthesis of the Li$_6$O$_6$ compound using a simple procedure and study of its electrochemical properties has been reported. Further, the single-crystal structure is determined and simulated its physical properties using the molecular dynamics method. The dielectric constant, conductivity, and dielectric loss were determined as a function of ac frequency and varying temperature, and the results were analyzed. Finally, the obtained results were compared with the experimental values, which show a broad agreement.

2. Materials and Methods

2.1. Synthesis of the sample.

1g (3.47 mmol) of hexachlorocyclohexane (lindane) and 0.89 mL (20 mmol) of lithium methoxide was taken in a Teflon liner and placed in an autoclave. The autoclave was kept in the oven for 6 hours at 70°C. After the completion of the reaction, the autoclave was allowed to cool to room temperature, and the resultant crude product was recrystallized using ethanol to obtain a pure crystalline solid. The synthesis procedure is shown in Figure 1. The considered compound is basically salt, and Li (+) and O (-) are the reasons for the obtained structure, as shown in Figure 1.

![Figure 1. Graphical representation of synthesis procedure.](image)

2.2. Single crystal data collection and analysis.

The purity of the compound was checked by determining its melting point. Table 1 summarizes the crystal data, data collection, and structure refinement parameters.

| Molecular formula | Li$_6$O$_6$ |
|-------------------|------------|
| Molecular weight  | 137.64     |
| Crystal system and space group | Monoclinic, P21/n |
| Temperature       | 293 K      |
| a, b, c (Å)       | 8.485(3), 10.237(3), 11.946(4) |
| β (°)             | 96.208(7)  |
| V (Å$^3$)         | 1031.6(6)  |
| Z                 | 4          |
| Radiation type    | MoKα       |
| μ (mm$^{-1}$)     | 0.81       |
| Wavelength (Å)    | 0.71075    |
| Data Collection   |            |
| Reflections Collected | 2274 |
| Theta range for data parameters | 3.11-27.49 |
| Refinement method | Full-matrix least-squares on F$^2$ |
| Final R indices   | R = 0.098, wR = 0.240 |

https://biointerfaceresearch.com/
After confirming the suitability with a polarizing microscope (Vacuum base module, Model-bx51 trf), a single crystal was selected and used for X-ray data collection employing Rigaku XtaLAB Mini CCD diffractometer operating at 50 kV and 12 mA. SHELX was used to solve the crystal structure by using the full-matrix least-squares technique. The data was submitted to the CCDC, and the deposition number is 2081482. The ortep diagram is shown in Figure 2.

![Figure 2. Ball and Stick representation of Li$_6$O$_6$ compound Li$_6$O$_6$](https://biointerfaceresearch.com/)

### 2.3. Electrochemical properties of Li$_6$O$_6$

Electrochemical charge-discharge experiments were performed with Swagelok-type cells. The working electrode was prepared by hand grinding a mixture of active material. Super-P Carbon (Timcal Belgium) in the ratio 85:15 (weight ratio) was assembled inside the argon-filled glovebox using Lithium foil as the counter electrode and reference electrode. The Whatman glass microfiber film was used as a separator, and 1M LiPF6 in a solution of ethylene carbonate and dimethyl carbonate (1:1 ratio by volume) was used as an electrolyte. The galvanostatic charge-discharge was performed at room temperature, at a C/5 rate (C corresponding to the theoretical exchange of one electron in 1 h) between 2.4 V to 4.4 V versus Li / Li$^+$. All the electrochemical experiments were carried out using VMP3Z biologic multi-channel potentiostat/galvanostat.

### 2.4. Raman and FTIR spectra of Li$_6$O$_6$

Raman shift recordings were carried out using the instrument Horiba scientific with model Xplora Plus, and the readings were recorded. It is shown in Figure 6 (a). The recorded FTIR spectra in the transmission mode with spectrophotometer model FTIR-4100 type A, a resolution of 4 cm$^{-1}$ in the wavelength range of 400 to 800 cm$^{-1}$, are shown in Figure 6 (b).

### 2.5. Dielectric constant, ac conductivity, and dielectric loss of Li$_6$O$_6$

Employing an Impedance analyzer (ZM 2376), the dielectric constant, ac conductivity, and dielectric loss have been determined as a function of frequency from 50Hz to 5MHz for various temperatures 25 °C, 50 °C, 75 °C, and 100 °C. The obtained results are analyzed and shown in Figures 7 to 9.
3. Results and Discussion

The Li₆O₆ compound crystallizes in the monoclinic system with space groups P₂₁/n and Z=4. Its ORTEP diagram is shown in Figure 2. Using crystal structure data and molecular dynamics with GULP SOFTWARE [21], we have simulated various physical parameters which are shown in Table 2.

Table 2. Physical parameters computed with GULP software and crystal structure data of Li₆O₆ compound.

| Physical parameter       | Values         | Li₂O₂ [24] |
|--------------------------|----------------|------------|
| Electronegativity        | 8.5 eV         |            |
| Lattice energy           | -0.05eV        | 30.26kJ/mol|
| Elastic constants (GPa)  |                |            |
| C11,C12,C13              | 0.151, 0.071, 0.11 | 163,54,12  |
| C33,C44,C55,C66          | 0.171,0.038,0.031,0.031 | 166,36,36,64 |
| Space group              | Fm3m           | P6₃/mmc(194)|
| Bulk, Young's, Shear     | 0.967, 7.67, 21.93, -0.83 | 72, -0.53, 0.21 |
| (Voigt in GPa)           |                |            |
| Velcocity of             | 0.605 and 1.283 |            |
| S- and P-waves (km/s)    |                |            |
| Zero-point energy        | 0.068 eV       |            |
| Entropy                  | 0.051 eV/K     | -1.492J/K/mol |
| Helmholtz Free Energy    | -11.89 eV      | -633kJ/mol  |
| Heat capacity            | 0.012 eV/K     | 1.603J/mol*K |
| constant volume          |                |            |

Using these values and employing an online ELATE three-dimension program we have plotted the 3-D variation of elastic moduli, namely young’s modulus (E), rigidity modulus (G), liner compressibility (β), and Poisson’s ratio (ν) of Li₆O₆ as shown in Figure 3.

Figure 3. 3-D perspective of (a) Young’s, (b) shear, (c) linear compressibility, and (d) Poisson's ratio. See also Table 2.
Due to the convolution of a Lorentzian and a Gaussian density, the Voigt approximation has been used to estimate these elastic moduli. Here, the young's modulus is the measurement of materials stiffness, which portrays the strain reaction whenever uniaxial stress is applied in the same direction, the rigidity modulus determines the mechanical resistance or hardness to the plastic deformation of a solid material [22]. Poisson's ratio gives the proportion of transverse strain to the axial strain, and the linear compressibility is the compression along an axis upon isostatic compression [23].

The calculated values of these elastic moduli are represented in Table 2. Our results are in reasonable agreement with Li-O based compound [24, 25] and demonstrate the changes in values near the surface boundary. From the obtained spatial variation of elastic moduli, it can be implemented that the green shape shows the minimum variation for a particular parameter, and the blue indicates the maximum variation. If the material is isotropic, then the shape of elastic moduli would be spherical. If there is any distortion from the spherical shape, it shows anisotropic behavior [25]. In our study, the directional dependent young's modus and linear moduli show isotropic behavior. The shear modulus and Poisson's ratio slightly distort from the spherical shape, which shows partial anisotropic behavior.

![image]

Figure 4. (a) The discharge voltage curve at different cycles, (b) Charge-discharge profile of Li6O6 material cycled in the voltage range of 2.4 - 4.4 V at a rate of C/5, (c) The profile of the cycle vs. discharge capacity performances of the Li6O6 material cycled between 1.3 and 4.4 V at C/5 rate and (d) The charging characteristics of Li6O6 material.

Figure 4 (a) shows the rate capabilities of all samples at different cycles between 2.4 and 4.4 V. The cells were all charged/discharged at the rate from C/5, for 100 cycles. It was observed that the cell, when discharged at a low rate, no significant change in its capacity was exhibited. The plateau x of the profile becomes lower with the increase of current density. When the current density comes to C/5, the capacities for all the samples showed a dramatic
drop. Figure 4 (b) shows the charge-discharge profiles of the Li$_6$O$_6$ material at a rate of C/5 in the voltage window of 2.4 to 4.4V. The graph shows the long voltage plateau, which corresponds to the removal of lithium from the transition metal layer phase during the initial charge. This phenomenon is accompanied by the removal of oxygen from the structure. The initial charge and discharge capacities are 1.5 and 0.7 mAh/g, respectively. Figure 4 (c) shows the profile of the cycle number v/s discharge capacity of the material. The discharge capacity is delivered first at around 1.6 mAh/g, whereas as an example for comparison with Li0.5VO2, it is 415 mAh/g and voltage of 1.12V [26]. It decreases gradually till 20 cycles and then remains stable for the rest of the range. The reversible capacity is around 0.8 mAh/g after 20 cycles, about 50 percent of the capacity at the C/5-rate. Figure 4 (d) shows the charge characteristics of Li$_6$O$_6$. For LiNiO$_2$, it was reported that discharge capacity changes from 200mAhg$^{-1}$ to 150mAhg$^{-1}$ for different cycles, which is much higher and more stable than what is reported here. Our emphasis is that this sample has a viable crystal structure that can play an important role in modifying other substitutes with rare earth elements to improve battery performance [27].

![Figure 5](https://biointerfareresearch.com/) Two different modes of Li$_6$O$_6$ molecule.

The normally observed charge/discharge profile obtained for the Li$_6$O$_6$ compound is shown in Figure 3 (a) for a window of 0 to 4.4 V at a rate of C/5, which we concur that it is very weak compared to other materials. We attribute this behavior to the fluctuations between the two modes given in Figure 5. These modes are equivalent to two weakly coupled harmonic oscillators with a Raman Shift frequency given in terms of the wavenumber 684 cm$^{-1}$ and an individual harmonic oscillator of Raman Shift frequency corresponding to the wavenumber 353 cm$^{-1}$. Thus, the individual frequency is nearly half of the coupled harmonic oscillator frequency.

$$\omega^2 = \frac{k_1 + k_2}{M}$$

It would be interesting to synthesize a compound Li$_3$O$_3$ with a stable mode at 325 cm$^{-1}$, which would be useful for energy storage [28]. Figure 4 (b) compares the charge/discharge profiles at the rate C/5 and shows weak electrochemical performance, which we attribute to a smaller crystallinity region. Figure 4 (c) shows that the sample under consideration exhibits a stable cycle life, which is reasonably comparable to earlier reports on Li-O-based compounds [29]. Charging characteristics with charging time show an encouraging result regarding the electrochemical properties of the material.

The importance of studying Li$_6$O$_6$ is brought out by the Raman spectra shown in Figure 6 (a), similar to the one reported by [31] at 531 cm$^{-1}$ for Li-O compounds. In FTIR spectra, we observe sharp peaks at 407.75, 422.53, 440.66, 478.09, 554.49, 576.2, 619.25, 684.59 cm$^{-1}$ which is normally due to metal ions like Li$^+$. This agrees with the reported values of the Li-O-based compound [32].
If a varying electric field $E$ is applied to a dielectric material, its phase lag slightly behind the applied field, whereas the polarization charges will vary in a periodic manner. The material can be characterized by \[ \epsilon = \epsilon' - j\epsilon'' \]
where $\epsilon'$ and $\epsilon''$ represent the dielectric constant and dielectric loss, respectively. The energy loss is given by \[ L = \omega \epsilon_0 \epsilon'' \left( \frac{A}{t} \right) E^2 \]
where $A$ and $t$ are the area and the thickness of the sample. $\epsilon_0$ is the permittivity of the free space. When we examine the ac conductivity or dielectric constant of a material, it is significant to analyze these properties in terms of electric polarization as a function of ac frequency. The total polarization in any material is due to electronic, ionic, and dipolar contributions. The dipolar contribution can be seen only in materials having permanent dipole moments in lower frequencies [33].
Figure 8. Variation of conductivity as a function of frequency for different temperatures.

Figure 9. Variation of dielectric loss as a function of frequency for different temperatures.

The ac conductivity, dielectric constant, and dielectric loss were examined from the frequency range 50 Hz to 5 MHz at different temperatures from 25 °C to 100 °C. The obtained results are shown in Figures 7, 8, and 9. From Figure 7, our sample has shown a high dielectric value and is independent of frequency up to 3kHz at all temperatures. After 100kHz, the constant dielectric increases sharply for all the temperatures due to the relaxation process, or friction against dipole motion drops with frequency. The dielectric constant versus frequency graph revealed that the dielectric constant reaches a maximum value of 25 °C and 50 °C at 3.5 MHz because of dipoles orientation along the applied electric field, electrode effects, and interfacial effect [34]. Further, it tends to decrease due to difficulty in orientation dipoles on their own at higher temperatures and frequencies. Figure 8 shows the results of ac conductivity versus frequency for different temperatures. The ac conductivity has been calculated using the relation [34].
Here, $G$ is the conductance in siemens, $A$ is the area in $m^2$, $t$ is the thickness of the sample in $m$. In our study, the area of the sample was $7 \times 3 \, mm^2$. The graph of $\log (F)$ versus ac conductivity shows an almost frequency independent region in lesser frequency and has a high conductivity value at 25 °C, 50 °C, and followed by 75 °C. The increase in ac conductivity value at a higher frequency for a given specific temperature may be due to the enhancement in the conductance mechanism. With a further increase in frequency, there is a decrease in conductivity due to structural disorder produced in the sample [35-38]. Figure 9 represents the dielectric loss as a function of frequency for various temperatures. Initially, the dielectric loss decreases as frequency increases, showing dispersion at a lower frequency range [39-41]. Afterward, it remained constant at higher frequencies. It is tracked down that, with the increase in temperature, the dielectric loss increases for temperatures less than 75 °C. As the temperature increases, the mobility of charge carriers increases in turn, which increases the polarization of charges, leading to an increase in the dielectric loss [42].

4. Conclusions

We have synthesized the Li$_6$O$_6$ compound, which shows several interesting structural, physical, and electrochemical properties. The salient features of our investigation are: It is a monoclinic crystal belonging to the space group P2$_1$/n. Electrochemical studies of Li$_6$O$_6$ show a weak charging and discharging property that can be improved with a modification of the synthesis, retaining a basic benzene-like structure having Lithium and Oxygen atoms at the appropriate places. The simulated physical properties using crystal structure data are in broad agreement with experimental values for Li-O-based compounds. A three-dimensional spatial variation of moduli parameters and Poisson's ratio indicate the behavior near the sample boundaries. A coupled harmonic oscillator like the behavior of the compound is conjectured based on the experimental observation of Raman Shift to explain the weak electrochemical properties of the sample. The dielectric constant, ac conductivity, and dielectric loss have been determined as a function of frequency and temperature and observed high conductivity value at 25 °C, 50 °C and followed by 75 °C and variation of dielectric constant and loss were identified due to orientation of dipoles at different ac frequency and temperatures. We have prepared a new type of Li-O-based compound with a hexagonal-like chemical structure, and this will pave the way for developing a new type of battery material which is the main intention of this paper.

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Conflicts of Interest

The authors declare no conflict of interest.
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