

# CO<sub>2</sub> Transformation at Controlled Temperature with Lithium Hydroxide Solution and Metallic Lithium

Elizabeth Teresita Romero-Guzmán, José Luis Iturbe-García\*

Departamento de Química, Gerencia de Ciencias Básicas, Instituto Nacional de Investigaciones Nucleares, Carretera México-Toluca, S/N. La Marquesa Ocoyoacác, Estado de México, Mexico  
Email: elizabeth.romero@inin.gob.mx, \*joseluis.iturbe@inin.gob.mx

**How to cite this paper:** Romero-Guzmán, E.T. and Iturbe-García, J.L. (2024) CO<sub>2</sub> Transformation at Controlled Temperature with Lithium Hydroxide Solution and Metallic Lithium. *Journal of Minerals and Materials Characterization and Engineering*, 12, 189-203.

<https://doi.org/10.4236/jmmce.2024.122012>

**Received:** March 16, 2024

**Accepted:** April 27, 2024

**Published:** April 30, 2024

Copyright © 2024 by author(s) and Scientific Research Publishing Inc. This work is licensed under the Creative Commons Attribution International License (CC BY 4.0).

<http://creativecommons.org/licenses/by/4.0/>



Open Access

## Abstract

This paper presents a study on CO<sub>2</sub> atmospheric transformation which was reacted directly with lithium hydroxide solution and metallic lithium. This solution was obtained through the reaction between metallic lithium and deionized water where hydrogen is produced and by exposing the metal at ambient conditions. In the transformation process, atmospheric CO<sub>2</sub> gas reacts directly with LiOH solution, in both cases, the CO<sub>2</sub> transformation kinetics was different. For this purpose, reactions between CO<sub>2</sub> and LiOH solution were carried out under controlled temperature and the second process only with metallic lithium, which was exposed at room temperature, however, in these two processes lithium carbonate oxide was formed and identified. According to the results, the efficiency in CO<sub>2</sub> transformation is a function of temperature value which was variable until completely obtaining the by-product, its XRD characterization indicated the formation only of Li<sub>2</sub>CO<sub>3</sub> in both procedures. Under laboratory conditions lithium compounds selectively reacted with CO<sub>2</sub>. In the same way, there is an alternative procedure to obtain LiOH and Li<sub>2</sub>CO<sub>3</sub> for different applications in various areas.

## Keywords

Metallic Lithium, Lithium Hydroxide Solution, Hydrogen, Atmospheric CO<sub>2</sub> Transformation, Lithium Carbonate

## 1. Introduction

Currently, air pollution is considered one of the most important problems for humanity because in recent decades atmosphere deterioration has been increas-

ing. Hence the interest in improving air quality both inside housing, offices, supermarkets and in general all closed spaces used by people, as well as externally. Unfortunately, the emissions of pollutants released into atmosphere will continue as long as fossil fuels continue to be burned, particularly in transportation and industry sectors, among others. In particular, the concentration of carbon dioxide (CO<sub>2</sub>) has drawn a lot of attention because it has significant impacts on environmental problems and, as consequence, on human health [1]. CO<sub>2</sub> is the main indicator that allows knowing air quality inside closed spaces, also considered as one of main greenhouse gases [2]. Unfortunately, CO<sub>2</sub> concentration in atmosphere has been increasing despite the agreements obtained in various political and economic forums worldwide to reduce these gas emissions and natural disasters that can occur with temperatures above 1.5°C caused by the greenhouse effect [3] [4]. In order to maintain an adequate quality of air inside closed spaces, CO<sub>2</sub> capture found in the atmospheric air commonly called “air capture” is an effective method to control the concentration of ambient CO<sub>2</sub> [5] [6] [7]. Its capture and concentration is a very promising strategy to mitigate CO<sub>2</sub> emissions, while at the same time having a benefit related to the production of value-added products, for example, obtaining fuel or its use in various industries [8]. On the other hand, in relation to the availability of lithium hydroxide, various methods for its synthesis have been studied, including thermochemical, ion exchange, Bipolar membrane electrodialysis (BMED), electrolysis, among others [9] [10]. The precipitation method to synthesize high purity LiOH has also been reported [11]. Subsequently, lithium hydroxide monohydrate (LiOH·H<sub>2</sub>O), an important lithium salt, is the most widely used CO<sub>2</sub> adsorbent in the last 40 years due to its high storage capacity whose reported value has been ~30% by weight [12] [13]. The main reaction mechanism between LiOH and CO<sub>2</sub> is described in Equation (1):



Other important applications of this hydroxide have also been reported, for example it is considered a crucial precursor for the production of cathode material for lithium-ion batteries [14] [15]. Multiple technological applications of lithium compounds have been investigated, where some of them, such as lithium ion, play an important role in energy storage systems [16]. Thus, development of new, high-capacity CO<sub>2</sub> capture materials (dry adsorption) is necessary for improvement of CO<sub>2</sub> capture and storage technology. It is one of a few technology solutions that can reduce energy-related CO<sub>2</sub> emissions and this process should operate under room temperature and ambient conditions [17] [18]. By other hand, hydrogen is considered a vector of clean and renewable energy, being a very important and promising alternative to replace fossil fuels. Hydrogen can store and provide energy that can be used in various sectors, mainly in industry, but normally it does not exist in nature and must be produced from compounds that contain it, including oil derivatives or in water as a renewable resource. Hydrogen is a very abundant element in many hydrogenated compounds, including

water, and the most available renewable energy vector for future energy systems, mainly fuel cells [19] [20]. In hydrogen production from any type of fossil fuels, mainly reforming process of natural gas or methane, the products of hydrocarbon gasification with water mainly include not only hydrogen, but also carbon monoxide and CO<sub>2</sub>. CO<sub>2</sub> adsorption has been carried out using different technologies focused on materials whose mechanisms are mainly focused as good absorbents or/and adsorbents, such is the case of amines, zeolites, carbons, aluminas, organometallic compounds, basic oxides, hydrotalcites, etc.; each of these materials has its own advantages and disadvantages in trapping this gas [21] [22] [23] [24] [25]. Therefore, the development of technologies to mitigate CO<sub>2</sub> concentrations has been of great interest from the practical point of view. The objective of this work was to use lithium compounds in two different forms, to carry out the reaction under certain temperature conditions with atmospheric CO<sub>2</sub>, one as lithium hydroxide solution and as metallic lithium where hydrogen was generated, and in both cases Li<sub>2</sub>CO<sub>3</sub> was formed as a by-product.

## 2. Experimental

### 2.1. Lithium Hydroxide Preparation

To prepare lithium hydroxide solution, following procedure was carried out: quantities of 100 mg of metallic lithium were weighed (Alfa Aesar, granular particle sizes of 1 - 3 mm and purity 99.4%), which were placed in 20 mL glass vial. The container was sealed with a rubber stopper and an aluminum sealing ring. This process was carried out in a glove box with controlled atmosphere to avoid direct contact between metal and ambient gases. Subsequently, 3 mL of deionized water were added with a syringe, which is at average temperature of 20 °C. The reaction is exothermic and kinetics was very fast, the time to completely react was on average 2.5 min. During the reaction between lithium and water hydrogen was generated. The system where the reaction is carried out has a rubber plug with a device through which hydrogen generated is released without exposing solution to environment. After reaction, a transparent solution was obtained. Later, when temperatures of system and environment were equal, the 20 mL glass vial was opened and pH of solution was measured. Finally, this solution was used to transform atmospheric CO<sub>2</sub> by evaporation. In some experiments, the solution evaporation was carried out depending on temperature and under vacuum, that is, without presence of CO<sub>2</sub> to avoid Li<sub>2</sub>CO<sub>3</sub> formation during this process and to obtain only lithium hydroxide in solid form.

### 2.2. CO<sub>2</sub> Transformation

The lithium hydroxide solution obtained in this process was used to carry out CO<sub>2</sub> transformation from environment. The transparent lithium solution (3 mL) was placed in a petri dish, which was put in contact with environment laboratory conditions. Subsequently, the petri dish was placed on a temperature-controlled heating rack, it was carried to complete evaporation at a tem-

perature of 25°C which was maintained for 2 hours. To know environmental CO<sub>2</sub> concentration, laboratory was monitored with a Testo 535 probe that presents high precision and efficiency, it has two LCD lines, it has a measurement range of 0 to 9999 ppm, its resolution is 1 ppm, and operating temperature 0°C to 50°C. On the other hand, in another series of experiments, CO<sub>2</sub> transformation process was carried out quickly, for which Li solution in petri dish was heated on the electric grill, programming different temperature intervals which were from 25°C to 50°C, each was evaporated to dryness. At these temperatures CO<sub>2</sub> atmospheric reacted and a transparent solid was obtained. Secondly, to determine behavior of lithium in environment, metallic Li particles were placed in a glass container and exposed to atmospheric air of laboratory for 60 days where average temperature was 20°C. Under these conditions, after one week the particles began to form a white film on their surface, as time passed, a white powder was formed until its complete transformation. Subsequently, all solids were characterized.

### 2.3. Materials Characterization

The lithium solids obtained at different temperatures and white powder produced from metallic lithium exposed to environment were characterized by X-ray diffraction. The samples were placed in a holder of lucite and then on the goniometer of the diffractometer. Some parameters used in determination by this technique were, a K $\alpha$  radiation source from Cu anode was selected with a diffracted beam monochromator at 40 kV and 40 mA,  $2\theta$  steps of 0.02°, and programmed times of 20 min to acquire the data X-ray patterns, with intensities high enough for further identification. The interval considered to acquire the spectrum was from 15° to 80° in  $2\theta$ . The diffractograms were collected by a Bruker D8 Advance X-ray powder diffractometer and an energy-dispersive one-dimensional detector in order to identify the phases formed. Identification and quantification of crystalline phases were carried out by DIFFRAC.EVA and TOPAS software. This software supports a reference pattern database derived from Crystallography Open Database (COD) and the Powder Diffraction File (PDF) for phase identifications.

Morphology and elemental composition. Another technique such as Scanning Electron Microscopy (SEM) to characterize the different solids was also used to study the morphology of the lithium-based materials through a scanning electron microscope, JEOL 5900 LV, at 20 kV. The samples were mounted on an aluminum holder with aluminum conductive tape and later covered with a gold layer approximately 200 Å thick using a sputtering mark Denton Vacuum model Desk II, this procedure was for to avoid an electrical overload on the powder surfaces. In all cases, with a backscattered electron detector the images were obtained. The electron microscope is equipped with a microanalysis energy dispersive X-ray (EDAX) probe to determine the morphology and semi-quantitative elemental composition of the samples with an EDAX-4 spectrometer.

## 2.4. Hydrogen Generation and Analysis

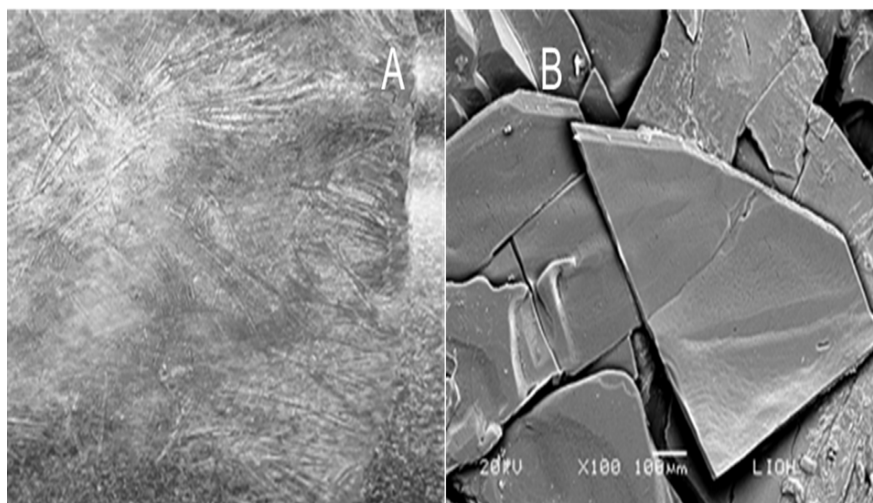
The reaction between metallic Li and humidity of environment to first form lithium hydroxide, which in turn reacts with atmospheric CO<sub>2</sub> and forms lithium carbonate, was carried out as follows: particles of metallic lithium were placed in a plastic tube, with small holes in the bottom for direct air contact with particles. The tube was attached to a plastic jar and perforated with four openings around it to allow interaction with the environment. An inverted glass vial was placed on top of the plastic jar, which wraps the plastic tube to contain the hydrogen generated by metallic lithium during the time exposed to environment. In this series of procedures, three systems were used to perform these reactions. The lithium material was left in the laboratory for 3 months, to determine the presence of hydrogen, the vials were analyzed after 30, 60 and 90 days. After programmed time, the vial was hermetically covered with a rubber stopper and an aluminum ring to prevent the release of hydrogen before analysis. In order to characterize the produced gas, gas chromatography (GC) and mass spectrometry (MS) measurements were performed. The gas generated after the programmed time was repeatedly injected and analyzed using a chromatograph (Gow-Mac 580 instrument) equipped with a 5 Å molecular sieve column at 35°C and an injector controlled by Clarity V.7.0.01.402 software. Argon was used as carrier gas at 20 mL·min<sup>-1</sup>. The effluent gases were monitored with a portable mass spectrometer (BELMass, MicrotracBEL Corp.).

## 3. Results and Discussion

### 3.1. Physicochemical Characterization of LiOH and Li<sub>2</sub>CO<sub>3</sub>

#### Morphology and Elemental Composition

The LiOH and Li<sub>2</sub>CO<sub>3</sub> considered in this work were analysed in powders. In conjunction with electron microscopy, elemental composition was determined. **Figure 1** represents two images of lithium hydroxide crystals. Image A shows a photo which was taken with a cell phone, on the surface of the Petri dish during the evaporation of the LiOH solution at a temperature of 25°C. On image, a series of channels appear which are distributed in all directions. At beginning of crystallization, small crystals such as those that appear in lower right part of image were observed and then fused to form the crystalline structure. The time considered during evaporation to form lithium hydroxide crystals was approximately 2 h, under these temperature conditions and the time considered, a small amount of lithium carbonate could be formed, as observed in the analysis carried out by X ray diffraction. **Figure 1(B)** corresponds to LiOH crystals once removed from Petri dish, they do not present a specific morphology, the particle size depends on the way in which they were separated from Petri dish, particle surfaces appears to be a homogeneous sample. The image was carried out at 100 magnification. In this Figure, it can be observed that surface is mostly smooth and compact, apparently with free spaces. Another analysis performed on this sample was by EDAX to determine elemental composition. According to results,



**Figure 1.** Lithium hydroxide during evaporation, photo (A) and its particles micrograph (B).

in LiOH sample the quantified elements were O, C and Au, which are reported in atomic percentages. The presence of O corresponds to the one that forms the hydroxide, the C may be due to lithium carbonate formed with low percentage under these temperature conditions, and Au is due to the coating that was done on sample to avoid an electrical overload at time of analysis.

**Figure 2** corresponds to a lithium carbonate micrograph. In the image, clusters of various sizes are observed, their crystals do not present a defined morphology and according to the scale the size of the particles are smaller than 10 microns. This material was evaporated at 50°C.

The image was obtained at 1000 magnification. On the right side of the micrograph is represented the X-ray spectrum of  $\text{Li}_2\text{CO}_3$ . The spectrum was obtained by EDAX to know the elemental composition, the C, O peaks at low energies as components of lithium carbonate were recorded. The third peak that appears at an energy of 2.17 keV corresponds to Au, which was used as a protective layer on the sample to avoid an electrical overload when carrying out the analysis. Although the analysis is semi-quantitative, the results give a good approximation of its percentage composition.

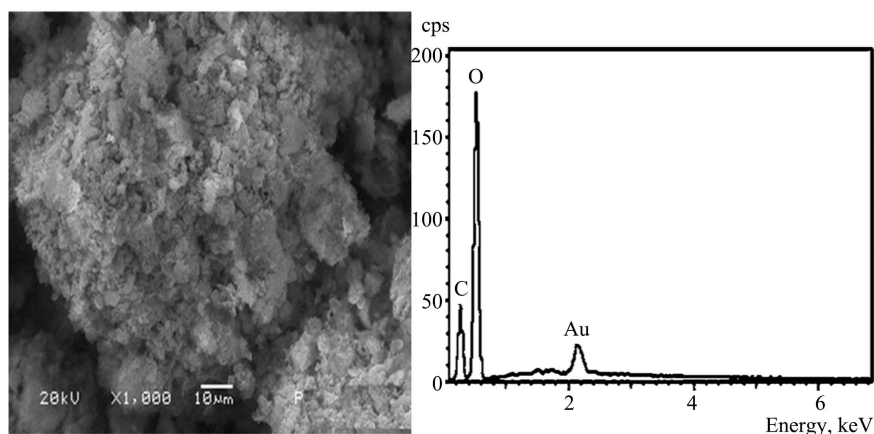
According to the results expressed in atomic percentages, the atomic ratio between carbon and oxygen in the lithium carbonate molecule agrees with the theoretical value. Therefore, in the  $\text{Li}_2\text{CO}_3$  molecule, the C/O atomic ratio is 3, and the one obtained in this work according to the experimental values of  $76.44 \pm 1.35$  for carbon and  $23.56 \pm 1.34$  for oxygen was 3.24 in average, that is, the material is homogeneous and only one phase was formed.

### 3.2. Lithium Hydroxide XRD Characterization Units

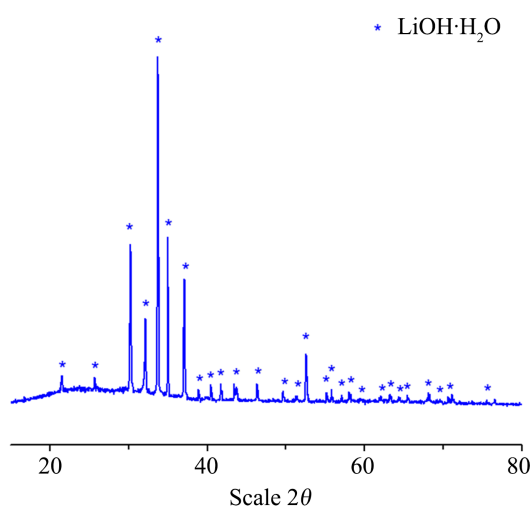
The LiOH and  $\text{Li}_2\text{CO}_3$  considered in this work were analyzed in powders. In conjunction with electron microscopy, elemental composition was determined.

**Figure 3** shows the diffraction spectrum of the solid LiOH sample.





**Figure 2.** Micrograph and X-ray spectrum of lithium carbonate.



**Figure 3.** X-ray Powder Diffraction (XRD) of the solid LiOH hydrate sample.

The image shows 6 peaks of higher intensity, 5 of which are in an interval of 30 to 40 in  $2\theta$  degrees, as well as many of small intensities but all correspond to the same analyzed species. Through card PDF 25-0486, its identification was carried out, which indicates hydrated lithium hydroxide as only phase. Likewise, by means of this card, its crystalline form is reported, which indicates that it is a monoclinic system and whose space group is determined by the number 183, also its reported crystal lattice parameters are:  $a = 6.95000 \text{ \AA}$ ,  $b = 8.28000 \text{ \AA}$ ,  $c = 3.20000 \text{ \AA}$ ,  $\beta = 95.230^\circ$ ,  $\gamma = 120^\circ$ . The 6 peaks whose values in  $2\theta$  angles are: 30.064, 31.937, 33.730, 34.971, 36.963, and 52.488, to which diffraction are attributed to planes (011), (101), (220), (130), (-121), (231), respectively. The spectrum corresponds to the product obtained after evaporation of the lithium solution, In this series of experiments, when the lithium hydroxide solution evaporates without  $\text{CO}_2$ , result LiOH crystals formation, the evaporation was performed at certain temperature and under vacuum to avoid the formation of  $\text{Li}_2\text{CO}_3$ . Therefore, only in the spectrum the LiOH crystals were identified. The LiOH solution was prepared by reacting metallic Li and deionized water. It is

well known that the metallic elements that are indicated in the first group of the periodic table react easily with water to generate hydrogen and as a by-product form the corresponding hydroxide. In the case of the reaction of lithium with deionized water, its behavior as a hydroxide is more similar to physicochemical properties of hydroxides of the second group. The reaction carried out between metallic lithium and deionized water is represented in Equation (2):



where for every 2 moles of Li, one mole of hydrogen is generated and 2 of lithium hydroxide.

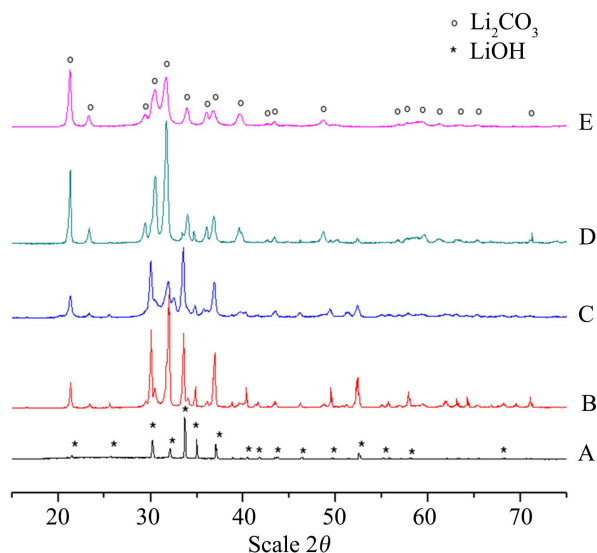
The transformation from the liquid phase by evaporation at low temperature to the solid phase is carried out where the same compound is maintained, that is, lithium hydroxide crystals. In this type of reaction, hydrogen was generated which was released through a syringe needle connected to a rubber hose. With this gas release procedure, exposing the solution to the environment with the probability of reacting with CO<sub>2</sub> was avoided, since the reaction between Li and water is exothermic. Thus, lithium hydroxide solution was obtained. The pH of the solution was 14, according to this value it is a strongly basic solution which easily reacts with CO<sub>2</sub> as described later. The water used in the reaction does not contain other types of ions, especially carbonates that could react with the LiOH solution. All peaks observed in the spectrum correspond to the crystalline phase of LiOH. It is important to note that neither phase appeared in the spectrum indicating that the reaction between metallic lithium and water formed only one by-product after hydrogen production.

### 3.3. CO<sub>2</sub> Transformation

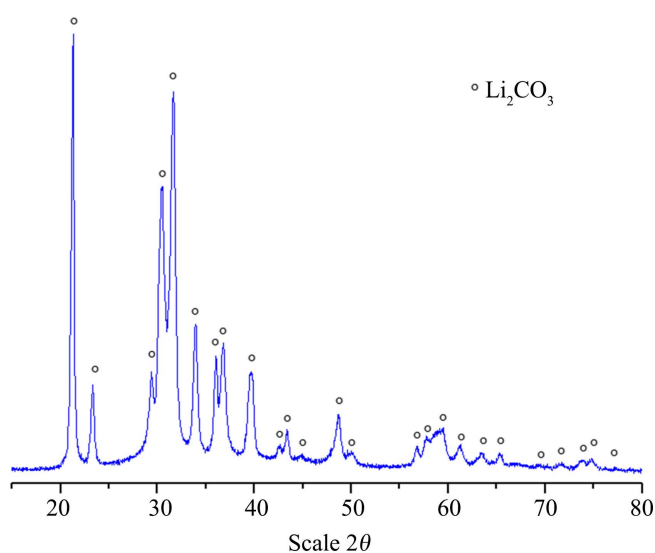
To know the CO<sub>2</sub> concentration inside the laboratory, 5 measurements were carried out per day during the months that metallic Li was exposed to environment as well as during evaporation of Li hydroxide solution, to keep a statistic during experimental part and take into account the concentration of this gas that reacted with lithium compounds. Both in solid and liquid form. The average CO<sub>2</sub> values that prevailed during the experimentation were  $552.32 \pm 12.46$  ppm. **Figure 4** shows the X-ray spectra according to evolution in CO<sub>2</sub> transformation with LiOH solution at different temperature values.

Spectrum A corresponds to lithium hydroxide that crystallized at temperature of 25°C in laboratory conditions. 6 most important intensities of this phase appear in interval from 30 to 55 degrees in 2 theta, the rest of peaks cannot be appreciated well due to scale when plotting all the spectra in this way. However, **Figure 5** shows individual spectrum with each lines which correspond to Li<sub>2</sub>CO<sub>3</sub> spectrum solid phase. In order to know if at higher temperatures the reaction between LiOH solution and atmospheric CO<sub>2</sub> increases carbonate formation, solution evaporation was thermally controlled for which crystallization was programmed at a higher temperature. Spectrum B is the result of analysis whose Li solution evaporation was carried out at 27°C. In diffractogram two phases appear,





**Figure 4.** X-ray diffractogram of lithium carbonate and lithium hydroxide in atmospheric  $\text{CO}_2$  transformation as function of temperature.

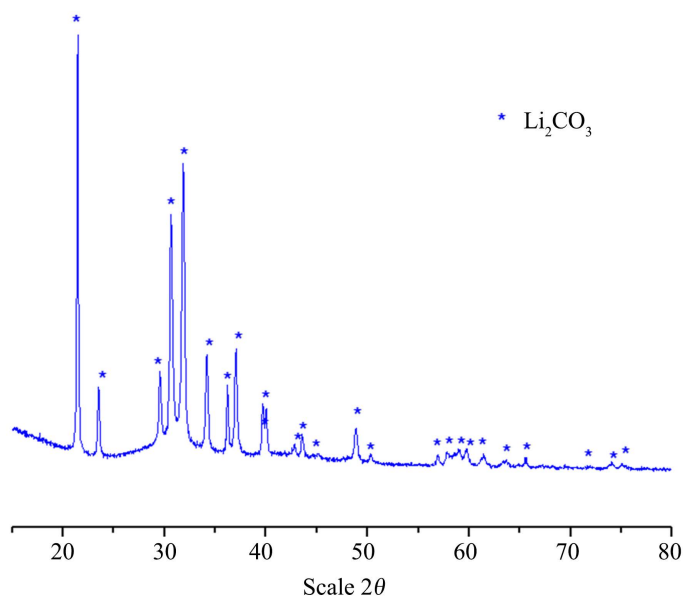


**Figure 5.** X-ray diffractogram of  $\text{Li}_2\text{CO}_3$  formed from lithium hydroxide solution exposed to atmospheric  $\text{CO}_2$  evaporated at  $50^\circ\text{C}$ .

on one hand LiOH and on the other small intensities are observed which correspond to  $\text{Li}_2\text{CO}_3$  phase identified with their corresponding PDF cards. Under these temperature conditions, the  $\text{CO}_2$  reaction with LiOH was favored despite minimal difference in temperature ( $2^\circ\text{C}$ ), the additional energy was enough to carry out  $\text{CO}_2$  transformation more efficiently. As indicated by first peak that appears in spectrum with a value of 21.239 in 2 theta degrees, which corresponds to  $\text{Li}_2\text{CO}_3$ . Spectrum C corresponds to one obtained at  $30^\circ\text{C}$ . In this spectrum, mixture of two lithium phases (LiOH and  $\text{Li}_2\text{CO}_3$ ) appears more clearly. Under these conditions,  $\text{CO}_2$  transformation with LiOH solution was carried out more efficiently. As seen on spectrum, highest intensity of LiOH peaks have signifi-

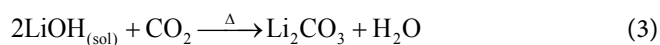
cantly decreased, while those of  $\text{Li}_2\text{CO}_3$  have increased. Spectrum D corresponds to that obtained when Li solution was evaporated at  $40^\circ\text{C}$ , at this temperature LiOH solution has practically reacted with atmospheric  $\text{CO}_2$ , however signals are observed that correspond to two LiOH greater intensity peaks whose values appear at 2 theta angles of  $30.064^\circ$  and  $33.730^\circ$ , indicating that lithium hydroxide solution has not fully reacted. At this temperature, practically all  $\text{Li}_2\text{CO}_3$  peaks are observed. Finally, spectrum E corresponds to lithium carbonate sample. On this occasion lithium hydroxide solution reacted completely, where evaporation was carried out at  $50^\circ\text{C}$ . At this temperature,  $\text{CO}_2$  transformation with lithium hydroxide solution was complete as indicated by this spectrum, where all peaks correspond to lithium carbonate verified with PDF card 09-0359. From this temperature, it was possible to obtain lithium carbonate under environmental conditions that prevail in laboratory from lithium hydroxide solution.

According to these results, a relative approximation of reaction was made to know the percentage of lithium carbonate formation as function of temperature, for which the area under the peak was considered whose value is 23.329 degrees in 2 theta. To determine the area, ten values of each side of this intensity were taken. This peak is located in a region where no other has an influence, that is, the peak is isolated and corresponds to lithium carbonate. Another parameter considered was the counting time, which was the same for each sample. Therefore, as the carbonate forms with increasing temperature, there is no interference with hydroxide peaks. Lithium solution reacts very little with  $\text{CO}_2$  at a temperature of  $25^\circ\text{C}$ , therefore percentage formation was 5%. By increasing evaporation temperature to  $27^\circ\text{C}$ , the reaction was favored with additional energy despite small temperature difference between these two values, increase in carbonate formation was 11.32% on this occasion. Subsequently, when evaporating solution at  $30^\circ\text{C}$ , transformation percentage reached 13.5%, as can be seen in spectrum C (**Figure 6**) where two phases (LiOH and  $\text{Li}_2\text{CO}_3$ ) appear mixed. At  $40^\circ\text{C}$  the  $\text{Li}_2\text{CO}_3$  presence is clearly noticeable, however a small LiOH fraction is still present as noted in peaks whose values are at  $30.064^\circ$  and  $33.730^\circ$  in 2 theta, carbonate formation percentage was 32.61. And finally at  $50^\circ\text{C}$  the reaction was carried out completely as observed in spectrum **Figure 6(e)** where only one phase was identified which corresponds to  $\text{Li}_2\text{CO}_3$ . Under these temperature conditions, reaction percentage was 33.4%. With these values, a good approximation in lithium carbonate formation was obtained as a function of temperature and according to  $\text{CO}_2$  concentration that prevails in laboratory environment. In kinetics of carbonate formation, a high temperature is not required, according to experimentation carried out in this work, reaction is slow when evaporating it at  $25^\circ\text{C}$  and when applying more thermal energy, lithium hydroxide solution and atmospheric  $\text{CO}_2$  react faster. **Figure 6** represents individual  $\text{Li}_2\text{CO}_3$  diffraction spectrum. The analyzed sample corresponds to LiOH solution evaporation in presence of atmospheric  $\text{CO}_2$  at  $50^\circ\text{C}$ . It can be seen that spectrum corresponds to a single phase, each of intensities are part of lithium carbonate according to PDF card 09-0359.



**Figure 6.** Diffraction spectrum of lithium carbonate obtained from atmospheric CO<sub>2</sub> with metallic lithium.

In this way, the reaction is carried out at a moderate temperature to prepare lithium carbonate. The reaction carried out between CO<sub>2</sub> and LiOH solution Li carbonate formation is described in Equation (3):



where  $\Delta$  corresponds to different programmed temperatures to evaporate Li solution whose values were from 25 °C to 50 °C.

In the same way, reactions with metallic lithium particles that were exposed to the environment laboratory are presented to know what type of reactions are carried out for long periods in CO<sub>2</sub> transformation. Lithium carbonate was also formed in this other process.

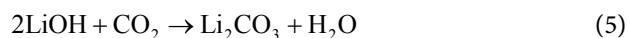
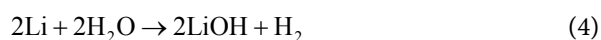
**Figure 6** shows the diffraction spectrum of lithium carbonate, which was obtained from metallic Li exposed to laboratory environmental conditions. The identification of this sample was made with PDF card 09-0359, indicating that it is also Lithium carbonate phase where characteristic peaks of this compound are shown in the spectrum. According this card it has a monoclinic crystalline structure with space group number 237, whose crystal lattice parameters are:  $a = 8.39000 \text{ \AA}$ ,  $b = 5.00000 \text{ \AA}$ ,  $c = 6.21000 \text{ \AA}$ ,  $\beta = 114.500^\circ$ . The main peaks are at beginning of spectrum whose values at 2 theta angles are: 21.239, 23.329, 29.356, 30.485, 31.589, 33.929, 35.892, 36.806 with its diffraction planes (110), (200), (111), (−202), (002), (−112), (020), (−311) respectively. No other phase was identified, which indicates that only one product was obtained, therefore, under these conditions, metallic lithium reacted during the time it was exposed with atmospheric CO<sub>2</sub>. This spectrum was similar to that obtained from evaporation of LiOH solution at 50 °C, no other phase was identified indicating only the presence of a product. Therefore in these conditions metallic lithium reacted

during exposed time with atmospheric CO<sub>2</sub>. The difference lies in how atmospheric CO<sub>2</sub> is transformed, but both compounds form the same carbonate. The peaks of this spectrum were recorded with higher resolution, indicating a crystalline material. The kinetics was very slow, because ambient temperature was also low (20 °C) on average, which remained constant during exposure of metal in ambient conditions (3 months).

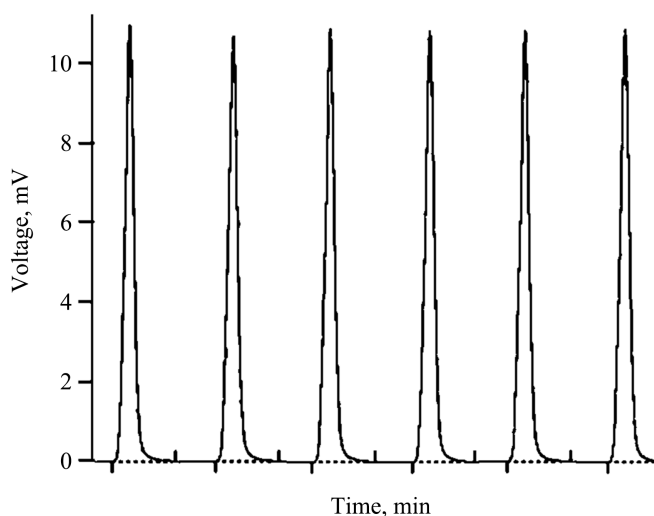
### 3.4. Hydrogen Generation

**Figure 7** shows the peaks obtained by gas chromatography, which correspond to the hydrogen generated after two months where each peak represents an analysis carried out from the same vial. The retention time for hydrogen was 1.5 min. In order to corroborate the presence of hydrogen, a standard was injected prior to the analysis of the samples. In each analysis, only the presence of this gas was observed, that is, no gaseous impurity was detected. The three considered vials presented the same chromatograms, the difference between them was the height of the peaks for each determination, the ones with the least intensity corresponded to the analyzes carried out after 30 days and the most intense ones at 90 days, indicating the generation of hydrogen in function of time from metallic Li exposed to the environment.

The reactions carried out between metallic particles lithium, humidity and CO<sub>2</sub> to form Li carbonate are described in Equations (4) and (5):



The equations indicate the reactions that take place during lithium carbonate formation. The humidity inside laboratory registered an average value of 65% during the time that metallic lithium was exposed to environment, therefore humidity reacted first with surface of particles, forming lithium hydroxide and



**Figure 7.** Chromatograms of hydrogen generated with metallic lithium exposed to the environment.

H<sub>2</sub> was generated as a byproduct according to Equation (4). On the other hand, two lithium hydroxide molecules react with one CO<sub>2</sub> molecule to form a hydrated lithium carbonate molecule, Equation (5). According to environmental conditions the temperature recorded on average 20°C, and time also prolonged therefore with these conditions the reaction kinetics was slow. According to these reactions, the mechanism to transform CO<sub>2</sub> from the environment using lithium metal was considered. With the hydrogen inside the glass vial, the transformation of CO<sub>2</sub> was verified during the programmed time.

It is interesting to know how atmospheric CO<sub>2</sub> reacts with lithium compounds. On the one hand, the strongly basic lithium hydroxide solution transforms CO<sub>2</sub> depending on the temperature and on the other hand, it was shown that metallic lithium forms LiOH with humidity and subsequently also reacts with atmospheric CO<sub>2</sub> at room temperature. In this sense, the kinetics in both procedures was a function of temperature, which was very efficient because in first instance hydrogen was produced through reaction of metallic lithium with deionized water when preparing hydroxide solution. This procedure can be an alternative to obtain lithium compounds easily and efficiently, which are considered for use in various areas.

#### 4. Conclusion

Solutions of lithium hydroxide with metallic Li particles and deionized water were prepared. The lithium solution reacted with CO<sub>2</sub> at various temperature values under laboratory conditions. These conditions were determined to synthesize lithium carbonate, where lithium solution completely reacted with atmospheric CO<sub>2</sub> by applying 50°C for evaporation. In the same way, lithium hydroxide solution was evaporated without presence of CO<sub>2</sub> to obtain solid LiOH. Another way to obtain Li<sub>2</sub>CO<sub>3</sub> was through reaction carried out between metallic lithium particles that were exposed to environment for a long time. Under these conditions, Li reacted with humidity and atmospheric CO<sub>2</sub> to form Li<sub>2</sub>CO<sub>3</sub>. By this method, clean hydrogen was generated, which is essential in the clean energy economy, providing a valuable resource to mitigate the climate change crisis that currently exists globally, this hydrogen can be used directly in fuel cells. In this same sense, lithium hydroxide and lithium carbonate are considered as precursors to manufacture lithium batteries, energy that is also classified as clean to reduce greenhouse gas emissions produced by the use of fossil fuels in all transportation, This procedure can be an alternative to obtaining lithium compounds easily and efficiently, that can also be used in other applications.

#### Acknowledgements

Thanks to the XRD and SEM staff of ININ, for their valuable support in the analysis of the samples characterized in this work.

#### Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

## References

- [1] Kim, S., Choi, M., Kang, J.S., Joo, H., Park, B.H., Sung, Y.E. and Yoon, J. (2021) Electrochemical Recovery of LiOH from Used CO<sub>2</sub> Adsorbents. *Catalysis Today*, **359**, 83-89. <https://doi.org/10.1016/j.cattod.2019.06.056>
- [2] Zilberman, P. (2015) The CO<sub>2</sub> Absorber Based on LiOH. *Acta Medica Marisensis*, **61**, 4-6. <https://doi.org/10.1515/amma-2015-0023>
- [3] Kaneco, S., Katsumata, H., Suzuki, T. and Ohta, K. (2006) Photoelectrocatalytic Reduction of CO<sub>2</sub> in LiOH/Methanol at Metal-Modified p-InP Electrodes. *Applied Catalysis B: Environmental*, **64**, 139-145. <https://doi.org/10.1016/j.apcatb.2005.11.012>
- [4] Yang, X., Li, S., Zhao, J., Huang, H. and Deng, L. (2022) Development of Covalent-Organic Frameworks Derived Hierarchical Porous Hollow Carbon Spheres Based LiOH Composites for Thermochemical Heat Storage. *Energy Chemistry*, **73**, 301-310. <https://doi.org/10.1016/j.jechem.2022.06.022>
- [5] Cho, Y., Lee, J.Y., Bokare, A.D., Kwon, S.B., Park, D.S., Jung, W.S. and Choi, W. (2015) LiOH-Embedded Zeolite for Carbon Dioxide Capture under Ambient Conditions. *Journal of Industrial and Engineering Chemistry*, **22**, 350-356. <https://doi.org/10.1016/j.jiec.2014.07.030>
- [6] Izquierdo, M.T., Gasquet, V., Sansom, E., Ojeda, M., Garcia, S. and Maroto-Valer, M.M. (2018) Lithium-Based Sorbents for High Temperature CO<sub>2</sub> Capture: Effect of Precursor Materials and Synthesis Method. *Fuel*, **230**, 45-51. <https://doi.org/10.1016/j.fuel.2018.05.041>
- [7] Chang, Y., Huang, H., Wang, L., Li, Y. and Zhong, C. (2020) Synergistic Dual-Li+ Sites for CO<sub>2</sub> Separation in Metal-Organic Framework Composites. *Chemical Engineering Journal*, **402**, Article ID: 126201. <https://doi.org/10.1016/j.cej.2020.126201>
- [8] Grasso, M.L., Arneodo, L.P. and Gennari, F.C. (2020) CO<sub>2</sub> Capture Properties of Li<sub>4</sub>SiO<sub>4</sub> after Aging in Air at Room Temperature. *Journal of CO<sub>2</sub> Utilization*, **38**, 232-240. <https://doi.org/10.1016/j.jcou.2020.02.002>
- [9] Yang, Y., Yao, S., Hu, Y., Sun, J., Cao, J., Li, Q. and Liu W. (2020) Mechanochemically Activated Li<sub>4</sub>SiO<sub>4</sub>-Based Adsorbent with Enhanced CO<sub>2</sub> Capture Performance and Its Modification Mechanisms. *Fuel*, **273**, Article ID: 117749. <https://doi.org/10.1016/j.fuel.2020.117749>
- [10] Zhao, Y., Xiang, X., Wang, M., Wang, H., Li, Y., Li, J. and Yang, H. (2021) Preparation of LiOH through BMED Process from Lithium-Containing Solutions: Effects of Coexisting Ions and Competition between Na<sup>+</sup> and Li<sup>+</sup>. *Desalination*, **512**, Article ID: 115126. <https://doi.org/10.1016/j.desal.2021.115126>
- [11] Joo, S., Shim, H.W., Choi, J.J., Lee, C.G. and Kim, D.G. (2020) A Method of Synthesizing Lithium Hydroxide Nanoparticles Using Lithium Sulfate from Spent Batteries by 2-Step Precipitation Method. *Korean Journal of Metals and Materials*, **58**, 286-291. <https://doi.org/10.3365/KJMM.2020.58.4.286>
- [12] Lin, J., Li, Q., Chen, X., Li, C., Lu, S. and Liew, K.M. (2019) Sorption-Enhanced CO Capture over Cu-Mn-Ce Composite Oxides with LiOH Addition: CO Oxidation and *in-Situ* CO<sub>2</sub> Sorption. *Chemical Engineering Journal*, **371**, 267-275. <https://doi.org/10.1016/j.cej.2019.04.049>
- [13] Zhao, Y., Wang, H., Li, Y., Wang, M. and Xiang, X. (2020) An Integrated Membrane Process for Preparation of Lithium Hydroxide from High Mg/Li Ratio Salt Lake Brine. *Desalination*, **493**, Article ID: 114620. <https://doi.org/10.1016/j.desal.2020.114620>



- [14] Gallant, B.M. (2022) Unlocking Reversibility of LiOH-Based Li-Air Batteries. *Joule*, **4**, 2254-2256. <https://doi.org/10.1016/j.joule.2020.10.018>
- [15] Liu, H. and Azimi, G. (2022) Production of Battery Grade Lithium Hydroxide Monohydrate Using Barium Hydroxide Causticizing Agent. *Resources, Conservation and Recycling*, **179**, Article ID: 106115. <https://doi.org/10.1016/j.resconrec.2021.106115>
- [16] Stefanelli, E., Puccini, M., Vitolo, S. and Seggiani, M. (2020) CO<sub>2</sub> Sorption Kinetic Study and Modeling on Doped-Li<sub>4</sub>SiO<sub>4</sub> under Different Temperatures and CO<sub>2</sub> Partial Pressures. *Chemical Engineering Journal*, **379**, Article ID: 122307. <https://doi.org/10.1016/j.cej.2019.122307>
- [17] Miao, Y., Pudukudy, M., Zhi, Y., Miao, Y., Shan, S., Jia, Q. and Ni, Y. (2020) A Facile Method for *in Situ* Fabrication of Silica/Cellulose Aerogels and Their Application in CO<sub>2</sub> Capture. *Carbohydrate Polymers*, **236**, Article ID: 116079. <https://doi.org/10.1016/j.carbpol.2020.116079>
- [18] Wang, J., Park, Y.K. and Jo, Y.M. (2020) Sequential Improvement of Activated Carbon Fiber Properties for Enhanced Removal Efficiency of Indoor CO<sub>2</sub>. *Journal of Industrial and Engineering Chemistry*, **89**, 400-408. <https://doi.org/10.1016/j.jiec.2020.06.011>
- [19] Chen, X., Zhao, Z., Hao, M. and Wang, D. (2013) Research of Hydrogen Generation by the Reaction of Al-Based Materials with Water. *Journal of Power Sources*, **222**, 188-195. <https://doi.org/10.1016/j.jpowsour.2012.08.078>
- [20] Khzouz, M., Gkanas, E.I., Girella, A., Statheros, T. and Milanese, C. (2020) Sustainable Hydrogen Production via LiH Hydrolysis for Unmanned Air Vehicle (UAV) Applications. *International Journal of Hydrogen Energy*, **45**, 5384-5394. <https://doi.org/10.1016/j.ijhydene.2019.05.189>
- [21] Li, J.R., Ma, Y., McCarthy, M.C., Sculley, J., Yu, J., Jeong, H.K., Balbuena, P.B. and Zhou, H. (2011) Carbon Dioxide Capture-Related Gas Adsorption and Separation in Metal-Organic Frameworks. *Coordination Chemistry Reviews*, **255**, 1791-1823. <https://doi.org/10.1016/j.ccr.2011.02.012>
- [22] Liu, Y., Wang, Z.U. and Zhou, H.C. (2012) Recent Advances in Carbon Dioxide Capture with Metal-Organic Frameworks. *Greenhouse Gases: Science and Technology*, **2**, 239-259. <https://doi.org/10.1002/ghg.1296>
- [23] Park, Y., Moon, D.K., Kim, Y.N., Ahn, H. and Lee, C.H. (2014) Adsorption Isotherms of CO<sub>2</sub>, CO, N<sub>2</sub>, CH<sub>4</sub>, Ar and H<sub>2</sub> on Activated Carbon and Zeolite LiX up to 1.0 MPa. *Adsorption*, **20**, 631-647. <https://doi.org/10.1007/s10450-014-9608-x>
- [24] Rashidi, N.A. and Yusup, S. (2016) An Overview of Activated Carbons Utilization for the Post-Combustion Carbon Dioxide Capture. *Journal of CO<sub>2</sub> Utilization*, **13**, 1-16. <https://doi.org/10.1016/j.jcou.2015.11.002>
- [25] Iturbe-García, J.L., Bonifacio, J., Granados, F. and López-Muñoz, B.E. (2019) Behavior of a Hydrotalcite Type Material Obtained from MgAl Alloy for CO<sub>2</sub> Adsorption. *Applied Clay Science*, **183**, Article ID: 105296. <https://doi.org/10.1016/j.clay.2019.105296>