Characterization and Thermal Dehydration Kinetics of Highly Crystalline Mcallisterite, Synthesized at Low Temperatures

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The hydrothermal synthesis of a mcallisterite (Mg$_2$(B$_6$O$_7$(OH)$_6$)$_2$·9(H$_2$O)) mineral at low temperatures was characterized. For this purpose, several reaction temperatures (0–70°C) and reaction times (30–240 min) were studied. Synthesized minerals were subjected to X-ray diffraction (XRD), fourier transform infrared (FT-IR), and Raman spectroscopies and scanning electron microscopy (SEM). Additionally, experimental analyses of boron trioxide (B$_2$O$_3$) content and reaction yields were performed. Furthermore, thermal gravimetry and differential thermal analysis (TG/DTA) were used for the determination of thermal dehydration kinetics. According to the XRD results, mcallisterite, which has a powder diffraction file (pdf) number of "01-070-1902," was formed under certain reaction parameters. Pure crystalline mcallisterite had diagnostic FT-IR and Raman vibration peaks and according to the SEM analysis, for the minerals which were synthesized at 60°C and 30 min of reaction time, particle size was between 398.30 and 700.06 nm. Its B$_2$O$_3$ content and reaction yield were 50.80 ± 1.12% and 85.80 ± 0.61%, respectively. Finally, average activation energies (conversion values (α) that were selected between 0.1 and 0.6) were calculated as 100.40 kJ/mol and 98.31 kJ/mol according to Ozawa and Kissinger-Akahira-Sunose (KAS) methods, respectively.

1. Introduction

Boron most often occurs in nature as borates which can be classified by the kind of metal it is complexed with. Magnesium borate minerals, which are a subclass of boron minerals, are inorganic compounds containing magnesium and boron. They are excellent additives for industry due to their high elasticity coefficient, heat resistance, and corrosion resistance [1]. Magnesium borates have specific applications in modified glass compositions, reinforcements in electronic ceramics, wide band gap semiconductors, aluminum/magnesium matrix alloys, antiwear additives such as thermoluminescence dosimeters, catalysts for the conversion of hydrocarbons, cathode ray tube screens, and X-ray screens [2–5].

Many kinds of magnesium borates having xMgO·yB$_2$O$_3$·zH$_2$O compositions can be found naturally in mixture with other metal borates or can be obtained in the laboratory by synthetic methods. Some examples of this type of borate hydrate minerals that have been synthesized are 2MgO·3B$_2$O$_3$·17H$_2$O, MgO·3B$_2$O$_3$·3.5H$_2$O, 2MgO·B$_2$O$_3$·H$_2$O, 2MgO·6B$_2$O$_3$·15H$_2$O, and MgO·3B$_2$O$_3$·7H$_2$O [6–13]. Mcallisterite is a type of magnesium borate with the chemical formula Mg$_2$(B$_6$O$_7$(OH)$_6$)$_2$·9H$_2$O. It has the appearance of very fine aggregates and white-colorless crystals, hardness of 2.5 Mohs, and low water solubility. Mcallisterite reserves are found in Argentina, China, Kazakhstan, and USA; however, in these reserves, magnesium and calcium borates are found in a mixture and purification is needed [14]. General hydrothermal synthesis procedures for magnesium borates involve the reactions of suitable raw materials at high temperatures such as >100°C or by double salt phase transformation. The type of experimental procedure used has effects on the product’s crystal properties and size.

In literature, there are some examples of materials’ surface modification by changing the reaction temperatures and reaction times. According to these studies, nanoscale materials can be synthesized as different crystal types [6–13, 15].

Hydrothermal processes have several advantages over the other types of conventional synthesis processes such as...
solid-state method in regard to energy conservation, better nucleation control, and lower temperature and pressure of operation [16, 17]. Higher reaction temperatures and longer reaction times cause increases in process cost.

Dehydrations of crystalline solids represent an important group of heterogeneous reactions. Characteristic dehydration features of materials should be known in order to determine design parameters of equipment and to decrease mass of required materials, thus reducing the transportation costs. The decomposition process of the hydrated boron mineral, which usually involves dehydration and dehydroxylation, can be explained by the removal of crystal water from structure [5–19]. Dehydration behaviors of different types of metal borate minerals have been determined by thermogravimetric analyses such as TG/DTA [1].

The effects of different nonisothermal kinetic methods on the thermal dehydration of indiderite were examined by Zhu et al. [7]. Changes in ulexite structure resulting from heating and the reaction kinetic parameters were studied by Ener et al. [20] and Tunç et al. [21]; their results showed that ulexite could be turned to amorphous phase of NaB(OH)$_2$.8H$_2$O at 855°C. Waclawska [22] studied the effect of mechanical treatment on phase transitions of calcium borate and colemanite and internal structure reconstitution processes of ground colemanite. There have also been some studies regarding dehydration kinetics of synthesized boron compounds. Kanturk et al. [23] studied dehydration kinetic parameters such as activation energy and preexponential factors of synthesized sodium metaborate tetrahydrate (NaB(OH)$_2$.2H$_2$O). Kinetic analyses of boric acid thermal decomposition were studied by thermogravimetric analysis and different kinds of nonisothermal kinetic methods were used for the calculation of parameters [24]. Guo et al. [25] have investigated the decomposition and oxidation behavior of MgB$_2$ using TG, XRD, and SEM-EDS.

In literature, despite the extensively reported synthesis of magnesium borates, only indiderite minerals’ kinetic behavior has been studied. To date, there have been no studies regarding the kinetic behavior of mcallisterite.

In this study, the low temperature (0–70°C) synthesis of a specific kind of magnesium borate mineral, namely, mcallisterite, is aimed. Therefore, in literature, Derun et al. [1] studied the magnesium borates between 80 and 100°C and synthesized a specific kind of magnesium borate mineral, namely, admontite. The other aim of this study is to determine the kinetic parameters (activation energy and coefficient factor) of mcallisterite mineral which was not studied before, with both Ozawa [26] and KAS [27, 28] nonisothermal kinetic methods.

2. Materials and Methods

2.1. Synthesis of Mcallisterite. The raw materials used in synthesis were boric acid (H$_3$BO$_3$), which was provided from Kırka Boron Management Plant (ETi Mine Kırka Works) in Eskisehir, Turkey, and magnesium oxide (MgO), which was provided from Merck Chemicals. H$_3$BO$_3$ was crushed, ground, and sieved and MgO was used as supplied.

The synthesis procedure of magnesium borates is given in Figure 1. Experiments were carried out at the reaction temperatures between 0 and 70°C and reaction time between 30 and 240 minutes. Each product was coded by initial letters of the raw materials (M: MgO and H: H$_3$BO$_3$), reaction temperature, and reaction time. For instance, “MH-60-30” indicated the product synthesized at a reaction temperature of 60°C and at a reaction time of 30 min.

2.2. Instrumental Analyses. Philips PANalytical XRD was used for identification of reaction products. X-rays were produced from a Cu-Kα tube at 45 kV and 40 mA. The parameters used in the analyses were 0.030° step, 0.50 s time for step, 0.060° C/s scan speed, and 0–60° range. ICSD patterns were scanned using the inorganic library built into the instrument’s program. Synthesized minerals were then subjected to FT-IR analyses using a Perkin Elmer FT-IR with universal attenuation total reflectance (ATR) sampling.
accessory with a diamond/ZnSe crystal. The measurement range was 1800–650 cm\(^{-1}\), scan number was 4, and resolution was 4 cm\(^{-1}\). For further analysis, Perkin Elmer Brand Raman Station 400 F was used for Raman spectroscopy. In these analyses, the exposure time was 4 seconds and the number of exposures was 4. Measurement range was 1800–250 cm\(^{-1}\) and the data interval was 2 cm\(^{-1}\). During the experiments, 100% laser power was used. Surface morphologies of synthesized minerals were obtained using a CamScan Apollo 300 field-emission SEM (20 kV and magnification 20000).

2.3. \(B_2O_3\) Analyses and Reaction Yields. Both \(B_2O_3\) analyses and calculations of reaction yields were performed according to Derun et al. [1].

2.4. Thermal Dehydration Kinetics. Thermal dehydration behavior of highly crystalline pure mcallisterite was studied between the temperature ranges of 20 and 720\(^\circ\)C with a Perkin Elmer Diamond TG/DTA. Purely obtained mcallisterite mineral was subjected to five different heating rates (2\(^\circ\)/min, 5\(^\circ\)/min, 10\(^\circ\)/min, 15\(^\circ\)/min, and 20\(^\circ\)/min) in an inert (nitrogen) atmosphere. Kinetic parameters such as activation energy \((E_a)\) and coefficient constants \((k_0)\) were calculated by Ozawa and KAS nonisothermal kinetic methods.

In the Ozawa kinetic method (1), values of \(1/T\) are plotted against \(\log \beta\) for each conversion value \((\alpha)\), where \(T\) is the thermodynamic temperature and \(\beta\) is heating rate. Activation energy \((E_a)\) is calculated from the slope of parallel lines. \(R\) is the gas constant. Consider

\[
\log \beta = \log \left( \frac{k_0 E_a}{R} \right) - 2.315 - 0.4567 \left( \frac{E_a}{RT} \right) - \log (g(\alpha)).
\]

In the KAS kinetic method (2), the kinetic parameters are determined from the plot of \(1/T\) against the left side of equation for each \(\alpha\) value:

\[
\ln \left( \frac{\beta}{T^2} \right) = \ln \left( \frac{k_0 E_a}{R \cdot g(\alpha)} \right) - \frac{E_a}{RT}.
\]

2.5. Thermal Conversion of Mcallisterite. In order to investigate and characterize the product obtained after the thermal dehydration kinetics study, mcallisterite mineral was placed in a Protherm MOS 180/4 high temperature furnace with 10\(^\circ\)/min temperature increment to a maximum temperature of 720\(^\circ\)C in nitrogen flowing (5 mL/min) atmosphere. After the thermal conversion, the product was analyzed by XRD with the same parameters given in Section 2.2.

3. Results and Discussion

3.1. XRD Results. The magnesium and boron sources used in the experiments were found to be periclase [MgO] and sassolette [H\(_3\)BO\(_3\)] with powder diffraction file (pdf) numbers of 01-087-0651 and 01-073-2158, respectively.
Table 1: XRD results of the synthesized magnesium borate minerals.

| Reaction temperature (°C) | Reaction time (min) | XRD scores of 01-070-1902 | XRD scores of 01-076-0540 | XRD scores of 01-073-0638 |
|---------------------------|---------------------|----------------------------|---------------------------|---------------------------|
|                           | 30                  | 78                         | 30                        | —                         |
|                           | 60                  | 80                         | —                         | —                         |
|                           | 120                 | 84                         | 25                        | —                         |
|                           | 240                 | 76                         | 45                        | —                         |
| 10                        | 30                  | 72                         | —                         | —                         |
|                           | 60                  | 8                          | 6                         | —                         |
|                           | 120                 | 69                         | 61                        | —                         |
|                           | 240                 | 76                         | 45                        | —                         |
| 20                        | 30                  | 85                         | 31                        | —                         |
|                           | 60                  | 77                         | 51                        | —                         |
|                           | 120                 | —                          | 71                        | —                         |
|                           | 240                 | —                          | 73                        | —                         |
| 30                        | 30                  | 77                         | 70                        | —                         |
|                           | 60                  | 84                         | 71                        | —                         |
|                           | 120                 | 50                         | 79                        | —                         |
|                           | 240                 | —                          | 81                        | —                         |
| 40                        | 30                  | 52                         | 81                        | —                         |
|                           | 60                  | 29                         | 80                        | —                         |
|                           | 120                 | 39                         | 80                        | —                         |
|                           | 240                 | —                          | 81                        | —                         |
| 50                        | 30                  | 66                         | 78                        | —                         |
|                           | 60                  | 86                         | 59                        | —                         |
|                           | 120                 | 88                         | 52                        | —                         |
|                           | 240                 | 45                         | 79                        | —                         |
| 60                        | 30                  | 84                         | —                         | —                         |
|                           | 60                  | 89                         | 16                        | —                         |
|                           | 120                 | 85                         | 63                        | —                         |
|                           | 240                 | 82                         | 82                        | —                         |
| 70                        | 30                  | 87                         | 18                        | —                         |
|                           | 60                  | 85                         | —                         | —                         |
|                           | 120                 | 85                         | 56                        | —                         |
|                           | 240                 | 57                         | 84                        | 23                        |

pdf number = 01-070-1902, mcallisterite, $\text{Mg}_2(\text{B}_6\text{O}_7(\text{OH})_6)_2 \cdot 9(\text{H}_2\text{O})$.
pdf number = 01-076-0540, admontite, $\text{MgO}(\text{B}_2\text{O}_3)_3 \cdot 7(\text{H}_2\text{O})$.
pdf number = 01-073-0638, $\text{MgB}_6\text{O}_7(\text{OH})_6 \cdot 3(\text{H}_2\text{O})$.

XRD patterns of synthesized pure mcallisterite minerals are given in Figure 3. As seen in Figure 3, all the characteristic peaks of mcallisterite were seen and higher count values were observed for MH-60-30 and MH-70-60 which is consistent with their higher crystal scores.

3.2. FT-IR and Raman Spectrum Results. FT-IR spectrum of product is given in Figure 4. The first peak at about 1650–1660 cm⁻¹ is the bending of H–O–H [δ(H–O–H)]. The peaks at 1412–1337 cm⁻¹ can be explained by asymmetric stretching of 3-coordinate boron [$v_a(\text{B}_3(3)-\text{O})$]. The peak around 1238 cm⁻¹ represents the bending of B–O–H [δ(B–O–H)]. Asymmetric and symmetric stretching of 4-coordinate boron [$v_a(\text{B}_4(4)-\text{O})$], [$v_s(\text{B}_4(4)-\text{O})$] were seen between the peaks of 1080–961 cm⁻¹ and 857–812 cm⁻¹, respectively. The last peak of 671 cm⁻¹ was the bending of 3-coordinate boron [δ(B(3)-O)].

Raman spectrum of the pure mcallisterite minerals is given in Figure 5. From the Raman results, symmetric stretching of 3-coordinate boron [$v_s(\text{B}_3(3)-\text{O})$] was seen at the peaks between 951 and 879 cm⁻¹, δ(B(3)-O) was seen at the peaks between 680 and 678 cm⁻¹. The characteristic peaks of magnesium borates, which are $v_p[\text{B}_6\text{O}_7(\text{OH})_6]^2-$ and $v_p[\text{B}_3\text{O}_4(\text{OH})_4]^-$, were seen at the peak values around 640 cm⁻¹. At the peak of 528 cm⁻¹, δ(B(3)-O) and bending of 4-coordinate boron [δ(B(4)-O)] were seen. The last peaks which are lower than the 490 cm⁻¹ can be explained by the δ(B(4)-O).
Figure 3: XRD patterns of synthesized pure mcallisterite minerals.

The FT-IR and Raman results are both consistent with the literature [29, 30].

3.3. SEM Results. SEM surface morphologies of the synthesized pure mcallisterite minerals are given in Figure 6. At 10°C and 0°C, crystals were seen as rectangular shapes due to overlapping of layers and single crystals. Particle sizes of the crystals at 10°C and 0°C were between 348 nm–1.32 μm and 285–544 nm, respectively. Cylindrical crystal formations occurred at 60°C and 70°C, where particle sizes were 344–719 nm and 398–700 nm, respectively.

3.4. B₂O₃ Results and Reaction Yields. B₂O₃ contents of the synthesized minerals are given in Table 2. Highest and lowest B₂O₃ were seen in MH-50-30 (51.62 ± 1.07%) and MH-0-30 (44.59 ± 1.34%). Pure mcallisterite minerals B₂O₃ contents were 53.25 ± 1.20% in MH-70-60, 54.17 ± 0.87% in MH-60-30, 49.91 ± 1.28% in MH-10-30, and 45.92 ± 0.54% in MH-0-60. These results were in mutual agreement with theoretical B₂O₃ content of mcallisterite mineral (54.35%).

Average reaction yield of the MH-60-30 was 85.80 ± 0.61% as calculated from the four repeated syntheses.

3.5. Kinetic Analysis Results. TG and DTG analyses of MH-60-30 are shown in Figures 7 and 8, respectively. The analyses showed that mcallisterite lost its crystal water via a two-step process at the heating rate of 2°C/min and by a single-step process at heating rates of greater than 2°C/min (>2°C/min, 5°C/min, 10°C/min, and 20°C/min).

The first step at the heating rate of 2°C/min was a rapid dehydration, where the initial, peak, and final temperatures were 90.81°C, 150.64°C, and 155.94°C, respectively. Weight decreases were 16.416% and 19.359% for the first and second steps, respectively. Total weight loss was 35.775%.

The initial, peak, and final temperatures and weight losses at other heating rates are given in Table 3. The average weight loss, calculated using all of the heating rates, was 35.379%, which is close to structural water content (35.16%) of mcallisterite mineral.
Figure 6: SEM surface morphologies of synthesized pure mcallisterite minerals at 20000x magnification.

Figure 7: TG curve of synthesized pure mcallisterite.

Figure 8: DTG curve of synthesized pure mcallisterite.

Ozawa and KAS nonisothermal kinetic methods were applied for conversion values (α) between 0.1 and 0.9. In the Ozawa kinetic method, \( \log(\beta) \) values were plotted against \( 1/T \) values for each \( \alpha \) value (Figure 9). For each heating rate kinetic parameter of \( E_a \) was calculated from the slope of the curves.

Likewise, in the KAS kinetic method, \( \ln(\beta/T^2) \) was plotted against \( 1/T \) for each \( \alpha \) value (Figure 10). Kinetic parameters of \( E_a \) and \( k_0 \) for each heating rate were calculated from the intercept and slopes of the curves, respectively. \( E_a \), \( k_0 \), and the correlation coefficient \( (R^2) \) values obtained for each curve are shown in Table 4.

The activation energy values were calculated as 47.81–101.18 kJ/mol and 53.91–103.95 kJ/mol according to Ozawa and KAS methods, respectively. \( k_0 \) values were between 0.0002 and 2913.89 according to KAS.
Average activation energies of mcallisterite mineral calculated for the conversion values between 0.1 and 0.6 were 100.40 kJ/mol and 98.31 kJ/mol according to Ozawa and KAS, respectively.

### 3.6. Thermal Conversion Results of Mcallisterite

Thermal conversion results showed that mcallisterite mineral lost 35.74 ± 0.32% of its weight. This was in agreement with the TG analyses and mcallisterite’s theoretical structural water content of 35.16%, which is equal to 15 molar equivalent of water.

Also, XRD analysis showed that the mcallisterite mineral had lost all of its structure water and changed to dehydrated magnesium minerals Mg(B$_2$O$_3$)$_2$ (pdf 01-076-0666) and B$_2$O$_3$ (pdf 01-072-0626). The obtained Mg(B$_2$O$_3$)$_2$ and B$_2$O$_3$ crystal scores were 71 and 24, respectively. At this step, in order to obtain pure Mg(B$_2$O$_3$)$_2$, the mixture was washed with pure ethanol and then filtered and dried at 40°C. Dried mineral was again subjected to XRD analyses and found as the same dehydrated magnesium mineral Mg(B$_2$O$_3$)$_2$ with a crystal score of 83. The increase in the crystal score means that the excess B$_2$O$_3$ content was removed and pure Mg(B$_2$O$_3$)$_2$ was obtained. Also, according to the weight changes, before and after the washing step, Mg(B$_2$O$_3$)$_2$ and B$_2$O$_3$ were found to be equimolar.

The crystallographic data obtained from XRD are shown in Table 5 for mcallisterite and Mg(B$_2$O$_3$)$_2$. The Mg(B$_2$O$_3$)$_2$
Table 3: Dehydration temperatures and weight losses of pure mcallisterite (MH-60-30).

| Heating rate (°C/min) | 2   | 5   | 10  | 15  | 20  |
|----------------------|-----|-----|-----|-----|-----|
| Step                 | 1st | 2nd | 1st | 1st | 1st | 1st |
| \( T_i \) (°C)       | 90.81 | 155.94 | 100.00 | 106.51 | 111.88 | 119.74 |
| \( T_p \) (°C)       | 150.64 | 165.79 | 172.14 | 182.94 | 184.86 | 186.22 |
| \( T_f \) (°C)       | 155.94 | 300.00 | 347.79 | 394.36 | 396.80 | 497.95 |
| \( \Delta m \) (%)   | 16.416 | 19.359 | 35.109 | 35.537 | 35.517 | 34.958 |
| \( \Sigma \Delta m \) (%) | 35.775 | 35.109 | 35.537 | 35.517 | 34.958 |

Average \( \Delta m \) (%) = 35.379

\( i \): initial; \( p \): peak; \( f \): final; \( m \): weight.

Table 4: Calculated kinetic parameters for KAS and Ozawa method.

| \( \alpha \) | Ozawa | Method | KAS |
|------------|-------|--------|-----|
|            | \( E_a \) (kJ/mol) | \( R^2 \) | \( k_0 \) | \( E_a \) (kJ/mol) | \( R^2 \) |
|            | \( E_a \) (kJ/mol) | \( k_0 \) | \( R^2 \) | \( E_a \) (kJ/mol) | \( k_0 \) | \( R^2 \) |
| 0.1        | 97.49 | 0.9909 | 95.58 | 2913.89 | 0.9896 |
| 0.2        | 98.42 | 0.9888 | 96.38 | 1695.83 | 0.9872 |
| 0.3        | 100.02 | 0.9871 | 97.95 | 1965.44 | 0.9872 |
| 0.4        | 102.24 | 0.9869 | 100.18 | 1989.34 | 0.9849 |
| 0.5        | 103.95 | 0.9914 | 97.88 | 470.80 | 0.9900 |
| 0.6        | 83.07 | 0.9794 | 79.64 | 3.0520 | 0.9750 |
| 0.7        | 64.07 | 0.9736 | 59.32 | 0.0106 | 0.9656 |
| 0.8        | 53.91 | 0.9674 | 47.81 | 0.0002 | 0.9533 |
| 0.9        | 35.775 | 35.109 | 35.537 | 35.517 | 34.958 |

Average \( \Delta m \) (%) = 35.379

\( \alpha \): activation energy; \( k \): pre-exponential factor; \( R^2 \): correlation coefficient.

4. Conclusions

From the results of this study, it is seen that the pure mcallisterite minerals can be synthesized at a reaction temperature of 60°C with a 30 min reaction time by a hydrothermal method from the raw materials of MgO and H_3BO_3.

According to the XRD results, “01-070-1902” coded mcallisterite mineral [Mg_2(B_6O_7(OH)_6)•9H_2O] was synthesized. FT-IR and Raman spectrum had the characteristic bands of magnesium borates [29, 30]. Surface morphologies revealed that proper crystals in nanoscale were obtained with particle size ranges of 398.30–700.06 nm. The B_2O_3 content of the MH-60-30 was 54.17 ± 0.87%, which is very close to the theoretical value of mcallisterite (54.35%). The average reaction yield of MH-60-30 was 85.80 ± 0.61%.

In thermal analysis at 2°C/min, mcallisterite lost its structure water content in a two-step process with the reaction scheme shown in (3) and (4):

1st step:

\[
\text{Mg}_2(\text{B}_6\text{O}_7(\text{OH})_6)\cdot 9\text{H}_2\text{O} \rightarrow \text{Mg}_2(\text{B}_6\text{O}_7(\text{OH})_6)\cdot 2\text{H}_2\text{O} + 7\text{H}_2\text{O}
\]

2nd step:

\[
\text{Mg}_2(\text{B}_6\text{O}_7(\text{OH})_6)\cdot 2\text{H}_2\text{O} \rightarrow 2(\text{MgO}\cdot \text{B}_2\text{O}_3) + 2\text{B}_2\text{O}_3 + 8\text{H}_2\text{O}
\]

In the first step, mcallisterite lost approximately 7 moles of its structure water and in the second step the remaining 8 moles of structural water were lost. According to the thermal conversion results, the final components were equimolar Mg(B_2O_3)_2 and B_2O_3.

In the thermal analyses at heating rates greater than 2°C/min, mcallisterite lost all 15 moles of structure water
Table 5: Crystallographic data of synthesized mcallisterite and MgO(B$_2$O$_3$)$_2$.

| Mineral name | Mcallisterite | Magnesium borate |
|--------------|---------------|------------------|
| pdf number   | 01-070-1902   | 01-076-0666      |
| Chemical formula | Mg$_2$(B$_6$O$_7$(OH)$_6$)$_2$·9(H$_2$O) | MgO(B$_2$O$_3$)$_2$ |
| Molecular weight (g/mole) | 768.56 | 179.55 |
| Crystal system | Rhombohedral | Orthorhombic |
| Space group | Pr3c (No. 167) | Pbca (No. 61) |
| a (Å) | 11.5490 | 13.7300 |
| b (Å) | 11.5490 | 7.9700 |
| c (Å) | 35.5670 | 8.6200 |
| α (°) | 90.00 | 90.00 |
| β (°) | 90.00 | 90.00 |
| γ (°) | 120.00 | 90.00 |
| z | 6.00 | 8.00 |
| Density (calculated) (g·cm$^{-3}$) | 1.86 | 2.53 |
| Characteristic peaks I (%)/2θ (°) | 35.7/15.332 | 94.4/17.033 |
|  | 32.9/31.875 | 80.9/19.921 |

content in a single step, turning into Mg(B$_2$O$_3$)$_2$ and B$_2$O$_3$ by the reaction scheme shown in (5):

1st step:

$$
\text{Mg}_2(B_6O_7(OH)_6)_2\cdot9\text{H}_2\text{O} \rightarrow 2(\text{MgO(B}_2\text{O}_3)_2) + 2\text{B}_2\text{O}_3 + 15\text{H}_2\text{O} \tag{5}
$$

In the kinetic study, for the conversion values between 0.1 and 0.6, $R^2$ values varied in the range of 0.9909–0.9869 and 0.990–0.9849 in Ozawa and KAS method, respectively. Average $E_a$ values of Ozawa and KAS methods were calculated as 100.40 KJ/mol and 98.31 KJ/mol, respectively.

In conclusion, the kinetic study of mcallisterite was reasonable considering that the Ozawa and KAS methods activation energy values were approximately the same.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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