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# MAGNETIC WATER TREATMENT FOR SCALE PREVENTION ON WATER HEATER ELEMENTS

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# MAGNETIC WATER TREATMENT FOR SCALE PREVENTION ON WATER HEATER ELEMENTS

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# MAGNETIC WATER TREATMENT FOR SCALE PREVENTION ON WATER HEATER ELEMENTS

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Calcium carbonates is one of the main components of scale that is commonly found in industrial equipment such as hot water systems. Scale formation on heater elements may lead to reduce heat efficiency and shorten the heat service life. Ion exchange softened water are used to reduce the scale formation, but excess salt during regeneration discharged to the wastewater stream, limits the reuse of wastewater for industrial purposes. As a result, non-salt alternative devices would provide consumers with the ability to reduce the impacts of ion exchange softened water without creating negative salinity impacts on wastewater stream. Magnetic water treatment device involves passing a hard water though a magnetic field. This method reduces amount of scale and favors the precipitations of aragonite, a softer type of scale rather than a hard scale, calcite.

A water heater system was constructed to quantify the scale formation with tap water by using one proprietary magnetic water treatment device, AkwaMag device, and compare it to untreated tap water at 60°C in systems with a tank with 70.4 $in^2$ of exposed iron and with a tank with little exposure of iron. Accelerated scale formation teste were performed on tanks with and without the magnetic device tested at 30 °C and 60 °C. Scale were collected and characterized by x-ray diffraction (XRD), and scanning electron microscopy (SEM) analysis.

The water heater simulation study from the experiment with a tank with little exposure of iron showed that the mass of scale was reduced on the magnetically treated water heater element. Aragonite was formed on both untreated and magnetically treated water heating elements, but the weight percentage of aragonite increased on the magnetically treated water heating elements based on the results obtained from XRD. Other compounds were also detected with XRD found in both heating elements. SEM of both heating elements showed the presence of calcium carbonate polymorphs. In accelerated scale study, the weight percentage of aragonite was higher than calcite at 60 °C and 30 °C. However, calcite was reduced in the magnetically treated water heater elements, which indicates the effects of magnetic fields on reducing calcite formation.

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Pursuing my master's degree has been a rewarding experience as I can attest to the fact that I have left the program with broader knowledge and the motivation to further succeed and constantly evolve. I would like to express my deep gratitude to my advisor Dr. Bruce Dvorak, who have been consistently providing help and support during the past two years especially in carrying out my research and writing my thesis. His advice and feedback acted as a catalyst that allowed me to further grow and evolve academically and professionally.

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# Chapter 1 Introduction

## 1.1 Background

The water sources in the United States are often classified to be hard water, containing high mineral content such as calcium and magnesium carbonates, bicarbonates and sulfates. Resulting in a need to treat the water before entering water line to avoid scale formation (USGS, 2019). Among the uses for ion exchange softened water is for reducing scale build-up on water heater elements, both for industrial and residential purposes. A study conducted by Water Quality Research Foundation (2011) showed that avoiding scale build-up using soften water can extend the life of the heating element and reduce energy costs by up to 25%.

Water softeners are regenerated with concentrated brine solution such as sodium chloride (NaCl), which is discharged to the sanitary sewer. Excess salt in the wastewater increases treatment cost and limits the reuse of wastewater for agricultural and industrial purposes (Asano et al. 2006). Reducing the use of ion exchange systems to soften hard water is a practical way to improve the quality of wastewater, but there's a limited research that has assessed the feasibility of Salt-Free Water "Softener" Alternatives.

A range of non-salt alternatives to minimize scale build-up have been developed, including electrically induced precipitation, template-assisted crystallization, capacitive deionization, and magnetic water treatment (Wiest et al. 2011). Magnetic water treatment devices are entering the market but often viewed as an unproven technology due to highly varied results in the literature and the contradictory claims about the treatment mechanism (Alabi et al. 2015). Magnetic water treatment is a device that's used to reduce the effects of hard water by passing it through a magnetic field. The magnetic field changes the crystal structure of the scale formed from calcite (hard scale) to aragonite

(soft scale) (Knez and Pohar, 2005). Magnetic devices are attractive due to their operating cost and affordability. Magnetic devices have smaller footprint when compared to most other systems and can be placed “in-line” on a water pipe to the desired industrial process.

### 1.2 Goal and Specific Research Objectives

The purpose of this research study was to investigate the viability of a physical device, which utilizes a magnetic field to minimize scale formation on water heater element. The primary objective of this study was to examine scale build-up on heating elements using a proprietary magnetic water treatment device, AkwaMag, and compare it to “untreated” tap water. This magnetic device uses a fast flow of water and a strong magnetic field. This was accomplished by constructing a water heater system simulating a real hot water system, and quantifying scale formation. The water heater system was used with two different conditions to model a real water system because some heater systems accidently or intentionally include exposed metals. The water heater system was used (1) with a tank with 70.4 $in^2$ of exposed iron and (2) with a tank with little exposure of iron. The impact of the corrosion in plumbing system was examined on both tanks. A secondary objective was to evaluate the calcium carbonate polymorphs with and without the use of AkwaMag device using a calcium carbonate supersaturated solution as an influent. The composition and the morphology of the scale formed was analyzed by using X-Ray Diffraction (XRD) and SEM analysis respectively.

### 1.3 Organization of thesis

This thesis is organized into five chapters. Chapter 1 provides an introduction of the thesis focusing on the background, research goals and objective. Chapter 2 provides a brief review of relevant literature sources, focusing on the scale problem and the factors affecting its formation as well as the mechanism of conventional water softening and Salt-Free Water “Softener” Alternatives. The properties of calcium carbonate polymorphs are discussed as well. Chapter 3 describes the methodology used in this research, along with the type of equipment apparatus used. Chapter 4 contains main findings and results of this study. Chapter 5 includes a brief summary of the primary conclusions and future work recommendations. Finally, the Appendices include detailed calculations related to hardness test results using a supersaturated solution as an influent, statistical analysis for influent tap water, and XRD analysis results.

# Chapter 2 Literature Review

## 2.1 Introduction

Scale deposits from hard water often causes technical and economic problems in industrial operations. When soluble minerals precipitate from hard water and deposit on hot surfaces, it affects the performance of industrial operations (Behbahani et al. 2008). Softened water is often used to remove hardness from water, as to reduce heat transfer loss from scale build-up on boilers and water heaters. However, water softeners are usually regenerated with concentrated sodium chloride solution, which is discharged to the sanitary sewer. Excess salt in wastewater, increases the treatment cost and reduces the potential of reusing treated wastewater for irrigation and industrial purposes.

Hard water is formed when water infiltrates through deposits of limestone, chalk or gypsum. Hard water is largely made up of calcium and magnesium carbonates, bicarbonates and sulfates (Larson and Buswell, 1942). Calcium is the fifth element and the third abundant metal in the earth's crust and the human body. It is not found in its metallic form on the earth's surface but associated with other elements and molecular species or ionized form complexed with a variety of other compounds (USGS, 2019). It is primarily found in igneous rocks as calcium silicates and in sedimentary (USGS, 2019). Soft waters are found in parts of New England, the South Atlantic-Gulf States, the Pacific Northwest, and Hawaii. Moderately hard waters are common in many rivers of Alaska and Tennessee. Hard and very hard waters are found in some streams in most of the regions throughout the country. A geography distribution of the hardness of groundwater is illustrated in Figure 2.1.

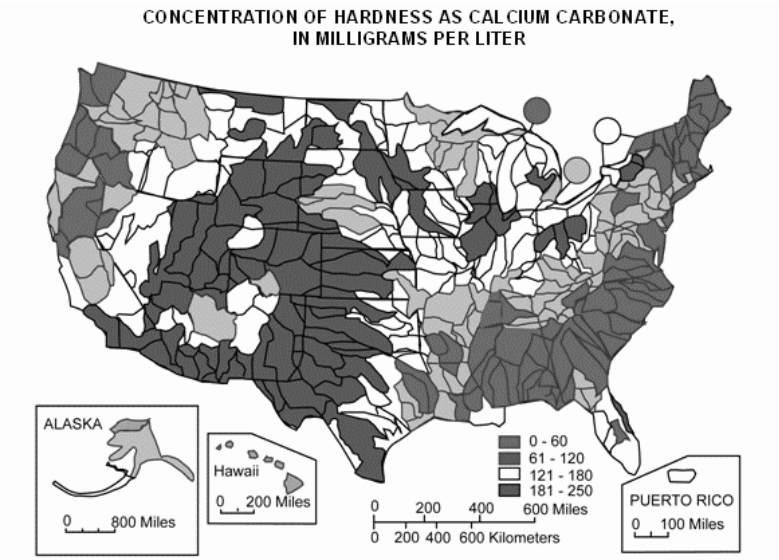


**Figure 2.1 Mean hardness as calcium carbonate concentration levels**. Source: USGS, (2019)

This chapter reviews key literature related to scale formation and prevention in hot water systems. Scale control methods like conventional ion exchange water softener and non-salt devices will be discussed. The mechanism of scale formation and the significant factors affecting its formation, and the properties of scales of calcium carbonate polymorphs will also be discussed.

## 2.2 Softening methods

Due to the desire to remove hardness without adding ions to the water, alternative treatment systems for scale prevention have been developed. Various non-salt devices have been proposed including capacitive deionization, electrically induced precipitation, template-assisted crystallization, and magnetic water treatment (Wiest et al. 2011). In particular, magnetic water treatments have attracted much attention. Conventional ion

exchange water softener and salt-free water softeners along with the limitation in the use of each method will be discussed.

### 2.2.1 Ion Exchange

Ion exchange is a process where dissolved ions in water are being removed and replaced with other similar charged ions from the surface of ion exchange resin (anion or cation exchange resins). When the capacity of the resin is exhausted, it needs to be restored by using a regenerant solution. Resins are mostly regenerated using a saturated brine solution such as sodium chloride or potassium chloride, other regenerant may also be used like strong acids such as hydrochloric acid and sulfuric acid or strong bases such as sodium hydroxide (Environmental Protection Agency, 2020).

For hardness removal from water, the process involves the exchange of hardness minerals (Calcium and Magnesium) with brine solution, often using sodium chloride as a regenerate brine since it is the most common approach in the US is to exchange sodium, from salt for calcium and magnesium ions. This process occurs in an Ion Exchange column where hard water is passed through a specialized resin beads that facilitates the exchange of ions based on their electrical charge. The specialized beads used here are called strong acid cation (SAC) resins. These resins are small, porous polymeric beads hold positively charged sodium ions and are displaced with calcium and magnesium as they flow inside the column. These beads have higher affinity for the hardness ions than for sodium ions (Naushad and Al-Othman, 2013). For example, during conventional ion exchange process, the displaced sodium ions flow downward the resin bead and leaves the water softener column's outlet; thus, a softened water is delivered (Skipton et al. 2008). This process is efficient in removing iron and manganese as well. After several

service cycles of this process, the resin becomes exhausted with hardness where no further softening can take place, thus, the ion exchange beads must be regenerated. The column is regenerated with brine solution of sodium chloride (NaCl) usually 8-10% by weight (Flodman and Dvorak, 2012). The exhausted resin beads are exchanged with sodium ions present in the brine solution. Excess sodium along with removed hardness are typically discharged to the sanitary sewer. The process of Ion Exchange process is depicted in Figure 2.2.

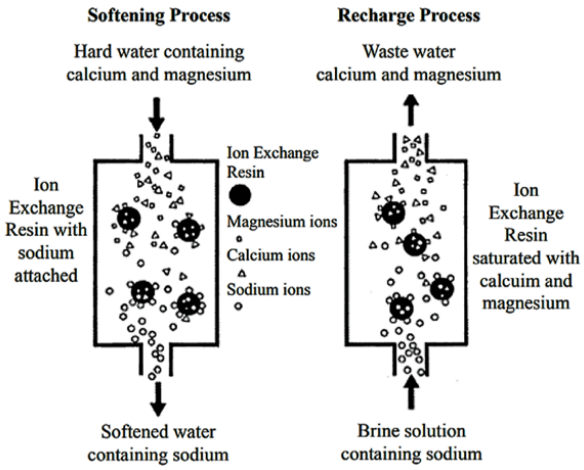


**Figure 2.2 Water Softening and Regeneration Process.**
Source: Skipton et al. (2008)

Softened water can significantly reduce the amount of scale build-up in water heaters compared with water heaters operated on hard water. A study has shown that water heaters operated on softened water experienced only around 1% on a mass basis of the scale build-up experienced by an identical water heater running on hard water (Stickford and Johnson, 1984). However, the major disadvantage of the water softener is associated with the excess salt discharged to the wastewater stream or septic leach field (Clifford, 1999). An increase in salt concertation in the wastewater treatment leads to

increased treatment cost which limits the reuse of wastewater for agricultural and industrial purposes. It can also leach to groundwater, eventually increasing the total dissolve solid (TDS) concertation (Provin and Pitt, 2017). Discharged salt might exceed the maximum concertation required by National Pollutant Discharge Elimination System (NDPES) permits.

### 2.2.2 Template assisted crystallization

Template assisted crystallization (TAC) is a technology that's relatively new to the water industry. TAC uses polymeric beads that contains a template for crystal growth. This template acts as nucleation sites which converts dissolved hardness into microscopic crystals. When the crystals are formed, are released from the polymeric beads, they become insoluble particles that will no longer attach to the surface (Wiest et al. 2011). Figure 2.3 illustrates the process of TAC. In Step 1, the dissolved hardness in water (Calcium and Magnesium) are converted into microscopic crystals. In Step 2, the seed crystal containing hardness are being released from the nucleation site into the solution.

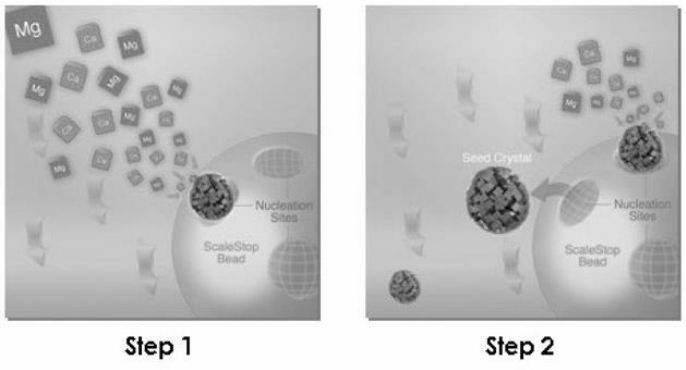


**Figure 2.3 Template Assisted Crystallization (TAC) process.** Source: Premier Water Technologies (2012)

This technology does not require chemicals or other regenerant for cleaning. However, pretreatment of the feed water is required prior using this technology if it

contains high level of iron and manganese. This technology has passed the German DVGW-512 test (German Gas and Water Corporation, 1996) to be applied for drinking water scale prevention. A study conducted by Wiest et al. (2011) following the German standard protocol DVGW Article W512, showed that TAC was the most efficient device with greater than 88% on a mass basis of scale reduction.

### 2.2.3 Capacitive deionization (CDI)

Capacitive deionization (CDI) is an electrochemical water process caused by the applied electrical current. The ions dissolved in water are absorbed into charged electrodes made of carbon porous material that have a high surface area (Oren, 2008). Negatively (anions) and positively (cations) charged ions are removed from water and are stored in anode and cathode, respectively as illustrated in Figure 2.4.

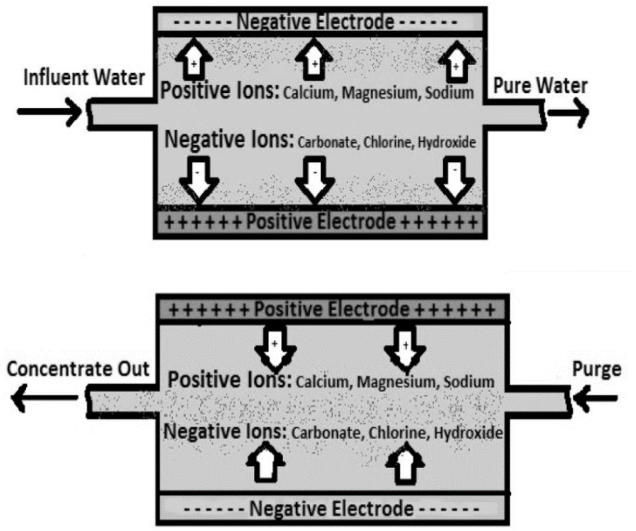


**Figure 2.4 Capacitive Deionization (CDI) Process, Purification step (Top), Backwash Step (Bottom).**
Source: Wiest et al. (2011)

This technology is not limited to the removal of hardness in water but also all charged ions present in water such as chloride, nitrates, nitrites, sulfates, fluorides, sodium, lead, and uranium (Dvorak, 2016). Backwashing is required for this technology for further purification use. CDI does not require high pressures when with membrane-based technologies such as reverse osmosis and nanofiltration. This attribute makes CDI a cost effective to be installed (Oren, 2008). According to results from Wiest et al. (2011), CDI reduced the mass of scale produced by about 80% in their tests.

### 2.2.4 Electrically induced precipitation

Electrically induced precipitation utilizes a direct electrical current to precipitate dissolved scale forming particles suspended in water. As the water enters a more scale forming environment, the calcium carbonate can react with suspended nucleation sites instead of surfaces and scale formation can be prevented (Wiest et al. 2011). The electric field affects the dissociation of bicarbonates in water which accelerates the formation of carbonates in water, inducting the precipitation of calcium carbonates on the electrode surface (Cho et al. 2005). Precipitate formed on an electrode must be cleaned periodically. A study showed that by using this technology, scale formation was reduced by 50% on mass basis (Wiest et al. 2011) which is lower in comparison with other non-salt technologies.

### 2.2.5 Magnetic Water Treatment

Magnetic water treatment devices are used to reduce the effects of hard water by passing it through a magnetic field to form a soft scale. It is becoming marketed more commonly but not always trusted due to the contradictory claims about the treatment mechanism. A number of mechanisms have been proposed in the literature to account for

the effectiveness of magnetic devices in reducing scale formation. The presence of aragonite could be used as a way of preventing scale because it is a softer type of scale and is less likely to form an adhesive scale on the surface (Kozic and Lipus, 2003).

The first proposed mechanism is related to the presence of iron impurities. Scale by magnetic treatment stems from the ferric hydroxide, $Fe(OH)_3$, generated by magnetically induced corrosion from an iron pipe. Magnetic unites that are equipped with brass compression fitting could cause iron pipe to be corroded resulting in increasing corrosion rate for the iron. Ferric hydroxide (Crystal structure: Goethite) is isomorphic with aragonite, the goethite particles would provide extremely effective sites for heterogeneous nucleation for aragonite (Duffy et al. 1977; Esmaeilnezhad et al. 2017).

The second proposed mechanism states that, the hydration of dissolved ions is deformed under the effects of magnetic field which alters their distribution in the water (Mosin and Ignatov, 2014). The magnetic field is proposed to decrease the hydration of the ions which is an important factor to the solubility of the dissolved salts in water. Lorentz force is responsible for the deformation of hydration shell (Mosin and Ignatov, 2014). Lorentz force is a magnetic force on a point charge due to magnetic field as shown in the following equation:

$$\vec{F} = q(\vec{v} \times \vec{B}) \qquad (2.1)$$

Where,

$\vec{F}$ = force on the ions- Newton(N)

q = Charge of ions- Coulomb (C)

$\vec{v}$= velocity of the ions– (m/s)

$\vec{B}$= Magnetic field intensity- Tesla (T) [1 T → 10000 Gauss (G)]

With the flow of water molecules in the magnetic field perpendicular to the magnetic field lines as shown in Figure 2.5, Lorentz forces F1,F2 occurs which influences the behavior of the dissolved ions in water.

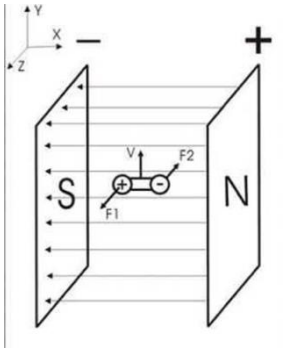


**Figure 2.5 Physical Behavior.** Source: Mosin and Ignatov, (2014)

## 2.3 Scale Produced by Hard Water

Natural waters contain alkaline earth metal such as magnesium, calcium and barium, and anions such as carbonate, silicate and sulfate, etc. Different combination of these cations and anions will potentially cause scale issues such as calcium carbonate, calcium silicate, calcium sulfate, barium sulfate, magnesium sulfate, etc. The scale problem occurs when such compounds exceeds their solubility limits at higher temperature (Cho et al. 2005). The most common occurring scale forming mineral in industrial water systems is calcium carbonate. The dissociation of bicarbonates ($HCO_3^-$) is the first step that leads to the precipitation of calcium carbonate ($CaCO_3$) as shown in the following equilibria reactions (Cho et al. 2005):

$$HCO_3^-{}_{(aq)} \rightleftharpoons OH^-{}_{(aq)} + CO_{2\,(aq)} \quad (2.2)$$

$$OH^-{}_{(aq)} + HCO_3^-{}_{(aq)} \rightleftharpoons CO_3^{2-}{}_{(aq)} + H_2O \quad (2.3)$$

$$Ca^{2+}_{(aq)} + CO_3^{2-}{}_{(aq)} \rightleftharpoons CaCO_{3(s)} \quad (2.4)$$

**Overall reaction**

$$Ca^{2+}_{(aq)} + 2HCO_3^{-}{}_{(aq)} \rightleftharpoons CaCO_{3(s)} + H_2O + CO_{2\,(aq)} \quad (2.5)$$

As water enters to a high temperature environment such as a heat exchange or a boiler, the precipitation of calcium carbonate occurs as shown in the overall reaction above. The formation of calcium carbonate precipitants at elevated temperature is associated with the reduction of carbon dioxide in the solution. At high temperature, the solubility of carbon dioxide in the solution decreases and leaves the system (Glater et al. 1980). The reduction of carbon dioxide in the solution results in shifting the overall reaction to the right, forming more calcium carbonates solid. Scale build-up in the surface of the hot element limits the flow of water, prevents effective heat transfer in heating devices, and causes additional energy load thereby increasing normal energy demand.

Calcium carbonate ($CaCO_3$) exhibits plenty of variation in nature. It occurs as three anhydrous crystalline polymorphs where the solid material has the ability to exist in more than one form of crystal structure (i.e., same chemistry but a different structure, different symmetry and crystal shapes): calcite, aragonite, and vaterite (Meldrum, 2003).

### 2.3.1 Main Factors Affecting Scale Formation

Scale formation is significantly affected by a variety of factors such hardness concentration, water temperature, pH of water, and induction time.

- **Effect of hardness concentration**

Supersaturation is the primary driving force for crystallization. As the concentration of hardness in the solution is increased, it will result in an increase in the

rate of nucleation and growth. At higher concentrations, more scale-forming components are available in the solution (Muryanto et al. 2014)

- **Effect of water temperature**

Calcium carbonate phase transformation is affected by temperature. Higher temperatures provide sufficient energy to the molecules or ions and result in a faster reaction rate moving the equilibrium to the right (Equation 2.5) producing calcium carbonate. Thus, as the temperature increases, the scale formation increase (Muryanto et al. 2012).

- **Effect of water pH**

As the pH of a water increases, the conversion of bicarbonate to calcium carbonate, as shown in reaction (2.5), increases. Several research studies (Andritsos and Karabelas, 1999) reported the effect of pH on the formation of a calcium carbonate scale and showed that by increasing the pH from 8 to 10 the, the scale formation increases.

- **Effect of induction time**

Induction time is the time required for the nuclei crystal to grow to a detectable size and form a scale. The induction time is determined by measuring the change in the conductivity of the solution over time. Such procedure has been widely used to monitor nucleation and crystal growth. As the induction time increases, the conductivity of the water decreases indicating that a substantial number of crystal-forming ions start leaving the solution to form crystals (Hoang et al. 2007; Muryanto et al. 2014).

### 2.3.2 Properties of Calcium Carbonate Polymorphs

Calcite has a trigonal symmetry, while aragonite and vaterite have an orthorhombic and a hexagonal symmetry, respectively. Scale is consisting largely of calcite, which is

the most thermodynamically stable form of calcium carbonates at room temperature, and forms hard layers, which are difficult to remove.

The other two of crystalline forms are unstable, with vaterite being specifically thermodynamically unstable at standard temperature and pressure. It has higher solubility than either crystalline forms, which is easily converted to calcite at low temperature or aragonite at high temperature. Aragonite is more stable at high pressure (Sarkar and Mahapatra, 2012).

Aragonite has a more compact structure than calcite and is composed of triangular carbonate ion groups ($CO_3$), where the carbon is located at the center of the triangle and the three oxygens at each corner. The carbonate ions are perpendicular to each other in two planes. The carbonate ions in calcite lie in a single plane pointing in the same direction, giving it the symmetry of the trigonal (Amethyst Galleries, Inc., 2019).

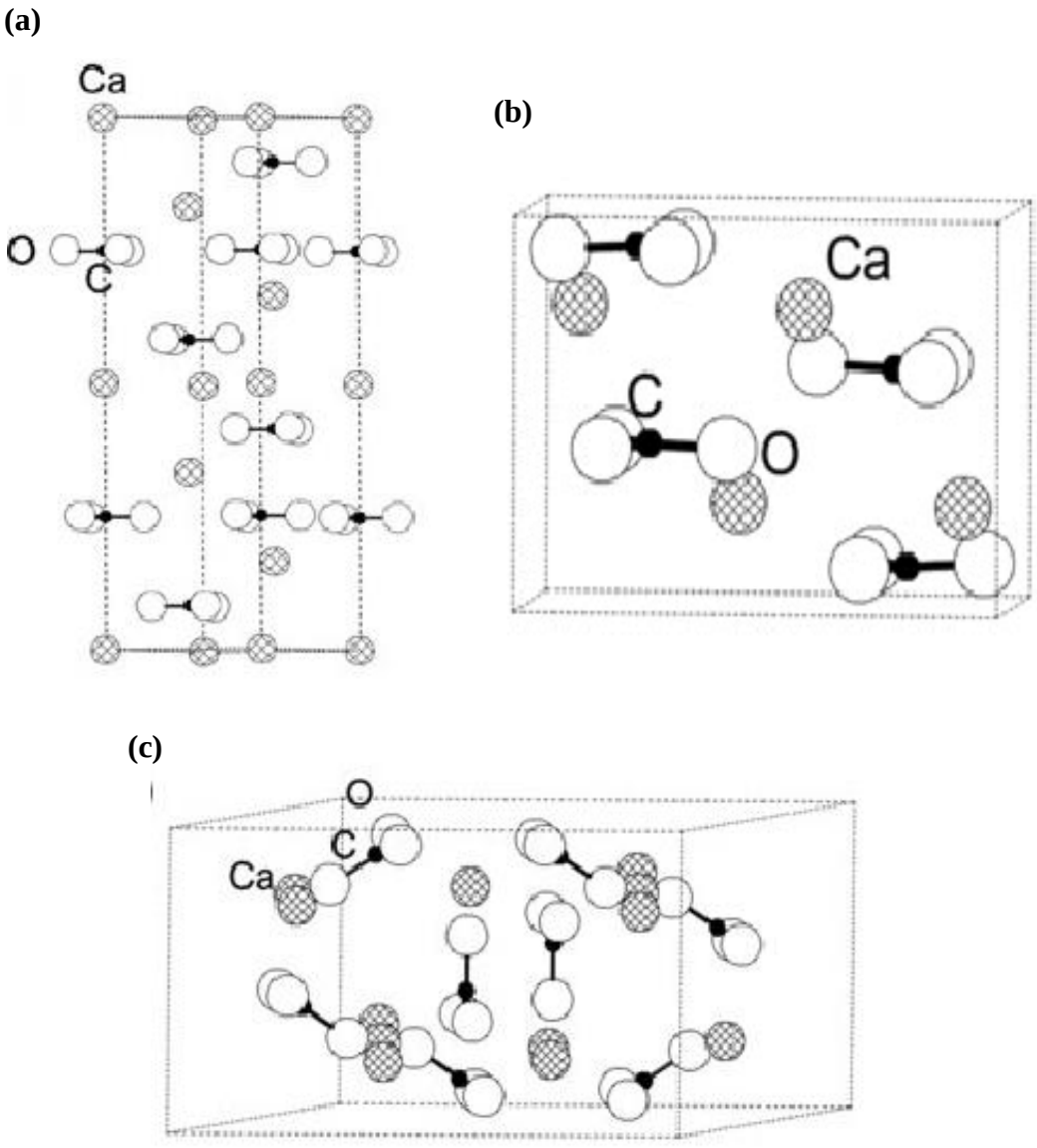


**Figure 2.6 Schematic representation of crystallographic unit cells for (a) Calcite (b) Aragonite and (c) Vaterite.** Source: Xu and Poduska, (2014)

# Chapter 3 Methodology

## 3.1 Introduction

This chapter describes the analysis methods used to test water quality and scale composition, and to present a description of the apparatus used during the experiments namely, the water heater simulation and accelerated scale simulation. The purpose of each study was to examine the scale formation using influent of (1) tap water and (2) calcium carbonate supersaturated water.

The water heater simulation study was constructed to mimic a real hot water system. The scale formation was monitored for 34 to 43 days with an operating temperature of 60 $^{\circ}$C. The total hardness and conductivity of influent tap water, magnetically treated water and untreated water was monitored throughout the experimental operation. This study was conducted twice, water heater test with a tank with 70.4 $in^2$ of exposed iron and with a tank with little exposure of iron. The source of iron impurities was from the metal pail made of steel that was used to mount the heater element, it corroded over time due to high operating temperature. In the water heater test with a tank with little exposure of iron, the metal pail was coated, and the scale formation was monitored for 25 days.

The accelerated scale simulation was performed in a batch process to have a sufficient amount of scale build-up on heating elements. The influent water of the supersaturated solution was set to be approximately 400 mg/L as $CaCO_3$. The total hardness and conductivity of the influent water was measured prior to starting the experiment. In addition to that, the scale formation process was monitored through testing the conductivity and the pH of the solution during the experiment. At the end of each test, the scale formed was measured through filtration process and gravimetric measurement.

The samples were also characterized using scanning electron microscopy (SEM) and X-Ray Diffraction (XRD) analysis.

### 3.2 Water Quality Testing

The influent water for water heater simulation study was from the City of Lincoln drinking water system. The Lincoln water source is groundwater, which is naturally high in quality and comes from wells along the Platte River near Ashland, Nebraska. The water contains detectable levels of iron and manganese and is further treated before it is distributed to homes and businesses. However, trace amounts of these elements can still be found in tap water after treatment (Lincoln Water System, 2019). A synthetic calcium carbonate influent water was prepared using high purity water as a base for the accelerated scale simulation study. Both water types were monitored for total hardness concentration, conductivity, and pH during this study. The water testing methods used are described subsequently.

#### 3.2.1 Hardness

The concentration of total hardness of the influent water was monitored everyday throughout the experimental operation. Hach EDTA Standard Method for Water, Wastewater and Seawater (SM) 8204 was used to measure the hardness (Water Analysis Handbook Hardness, Calcium-Titration Method using EDTA Method 8204, 1983). SM 8204 uses the digital titration of a measured sample with potassium hydroxide. Hydroxynaphthol blue indicator is used to measure the calcium hardness. Digital titrators uses highly precisely dispensation device and titrant cartridges (0.800 M EDTA), corresponding to the expected sample concentration. The concentration of hardness at the

end point is determined by recording the number of digits appears in the device's digital counter multiplied by a digit multiplier available in manual.

### 3.2.2 Conductivity

The conductivity of the influent water was monitored throughout the experimental operation. Electrical conductivity is the measure of water capacity to conduct electrical current, which implies the total dissolved inorganic salt and salinity levels in water. The water conductivity is directly correlated with calcium hardness concentration. Hach Standard Method for Water and Wastewater (SM) 8160 was used to measure the conductivity (Water Analysis Handbook Conductivity, 1983). The conductivity probe was calibrated (919 μS/cm-1000 μS/cm) using sodium chloride standard solution, 1000 ± 10 μS/cm.

### 3.2.3 pH

The pH of the influent water was monitored throughout the accelerated experimental scale simulation. The pH was measured using 4-Star Plus pH/DO probe meter from Thermo Fisher Scientific Inc under Standard Method for Water and Wastewater (SM) 4500 (APHA et al. 2005). A 3-point calibration using 3 different buffer solutions was used to calibrate the pH probe.

### 3.2.4 Iron, Manganese and other Different/Unknown Elements

Tap water sample was collected at faucet while magnetically treated water sample was collected as it entered the tank to detect for Iron and Manganese. Besides detecting for iron and manganese in both water samples, they were also detected if there appear to be different/unknown elements that are being added to the magnetically treated water as it passes through a magnetic treatment unit and compared with the tap water. All samples

collected were sent to the University of Nebraska-Lincoln (UNL) Water Science laboratory (Nebraska Water Center, 2020).

The method used at the water science laboratory for iron and manganese and other unknown elements were Inductively Coupled Plasma - Mass Spectrometry (ICP-MS) SM 6020A and semi-quantitative elemental analysis SM 200.8 respectively. The reporting limits provided by the UNL Water Science laboratory were 0.1 µg/L and 0.04 µg/L for iron and manganese respectively. The reporting limit using semi-quantitative elemental analysis is not identified yet.

### 3.3 Scale Analysis

The quantity of scale formed for each experimental test was determined by a combination of the filtration process and gravimetric measurement. The characterization of the scale was performed by X-ray Powder diffraction (XRD), and scanning electron microscopy (SEM) at Nebraska Center for Materials and Nanoscience laboratory (Nebraska Center for Materials & Nanoscience, 2020). SEM scans the surface of the sample by using electron beams to interact with the atoms and produce information regarding the surface morphology of the sample (Tung et al. 2003).

The solid scale was separated from the solution by means of filtration after the completion of each test and air-dried at room temperature while waiting for XRD and SEM analysis of the precipitates to be performed. The solid scale was removed from the heating element by scraping with a stainless-steel tool and combined with loose scale from the tank and weighed using a laboratory analytical balance.

### 3.3.1 X-ray Diffraction (XRD)

X-ray diffraction was used to analyze the precipitates formed at each test to identify the crystalline phases present on the sample. The proportion of calcite and aragonite were quantitively identified as well. The equipment used for this analysis is called PANalytical Empyrean. Each sample took almost 20 minutes to be analyzed.

X-rays beams (Cu kα radiation, $\lambda = 1.54056$ Å) were directed onto the sample and the scattered intensity is measured as a function of outgoing direction. $2\theta$ is the angle between the incoming and outgoing beams direction. The lattice spacing, d, were calculated from the $2\theta$ values using Braggs Law: $n\lambda = 2d \sin(\theta)$, where n is a positive integer (1, 2, 3, ...) $\lambda$ is the wavelength of the x-ray beam. For iron-containing samples, a monochromator was used to reduce the fluorescence signals enhanced by iron during analysis. A monochromator is an optical device that transmits a narrow band of wavelengths selected from a wide range of wavelengths to illuminate the sample. The ICDD (International Commission for Diffraction Data) database for phase identification was used to compare with the d spacing and intensity data (S. Valloppilly, Personal Communication, March 4$^{th}$, 2020).

### 3.3.2 Scanning Electron Microscopy (SEM)

The morphology of the precipitates was examined by FEI NanoSEM 450 equipment. Based on the shape of crystals formed, the crystal structure is identified and compared with the results found from the XRD analysis. Each sample took between 30 minutes to 2 hours to be analyzed.

SEM uses a focused electron beams to interact with a surface of the sample to create an image. The SEM chamber was allowed to reach nominal pressure by venting

the chamber. Few particles of the sample were needed to perform the analysis. A carbon tape was used to adhesively bond the sample onto sample stub and placed into sample stage inside the SEM chamber. The system was allowed to reach vacuum by turning on the pump. The operating voltage was selected to give a better image by using the SEM software. To capture the SEM image, the magnification level was optimized until the desired feature is observed in the sample (X. Li, Personal Communication, March 9$^{th}$, 2020).

### 3.4 Magnetic Device

AkwaMag device was used in this study to facilitate scale control by directing water through a strong, proprietary magnetic field, known as the High Intensity Multipass system. This process changes the structure of the calcium carbonate, diminishing its ability to stick to surfaces instead of inhibiting the scale formation in water. Table 3.1. lists product specifications of the AkwaMag device (AkwaMag, Inc, 2014). The device was installed according to the manufacturer's instructions.

**Table 3.1 Product Specifications for the AkwaMag Device**

| **Specification** | **Operating Condition** |
|---|---|
| Assembled (H xW x D) | 18 inches x 14 inches x 8 inches |
| Service Flow Rate | Up to 11.5 gallons per minutes |
| Water Pressure Limits | 30-80 lb./inch$^2$ |
| Water Temperature Limits | 40-120 $^{\circ}$F |

The effect of magnetic softening using an AkwaMag device on tap water samples vs untreated tap water samples were measured by the use of electrochemical impedance spectroscopy (EIS) as shown in Figure 3.1. EIS is an analytical technique that allows the simulation of a liquid as an electrical circuit (Sammer et al. 2016). The data was obtained from a collaborative study between the AkwaMag Company and Wetsus, the European Center for Sustainable Water Technologies.

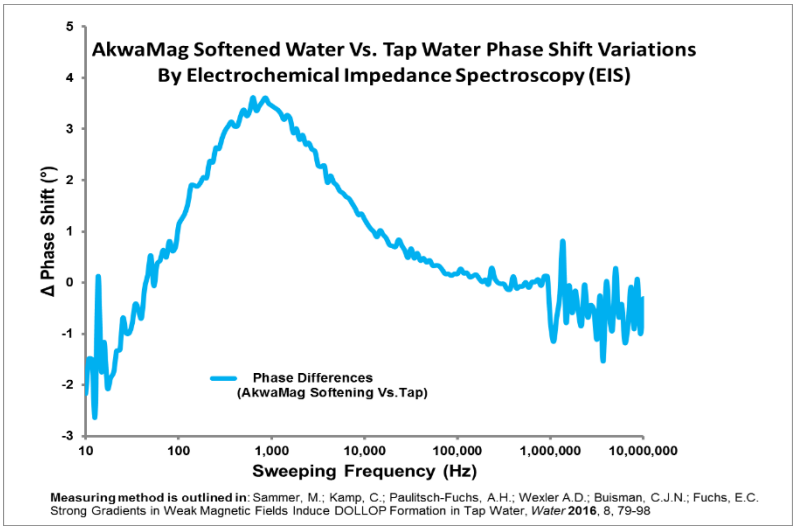


**Figure 3.1 Impedance phase shift spectra of AkwaMag vs Tap water**

At frequency below $10^6$ Hz, ions in tap water move faster along with the field and eventually form layers at the electrodes causing electrode polarization. This causes the impedance phase to increase and eventually decrease at higher frequency unlike the AkwaMag softened water. Since the hydration shell of dissolved ions are deformed under the effects of magnetic field, which alters their distribution in the water, they cannot follow the field as quickly as ions in tap water to cause the same electrode polarization.

Thus, the peaks showing up at different frequencies in the previously provided figure illustrates the difference of impedance phase shift of both water types. Noisy data exists at frequencies below 100 Hz and between $10^6$-$10^7$ Hz due to the limitations of the instrument used for analysis.

### 3.5 Water Heater Simulation

The testing procedure for the water heater experiment was similar to German standard protocol DVGW Article W512, "Verification of a Water Treatment Device for the Reduction of Scale Formation" (German Gas and Water Corporation, 1996), to evaluate salt-free water conditioning devices to control scale formation. The protocol consists of four test rigs that all receive the same type of water, two of the rigs include non-salt water devices while the other two test rigs are controls. The testing duration for this protocol is 20 days at a temperature of 80 $^{\circ}$C, where the flow of water is controlled by a timer to simulate daily water use. In this experiment, a similar approach was taken using two test rigs with an operating temperature of 60 $^{\circ}$C.

#### 3.5.1 Experimental Apparatus

A heating system connected to the tap water, mimicking a real hot water system was constructed. The heating system schematic and a photograph of experimental set-up apparatus are shown in Figure 3.2 and Figure 3.3 The pressure-regulating valve was directly connected to the tap water faucet to keep the water pressure under control before it reaches into the heating system. The municipal water supply enters the building at a very high pressure, where water pressure could be irregular which could cause failure to the system due to irregular flow of water. Thus, the water pressure coming from the water supply was adjusted and set at a pressure of about 35 psi (pounds per square inch). A

programmable water timer was used to simulate watering duration and frequency throughout the experimental period. A garden hose pipe was used to convey the water from the outlet of the pressure regulating valve to the timer. Parallel systems made of polyvinyl chloride (PVC) pipe were constructed. Two situations were tested, untreated tap water and tap water treated with the AkwaMag to run two tests at a time. A globe valve was used to regulate the water flow in both pipes.

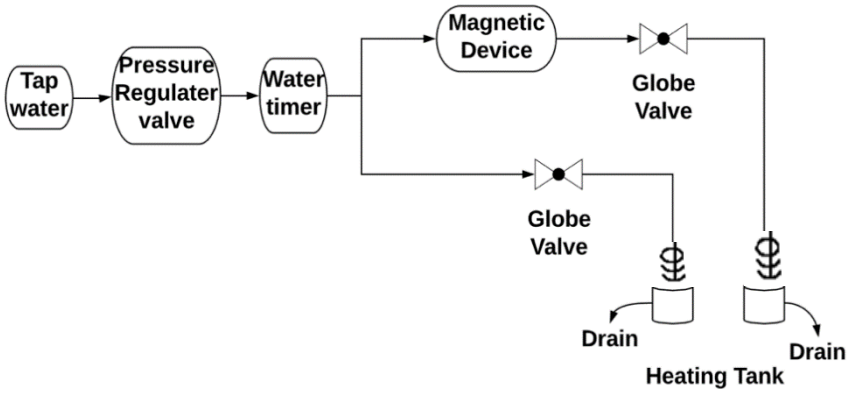


**Figure 3.2 Heating System Apparatus Schematic**

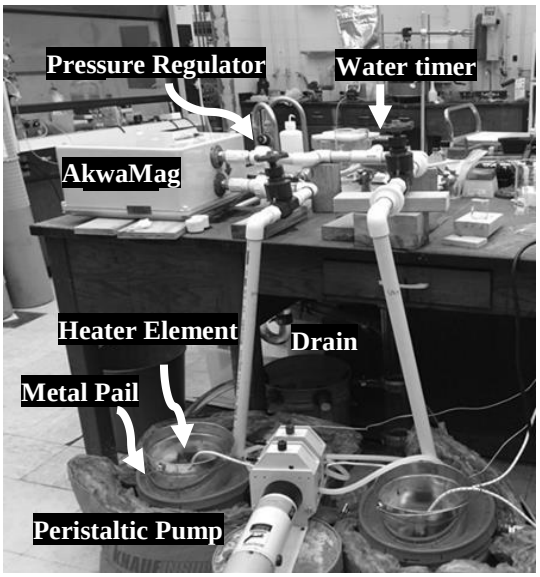


**Figure 3.3 Experimental Set-Up for Water Heater Simulation test**

A PVC pipe with ¾-inch nominal inside diameter was installed at the outlet of the timer and connected to tee fitting to allow the water line to be split into two lines with a connection that is at a 90-degree angle. A 1-inch nominal inside diameter PVC pipe was then connected to it. To run two tests at a time with equal flow of water from the water source, same amount of 1-inch nominal inside diameter PVC pipes installed in both sides with different head loss. Additional fittings were added into the AkwMag line.

The heating tank capacity was 5 gallons (18.92 L), but the water filled into tank was about 4 gallons (15.14 L). The wattage of the heating element was 1500 W and mounted on a small metal pail. The elements were connected to a temperature controller. The controller allowed the elements to heat the water to the desired temperature. The water inside was circulated using a peristaltic pump to maintain an even temperature. Due to the high operating temperature at the heating tank, a thick insulator was rolled around the tank. The drain line was directly connected downstream in a drainage basin. Table 3.2 provides a list of the equipment used, including model and specifications used for this experiment. In addition to the items listed in Table 3.2, various fittings and tubing were also used.

**Table 3.2 Experimental Set-up Equipment for Water Heater Simulation**

| Equipment | Type | Vendor/Model | Specifications |
|---|---|---|---|
| Pressure Regulator Valve | Adjustable Water Pressure Reducer with Gauge | Renator M11-0660R | ¾ inch Garden hose threads and NH threads |
| Water Timer | Digital Watering Timer for Garden Lawn | Homitt | ¾ inch Hose thread top and bottom connector |
| Globe Valve | Threaded PVC Globe Valve | Asahi/America ® | Pressure rating @ 70°F: 150 psi, 1 inch ID |
| Heater Element | Bolt On Style, High-Watt Density | Grainger, 1500 W, 120 V | L: 7-5/8 inches |
| Temperature controller | PID Temperature Controller | Inkbird | With Heat Sink, Solid State Relay and type K sensor |
| Metal Pail | leaktite | Home Depot | 5-qt. Metal Pail |
| Water circulating pump | Rotary Peristaltic | Masterflex I/P | With controller |
| Heater Tank | 5 Gal. Bucket | Home Depot | 20-qt |
| Drain Line | Clear PVC Vinyl Tubing | Everbilt | 1-1/4 inches O.D. x 1inches I.D. x 10 ft |
| Insulator | Fiberglass Insulation | Knauf Insulation Roll | 15 inches x 32ft. |

### 3.5.2 Operational Schedule for Water Heater Simulation

The water heater system study testing consisted of water being flowing from tap water alternately through the system at a constant flowrate. To achieve equal flowrate in both treatment lines, the length of the pipes after tee fitting were equal. To simulate the turning on of faucets in a home setting, at half flow or more, which is at least 2.0 to 2.5 L/min, the flowrate was set accordingly. The flowrate was controlled manually using globe valve. The flowrate for AkwaMag line and control line were set at 2.40 L/min and

2.50 L/min respectively. The flowrate of the treatment line was slightly lower than the control line due to water flowing inside the magnetic device.

After calibrating both globe valves to achieve the desired flowrate, the time it takes for the water to fill up both tanks to the drain line was measured. It took 5 minutes to fill up both tanks to the desired level. It took approximately 50 minutes to heat the water in the tank to the desired temperature at 60°C. A peristaltic pump was used to circulate the water inside both tanks to maintain an even temperature. The timer was used to set a cycle of 2 hours. The cycle consists of 5 minutes for watering, 50 minutes for heating, and the rest of the time for scale formation. The cycles were continuously repeated during the experimental period.

Throughout the testing, water samples were taken to measure for hardness and conductivity. Table 3.3 lists the sampling location and frequency.

**Table 3.3 Sampling Location and Frequency for Water Heater Simulation experiment**

| **Sampling Location** | **Sampling Frequency** |
|---|---|
| Influent service (Tap water faucet) | Sample tested in triplicate per day at the beginning of the cycle (50mL) |
| Influent untreated water bucket | Sample tested in triplicate per day at the beginning of the cycle (50 mL) |
| Influent magnetically treated water bucket | Sample tested in triplicate at the beginning of the cycle (50mL) |

The water heater study was originally planned for 21 days; however, several issues occurred during the testing. The retainer teeth in the pump head caused leaks on the tube connected to untreated water tank. The water level in the tank decreased overtime which caused the heater element to burn out. Thus, the experiment was on hold for two days to replace the heater element and pump tube for that tank. In addition to that,

the amount of scale built on the elements was not sufficient to do XRD analysis, thus; the test was running for a longer time. Due to the experimental failure and lack of adequate scale for analysis, the test duration for both treated and control line differed so that they can end at the same time. The control line test lasted for 34 days while the untreated water line lasted for 43 days. Despite extending the test duration, the scale formed on the water heater elements were not sufficient to perform XRD analysis.

This water heater test was exposed to iron due to the corrosion of metal pail that is made of steel. The amount of iron added in both tanks were not quantified, but the area of the corroded metal pail exposed to the tank was determined, 70.4 $in^2$. The presence of iron impurities inhibited the scale formation resulting in having less scale formed on water heater elements (Muryanto et al. 2012). The metal pail was coated with high-temperature paint to reduce the chances of developing significant rust. The water heater test with a tank with little exposure of iron was operated for 25 days, keeping other operating parameters the same as the water heater test with exposed iron in the tank.

### 3.6 Accelerated Experimental Scale Simulation

Scale formation using tap water as an influent normally takes months or years to be formed due its low saturation index leading to decline its scale-forming ability (Smith et al. 2004). In order to have a sufficient amount of scale build-up on heating elements faster, a simple bench-top system is built using a supersaturated calcium carbonate synthetic water. In supersaturated solution, the formation and transformation mechanism of calcium carbonate under different temperatures can be observed in a shorter time period (Ogino et al. 1987). The objective of this study is to determine the calcium carbonate polymorphs at 30°C and 60°C with and without the use of AkwaMag device.

### 3.6.1 Experimental Apparatus for Feed Preparation

A carbonized aqueous solution, containing only $Ca^{2+}$, $CO_3^{2-}$ and $HCO_3^-$ ions was prepared by dissolving reagent grade $CaCO_3$ in high purity water, and bubbling carbon dioxide according to:

$$CO_2+H_2O+CaCO_3 \rightarrow Ca^{2+}+2HCO_3^-. \quad (3.1)$$

This method is proved to yield better results in terms of accelerating scaling process as the dissolved $CO_2$ increases the solubility of calcium carbonate in water (Fathi et al. 2006; Knez and Pohar, 2005; Rathilal, 2004). The approximate total volume of the feed prepared was 8 L. The feed preparation set-up is illustrated in Figure 3.4.

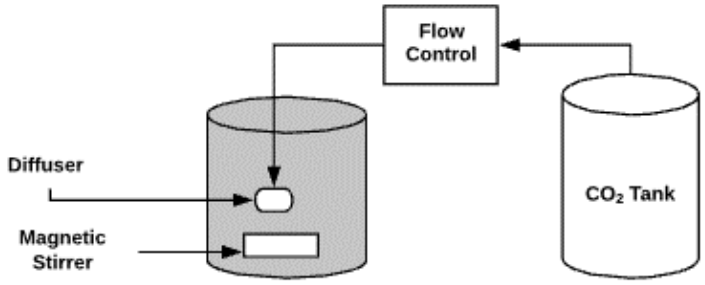


**Figure 3.4 Feed preparation Set-Up**

### 3.6.2 Operational Schedule for Feed Preparation

The desired total hardness of the feed was set to be approximately 400 mg/L as $CaCO_3$. The carbon dioxide gas was bubbled for two days; the hardness concentration, the pH and conductivity of the synthetic solution were tested. The pH of the water was adjusted to 6 to 7 to be neutral by exhausting a part of the dissolved $CO_2$ in the atmosphere using a strong stirring. The dissolving time for $CO_2$ could be reduced by

heating the water. The synthetic solution was then transferred into a different tank to run the experiment.

### 3.6.3 Apparatus for Accelerated Scale Formation

Accelerated scale formation on the heater element was carried out in a four different experiment at different conditions. Two of the experiments, which included untreated water and magnetically treated water, were operated at temperature of 60°C and the other two experiments were operated at 30°C. The heating tank capacity in this experiment was 2 gallons (7.5 L) while the 7 L of the water was filled into the tank. The flow rate of the water passing through magnetic water treatment was set at 2.0 L/min using a peristaltic pump.

### 3.6.4 Operational Schedule for Accelerated Scale Formation

The four experiments operated for three to six days to build enough scale on the heating element. The conductivity and the pH of the water were monitored throughout the experiment to detect the nucleation time. The conductivity and pH are proportional to the water hardness and degassing of $CO_2$ in the solution respectively. Table 3.4 illustrates the operation schedule for the experiments. There's a variation in terms of sampling procedure for monitoring both parameters. Due to low operating temperature at 30 °C, the conductivity of the solution showed less difference in the first five hours of the experiments which indicates a slow nucleation and scale formation. Based on that, the samples were taken and tested in triplicate at three hours interval every 24 hours during the testing period to allow more time for the scale to be formed. Same procedure was followed with the magnetically treated water, however, the test lasted for six days to observe the difference in conductivity of the solution.

**Table 3.4 Operation Schedule for Accelerated Scale Formation**

| **Water Type** | **Temperature (Test Duration)** | **Sampling Frequency** |
|---|---|---|
| Untreated Water | 60 ˚C (3 days) | 1 per hour at the beginning of the first 5 hours of the test (50 mL) |
| Untreated Water | 30 ˚C (3 days) | 3 per day at every 24 hours (50 mL) |
| Magnetically treated Water | 60 ˚C (3 days) | 1 per hour at the beginning of the first 5 hours of the test (50 mL) |
| Magnetically treated Water | 30 ˚C (6 days) | 3 per day at every 24 hours (50mL) |

At the end of the test, the solids were separated from the solution through the filtration process, the pH, and the conductivity were analyzed to evaluate the difference between the initial and final readings. The scale formed on the element and tank were scrapped off using a stainless-steel tool and measured. All samples were collected and characterized with XRD and SEM analysis.

# Chapter 4 Results and Discussion

## 4.1 Introduction

Experiments were performed to investigate the scale formation build-up on water heater elements with and without the use of AkwaMag device. Water Heater Simulation test, which included experiment with a tank with 70.4 $in^2$ of exposed iron and experiment with a tank with little exposure of iron, were carried out to quantify the amount of scale formed. From the experiment with a tank with 70.4 $in^2$ of exposed iron, the calcium carbonate and iron-containing compounds were present on untreated and magnetically treated water tanks. From the experiment with a tank with little exposure of iron, the reduction of calcite was observed under the effect of magnetic field.

The accelerated scale formation illustrated the reduction of calcite in both water types and temperature. However, the formation of aragonite was favored in high temperature condition in supersaturation condition.

## 4.2 Water Heater Simulation

This section provides the results from the water heater simulation tests, including influent water quality and scale formation analysis for the experiments with a tank with 70.4 $in^2$ of exposed iron , and with a tank with little exposure of iron. The influent water quality including total hardness and conductivity were monitored throughout the testing period. Tap water and magnetically treated water samples were taken after the experiment with exposed iron in the tank and detected for standard elements (Iron and Manganese) and also examined to identify if there appear to be different/unknown elements that is being added to the magnetically treated water as it passes through a magnetic treatment unit.

The scale deposits formed on the untreated and magnetically treated tap water heater elements and tanks were collected, measured, and characterized. The XRD measurement was only performed on the samples that had a sufficient amount of scale formed to be analyzed in the XRD equipment provided by the nanoscience laboratory. In the experiment with a tank with 70.4 $in^2$ of exposed iron, the samples analyzed were from the tanks only while in the experiment with a tank with little exposure of iron, the samples analyzed were from the tanks and the water heater elements. SEM analysis was only performed on the scale deposit formed in the water heater elements from both experiments.

### 4.2.1 Total Hardness and Conductivity of Influent Water

The influent water quality from the experiments with a tank with 70.4 $in^2$ of exposed iron and with a tank with little exposure of iron were monitored for hardness and conductivity throughout the testing period. Water samples were collected at the tap water faucet, and the influent untreated and magnetically treated water as it entered the tank respectively as shown in Figures 4.1.and 4.2.

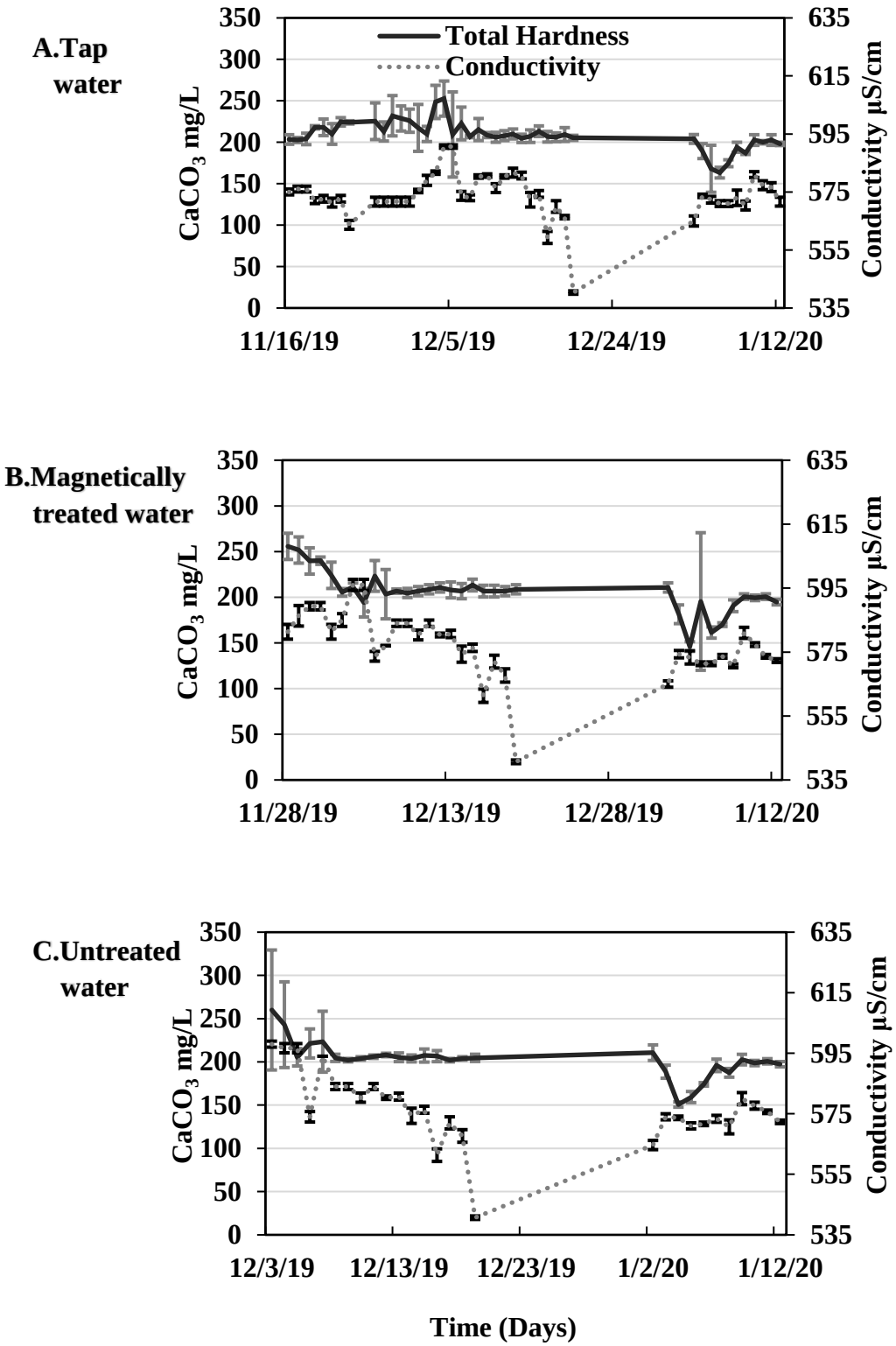


**Figure 4.1 Influent water quality results from the experiment with a tank with 70.4 in$^2$ of exposed iron of (A) Tap water, (B) Magnetically treated water, (C) Untreated water**

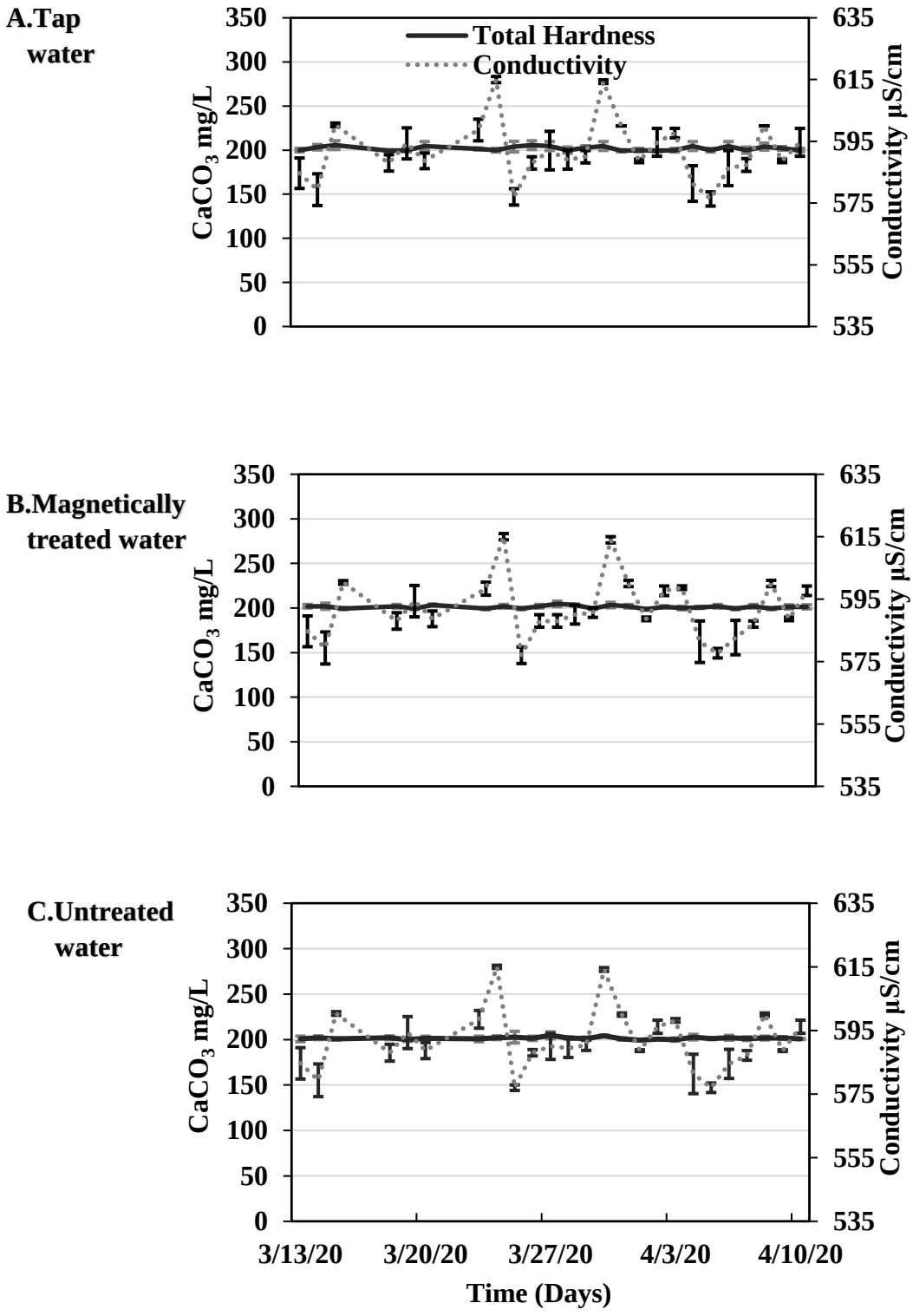


**Figure 4.2 Influent water quality results from the experiment with a tank with little exposure of iron of (A) Tap water, (B) Magnetically treated water, (C) Untreated water**

As shown in the previously provided figures, the influent total hardness and the conductivity of the solution did not change over the time. The statistical analysis using two-tail test (Dowdy et al. 2004) showed that the means of total hardness and conductivity are not statistically different between, tap water, magnetically treated water and untreated water. Regression slope analysis showed that the there was a slight decline in the concentration over time of the three types of water. Also, it showed a slight decline in the conductivity over time for magnetically treated water and untreated water.

### 4.2.2 Influent Iron and Manganese and other Different/Unknown Elements

The concentrations of Iron and Manganese and other unknown elements present in the influent water were determined by using ICP-MS analysis and semi-quantitative elemental analysis to confirm that there is no obvious dissolution of a trace element from the AkwaMag device that may be an indicator of a "hidden" template-induced precipitation. The water samples were collected at the tap water faucet and the influent magnetically treated water as it entered the tank. Table 4.1. lists the results of ICP-MS analysis for each water type and Figure 4.3 shows the semi-quantitative analysis results.

**Table 4.1 ICP-MS Analysis**

| Sampling Location | Iron (µg/L) | Manganese (µg/L) | Sampling date |
|---|---|---|---|
| **Tap water collected at faucet** | 6.42 | 2.40 | 02/14/2020- |
| **Influent magnetically treated water collected as it entered the tank** | 9.07 | 2.75 | 02/14/2020 |

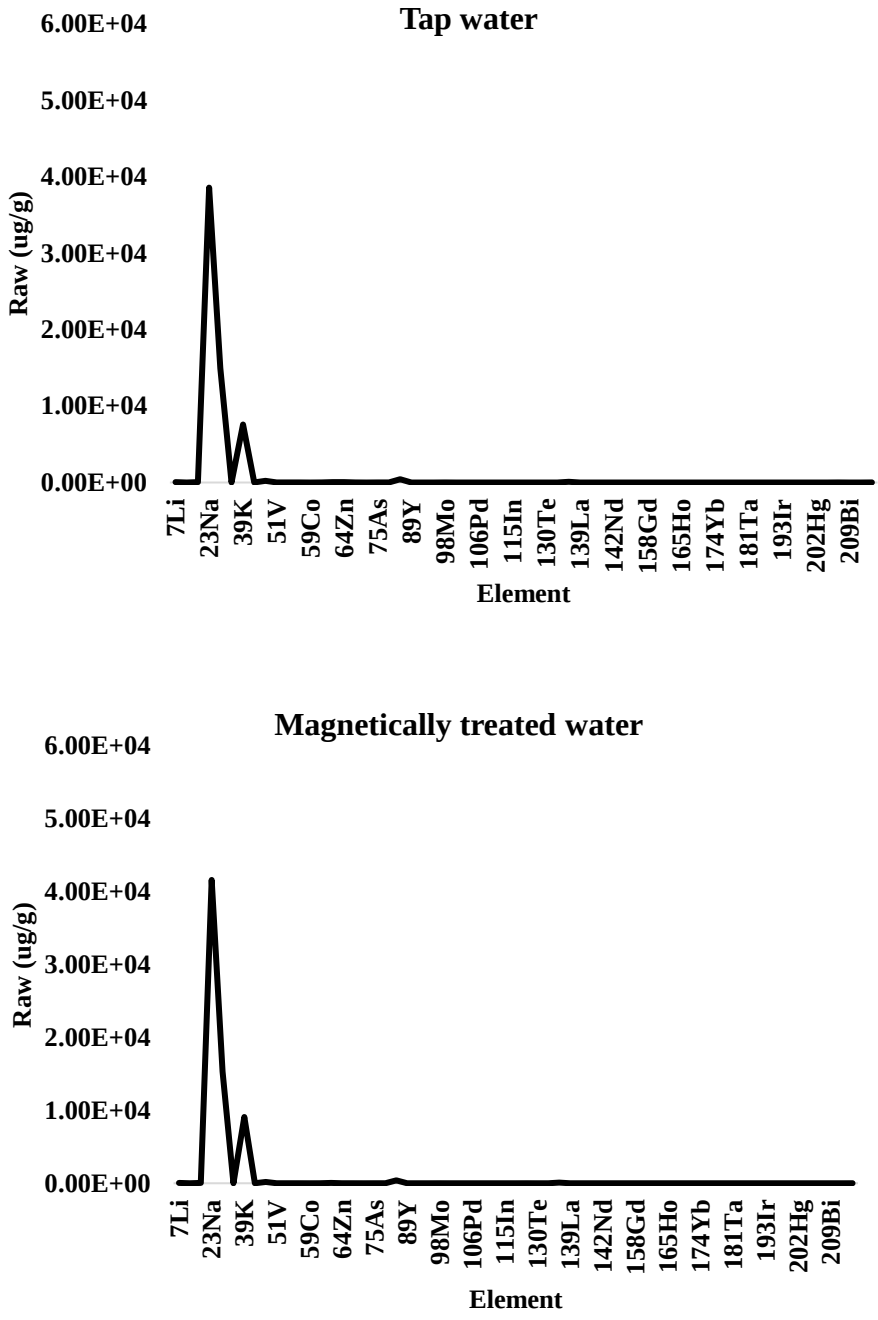


**Figure 4.3. Semi-quantitative results for different elements**

Based on the ICP-MS results, the concentrations of iron and manganese in the magnetically treated water is slightly higher than the tap water. In Figure 4.3, most of the elements have similar raw concentration between the tap water and magnetically treated water. However, sodium is slightly higher in the magnetically treated water sample.

Tap water was the first sample collected at the faucet by the time the water heater simulation experiment began, while the magnetically treated water sample were collected near the influent pipe as it entered and filled the tank up to the drain line for five minutes. A 5-minute detention time could possibly be associated with the increase in iron and manganese concentrations in the magnetically treated water sample. In addition, not flushing the water faucet for several minute prior starting the experiment and sampling could cause sediment/precipitant slowly builds up at the bottom of the water main over time, which will influence the overall water quality including iron and manganese.

### 4.2.3 Analysis of precipitates with a tank with 70.4 $in^2$ of exposed iron and with a tank with little exposure of iron

The precipitate that had gradually formed during the water heater simulation test were collected at the end of each experiment from the tank filtered and dried to find the mass of the solid as shown in Figure 4.4. The scale deposits formed on the water heater elements, as shown in Figure 4.5, were scrapped off and measured to find the mass. The color of the solid formed is mainly red which implies the presence of iron impurities in the samples.

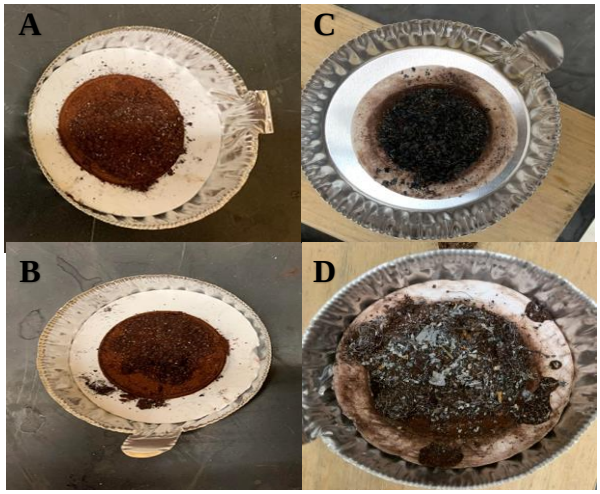


**Figure 4.4 Solids formed from the experiment with a tank with 70.4 $in^2$ of exposed iron of (A) Untreated water tank (B) Magnetically treated water tank, and the experiment with a tank with little exposure of iron of (C) Untreated water tank (D) Magnetically treated water tank**

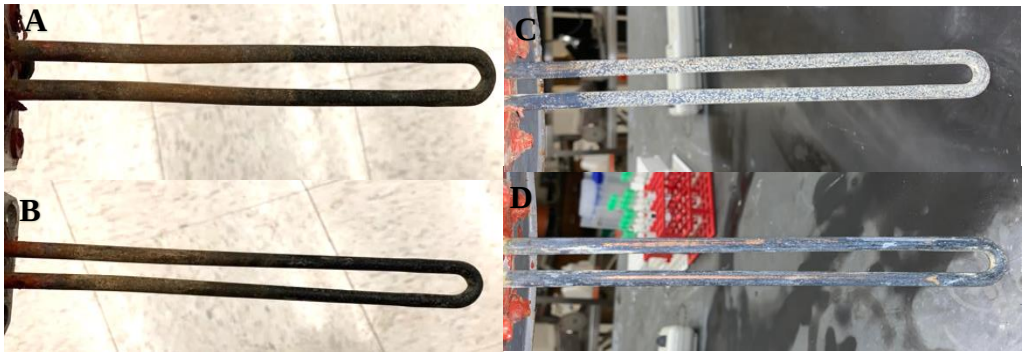


**Figure 4.5 Scale formed on heater element from the experiment with a tank with 70.4 $in^2$ of exposed iron of (A) Untreated water (B) Magnetically treated water, and from the experiment with a tank with little exposure of iron of (C) Untreated water (D) Magnetically treated water**

The difference in the amount of scale build-up on each heater element from the experiment with a tank with 70.4 $in^2$ of exposed iron is not clear due to the presence of iron impurities which inhibited the scale formation. However, the texture of the magnetically treated tap water heater element was smoother than the untreated tap water.

After coating the metal pail to run the experiment with a tank with little exposure of iron, the scale-build up increased significantly on the untreated water heater element. The texture of the untreated water heating element was rough with more mass of scale build-up.

The mass of solid formed on the untreated water tank is more than the magnetically treated water, which suggests that the mass of iron in each water is either similar or higher in the magnetically treated tap water. The amount of iron presented on each tank for experiments with a tank with 70.4 $in^2$ of exposed iron and with a tank with little exposure of iron is approximated and presented in Appendix B. Table 4.2 lists the mass of solid and scale formed from each experiment. The mass of scale formed on the magnetically treated water heater element was significantly reduced compared to untreated water heater element.

**Table 4.2 Mass of solid and scale formed**

| Location | Experiment with a tank with 70.4 $in^2$ of exposed iron | Experiment without significant exposed iron in tank |
|---|---|---|
| **Untreated water tank** | 1.35 (g) | 1.01 (g) |
| **Magnetically treated water tank** | 1.09 (g) | 0.52 (g) |
| **Untreated water heater element** | - | 0.26 (g) |
| **Magnetically treated water** | - | 0.017 (g) |

The scale formed were further analyzed using X-Ray Diffraction analysis. The X-ray diffractogram of the crystals obtained for each sample are provided in Appendix E,

where the peaks for each compound formed are distinguished with different colors. Experimental data are imported into ICDD (International Commission for Diffraction Data) powder diffraction file (PDF) database. The identification of crystalline phase for each compound was performed by the comparison of d values in the diffractogram with ICDD PDF database containing reference patterns. The file number of PDF card is listed next to each compound. The PDF card contains information regarding compound and mineral name, data on diffraction pattern where the three strongest lines are bolded, crystallographic and other data. The detailed PDF cards for each compound are provided in Appendix E.

Table 4.3 lists the results of X-ray diffraction analysis of the different proportions of compounds and their corresponding crystalline phase detected on sample collected from the tanks from the experiment with a tank with 70.4 $in^2$ of exposed iron at 60 °C. Calcite was mainly detected on the untreated tap water sample, while other carbonate and iron-containing compounds were detected on both water types. Neither calcite nor aragonite were detected in magnetically treated water sample. A study has shown that trace amount of $Fe^{3+}$ inhibits the growth of calcite in the presence of a magnetic field, which explains the absence of calcite in the magnetically treated water (Herzog et al. 1989).

**Table 4.3 Composition (Est Wt. %) of solid formed at 60 °C from the experiment with a tank with 70.4 $in^2$ of exposed iron**

| Compound Name/ Crystalline Phase | Untreated water | Magnetically treated water |
|---|---|---|
| **Calcium Carbonate (Calcite)** | 29 | ND |
| **Calcium Magnesium Iron Carbonate (Dolomite)** | ND | 53 |
| **Magnesium Carbonate (Magnesite)** | 23 | 11 |
| **Magnesium Manganese Oxide (Hausmannite, magnesian)** | 15 | ND |
| **Calcium Hydroxide (Portlandite)** | 7 | 3 |
| **Iron Oxide Hydroxide (Maghemite)** | ND | 11 |
| **Magnesium Iron Oxide (Magnesioferrite)** | 14 | 16 |
| **Iron Oxide (Magnetite)** | 12 | 5 |

**ND: Not detected** .

Table 4.4 lists the results of X-ray diffraction analysis of the different proportions of compounds detected on samples collected from the tanks from the experiment with a tank with little exposure of iron at 60 °C. Calcite and magnesian were mostly detected on the untreated tap water sample while aragonite and calcite were mostly detected on the magnetically treated tap water. The composition of calcite in magnetically treated tap water decreased with an increase in aragonite.

**Table 4.4 Composition (Est Wt. %) of solid formed at 60 °C from the experiment with a tank with little exposure of iron.**

| Compound Name/Crystalline Phase | Untreated water | Magnetically treated water |
|---|---|---|
| **Iron Oxide (Magnetite)** | 6 | 5 |
| **Magnesium Iron Oxide (Magnesioferrite)** | 6 | 7 |
| **Calcium Magnesium Carbonate (Calcite, Magnesian)** | 36 | 6 |
| **Calcium Carbonate (Calcite)** | 27 | 31 |
| **Magnesium Carbonate (Magnesite)** | 6 | ND |
| **Calcium Carbonate (Aragonite)** | 19 | 51 |

**ND: Not detected**

The composition of iron drastically decreased in the experiment with little exposure of iron in the tank. The metal pail corroded slightly towards the end of the experimental operation but had no effect on the scale formation in the heater elements.

Table 4.5 lists the results of X-ray diffraction analysis of the different proportions of compounds detected on samples collected from the heating elements from the experiment with a tank with little exposure of iron at 60 °C.

**Table 4.5 Composition (Est Wt. %) of scale formed in heating elements at 60 °C from the experiment with a tank with little exposure of iron.**

| Compound Name/Crystalline Phase | Untreated water | Magnetically treated water |
|---|---|---|
| **Magnesium Calcium Carbonate, (Calcite, Magnesian)** | 68 | ND |
| **Calcium Magnesium Carbonate (Calcite, Magnesian)** | ND | 36 |
| **Calcium Carbonate (Calcite)** | 12 | 25 |
| **Magnesium Carbonate (Magnesite)** | 5 | 12 |
| **Calcium Carbonate (Aragonite)** | 15 | 27 |

**ND: Not detected**

Calcite was the main constituent formed on the untreated water heating element which indicates the presence of hard scale. On the magnetically treated water heating element, the estimated weight percentage of aragonite increased by the use of the magnetic field in comparison with the untreated water. Results from XRD showed that there was a difference in the amount of the two crystallographic forms of $CaCO_3$ and other carbonate-containing compounds if the tap water was treated with a magnetic field. The increase in the amount of aragonite in the magnetically treated water samples was detected only on the experiments with a tank with little exposure of iron due to the reduction of the amount of iron-containing compounds in the sample.

The presence of metallic ions oriented from corrosion products made of iron affected the precipitation and scale formation of $CaCO_3$. Research has shown that the presence of metallic iron affects the crystallization process and the growth of crystal through adsorption of iron onto the active growth sites available on the surface of the crystals (Muryanto, 2002). High proportions of iron containing compounds presented in the tank retarded the crystal growth process in the experiment with a tank with 70.4 $in^2$ of exposed iron, which induced the scale reduction on the heating element. While in the experiment with a tank low levels of iron exposed in the tank, scale formation on heating element was not suppressed. Even though the amount of dissolved iron in both cases were not measured, other several studies has shown that higher concentrations of iron, results in more iron being adsorbed into crystal surface which reduces the mass of scale formed on heated surface and increase the precipitation of scale in the bulk solution (Muryanto, 2002; Muryanto et al. 2012; Pernot et al. 1998).

### 4.2.4 Scanning Electron Microscope (SEM) Images

Samples of precipitates from the water heater elements were scrapped off and observed under the Electron Microscope to identify the structure of the scale formed. Figure 4.6 illustrates the morphology of the scale formed on the untreated and magnetically treated water heater elements respectively.

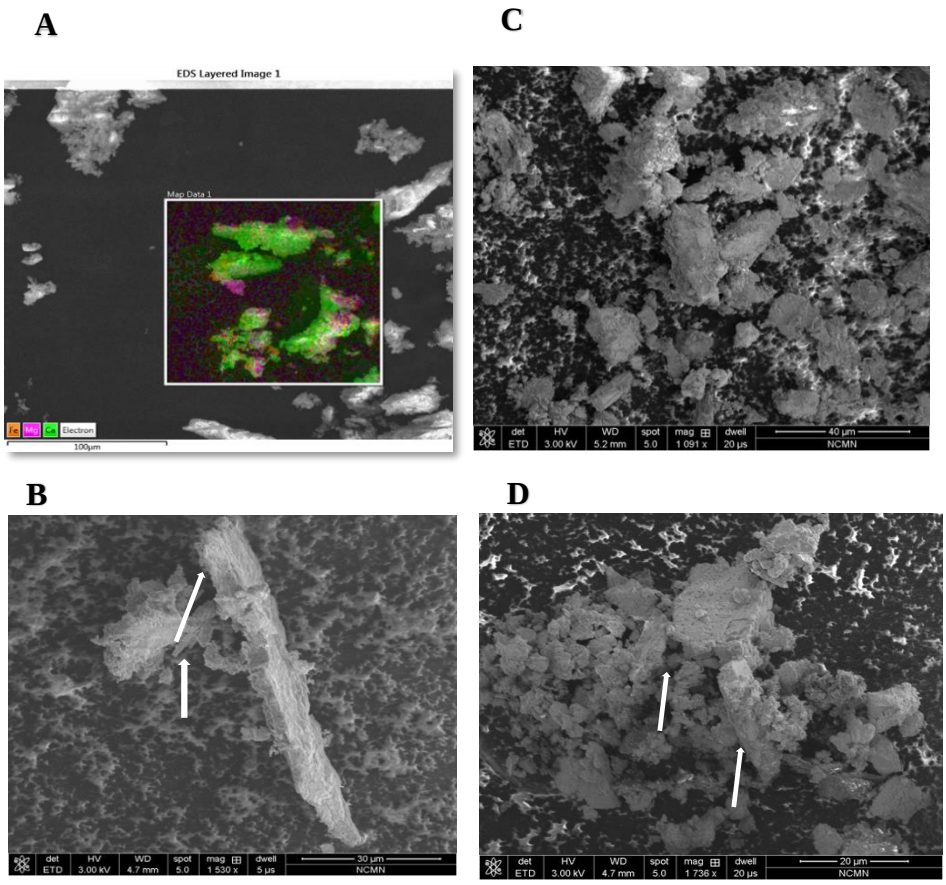


**Figure 4.6 SEM Image of heating element from the experiment with a tank with 70.4 in$^2$ of exposed iron of (A) Untreated water (Electron Layer Image), (B) Magnetically treated water, and from the experiment with a tank with little exposure of iron of (C) Untreated water (D) Magnetically treated water**

As shown in Figure 4.6 (A), the scale formed constitutes mainly of calcium with small proportions of magnesium and iron. The crystal shape of the scale formed appeared

to be with no substructure due to precipitation occurring on many nucleation sites, which then combines into a larger particle with no substructure (Cho et al. 2005). While in Figure 4.6 (B), the crystal shape of aragonite was detected under the microscope (white arrow). On the untreated water from the experiment with a tank with little exposure of iron, the crystal shape of calcite appears to be in a clustered appearance or are near cubic shape. The crystal shape of calcite and aragonite from the SEM analysis were similar to those found in literature (Ni and Ratner, 2008; Ogino et al. 1987).

### 4.3 Accelerated Experimental Scale Simulation

In this study, the influent water quality of the synthetic supersaturated calcium carbonate solution was prepared and tested for total hardness, pH, and conductivity for untreated water and magnetically treated water. The effect of induction time, which is between 6 days to 3 hours at 60 °C and 30 °C were examined for both water types by monitoring the conductivity of the solution over time. The proportion of calcite and aragonite as well as the morphology of the scale formed at 60 °C and 30 °C were determined by XRD and SEM analysis.

#### 4.3.1 Effect of pH with respect to Time

Figures. 4.7 shows how the pH of both water types in the reactor changes with respect to time at two different temperatures, 60°C and 30 °C, 30 minutes after temperature stabilization in the reactor. At 60 °C, the pH was monitored within the first five hours of the testing. At 30 °C, the pH readings were taken within an hour interval for three hours (1:30 PM, 2:30 PM, and 3:30 PM) per day during the testing period for untreated and magnetically treated water.

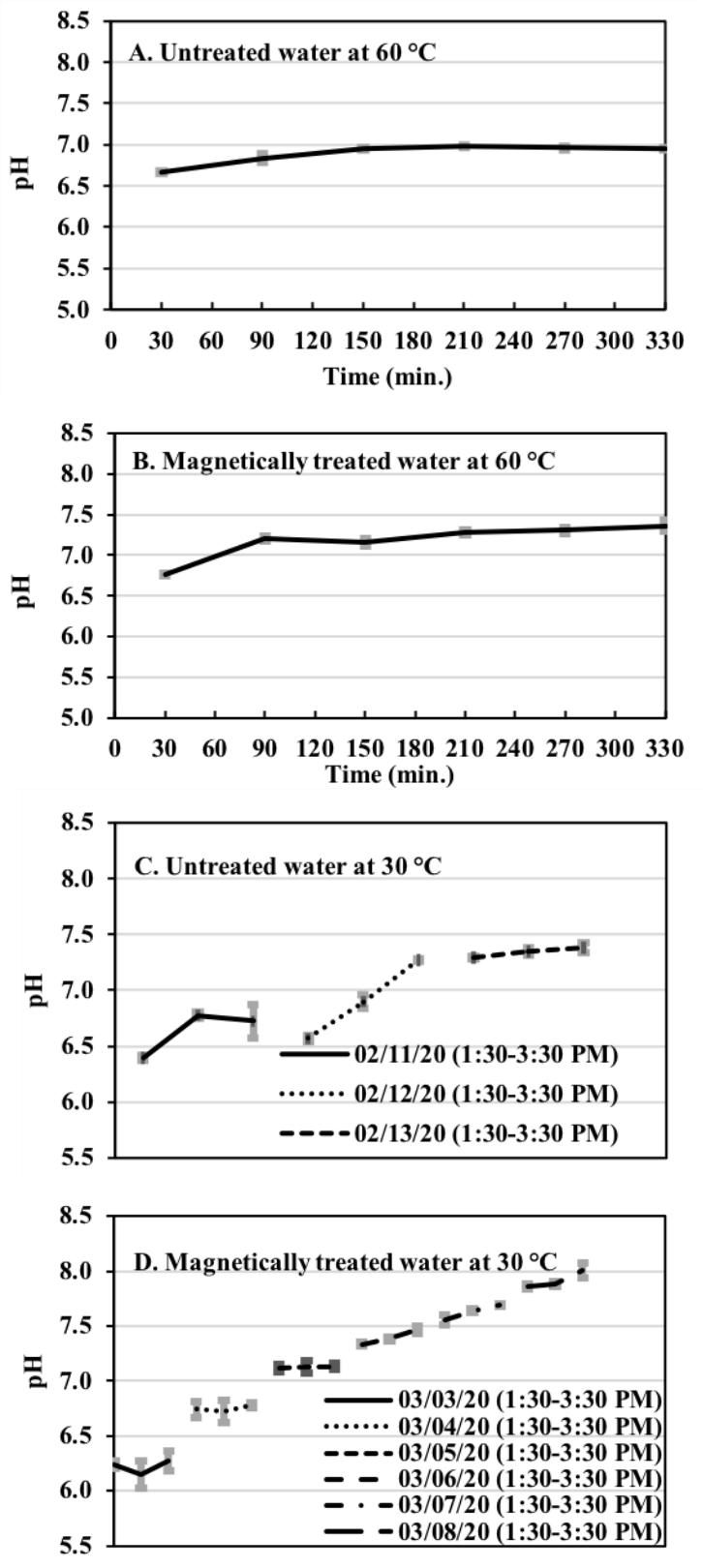


**Figure 4.7 Effect of pH on (A) untreated water at 60 °C (B) magnetically treated water at 60 °C and (C) untreated water at 30 °C (D) magnetically treated water at 30 °C**

As shown in the previously provided figures, the pH is increasing within the first 5 hours of the experiment, which indicates the degassing of carbon dioxide at 60°C. However, at 30°C the pH was slightly increasing each day. The degassing of carbon dioxide from the solution is directly proportional with the formation of calcium carbonate precipitants at both operating temperature over time.

### 4.3.2 Effect of Induction Time

The effect of induction time on both water types at 60 °C and 30 °C were monitored 30 minutes after temperature stabilization in the tank as shown in Figure 4.8 At 60 °C, the conductivity was monitored within the first five hours of the testing. At 30 °C, the conductivity readings were taken within an hour interval for three hours (1:30 PM, 2:30 PM, and 3:30 PM) per day during the testing period for untreated and magnetically treated water.

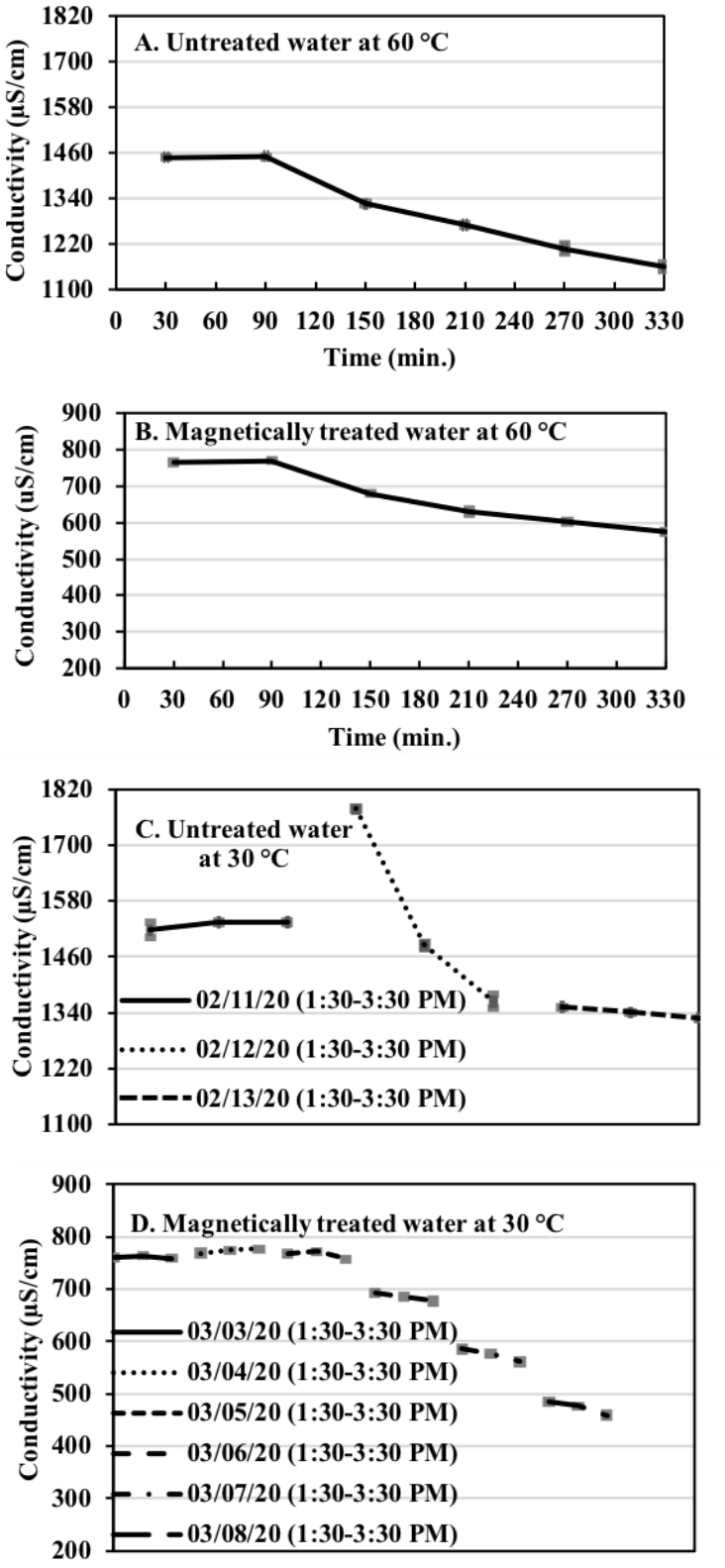


**Figure 4.8 Effect of Conductivity on (A) untreated water at 60 °C (B) magnetically treated water at 60 °C and (C) untreated water at 30 °C (D) magnetically treated water at 30 °C**

The conductivity readings over time of both water types is different due to the difference in the concentration of the calcium carbonate influent water as reported in Appendix C. Despite the difference in the conductivity readings, the trend is similar for both water types. At 60 °C the conductivity of the solution in reactor was significantly decreasing within the first 5 hours of the experiment. The abrupt decrease in the conductivity after 90 minutes indicates in the faster rate of nucleation and crystallization process at elevated temperature.

At 30 °C the conductivity of the solution was decreasing much slower for both water types. It took 3 days for the untreated water's conductivity to decrease while 6 days for magnetically treated water. This suggests that the induction time increases with decreasing the temperature which prolongs the onset of crystallization especially in the magnetically treated water at low temperature. In Day 2, the first sample of untreated water recorded showed a high value of conductivity due to the high temperature of the sample. This error is associated with the temperature controller which was operating somewhat higher than the set value.

### 4.3.4 X-Ray Diffraction and SEM analysis of the Accelerated Experimental Scale Simulation

The samples of scale from the heater element at each operating temperature were collected and analyzed by using XRD and SEM analysis. X-ray diffraction patterns of the crystals obtained from untreated and magnetically treated water samples at 60 °C are given in Figures 4.9 and 4.10 respectively while at 30 °C are provided in Appendix E.

The y-axis gives the peak intensity of the diffracted beam, which represents the atomic position in the crystal structure. The x-axis indicates the angle (2θ) at which the x-

ray beams were diffracted on the sample. The distance between planes of atoms in the sample that cause to diffraction peaks is called d-value and can be calculated from the 2θ values using Braggs Law. Some peaks are high in intensity than others because there is preferential growth of certain crystal orientation in the sample and are well crystallized. The experimental data/pattern represents in red while the graphical fit data of each reference phase represents in different colors corresponding to their respective PDF number.

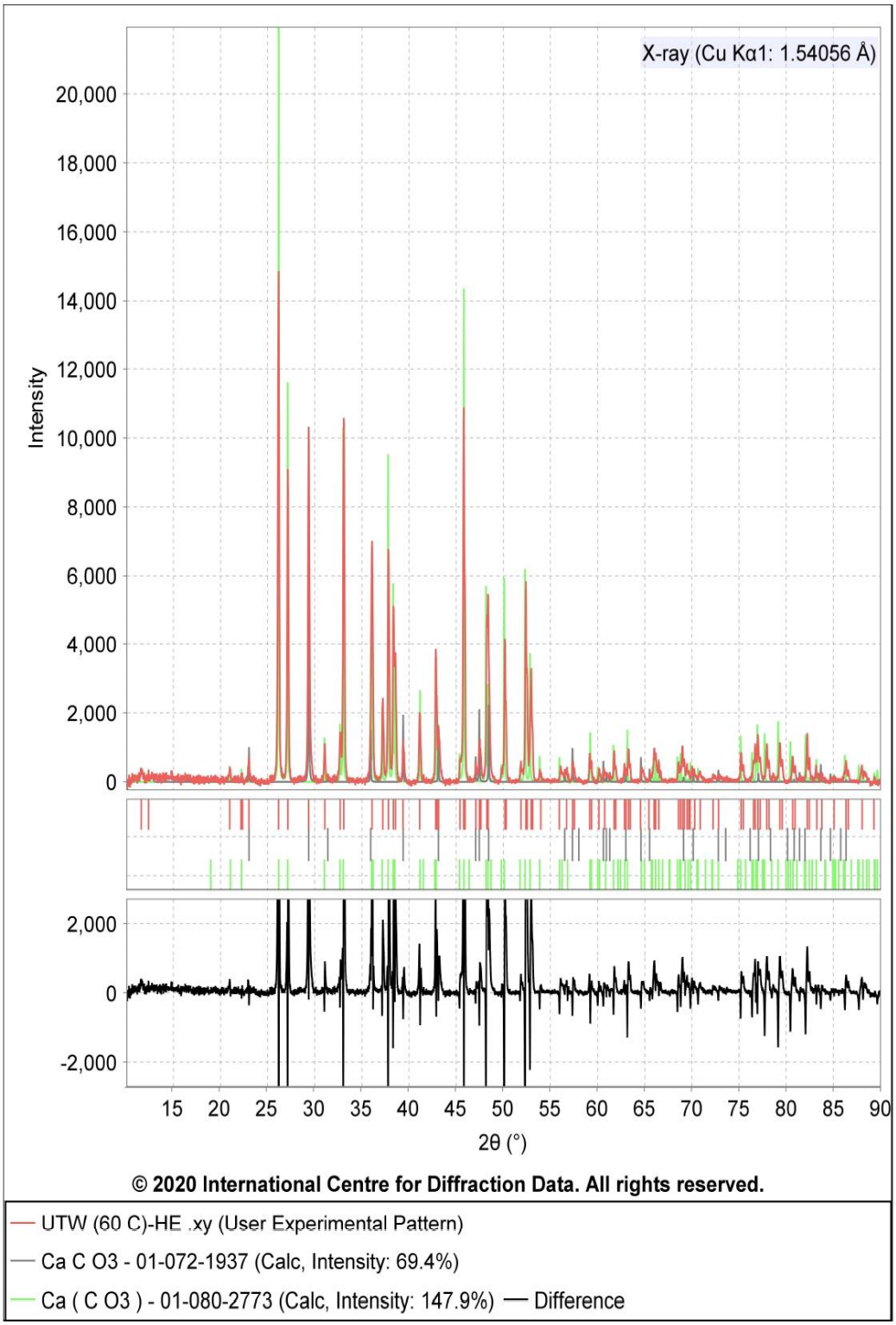


**Figure 4.9 XRD patterns of substances precipitated from Untreated Water (UTW) heating element (HE) at 60 °C. Aragonite-**PDF# 01-080-2773 **Calcite-**PDF# 01-072-1937

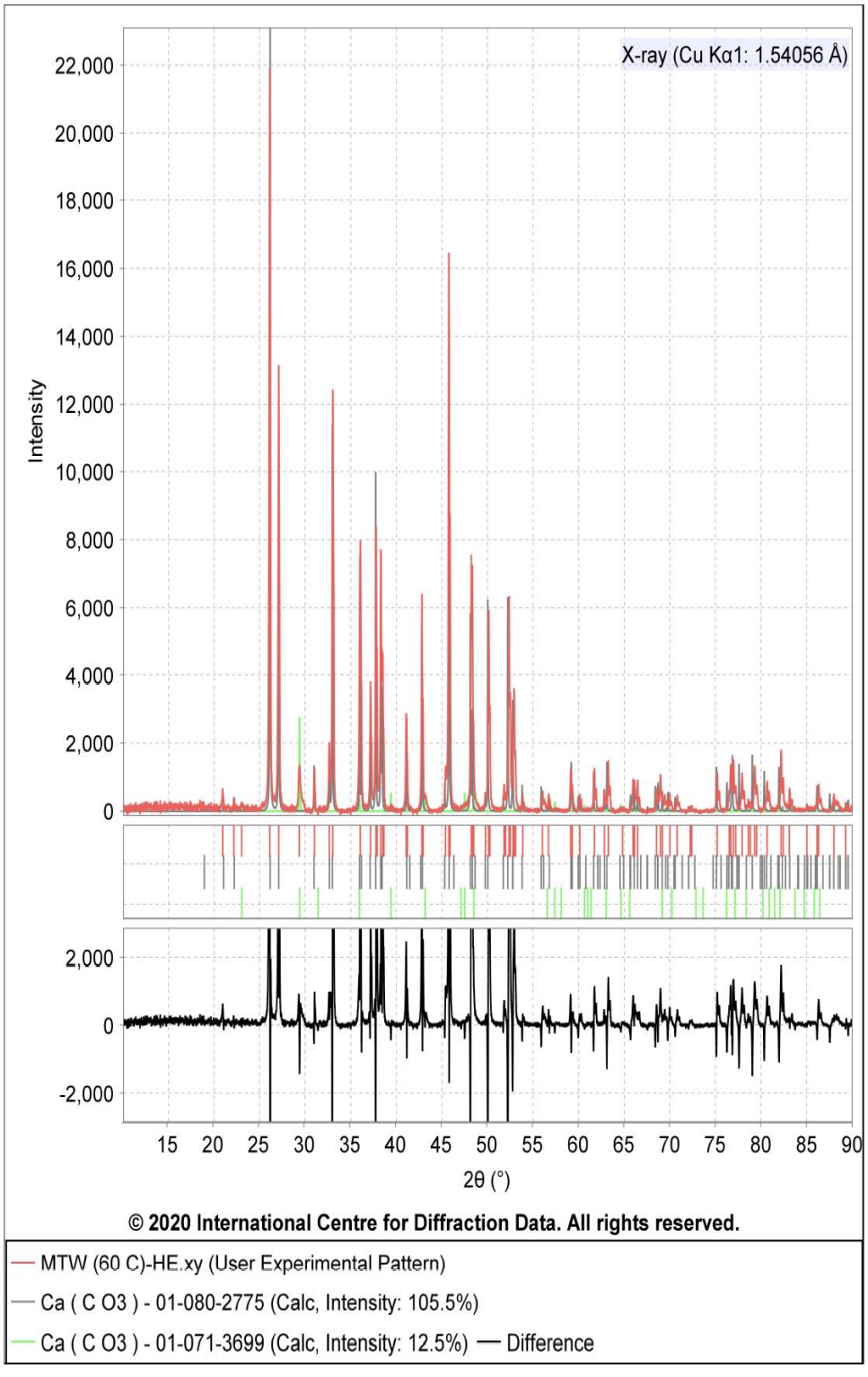


**Figure 4.10 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element (HE) at 60 °C. Aragonite**-PDF# 01-080-2775 **Calcite-** PDF# 01-071-3699

The figures above reveal that the crystals are aragonite and calcite. In Figure 4.9, aragonite formed at most intense peak of 26.17° 2θ (at d-value of 3.401 Å) while calcite formed at a most intense peak of 29.36° 2θ (at d-value of 3.038 Å). In Figure 4.10, aragonite formed at strongest peak of 26.19° 2θ (at d-value of 3.404 Å) while calcite formed at strongest peak of 29.39° 2θ (at d-value of 3.036 Å). The composition of each phase is estimated by the Reference Intensity Ratio method (RIR), in the ICCD database. It is determined by taking the ratio of the strongest line of the intensity for each phase of the strongest line of corundum, I/Ic. The PDF card of each are provided in Appendix E.

Table 4.6 lists the proportions of calcite and aragonite in both water types at 60 and 30 °C. The percentage of calcite is decreased in magnetically treated water at 60 °C which confirms the effect of magnetic field on the reduction of calcite formation. At 30 °C, aragonite was mostly formed in the magnetically treated water sample. At higher temperatures, the carbon dioxide was driven off at a faster rate and as a result, the precipitation was faster, favoring the aragonite structure.

**Table 4.6 Precipitates of scale formed composition at 60 and 30 °C**

| | **60 °C Est Wt. %** | | **30 °C Est Wt. %** | |
|---|---|---|---|---|
| **Compound Name/ Crystalline Phase** | **Untreated water** | **Magnetically treated water** | **Untreated water** | **Magnetically treated water** |
| **Calcium Carbonate (Aragonite)** | 86 | 96 | 92 | 100 |
| **Calcium Carbonate (Calcite)** | 14 | 4 | 8 | - |

.

The results provided in Table 4.6 were relatively similar between the two cases, favoring the formation of aragonite. The phase transformation in accelerated scale process depends on the level of supersaturation, which is different for different $CaCO_3$ polymorphs because they have different solubility products.

The supersaturation, Ω, depends on the ($Ca^{2+}$) and ($CO_3^{2-}$) ion activity according to the following equation:

$$\Omega = \frac{[Ca^{2+}][CO_3^{2-}]}{K_{so}} \qquad (4.1)$$

As the bulk solubility constant, $K_{so,}$ of vaterite, $K_{so}$ at 25 °C = $10^{-7.91}$, calcite, $K_{so}$ at 25 °C= $10^{-8.49}$ and aragonite, $K_{so}$ at 25 °C = $10^{-8.3}$ (Knez and Pohar, 2005). To initiate homogenous nucleation, the supersaturation must exceed critical value which is $\Omega_{critical}$ = 40 as reported by Gabrielli et al. (1999), this is governed mainly by degassing of $CO_2$ from the solution to increase the concentration of $CO_3^{2-}$. Several studies have shown that in supersaturated solution, calcite was predominantly formed at room temperature, while the formation of aragonite was favorable at higher temperature (Cherkas et al. 2018; Knez and Pohar, 2005). This finding is consistent with a previous study conducted by, Rathilal (2004) to investigate the scale formation on heated surface, with and without the use of magnetic water treatment device, between 30-80 °C. The formation of aragonite was predominant in both cases, and the reduction of calcite was observed under the effects of magnetic fields. The formation of calcite was suppressed at temperatures above 60 °C in both cases.

Figure 4.11 illustrates the SEM images of the scale formed at 60 °C and 30 °C of both water types. Aragonite has needle-like crystal structure while calcite had a clustered appearance or are near cubic shape.

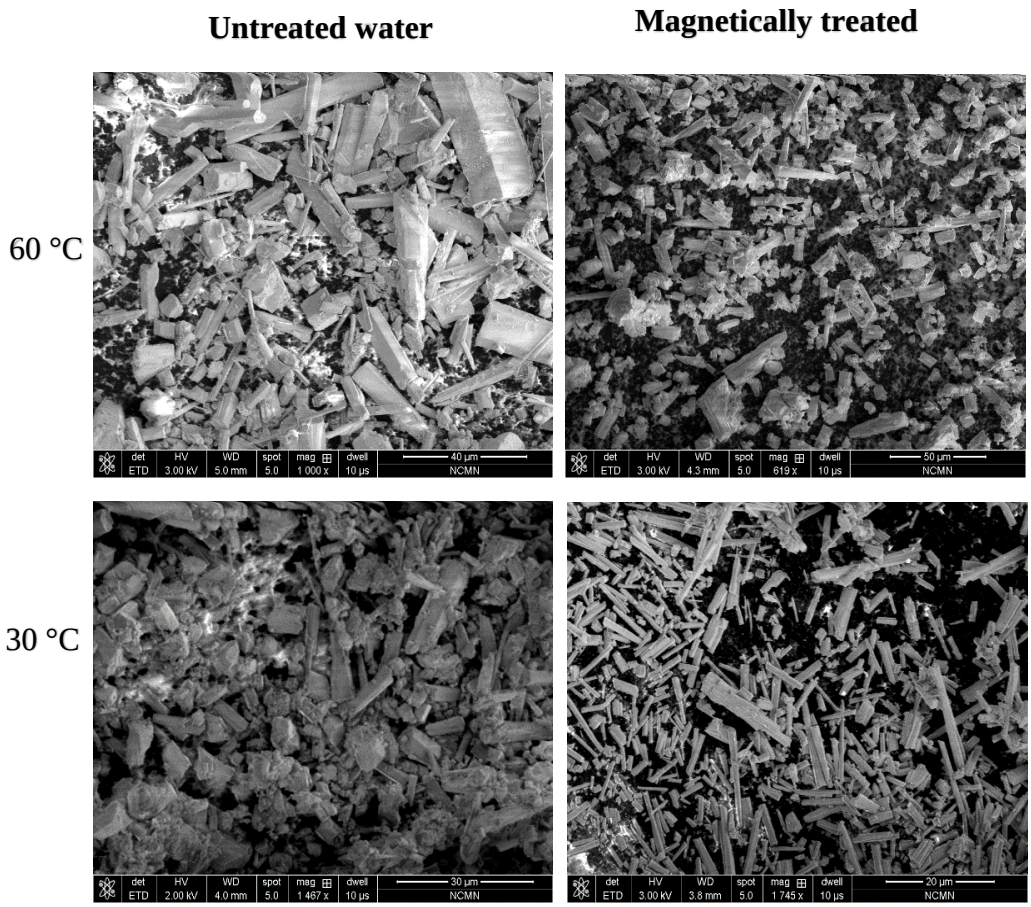


**Figure 4.11 SEM Images of Calcite and Aragonite**

The duration of the precipitation decreased as temperature was increased. The treated and untreated water samples gave rise to $CaCO_3$ precipitating in the aragonite form at both operating temperatures. The reduction of calcite is observed which indicates the effects of magnetic fields. Different proportions of calcite and aragonite can be observed in the SEM images provided in Figure 4.11. At 30 °C for magnetically treated water, aragonite is the only structure the can be observed which is confirmed by the results obtained from XRD analysis

# Chapter 5: Conclusion and Recommendation

## 5.1 Introduction

Scale formation is considered among the most significant problems affecting the performance and economics of industrial water systems especially in water heating systems, desalination plants and water treatment processes. Scale is made up of calcite, which is a hard scale. Softened water is often used to reduce scale build-up. However, the implication of using softened water is associated with the excess salt discharged by the water softener to the sanitary sewer, which affects the reuse of wastewater for agricultural and industrial purposes. Thus, the demand on non-salt alternatives devices is critical to reduce the impacts of water softener. The overall goal of this research was to examine the scale build-up and calcium carbonate polymorphs on heating elements from using a proprietary magnetic water treatment device, called AkwaMag, and compare it to "untreated" water. In addition, to evaluate the calcium carbonate polymorphs with and without the use of the magnetic water treatment device using a calcium carbonate supersaturated solution as a feed water. To accomplish this goal, several objectives needed to be met.

The first objective was to construct a water heating system to mimic a real hot water system to evaluate the scale build-up. This was accomplished by conducting water-heating tests with a tank with 70.4 $in^2$ of exposed iron and with a tank with little exposure of iron. Iron release from corrosive materials, like the metal pail that was used to mount the heater element, affects scale formation on the heating elements in contrast to the systems where corrosion resistant materials is being used. The amount of corrosive materials like iron in the tank affects the content and the mass of scale formed on heating elements. The second objective of this research was to perform an accelerated scale study

by using a supersaturated calcium carbonate solution as a feed at two operating temperatures 60 ˚C and 30 ˚C. The goal of this study was to have a sufficient amount of scale build-up on heating elements in a shorter time and compare the polymorphs of calcium carbonate at both temperatures with and without the use of AkwaMag device. The composition and morphology of the scale formed were characterized by using XRD and SEM analysis respectively.

**5.2 Key Conclusions**

Based on water heater simulation study where the system was exposed with iron in the tank, higher amount of iron resulted in the reduction of scale mass on heating elements. Scale were also formed at the bottom of both tanks, where the amount of scale formed on the untreated water tank was slightly higher than the magnetically treated water tank which affected the content of scale. The presence of iron containing compounds in the tank inhibited the presence of a soft type of scale, aragonite, on the magnetically treated water tank based on the results obtained from XRD analysis. However, SEM image of the magnetically treated water heating element showed the presence of aragonite.

The water heater simulation study from the experiment with a tank with little exposure of iron, showed the mass of scale was significantly reduced on treated heater element compared to untreated water heater element. Aragonite was formed on both untreated and magnetically treated water heating elements, but the composition of aragonite increased on the magnetically treated water heating elements based on the results obtained from the XRD analysis. Other compounds were also detected with XRD

found in both heating elements. SEM of both heating elements showed the presence of calcium carbonate polymorphs.

In accelerated scale study, the composition of aragonite was higher than calcite at 60 $^{\circ}$C and 30 $^{\circ}$C. However, the reduction of calcite was observed in the magnetically treated water, which indicates the effects of magnetic fields on suppressing calcite formation.

**5.3 Implications**

The results obtained in this study would be of interest to water and wastewater utilities considering low cost non-salt alternatives to ion exchange softening since the reduction of scale formation was observed under the effects of magnetic fields. The device might not be quite as good as an ion exchange water softener, but many industrial applications require a good but not perfect treatment system that is low cost and can be placed in-line before the equipment (parts rinse system, small water heater in isolated part of facility, etc.).The non-salt devices can reduce the amount of money used in purchasing salt for regenerating water softeners as well as reduce the time required for regular maintenance and cleaning.

**5.4 Recommendation for future work**

For future work, it is recommended to examine the effect of adding trace amounts of metal impurities in scale formation. Several research studies have shown that the presence of impurities affect the crystallization process, i.e., nucleation rate and crystal growth, of minerals like $CaCO_3$ and $CaSO_4$ (Muryanto, 2002; Sangwal, 1996). Effect of transition metals, that are normally found in trace amounts in mineral processing plants or released in certain magnetic devices (Coetzee et al. 1996; Muryanto et al. 2012) such as

Copper and Zinc, ($Cu^{2+}$, $Zn^{2+}$), on the nucleation rate and crystal morphology, can be investigated with and without the use of a magnetic device. The presence of these impurities can act as heterogenous nucleation centers that will eventually become the seeds for the formation of clustered scale crystal (Mosin and Ignatov, 2014; Tang et al. 2010).

A study conducted by Muryanto et al. (2012) showed that, the crystallization process is prolonged with increasing the concentration of $Cu^{2+}$, resulting in the reduction of the amount of scale produced. Another study by Chibowski et al. (2003) showed the amount of $CaCO_3$ deposited on copper plate was reduced in the absence of magnetic fields between 20-80 °C, and greater reduction was observed in the presence of magnetic field. However, MacAdam and Parsons (2009) observed that the inhibitory effects of zinc on scale formation was more significant than copper resulted to a 35% scale reduction on mass basis. This finding is consistent with previous studies on the great potentiality of zinc as a scale inhibitor (Coetzee et al. 1998; Parsiegla, 1998).

The feed (tap water) should be tested for its saturation index as an indicator of the degree of saturation of water with respect to calcium carbonate so that the precipitation takes a shorter time to occur within a week. This helps to identify if the water is under saturated, neutral or supersaturated with respect to calcium. If the solution is the supersaturated, the rate of scale formation increases producing a sufficient amount of scale build-up on the heating element, which could be further, analyzed with XRD and SEM analysis.

Besides determining the saturation index of the feed, increasing the rate of heat transfer from the heating element could accelerate the scale formation process. By using a

heating element with a greater surface area, the rate of heat transfer would increase since it is directly proportional to the surface area. Thus, more scale will be formed due high rate of heat being transferred from the element to the solution in the tank.

It is also recommended to test the water in three situations (tap water treated with the magnetic device, untreated tap water, soft water) at 60 $^{\circ}$C and 80 $^{\circ}$C. This will help to identify the difference in the type of scale formed for untreated tap water and the magnetically treated water, and the magnetically treated water and soft water would form less scale on the heating element surface. The effect of temperature would be helping to identify the different of mass formed in each situation.

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## APPENDIX A: Statistical Analysis for Water Heater Simulation Influent Water Quality

### Unpaired T- test for influent water quality

**Objective:**

To determine if there is a significant difference between the means of:

(1) Tap water and Magnetically treated water ( Total Hardness & Conductivity)

(2) Tap water and Untreated water ( Total Hardness & Conductivity)

**Assumptions:**

1. Unequal variances between the two data set
2. Independent means
3. Significance Level: 0.05

**Equations (MathPortal, 2020)**

$$t = \frac{\overline{X_1} - \overline{X_2}}{S_{\bar{X}_1 - \bar{X}_2}}$$

$$S_{\bar{X}_1 - \bar{X}_2} = \sqrt{\frac{S_{X_1}^2}{n_1} + \frac{S_{X_2}^2}{n_2}}$$

$$d.o.f = \frac{\left(\frac{S_{X_1}^2}{n_1} + \frac{S_{X_2}^2}{n_2}\right)^2}{\frac{\left(\frac{S_{X_1}^2}{n_1}\right)^2}{n_1 - 1} + \frac{\left(\frac{S_{X_2}^2}{n_2}\right)^2}{n_2 - 1}}$$

$$S_{X_1}^2 = \frac{1}{n-1}\sum_{i=1}^{n}\left(X_{1i} - \overline{X_1}\right)^2$$

$$S_{X_2}^2 = \frac{1}{n-1}\sum_{i=1}^{n}\left(X_{2i} - \overline{X_2}\right)^2$$

$\overline{X_1}$ = Mean of data for group 1
$\overline{X_2}$ = Mean of data for group 2
$S_{X_1}$ = Standard deviation of data for group 1
$S_{X_2}$ = Standard deviation of data for group 2
$d.o.f$ = degrees of freedom
$n_1$ = Total number of values in first dataset
$n_2$ = Total number of values in second dataset

**Table A.1. Unpaired T- test to compare Tap Water and Magnetically Treated Water (From the experiment with a tank with 70.4 $in^2$ of exposed iron ).**

| | Total Hardness $CaCO_3$ mg/L | | Conductivity µS/cm | |
|---|---|---|---|---|
| | **Tap Water** | **Magnetically Treated Water** | **Tap Water** | **Magnetically Treated Water** |
| **Mean** | 208.9 | 205.9 | 573.7 | 577 |
| **Variance** | 297.3 | 498.3 | 63.3 | 105.7 |
| **Stand. Dev.** | 17.3 | 22.3 | 8 | 10.3 |
| **n** | 43.0 | 33.0 | 43 | 33 |
| **t** | 0.6 | | -1.5 | |
| **d.o.f** | 59 | | 59 | |
| **Critical value from T-table** | 2.0 | | 2 | |
| **Conclusion** | \|t\| is smaller than critical value (0.6<2.0), so the means are not significantly different. | | \|t\| is smaller than critical value (1.5<2.0), so the means are not significantly different. | |

**Table A.2 Unpaired T- test to compare Tap Water and Untreated Water (From the experiment with a tank with 70.4 $in^2$ of exposed iron ).**

| | Total Hardness $CaCO_3$ mg/L | | Conductivity µS/cm | |
|---|---|---|---|---|
| | **Tap Water** | **Untreated Water** | **Tap Water** | **Untreated Water** |
| **Mean** | 208.9 | 202.8 | 573.7 | 576.8 |
| **Variance** | 297.7 | 435.6 | 63.3 | 137 |
| **Stand. Dev.** | 17.3 | 20.9 | 8 | 11.7 |
| **n** | 43.0 | 28.0 | 43 | 28 |
| **t** | 1.3 | | -1.2 | |
| **d.o.f** | 50.0 | | 43 | |
| **Critical value from T-table** | 2.0 | | 2 | |
| **Conclusion** | \|t\| is smaller than critical value (1.3<2.0), so the means are not significantly different. | | \|t\| is smaller than critical value (0.3<2.0), so the means are not significantly different. | |

**Table A.3. Unpaired T- test to compare Tap Water and Magnetically Treated Water (From the experiment with a tank with little exposure of iron).**

| | **Total Hardness $CaCO_3$ mg/L** | | **Conductivity µS/cm** | |
|---|---|---|---|---|
| | **Tap Water** | **Magnetically Treated Water** | **Tap Water** | **Magnetically Treated Water** |
| **Mean** | 202.0 | 201.0 | 591.8 | 591.9 |
| **Variance** | 6.3 | 2.3 | | |
| **Stand. Dev.** | 2.5 | 1.7 | 9.71 | 9.81 |
| **n** | 25 | 25 | 25 | 25 |
| **t** | 1.6 | | -0.04 | |
| **d.o.f** | 42.0 | | 48 | |
| **Critical value from T-table** | 2.00 | | 2.00 | |
| **Conclusion** | \|t\| is smaller than critical value (1.6<2.0), so the means are not significantly different. | | \|t\| is smaller than critical value (0.04<2.0), so the means are not significantly different. | |

**Table A.4 Unpaired T- test to compare Tap Water and Untreated Water (From the experiment with a tank with little exposure of iron.).**

| | **Total Hardness $CaCO_3$ mg/L** | | **Conductivity µS/cm** | |
|---|---|---|---|---|
| | **Tap Water** | **Untreated Water** | **Tap Water** | **Untreated Water** |
| **Mean** | 202.0 | 201.5 | 591.8 | 591.8 |
| **Variance** | 6.25 | | 94.2 | 19.4 |
| **Stand. Dev.** | 2.5 | 1.29 | 9.71 | 9.7 |
| **n** | 25 | 25 | 25 | 25 |
| **t** | 0.92 | | -0.01 | |
| **d.o.f** | 36 | | 48 | |
| **Critical value from T-table** | 2.04 | | 2 | |
| **Conclusion** | \|t\| is smaller than critical value (0.92<2.04), so the means are not significantly different. | | \|t\| is smaller than critical value (0.01<2.0), so the means are not significantly different. | |

## Regression Slope analysis for influent water quality

**Table A.5 Regression Slope for influent water Total Hardness $CaCO_3$ mg/L (From the experiment with a tank with 70.4 $in^2$ of exposed iron)**

| | Tap Water | Untreated Water | Magnetically Treated Water |
|---|---|---|---|
| **Linear regression Eqn** | y = -0.605x + 26715 | y = -0.9432x + 41535 | y = -1.0314x + 45397 |
| **Slope** | -0.61 | -0.94 | -1.03 |
| **standard error of the slope (SE)** | 0.12 | 0.22 | 0.19 |
| **t = slope/SE** | -5.13 | -4.22 | -5.52 |
| **d.o.f = n-2** | 41.00 | 26.00 | 31.00 |
| **Critical value from T-table** | 2.03 | 2.06 | 2.04 |
| **Conclusion** | \|t\| is greater than critical value (5.13>2.03), the slope is significantly different from zero | \|t\| is greater than critical value (4.22>2.06), the slope is significantly different from zero | \|t\| is lgreater than critical value (5.22>2.04), the slope is significantly different from zero |

**Table A.6 Regression Slope for influent water Conductivity µS/cm (From the experiment with a tank with 70.4 $in^2$ of exposed iron)**

| | Tap Water | Untreated Water | Magnetically Treated Water |
|---|---|---|---|
| **Linear regression Eqn** | y = -0.0454x + 2561.7 | y = -0.3678x + 16693 | y = -0.3238x + 14766 |
| **Slope** | -0.05 | -0.37 | -0.32 |
| **standard error of the slope (SE)** | 0.07 | 0.15 | 0.11 |
| **t = slope/SE** | -0.65 | -2.52 | -3.01 |
| **d.o.f = n-2** | 41.00 | 26.00 | 31.00 |
| **Critical value from T-table** | 2.03 | 2.06 | 2.04 |
| **Conclusion** | \|t\| is smaller than critical value (0.65<2.03), the slope is equal to zero | \|t\| is greater than critical value (2.52>2.06), the slope is significantly different from zero | \|t\| is greater than critical value (3.01>2.06), the slope is significantly different from zero |

**Table A.7 Regression Slope for influent water Total Hardness $CaCO_3$ mg/L (From the experiment with a tank with little exposure of iron)**

| | Tap Water | Untreated Water | Magnetically Treated Water |
|---|---|---|---|
| **Linear regression Eqn** | y = -0.0295x + 1497 | y = -0.0014x + 261.12 | y = -0.0208x + 1115.7 |
| **Slope** | -0.0295 | | |
| **standard error of the slope (SE)** | 4.54 | 0.03 | 0.04 |
| **t = slope/SE** | -0.001 | -1.570 | -12.889 |
| **d.o.f = n-2** | 23 | 23 | 23 |
| **Critical value from T-table** | 2.06 | 2.06 | 2.06 |
| **Conclusion** | \|t\| is smaller than critical value (0.001<2.06), the slope is equal to zero | \|t\| is smaller than critical value (1.570<2.06), the slope is equal to zero | \|t\| is greater than critical value (12.889<2.06), ), the slope is significantly different from zero |

**Table A.8 Regression Slope for influent water Conductivity µS/cm (From the experiment with a tank with little exposure of iron)**

| | Tap Water | Untreated Water | Magnetically Treated Water |
|---|---|---|---|
| **Linear regression Eqn** | y = 0.0231x - 421.87 | y = 0.0347x - 931.6 | y = 0.0463x - 1441.3 |
| **Slope** | 0.0231 | 0.0347 | 0.0463 |
| **standard error of the slope (SE)** | 0.23 | 0.24 | 0.24 |
| **t = slope/SE** | 0.4028 | 0.599 | 0.8 |
| **d.o.f = n-2** | 23 | 23 | 23 |
| **Critical value from T-table** | 2.06 | 2.06 | 2.06 |
| **Conclusion** | \|t\| is smaller than critical value (0.402<2.06), the slope is equal to zero | \|t\|is smaller than critical value (0.599<2.06), the slope is equal to zero | \|t\| is smaller than critical value (0.8<2.06), the slope is equal to zero |

# APPENDIX B: Calculation for iron content in experiments with a tank with 70.4 $in^2$ of exposed iron and with little exposure of iron in tank

**Assumptions:**
Assuming that the % of sample that is each type of compound as determined by XRD is accurate.
That the formulas for each type of compond is correct based on XRD analysis

**Experiment with exposed iron in tank**

**Untreated Tap water**

| MW Iron (g/mol) | 55.84 | Mass of Solid (g) | 1.35 | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Compound name** | **Chemical Formula** | **MW (g/mol)** | **Wt % in the sample** | **fraction** | **Molar Mass ratio** | **Molar Mass ratio** | **Mass of iron (g)** | **= Mass of solid*fraction*Molar Mass Ratio** |
| **Iron Oxide** | Fe3O4 | 231.55 | 12 | 0.12 | (Fe/Fe2O3) | 0.24 | 0.04 | |
| **Magnesium Iron Oxide** | MgFe2O4 | 200.00 | 14 | 0.14 | (Fe/MgFe2O4) | 0.28 | 0.05 | |
| | | | | | | **Sum** | **0.09** | |

**Magnetically Treated Tap water**

| MW Iron (g/mol) | 55.84 | Mass of Solid (g) | 1.09 | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Compound name** | **Formula** | **MW (g/mol)** | **Wt % in the sample** | **fraction** | **Molar Mass ratio** | **Molar Mass ratio** | **Mass of iron (g)** | **= Mass of solid*fraction*Molar Mass Ratio** |
| **Iron Oxide** | Fe3O4 | 231.55 | 5 | 0.05 | (Fe/Fe3O4) | 0.24 | 0.01 | |
| **Magnesium Iron Oxide** | MgFe2O4 | 200.00 | 16 | 0.16 | (Fe/MgFe2O4) | 0.28 | 0.05 | |
| **Calcium Magnesium Iron Carbonate** | CaMg0.6Fe0.4(CO3)2 | 197.00 | 53 | 0.53 | (Fe/CaMg0.6Fe0.4(CO3)2) | 0.28 | 0.16 | |
| **Iron Oxide Hydroxide** | Fe21O31(OH) | 1685.85 | 11 | 0.11 | (Fe/Fe21O31(OH)) | 0.03 | 0.00 | |
| | | | | | | **Sum** | **0.23** | |

**Experiment without significant exposed iron in tank**

**Untreated Tap water**

| MW Iron (g/mol) | 55.84 | Mass of Solid (g) | 1.01 | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Compound name** | **Formula** | **MW (g/mol)** | **Wt % in the sample** | **fraction** | **Molar Mass ratio** | **Molar Mass ratio** | **Mass of iron (g)** | **= Mass of solid*fraction*Molar Mass Ratio** |
| **Iron Oxide** | Fe3O4 | 231.55 | 6 | 0.06 | (Fe/Fe3O4) | 0.24 | 0.01 | |
| **Magnesium Iron Oxide** | MgFe2O4 | 200.00 | 6 | 0.06 | (Fe/MgFe2O4) | 0.28 | 0.02 | |
| | | | | | | **Sum** | **0.03** | |

**Magnetically Treated Tap water**

| MW Iron (g/mol) | 55.84 | Mass of Solid (g) | 0.52 | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Compound name** | **Formula** | **MW (g/mol)** | **Wt % in the sample** | **fraction** | **Molar Mass ratio** | **Molar Mass ratio** | **Mass of iron (g)** | **= Mass of solid*fraction*Molar Mass Ratio** |
| **Iron Oxide** | Fe3O4 | 231.55 | 5 | 0.05 | (Fe/Fe2O4) | 0.24 | 0.01 | |
| **Magnesium Iron Oxide** | MgFe2O4 | 199.99 | 7 | 0.07 | (Fe/MgFe2O4) | 0.28 | 0.01 | |
| | | | | | | **Sum** | **0.02** | |

## APPENDIX C: Calculation of Feed Preparation for Accelerated Experimental Scale Simulation

### (A) Untreated water influent (400 ppm as $Ca^{2+}$):

Number of moles of $CaC0_3$ = mass /molar mass

4 g/100g $mol^{-1}$ = 0.04 moles

Number of moles $Ca^{2+}$ = 0.04 moles

Therefore mass of $Ca^{2+}$ = no. of moles × molar mass

0.04 moles ×40 g/mol. = 1.6 g

Calcium conc. (mg/L as $Ca^{2+}$) = 1600 mg/4L = **400 ppm as $Ca^{2+}$**

Total Hardness (mg/L as $CaCO_3$) = 2.5 $\frac{\left(\frac{\text{mg as CaCO3}}{\text{mmol.}}\right)}{\left(\frac{\text{mg Ca2+}}{\text{mmol.}}\right)}$× Calcium conc. (mg/L as $Ca^{2+}$) +

4.12 $\frac{\left(\frac{\text{mg as CaCO3}}{\text{mmol.}}\right)}{\left(\frac{\text{mg Mg2+}}{\text{mmol.}}\right)}$ × Magnesium conc. (mg /L as $Mg^{2+}$) *0*

Total Hardness (mg/L as $CaCO_3$) = 2.50$\frac{\left(\frac{\text{mg CaCO3}}{\text{mmol.}}\right)}{\left(\frac{\text{mg Ca2+}}{\text{mmol.}}\right)}$ × 400 ppm as $Ca^{2+}$ = **1,000 ppm as $CaCO_3$**

### (B) Magnetically treated water influent (400 ppm as $CaCO_3$):

Mass of $CaCO_3$ powder required = 1.6 g

Volume of high purity water required = 4 L

Total Hardness concentration (mg/L as $CaCO_3$) = 1600 mg ÷ 4 L = **400 ppm as $CaCO_3$**

Molecular weight of $CaCO_3$: $\frac{100\text{ mg}}{\text{mmol.}}$, $Ca^{2+}$: $\frac{40\text{ mg}}{\text{mmol.}}$ , $Mg^{2+}$: $\frac{24.3\text{ mg}}{\text{mmol.}}$

Calcium conc. (mg/L as $Ca^{2+}$) = 400 ppm as $CaCO_3$ / 2.50 = 160 mg/L as $Ca^{2+}$

# APPENDIX D: Results of Feed Water for Accelerated Experimental Scale Simulation

The results of influent water quality analysis for accelerated experimental scale simulation test are presented in tables D.1 and D.2. The analysis was performed immediately after the feed has been prepared prior each experimental operating temperature, $T_1$=60 °C and $T_2$=30 °C.

## APPENDIX D.1: Influent water quality analysis for untreated water

**Table D.1. Influent water quality analysis for untreated water**

| | | Number of Replicate =3 | | | |
|---|---|---|---|---|---|
| | | $T_1$ | | $T_2$ | |
| **Parameter** | **Unit** | **Average** | **SD** | **Average** | **SD** |
| **Total Hardness** | $CaCO_3$ mg/L | ~1000 | 0 | ~1000 | 0 |
| **pH** | - | 6.14 | 0.03 | 6.13 | 0.05 |
| **Conductivity** | µS/cm | 1439 | 1.5 | 1509 | 1.5 |

**SD: Standard Deviation**

## APPENDIX D.2: Influent water quality analysis for magnetically treated water

For the magnetically treated water, the pH and conductivity were tested before and after the water flowed through the AkwaMag device to confirm that there is no significant change in water chemistry. The pH and conductivity readings slightly increased after passing through AkwaMag device, which could be due measurement error.

**Table D.2. Influent water quality analysis for magnetically treated water**

| | | Number of Replicate =3 | | | |
|---|---|---|---|---|---|
| | | $T_1$ | | $T_2$ | |
| **Parameter** | **Unit** | **Average** | **SD** | **Average** | **SD** |
| **Total Hardness** | $CaCO_3$ mg/L | 390 | 21 | 403 | 6.8 |
| **pH (Before)** | - | 6 | 0 | 6 | 0 |
| **pH (After)** | - | 6.21 | 0.04 | 6.03 | 0.05 |
| **Conductivity (Before)** | µS/cm | 766 | 3.5 | 721 | 1.5 |
| **Conductivity (After)** | µS/cm | 766 | 3.5 | 731 | 0.58 |

**SD: Standard Deviation**

# APPENDIX E: X-Ray Diffraction (Results)

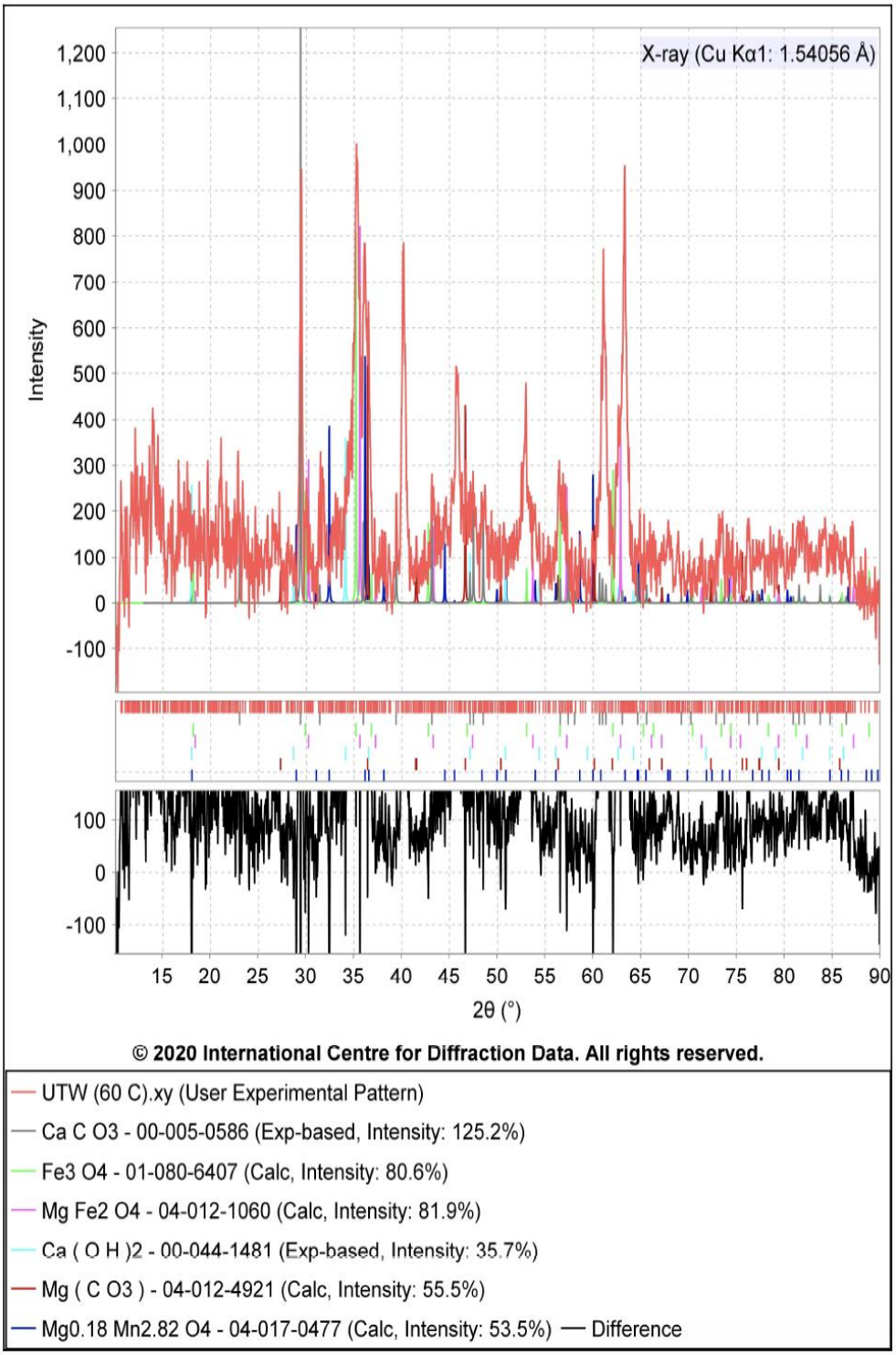


**Figure E.1 XRD patterns of substances precipitated from Untreated Water (UTW) tank at 60 ˚C from experiment with a tank with 70.4 in$^2$ of exposed iron**

# SIeve+ Report

## Experiment

**Search Line:** 1.467772 Å **D1 Range:** 1.465 Å - 1.471 Å
**Search Line:** 2.244214 Å **D1 Range:** 2.236 Å - 2.252 Å
**Search Line:** 1.470838 Å **D1 Range:** 1.468 Å - 1.474 Å
**Search Line:** 1.516026 Å **D1 Range:** 1.513 Å - 1.519 Å
**Search Line:** 1.464294 Å **D1 Range:** 1.461 Å - 1.467 Å
**Search Line:** 1.512200 Å **D1 Range:** 1.509 Å - 1.516 Å
**Search Line:** 2.458280 Å **D1 Range:** 2.449 Å - 2.468 Å
**Search Line:** 2.509879 Å **D1 Range:** 2.500 Å - 2.520 Å
**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (6)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 00-005-0586 | S | Calcium Carbonate | 1.252 | 28.96 | *3.23 | 29 |
| 2 | true | 01-080-6407 | S | Iron Oxide | 0.806 | 18.634 | *5.16 | 12 |
| 3 | true | 04-012-1060 | S | Magnesium Iron Oxide | 0.819 | 18.936 | *4.21 | 14 |
| 4 | true | 00-044-1481 | S | Calcium Hydroxide | 0.357 | 8.269 | *3.61 | 7 |
| 5 | true | 04-012-4921 | I | Magnesium Carbonate | 0.555 | 12.836 | *1.82 | 23 |
| 6 | true | 04-017-0477 | S | Magnesium Manganese Oxide | 0.535 | 12.365 | 2.64 | 15 |

**00-005-0586** Jun 9, 2020 2:37 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca C O3
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**Compound Name:** Calcium Carbonate **Mineral Name:** Calcite, syn

**Radiation:** CuKα1 **λ:** 1.5405 Å **Filter:** Ni Beta **Intensity:** Diffractometer **I/Ic:** 2

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.989 Å **AuthCell c:** 17.062 Å **AuthCell Vol:** 367.78 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 61.30 ] **Author's Cell Axial Ratio [ c/a:** 3.420 ]
**Density [ Dcalc:** 2.711 g/cm³ **Dmeas:** 2.71 g/cm³ ] **SS/FOM:** F(30) = 57.2(0.0159, 33)
**Temp:** 299.0 K (Author provided temperature) **Color:** Colorless

**Space Group:** R-3c (167) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 4.989 Å **XtlCell b:** 4.989 Å **XtlCell c:** 17.062 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 367.78 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.420 **a/b:** 1.000 **c/b:** 3.420 ]
**Reduced Cell [ RedCell a:** 4.989 Å **RedCell b:** 4.989 Å **RedCell c:** 6.375 Å **RedCell α:** 66.97°
**RedCell β:** 66.97° **RedCell γ:** 60.00° **RedCell Vol:** 122.59 Å³ ]

εα: =1.487 πωβ: =1.659 **Sign:** =-

**Atomic parameters are cross-referenced from PDF entry 04-012-8072** **ADP:** U
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | 0.01525 | |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | 0.02084 | |
| O | 3 | 18e | .2 | 0.25 | 0.0 | 0.25 | 1.0 | 0.02084 | |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Educational Pattern, Forensic, Inorganic, Mineral Related (Mineral , Synthetic), NBS Pattern, Pharmaceutical (Excipient), Pigment/Dye, Superconducting Material (Superconductor Related Materials)

**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 01-072-1937 (Alternate), 01-083-0577 (Alternate), 01-083-0578 (Alternate), ✓ 04-001-7249 (Alternate), ✓ 04-006-6528 (Alternate), ✓ 04-007-2808 (Alternate), ✓ 04-007-4388 (Alternate), ✓ 04-007-8659 (Primary), ✓ 04-008-0788 (Alternate), ✓ 04-012-0489 (Primary), ✓ 04-012-8072 (Alternate)

**CAS Number - PR:** 13397-26-7 **Entry Date:** 09/01/1955

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Swanson, Fuyat. Natl. Bur. Stand. (U. S. ), Circ. 539 II, 51 (1953). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Optical Data | | Dana's System of Mineralogy, 7th Ed. II, 142. |

**Database Comments:** Additional Patterns: See PDF 01-072-1214 , 01-072-1937, 01-081-2027, 01-083-0577 and 01-083-0578. Analysis: Spectroscopic analysis: <0.1% Sr; <0.01% Ba; <0.001% Al, B, Cs, Cu, K, Mg, Na, Si, Sn; <0.0001% Ag, Cr, Fe, Li, Mn. Color: Colorless. General Comments: Additional weak reflections (indicated by brackets) were observed. Other form: aragonite. Pattern reviewed by Parks, J., McCarthy, G., North Dakota State Univ., Fargo, North Dakota, USA, ICDD Grant-in-Aid (1992). Agrees well with experimental and calculated patterns. Antacid. Sample Source or Locality: Sample from Mallinckrodt Chemical Works. Temperature of Data Collection: Pattern taken at 299 K. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (45) - Ca C O3 - 00-005-0586 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.0218 | 3.860000 | 12 | 0 | 1 | 2 | | 48.5122 | 1.875000 | 17 | 1 | 1 | 6 | | 64.6765 | 1.440000 | 5 | 3 | 0 | 0 | |
| 29.4049 | **3.035000** | 100 | 1 | 0 | 4 | | 56.5530 | 1.626000 | 4 | 2 | 1 | 1 | | 65.5972 | 1.422000 | 3 | 0 | 0 | 12 | |
| 31.4176 | 2.845000 | 3 | 0 | 0 | 6 | | 57.4001 | 1.604000 | 8 | 1 | 2 | 2 | | 69.2291 | 1.356000 | 1 | 2 | 1 | 7 | |
| 35.9654 | 2.495000 | 14 | 1 | 1 | 0 | | 58.0733 | 1.587000 | 2 | 1 | 0 | 10 | | 70.2364 | 1.339000 | 2 | 0 | 2 | 10 | |
| 39.4009 | **2.285000** | 18 | 1 | 1 | 3 | | 60.6762 | 1.525000 | 5 | 2 | 1 | 4 | | 72.8676 | 1.297000 | 2 | 1 | 2 | 8 | |
| 43.1447 | **2.095000** | 18 | 2 | 0 | 2 | | 60.9857 | 1.518000 | 4 | 2 | 0 | 8 | | 73.7264 | 1.284000 | 1 | 3 | 0 | 6 | |
| 47.1226 | 1.927000 | 5 | 0 | 2 | 4 | | 61.3435 | 1.510000 | 3 | 1 | 1 | 9 | | 76.2977 | 1.247000 | 1 | 2 | 2 | 0 | |
| 47.4886 | 1.913000 | 17 | 0 | 1 | 8 | | 63.0584 | 1.473000 | 2 | 1 | 2 | 5 | | 77.1749 | 1.235000 | 2 | 1 | 1 | 12 | |

**00-005-0586** Jun 9, 2020 2:37 PM (fal-sharji2)

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 80.9302 | 1.186900 | <1 | 3 | 1 | 2 | E | 94.6975 | 1.047300 | 3 | 4 | 0 | 4 | | 103.8950 | 0.978200 | 1 | 1 | 3 | 10 | |
| 81.5449 | 1.179500 | 3 | 2 | 1 | 10 | | 95.0075 | 1.044700 | 4 | 3 | 1 | 8 | | 104.1201 | 0.976700 | 3 | 1 | 2 | 14 | |
| 82.1106 | 1.172600 | <1 | 0 | 1 | 14 | E | 96.1617 | 1.035200 | 2 | 1 | 0 | 16 | | 105.8419 | 0.965500 | 2 | 3 | 2 | 4 | |
| 83.7646 | 1.153600 | 3 | 1 | 3 | 4 | | 97.6440 | 1.023400 | <1 | 2 | 1 | 13 | | 106.1414 | 0.963600 | 4 | 0 | 4 | 8 | |
| 84.7850 | 1.142500 | 1 | 2 | 2 | 6 | | 99.1573 | 1.011800 | 2 | 3 | 0 | 12 | | 107.3295 | 0.956200 | <1 | 0 | 2 | 16 | |
| 86.4804 | 1.124400 | <1 | 1 | 2 | 11 | | 102.2384 | 0.989500 | <1 | 3 | 2 | 1 | | 109.5566 | 0.942900 | 2 | 4 | 1 | 0 | |
| 93.0691 | 1.061300 | 1 | 2 | 0 | 14 | | 102.9484 | 0.984600 | 1 | 2 | 3 | 2 | | 110.4794 | 0.937600 | 2 | 2 | 2 | 12 | |

**04-012-1060** Jun 9, 2020 2:38 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Pressure & Temperature (Non-ambient)
**Chemical Formula:** Mg Fe2 O4 **Empirical Formula:** Fe2 Mg O4 **Weight %:** Fe55.85 Mg12.15 O32.00
**Atomic %:** Fe28.57 Mg14.29 O57.14 **ANX:** A3X4 **Compound Name:** Magnesium Iron Oxide
**Mineral Name:** Magnesioferrite, Syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 4.07 **I/Ic - ND:** 1.5

**SYS:** Cubic **SPGR:** Fd-3m (227)
**Author's Cell [ AuthCell a:** 8.35460(9) Å **AuthCell Vol:** 583.15 Å³ **AuthCell Z:** 8.00 **AuthCell MolVol:** 72.89 ]
**Density [ Dcalc:** 4.556 g/cm³ **Dstruc:** 4.56 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0002, 30)
**Temp:** 920.0 K (Author provided temperature) **R-factor:** 0.074 **Color:** Brown

**Space Group:** Fd-3m (227) **Molecular Weight:** 200.00
**Crystal Data [ XtlCell a:** 8.355 Å **XtlCell b:** 8.355 Å **XtlCell c:** 8.355 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 583.15 Å³ **XtlCell Z:** 8.00 ]
**Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 ]
**Reduced Cell [ RedCell a:** 5.908 Å **RedCell b:** 5.908 Å **RedCell c:** 5.908 Å **RedCell α:** 60.00°
**RedCell β:** 60.00° **RedCell γ:** 60.00° **RedCell Vol:** 145.79 Å³ ]

**ADP:** U **Origin:** O2 **Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 11 | z,-x+1/4,-y+1/4 | 21 | -y+1/4,z,-x+1/4 | 31 | -x+1/4,-z+1/4,y | 41 | z,y,x |
| 2 | -x,-y,-z | 12 | -z,x+3/4,y+3/4 | 22 | y+3/4,-z,x+3/4 | 32 | x+3/4,z+3/4,-y | 42 | -z,-y,-x |
| 3 | x,-y+1/4,-z+1/4 | 13 | -z+1/4,x,-y+1/4 | 23 | -y+1/4,-z+1/4,x | 33 | y,x,z | 43 | z,-y+1/4,-x+1/4 |
| 4 | -x,y+3/4,z+3/4 | 14 | z+3/4,-x,y+3/4 | 24 | y+3/4,z+3/4,-x | 34 | -y,-x,-z | 44 | -z,y+3/4,x+3/4 |
| 5 | -x+1/4,y,-z+1/4 | 15 | -z+1/4,-x+1/4,y | 25 | x,z,y | 35 | y,-x+1/4,-z+1/4 | 45 | -z+1/4,y,-x+1/4 |
| 6 | x+3/4,-y,z+3/4 | 16 | z+3/4,x+3/4,-y | 26 | -x,-z,-y | 36 | -y,x+3/4,z+3/4 | 46 | z+3/4,-y,x+3/4 |
| 7 | -x+1/4,-y+1/4,z | 17 | y,z,x | 27 | x,-z+1/4,-y+1/4 | 37 | -y+1/4,x,-z+1/4 | 47 | -z+1/4,-y+1/4,x |
| 8 | x+3/4,y+3/4,-z | 18 | -y,-z,-x | 28 | -x,z+3/4,y+3/4 | 38 | y+3/4,-x,z+3/4 | 48 | z+3/4,y+3/4,-x |
| 9 | z,x,y | 19 | y,-z+1/4,-x+1/4 | 29 | -x+1/4,z,-y+1/4 | 39 | -y+1/4,-x+1/4,z | | |
| 10 | -z,-x,-y | 20 | -y,z+3/4,x+3/4 | 30 | x+3/4,-z,y+3/4 | 40 | y+3/4,x+3/4,-z | | |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Fe | 1 | 8a | -43m | 0.125 | 0.125 | 0.125 | 0.91 | 0.0088 | |
| Mg | 2 | 8a | -43m | 0.125 | 0.125 | 0.125 | 0.09 | 0.0088 | |
| Fe | 3 | 16d | .-3m | 0.5 | 0.5 | 0.5 | 0.545 | 0.0058 | |
| Mg | 4 | 16d | .-3m | 0.5 | 0.5 | 0.5 | 0.455 | 0.0058 | |
| O | 5 | 32e | .3m | 0.2567 | 0.2567 | 0.2567 | 1.0 | 0.0081 | |

**Subfile(s):** Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic) **Former PDF's #:** 01-076-9713
**LPF Prototype Structure [Formula Order]:** Mg Al2 O4,cF56,227
**LPF Prototype Structure [Alpha Order]:** Al2 Mg O4,cF56,227 **Pearson Symbol:** cF56.00

**04-012-1060** Jun 9, 2020 2:38 PM (fal-sharji2)

**Cross-Ref PDF #'s:**

00-017-0464 (Primary), 00-036-0398 (Primary), 01-073-1960 (Alternate), 01-073-2410 (Alternate), 01-075-9708 (Alternate), 01-078-5428 (Alternate), 01-082-9881 (Alternate), 01-088-1935 (Alternate), 01-088-1936 (Alternate), 01-088-1937 (Alternate), 01-088-1938 (Alternate), 01-088-1939 (Alternate), 01-088-1940 (Alternate), 01-088-1941 (Alternate), 01-088-1942 (Alternate), 01-088-1943 (Alternate), 01-089-3084 (Alternate), 01-089-4924 (Alternate), 01-089-6187 (Alternate), 01-089-6188 (Alternate), 01-089-6189 (Alternate), ✓ 04-001-7921 (Alternate), ✓ 04-001-9288 (Alternate), ✓ 04-002-0587 (Alternate), ✓ 04-002-0619 (Alternate), ✓ 04-002-2458 (Alternate), ✓ 04-002-2459 (Alternate), ✓ 04-002-3054 (Alternate), ✓ 04-002-3768 (Alternate), ✓ 04-002-3769 (Alternate), ✓ 04-002-5223 (Alternate), ✓ 04-002-5328 (Alternate), ✓ 04-002-5461 (Alternate), ✓ 04-002-5666 (Alternate), ✓ 04-002-5894 (Alternate), ✓ 04-002-5904 (Alternate), ✓ 04-002-6403 (Alternate), ✓ 04-002-8191 (Alternate), ✓ 04-002-8204 (Alternate), ✓ 04-005-7127 (Alternate), ✓ 04-005-8346 (Alternate), ✓ 04-005-8349 (Alternate), ✓ 04-006-0223 (Alternate), ✓ 04-006-0426 (Alternate), ✓ 04-006-0427 (Alternate), ✓ 04-006-1839 (Alternate), ✓ 04-006-2461 (Alternate), ✓ 04-006-2469 (Alternate), ✓ 04-006-4005 (Alternate), ✓ 04-006-6673 (Alternate), ✓ 04-006-6676 (Alternate), ✓ 04-006-6677 (Alternate), ✓ 04-006-6682 (Alternate), ✓ 04-007-4190 (Alternate), ✓ 04-007-4269 (Alternate), ✓ 04-007-5629 (Alternate), ✓ 04-007-5630 (Alternate), ✓ 04-008-2382 (Alternate), ✓ 04-010-6157 (Primary), ✓ 04-011-9002 (Alternate), ✓ 04-011-9003 (Alternate), ✓ 04-012-0908 (Alternate), ✓ 04-012-0909 (Alternate), ✓ 04-012-0910 (Alternate), ✓ 04-012-0911 (Alternate), ✓ 04-012-0912 (Alternate), ✓ 04-012-0913 (Alternate), ✓ 04-012-0914 (Alternate), ✓ 04-012-0915 (Alternate), ✓ 04-012-0916 (Alternate), ✓ 04-012-0917 (Alternate), ✓ 04-012-0918 (Alternate), ✓ 04-012-0919 (Alternate), ✓ 04-012-0920 (Alternate), ✓ 04-012-0921 (Alternate), ✓ 04-012-0922 (Alternate), ✓ 04-012-0923 (Alternate), ✓ 04-012-0924 (Alternate), ✓ 04-012-0925 (Alternate), ✓ 04-012-0926 (Alternate), ✓ 04-012-0927 (Alternate), ✓ 04-012-0928 (Alternate), ✓ 04-012-0929 (Alternate), ✓ 04-012-0930 (Alternate), ✓ 04-012-0931 (Alternate), ✓ 04-012-0932 (Alternate), ✓ 04-012-0933 (Alternate), ✓ 04-012-0934 (Alternate), ✓ 04-012-0935 (Alternate), ✓ 04-012-0936 (Alternate), ✓ 04-012-0937 (Alternate), ✓ 04-012-0938 (Alternate), ✓ 04-012-0939 (Alternate), ✓ 04-012-0940 (Alternate), ✓ 04-012-0941 (Alternate), ✓ 04-012-0942 (Alternate), ✓ 04-012-0943 (Alternate), ✓ 04-012-0944 (Alternate), ✓ 04-012-0945 (Alternate), ✓ 04-012-0946 (Alternate), ✓ 04-012-0947 (Alternate), ✓ 04-012-0948 (Alternate), ✓ 04-012-0949 (Alternate), ✓ 04-012-0950 (Alternate), ✓ 04-012-0951 (Alternate), ✓ 04-012-1050 (Alternate), ✓ 04-012-1051 (Alternate), ✓ 04-012-1052 (Alternate), ✓ 04-012-1053 (Alternate), ✓ 04-012-1054 (Alternate), ✓ 04-012-1055 (Alternate), ✓ 04-012-1056 (Alternate), ✓ 04-012-1057 (Alternate), ✓ 04-012-1058 (Alternate), ✓ 04-012-1059 (Alternate), ✓ 04-012-1061 (Alternate), ✓ 04-012-1062 (Alternate), ✓ 04-012-1063 (Alternate), ✓ 04-012-1064 (Alternate), ✓ 04-012-1065 (Alternate), ✓ 04-012-1066 (Alternate), ✓ 04-012-1067 (Alternate), ✓ 04-012-1068 (Alternate), ✓ 04-012-1069 (Alternate), ✓ 04-012-1070 (Alternate), ✓ 04-012-1071 (Alternate), ✓ 04-012-1072 (Alternate), ✓ 04-012-1073 (Alternate), ✓ 04-012-1074 (Alternate), ✓ 04-012-1075 (Alternate), ✓ 04-012-1076 (Alternate), ✓ 04-012-1077 (Alternate), ✓ 04-012-1078 (Alternate), ✓ 04-012-1079 (Alternate), ✓ 04-012-1080 (Alternate), ✓ 04-012-1081 (Alternate), ✓ 04-014-3057 (Alternate), ✓ 04-014-3693 (Alternate), ✓ 04-014-3694 (Alternate), ✓ 04-014-3695 (Alternate), ✓ 04-014-3696 (Alternate), ✓ 04-014-3697 (Alternate), ✓ 04-014-3698 (Alternate), ✓ 04-014-3699 (Alternate), ✓ 04-014-3700 (Alternate), ✓ 04-014-3701 (Alternate), ✓ 04-014-3702 (Alternate), ✓ 04-014-3703 (Alternate), ✓ 04-014-3704 (Alternate), ✓ 04-014-3705 (Alternate), ✓ 04-014-3706 (Alternate), ✓ 04-014-3707 (Alternate), ✓ 04-014-3708 (Alternate), ✓ 04-014-3709 (Alternate), ✓ 04-014-3710 (Alternate), ✓ 04-014-3711 (Alternate), ✓ 04-014-3712 (Alternate), ✓ 04-014-3713 (Alternate), ✓ 04-014-3714 (Alternate), ✓ 04-014-3715 (Alternate), ✓ 04-014-3716 (Alternate), ✓ 04-014-3717 (Alternate), ✓ 04-014-3718 (Alternate), ✓ 04-014-3719 (Alternate), ✓ 04-014-3720 (Alternate), ✓ 04-014-3721 (Alternate), ✓ 04-014-3722 (Alternate), ✓ 04-014-3723 (Alternate), ✓ 04-014-3724 (Alternate), ✓ 04-014-3725 (Alternate), ✓ 04-014-3726 (Alternate), ✓ 04-014-3727 (Alternate), ✓ 04-014-3728 (Alternate), ✓ 04-014-3729 (Alternate), ✓ 04-014-3730 (Alternate), ✓ 04-014-3731 (Alternate), ✓ 04-014-3732 (Alternate), ✓ 04-014-3733 (Alternate), ✓ 04-014-3734 (Alternate), ✓ 04-015-7027 (Alternate)

**Entry Date:** 09/01/2009 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Effects of high pressure and high temperature on cation ordering in magnesioferrite, MgFe2O4, using in situ synchrotron X-ray powder diffraction up to1430 K and 6 GPa". Antao S.M., Hassan I., Crichton W.A., Parise J.B. Am. Mineral. 90, 1500,1505 (2005). |

**Database Comments:** ANX: A3X4. Color: brown. In Situ Condition: In gold capsule (crimped closed). LPF Collection Code: 1601271. Sample Preparation: Compound Preparation: solid-state reaction. Sample dried at 423 K for 1 d. Pressure of Datacollection: 5 GPa. Temperature of Data Collection: 920 K. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (34) - Mg Fe2 O4 - 04-012-1060 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.3781 | 4.823530 | 29 | 1 | 1 | 1 | | 74.3982 | 1.274060 | 71 | 5 | 3 | 3 | | 111.1053 | 0.934073 | 22 | 8 | 4 | 0 | |
| 30.2322 | **2.953800** | 375 | 2 | 2 | 0 | | 75.4071 | 1.259500 | 16 | 6 | 2 | 2 | | 114.2731 | 0.917037 | 1 | 9 | 1 | 1 | |
| 35.6110 | **2.519010** | 999 | 3 | 1 | 1 | | 79.4003 | 1.205880 | 21 | 4 | 4 | 4 | | 115.3462 | 0.911562 | 1 | 8 | 4 | 2 | |
| 37.2513 | 2.411770 | 23 | 2 | 2 | 2 | | 82.3600 | 1.169880 | 3 | 7 | 1 | 1 | | 119.7419 | 0.890603 | 7 | 6 | 6 | 4 | |
| 43.2824 | 2.088650 | 192 | 4 | 0 | 0 | | 87.2522 | 1.116430 | 35 | 6 | 4 | 2 | | 123.1680 | 0.875800 | 43 | 9 | 3 | 1 | |
| 47.3918 | 1.916680 | 1 | 3 | 3 | 1 | | 90.1751 | 1.087680 | 99 | 7 | 3 | 1 | | 129.2053 | 0.852688 | 89 | 8 | 4 | 4 | |
| 53.7026 | 1.705380 | 109 | 4 | 2 | 2 | | 95.0530 | 1.044320 | 40 | 8 | 0 | 0 | | 133.0867 | 0.839669 | 1 | 9 | 3 | 3 | |
| 57.2503 | 1.607840 | 299 | 5 | 1 | 1 | | 97.9937 | 1.020680 | 1 | 7 | 3 | 3 | | 140.1844 | 0.819236 | 20 | 8 | 6 | 2 | |
| 62.8728 | **1.476900** | 401 | 4 | 4 | 0 | | 98.9795 | 1.013140 | 1 | 6 | 4 | 4 | | 144.9960 | 0.807670 | 55 | 9 | 5 | 1 | |
| 66.1109 | 1.412190 | 3 | 5 | 3 | 1 | | 102.9486 | 0.984599 | 16 | 8 | 2 | 2 | | 146.7319 | 0.803922 | 8 | 10 | 2 | 2 | |
| 67.1724 | 1.392430 | 1 | 4 | 4 | 2 | | 105.9668 | 0.964706 | 55 | 7 | 5 | 1 | | | | | | | | |
| 71.3396 | 1.320980 | 35 | 6 | 2 | 0 | | 106.9826 | 0.958338 | 7 | 6 | 6 | 2 | | | | | | | | |

**01-080-6407** Jun 9, 2020 2:38 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Temperature (Non-ambient) **Chemical Formula:** Fe3 O4
**Empirical Formula:** Fe3 O4 **Weight %:** Fe72.36 O27.64 **Atomic %:** Fe42.86 O57.14 **ANX:** A3X4
**Compound Name:** Iron Oxide **Mineral Name:** Magnetite **Common Name:** Iron(II) diiron(III) tetraoxide

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 4.72 **I/Ic - ND:** 1.25

**SYS:** Cubic **SPGR:** Fd-3m (227)
**Author's Cell [ AuthCell a:** 8.4499(5) Å **AuthCell Vol:** 603.33 Å³ **AuthCell Z:** 8.00 **AuthCell MolVol:** 75.42 ]
**Density [ Dcalc:** 5.098 g/cm³ **Dstruc:** 5.1 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 773.0 K (Author provided temperature) **R-factor:** 0.0264

**Space Group:** Fd-3m (227) **Molecular Weight:** 231.54
**Crystal Data [ XtlCell a:** 8.450 Å **XtlCell b:** 8.450 Å **XtlCell c:** 8.450 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 603.33 Å³ **XtlCell Z:** 8.00 ]
**Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 ]
**Reduced Cell [ RedCell a:** 5.975 Å **RedCell b:** 5.975 Å **RedCell c:** 5.975 Å **RedCell α:** 60.00°
**RedCell β:** 60.00° **RedCell γ:** 60.00° **RedCell Vol:** 150.83 Å³ ]

**Crystal (Symmetry Allowed):** Centrosymmetric

**Subfile(s):** Common Phase, Forensic, Inorganic, Metals & Alloys, Mineral Related (Mineral , Natural)
**Prototype Structure [Formula Order]:** Mg Al2 O4 **Prototype Structure [Alpha Order]:** Al2 Mg O4
**Pearson Symbol:** cF56.00

**Cross-Ref PDF #'s:**
00-001-1111 (Deleted), 00-002-1035 (Deleted), 00-003-0862 (Deleted), 00-007-0322 (Deleted), 00-011-0614 (Deleted), 00-019-0629 (Primary), 00-065-0731 (Primary), 01-071-4918 (Alternate), 01-072-2303 (Alternate), 01-074-1909 (Alternate), 01-074-1910 (Alternate), 01-075-0449 (Alternate), 01-075-1610 (Alternate), 01-075-9710 (Alternate), 01-076-1849 (Alternate), 01-076-5948 (Alternate), 01-078-6086 (Alternate), 01-080-6402 (Alternate), 01-080-6403 (Alternate), 01-080-6404 (Alternate), 01-080-6405 (Alternate), 01-080-6406 (Alternate), 01-080-6408 (Alternate), 01-080-6409 (Alternate), 01-080-6410 (Alternate), 01-080-7683 (Alternate), 01-087-2334 (Alternate), 01-088-0866 (Alternate), 01-089-3854 (Alternate), 01-089-4319 (Alternate), ✓ 03-065-3107 (Alternate), ✓ 04-001-7822 (Alternate), ✓ 04-001-7909 (Alternate), ✓ 04-001-9000 (Alternate), ✓ 04-001-9326 (Alternate), ✓ 04-002-0264 (Alternate), ✓ 04-002-0618 (Alternate), ✓ 04-002-0643 (Alternate), ✓ 04-002-1855 (Alternate), ✓ 04-002-2487 (Alternate), ✓ 04-002-2707 (Alternate), ✓ 04-002-2709 (Alternate), ✓ 04-002-2981 (Alternate), ✓ 04-002-3194 (Alternate), ✓ 04-002-3668 (Alternate), ✓ 04-002-5310 (Alternate), ✓ 04-002-5448 (Alternate), ✓ 04-002-5632 (Alternate), ✓ 04-002-5683 (Alternate), ✓ 04-002-5903 (Alternate), ✓ 04-002-6866 (Alternate), ✓ 04-002-6955 (Alternate), ✓ 04-002-8141 (Alternate), ✓ 04-002-8629 (Alternate), ✓ 04-002-9019 (Alternate), ✓ 04-002-9635 (Alternate), ✓ 04-003-1446 (Alternate), ✓ 04-004-2838 (Alternate), ✓ 04-005-4307 (Alternate), ✓ 04-005-4319 (Primary), ✓ 04-005-4404 (Alternate), ✓ 04-005-4551 (Alternate), ✓ 04-005-5733 (Alternate), ✓ 04-005-6268 (Alternate), ✓ 04-005-9786 (Alternate), ✓ 04-005-9788 (Alternate), ✓ 04-005-9815 (Alternate), ✓ 04-006-0225 (Alternate), ✓ 04-006-0424 (Alternate), ✓ 04-006-0425 (Alternate), ✓ 04-006-1668 (Alternate), ✓ 04-006-2406 (Alternate), ✓ 04-006-2467 (Alternate), ✓ 04-006-2752 (Alternate), ✓ 04-006-4615 (Alternate), ✓ 04-006-6497 (Alternate), ✓ 04-006-6550 (Alternate), ✓ 04-006-6692 (Alternate), ✓ 04-006-8076 (Alternate), ✓ 04-007-1427 (Alternate), ✓ 04-007-2718 (Alternate), ✓ 04-007-6010 (Alternate), ✓ 04-007-8567 (Alternate), ✓ 04-007-8976 (Alternate), ✓ 04-007-9093 (Alternate), ✓ 04-008-0315 (Alternate), ✓ 04-008-0777 (Alternate), ✓ 04-008-4423 (Alternate), ✓ 04-008-4511 (Alternate), ✓ 04-008-4512 (Alternate), ✓ 04-008-8145 (Alternate), ✓ 04-008-8146 (Alternate), ✓ 04-008-8147 (Alternate), ✓ 04-008-8148 (Alternate), ✓ 04-009-4225 (Alternate), ✓ 04-009-8417 (Alternate), ✓ 04-009-8418 (Alternate), ✓ 04-009-8419 (Alternate), ✓ 04-009-8420 (Alternate), ✓ 04-009-8421 (Alternate), ✓ 04-009-8422 (Alternate), ✓ 04-009-8423 (Alternate), ✓ 04-009-8424 (Alternate), ✓ 04-009-8425 (Alternate), ✓ 04-009-8426 (Alternate), ✓ 04-009-8427 (Alternate), ✓ 04-009-8428 (Alternate), ✓ 04-009-8429 (Alternate), ✓ 04-009-8430 (Alternate), ✓ 04-009-8431 (Alternate), ✓ 04-009-8432 (Alternate), ✓ 04-009-8433 (Alternate), ✓ 04-009-8434 (Alternate), ✓ 04-009-8435 (Alternate), ✓ 04-009-8436 (Alternate), ✓ 04-009-8437 (Alternate), ✓ 04-009-8438 (Alternate), ✓ 04-009-8439 (Alternate), ✓ 04-009-8440 (Alternate), ✓ 04-009-8441 (Alternate), ✓ 04-009-8442 (Alternate), ✓ 04-009-8443 (Alternate), ✓ 04-011-5952 (Alternate), ✓ 04-013-7099 (Alternate), ✓ 04-013-7100 (Alternate), ✓ 04-013-9806 (Alternate), ✓ 04-013-9807 (Alternate), ✓ 04-013-9808 (Alternate), ✓ 04-013-9809 (Alternate), ✓ 04-013-9810 (Alternate), ✓ 04-013-9811 (Alternate), ✓ 04-014-1396 (Alternate), ✓ 04-014-9664 (Alternate), ✓ 04-015-3100 (Alternate), ✓ 04-015-3101 (Alternate), ✓ 04-015-3102 (Alternate), ✓ 04-015-8200 (Alternate), ✓ 04-015-8203 (Alternate), ✓ 04-015-8204 (Alternate), ✓ 04-015-8207 (Alternate), ✓ 04-015-8209 (Alternate), ✓ 04-015-8211 (Alternate), ✓ 04-015-8213 (Alternate), ✓ 04-015-8214 (Alternate), ✓ 04-017-1024 (Alternate)

**Entry Date:** 09/01/2013

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Structure | | "Structure of magnetite (Fe3 O4) above the Curie temperature: a cation ordering study". Levy, D., Giustetto, R., Hoser, A. Phys. Chem. Miner. 39, 169 (2012). |

**01-080-6407** Jun 9, 2020 2:38 PM (fal-sharji2)

**Database Comments:** ANX: A3X4. Analysis: Fe3 O4. Formula from original source: Fe3 O4. ICSD Collection Code: 183974. Sample Source or Locality: Brosso mining area, Ivrea,Italy. Structures: Magnetic structure also determined. Temperature of Data Collection: 773 K. Wyckoff Sequence: e d a (FD3-MZ). Unit Cell Data Source: Powder Diffraction.

**d-Spacings (34) - Fe3 O4 - 01-080-6407 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.1690 | 4.878550 | 100 | 1 | 1 | 1 | | 73.4200 | 1.288600 | 58 | 5 | 3 | 3 | | 109.2431 | 0.944728 | 14 | 8 | 4 | 0 | |
| 29.8833 | **2.987490** | 296 | 2 | 2 | 0 | | 74.4112 | 1.273870 | 23 | 6 | 2 | 2 | | 112.2989 | 0.927497 | 1 | 9 | 1 | 1 | |
| 35.1962 | **2.547740** | 999 | 3 | 1 | 1 | | 78.3311 | 1.219640 | 17 | 4 | 4 | 4 | | 113.3319 | 0.921960 | 1 | 8 | 4 | 2 | |
| 36.8160 | 2.439280 | 75 | 2 | 2 | 2 | | 81.2346 | 1.183220 | 3 | 5 | 5 | 1 | | 117.5510 | 0.900762 | 4 | 6 | 6 | 4 | |
| 42.7702 | 2.112470 | 202 | 4 | 0 | 0 | | 86.0261 | 1.129170 | 23 | 6 | 4 | 2 | | 120.8236 | 0.885790 | 25 | 9 | 3 | 1 | |
| 46.8253 | 1.938540 | 4 | 3 | 3 | 1 | | 88.8867 | 1.100080 | 74 | 7 | 3 | 1 | | 126.5480 | 0.862414 | 48 | 8 | 4 | 4 | |
| 53.0493 | 1.724830 | 82 | 4 | 2 | 2 | | 93.6498 | 1.056240 | 27 | 8 | 0 | 0 | | 130.1922 | 0.849247 | 1 | 9 | 3 | 3 | |
| 56.5462 | 1.626180 | 263 | 5 | 1 | 1 | | 96.5183 | 1.032320 | 1 | 7 | 3 | 3 | | 136.7568 | 0.828581 | 10 | 8 | 6 | 2 | |
| 62.0843 | **1.493750** | 331 | 4 | 4 | 0 | | 97.4779 | 1.024700 | 1 | 6 | 4 | 4 | | 141.1061 | 0.816883 | 29 | 9 | 5 | 1 | |
| 65.2723 | 1.428290 | 7 | 5 | 3 | 1 | | 101.3395 | 0.996830 | 10 | 8 | 2 | 2 | | 142.6488 | 0.813092 | 5 | 10 | 2 | 2 | |
| 66.3160 | 1.408320 | 1 | 4 | 4 | 2 | | 104.2694 | 0.975710 | 36 | 7 | 5 | 1 | | | | | | | | |
| 70.4144 | 1.336050 | 24 | 6 | 2 | 0 | | 105.2541 | 0.969270 | 7 | 6 | 6 | 2 | | | | | | | | |

**04-012-4921** Jun 9, 2020 2:39 PM (fal-sharji2)

**Status** Alternate **QM:** Indexed **Pressure/Temperature:** Pressure (Non-ambient) **Chemical Formula:** Mg ( C O3 )
**Empirical Formula:** C Mg O3 **Weight %:** C14.25 Mg28.83 O56.93 **Atomic %:** C20.00 Mg20.00 O60.00
**ANX:** ABX3 **Compound Name:** Magnesium Carbonate **Mineral Name:** Magnesite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.24 **I/Ic - ND:** 1.15

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.3530(4) Å **AuthCell c:** 13.0325(29) Å **AuthCell Vol:** 213.86 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 35.64 ] **Author's Cell Axial Ratio [ c/a:** 2.994 ]
**Density [ Dcalc:** 3.928 g/cm³ **Dstruc:** 3.93 g/cm³ ] **SS/FOM:** F(30) = 93.6(0.0094, 34)
**Temp:** 293.0 K (Author provided temperature)

**Space Group:** R-3c (167) **Molecular Weight:** 84.31
**Crystal Data [ XtlCell a:** 4.353 Å **XtlCell b:** 4.353 Å **XtlCell c:** 13.033 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 213.86 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 2.994 **a/b:** 1.000 **c/b:** 2.994 ]
**Reduced Cell [ RedCell a:** 4.353 Å **RedCell b:** 4.353 Å **RedCell c:** 5.019 Å **RedCell α:** 64.30°
**RedCell β:** 64.30° **RedCell γ:** 60.00° **RedCell Vol:** 71.29 Å³ ]

**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | IDP | AET |
|---|---|---|---|---|---|---|---|---|---|
| O | 1 | 18e | .2 | 0.3066 | 0.0 | 0.25 | 1.0 | | |
| Mg | 2 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | | |
| C | 3 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | | |

**Subfile(s):** Inorganic, Mineral Related (Mineral , Natural) **Former PDF's #:** 01-070-8518
**LPF Prototype Structure [Formula Order]:** Ca ( C O3 ),hR30,167
**LPF Prototype Structure [Alpha Order]:** C Ca O3,hR30,167 **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 01-080-0101 (Alternate), 01-083-1761 (Alternate), 01-086-0175 (Alternate), ✓ 04-012-4916 (Alternate), ✓ 04-012-4917 (Alternate), ✓ 04-012-4918 (Alternate), ✓ 04-012-4919 (Alternate), ✓ 04-012-4920 (Alternate), ✓ 04-012-4922 (Alternate), ✓ 04-012-4923 (Alternate), ✓ 04-012-4924 (Alternate), ✓ 04-012-4925 (Alternate), ✓ 04-012-4926 (Alternate), ✓ 04-013-2017 (Alternate), ✓ 04-013-2018 (Alternate), ✓ 04-013-2019 (Alternate), ✓ 04-013-2020 (Alternate), ✓ 04-013-2021 (Alternate), ✓ 04-014-4830 (Primary), ✓ 04-014-4846 (Alternate)

**Entry Date:** 09/01/2009 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Structural refinements of magnesite at very high pressure". Fiquet G., Guyot F., Kunz M., Matas J., Andrault D., Hanfland M. Am. Mineral. 87, 1261,1265 (2002). |

**Database Comments:** ANX: ABX3. In Situ Condition: Powdered samples were placed in diamond anvil without pressure transmitting medium. Powdered platinum was used as pressure calibrant. At each pressure samples were annealed by heating with laser and allowed to cool before diffraction data was collected. LPF Collection Code: 1811866. Sample Preparation: Compound Preparation: annealed by local heating at 2000-2500 K by focused infrared laser beam at each pressure step. CRUCIBLE: diamond anvil pressure cell. Pressure of Datacollection: 56.6 GPa. Calculated Pattern Original Remarks: LPF Editor Comment: editor took fixed coordinates from the literature. Temperature of Data Collection: 293 K. Minor Warning: No R factors reported/abstracted. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (49) - Mg ( C O3 ) - 04-012-4921 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 27.3080 | 3.263090 | 111 | 0 | 1 | 2 | | 65.8889 | 1.416410 | 14 | 2 | 1 | 1 | | 90.1149 | 1.088250 | 15m | 0 | 3 | 6 | |
| 36.4176 | **2.465050** | 999 | 1 | 0 | 4 | | 67.1976 | 1.391970 | 57 | 1 | 2 | 2 | | 90.1149 | 1.088250 | m | 2 | 2 | 0 | |
| 41.4530 | 2.176500 | 81 | 1 | 1 | 0 | | 72.3197 | 1.305470 | 93 | 2 | 1 | 4 | | 90.3488 | 1.086040 | 34 | 0 | 0 | 12 | |
| 41.5413 | 2.172080 | 133 | 0 | 0 | 6 | | 75.6117 | 1.256600 | 187 | 3 | 0 | 0 | | 91.8137 | 1.072500 | 42m | 0 | 2 | 10 | |
| 46.6369 | **1.945930** | 760 | 1 | 1 | 3 | | 76.0646 | 1.250240 | 9 | 1 | 2 | 5 | | 91.8137 | 1.072500 | m | 1 | 2 | 8 | |
| 50.3534 | 1.810670 | 119 | 2 | 0 | 2 | | 77.3583 | 1.232530 | 31m | 1 | 0 | 10 | | 93.7204 | 1.055630 | 27 | 2 | 2 | 3 | |
| 56.3434 | 1.631550 | 97 | 0 | 2 | 4 | | 77.3583 | 1.232530 | m | 2 | 0 | 8 | | 95.3068 | 1.042210 | 1 | 1 | 3 | 1 | |
| 60.1339 | **1.537450** | 284 | 1 | 1 | 6 | | 79.4216 | 1.205610 | 65 | 1 | 1 | 9 | | 96.5146 | 1.032350 | 3 | 3 | 1 | 2 | |
| 62.0078 | 1.495410 | 133 | 0 | 1 | 8 | | 85.8052 | 1.131510 | 4 | 2 | 1 | 7 | | 101.3787 | 0.995551 | 49 | 1 | 3 | 4 | |




**04-012-4921** Jun 9, 2020 2:39 PM (fal-sharji2)

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 104.6862 | 0.972965 | 29 | 2 | 2 | 6 | | 116.9294 | 0.903747 | 2 | 0 | 1 | 14 | | 139.2518 | 0.821685 | 73 | 0 | 3 | 12 | |
| 104.8676 | 0.971779 | 9 | 1 | 1 | 12 | | 122.1849 | 0.879917 | 33 | 3 | 1 | 8 | | 139.9297 | 0.819898 | 3 | 2 | 1 | 13 | |
| 105.0803 | 0.970395 | 2 | 3 | 1 | 5 | | 124.6058 | 0.869963 | 13 | 2 | 2 | 9 | | 141.5502 | 0.815773 | 20m | 0 | 4 | 8 | |
| 106.4496 | 0.961659 | 9 | 2 | 1 | 10 | | 126.4055 | 0.862955 | 2 | 3 | 2 | 1 | | 141.5502 | 0.815773 | m | 1 | 3 | 10 | |
| 111.3432 | 0.932747 | 1 | 0 | 4 | 2 | | 127.9124 | 0.857335 | 12 | 2 | 3 | 2 | | 144.7250 | 0.808275 | 21 | 4 | 1 | 3 | |
| 115.4608 | 0.910986 | 2m | 1 | 2 | 11 | | 134.2905 | 0.835905 | 10 | 3 | 2 | 4 | | 145.3367 | 0.806917 | 15 | 1 | 1 | 15 | |
| 115.4608 | 0.910986 | m | 1 | 3 | 7 | | 134.7000 | 0.834653 | 4 | 2 | 0 | 14 | | | | | | | | |
| 116.6022 | 0.905337 | 25 | 4 | 0 | 4 | | 138.8951 | 0.822640 | 11 | 4 | 1 | 0 | | | | | | | | |

**00-044-1481** Jun 9, 2020 2:38 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca ( O H )2
**Empirical Formula:** Ca H2 O2 **Weight %:** Ca54.09 H2.72 O43.19 **Atomic %:** Ca20.00 H40.00 O40.00
**Compound Name:** Calcium Hydroxide **Mineral Name:** Portlandite, syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **Filter:** Graph Mono **d-Spacing:** Diff. **Cutoff:** 15.00
**Intensity:** Diffractometer **I/Ic:** 2.9

**SYS:** Hexagonal **SPGR:** P-3m1 (164)
**Author's Cell [ AuthCell a:** 3.5899(4) Å **AuthCell c:** 4.916(3) Å **AuthCell Vol:** 54.87 Å³ **AuthCell Z:** 1.00
**AuthCell MolVol:** 54.87 ] **Author's Cell Axial Ratio [ c/a:** 1.369 ] **Density [ Dcalc:** 2.242 g/cm³ ]
**SS/FOM:** F(25) = 51.7(0.0167, 29) **Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **Color:** White

**Space Group:** P-3m1 (164) **Molecular Weight:** 74.09
**Crystal Data [ XtlCell a:** 3.590 Å **XtlCell b:** 3.590 Å **XtlCell c:** 4.916 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 54.87 Å³ **XtlCell Z:** 1.00 ]
**Crystal Data Axial Ratio [ c/a:** 1.369 **a/b:** 1.000 **c/b:** 1.369 ]
**Reduced Cell [ RedCell a:** 3.590 Å **RedCell b:** 3.590 Å **RedCell c:** 4.916 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 120.00° **RedCell Vol:** 54.87 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-006-9147** **ADP:** U
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z | 9 | x,x-y,z | 11 | -x+y,y,z |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z | 10 | -x,-x+y,-z | 12 | x-y,-y,-z |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 1a | -3m. | 0.0 | 0.0 | 0.0 | 1.0 | 0.01194 | |
| O | 2 | 2d | 3m. | 0.33333 | 0.66666 | 0.234 | 1.0 | 0.01203 | |
| H | 3 | 2d | 3m. | 0.33333 | 0.66666 | 0.4256 | 1.0 | 0.04203 | |

**Anisotropic Displacement Parameters:**

| Atom | Num | Uani11 | Uani22 | Uani33 | Uani12 | Uani13 | Uani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.0083 | 0.0083 | 0.0193 | 0.0042 | 0.0 | 0.0 |
| O | 2 | 0.0106 | 0.0106 | 0.0149 | 0.0053 | 0.0 | 0.0 |
| H | 3 | 0.0528 | 0.0528 | 0.0205 | 0.0264 | 0.0 | 0.0 |

**Subfile(s):** Cement and Hydration Product, Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic), Pharmaceutical (Excipient)

**Mineral Classification:** Brucite (Group), hydroxide (Subgroup) **Pearson Symbol:** hP5.00
**Pearson Symbol w/o H:** hP3

**Cross-Ref PDF #'s:** ✓ 04-006-9147 (Alternate), ✓ 04-006-9148 (Alternate), ✓ 04-006-9149 (Alternate), ✓ 04-006-9150 (Alternate), ✓ 04-006-9151 (Alternate), ✓ 04-006-9152 (Alternate), ✓ 04-007-5231 (Alternate), ✓ 04-008-0220 (Alternate), ✓ 04-010-3117 (Primary)

**CAS Number - PR:** 1305-62-0 **Entry Date:** 09/01/1994

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA. ICDD Grant-in-Aid (1992). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Optical Data | | Winchell, A., Winchell, H. Microscopic Character of Artificial Inorg. Solid Sub. 69 (1964). |

**Database Comments:** Additional Patterns: Validated by a calculated pattern. Color: White. General Comments: Average relative standard deviation in intensity of the ten strongest reflections for three specimen mounts = 2.2%. Astringent. Sample Source or Locality: Sample obtained from Sigma Chemical Co. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (28) - Ca ( O H )2 - 00-044-1481 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.0073 | **4.922000** | 72 | 0 | 0 | 1 | | 56.0907 | 1.638300 | 1 | 0 | 0 | 3 | | 79.0924 | 1.209800 | 2 | 1 | 1 | 3 | |
| 28.6709 | 3.111000 | 27 | 1 | 0 | 0 | | 59.4244 | 1.554100 | 3 | 2 | 0 | 0 | | 81.9069 | 1.175200 | 2 | 2 | 1 | 0 | |
| 34.1013 | **2.627000** | 100 | 1 | 0 | 1 | | 62.6319 | 1.482000 | 9 | 2 | 0 | 1 | | 84.7484 | 1.142900 | 5m | 1 | 0 | 4 | |
| 36.5257 | 2.458000 | 1 | 0 | 0 | 2 | | 64.2314 | 1.448900 | 7m | 1 | 0 | 3 | | 84.7484 | 1.142900 | m | 2 | 1 | 1 | |
| 47.1200 | 1.927100 | 30 | 1 | 0 | 2 | | 64.2314 | 1.448900 | m | 1 | 1 | 2 | | 86.1940 | 1.127400 | 2 | 2 | 0 | 3 | |
| 50.8120 | **1.795400** | 31 | 1 | 1 | 0 | | 71.8086 | 1.313500 | 6 | 2 | 0 | 2 | | 93.2060 | 1.060100 | 3 | 2 | 1 | 2 | |
| 54.3565 | 1.686400 | 14 | 1 | 1 | 1 | | 77.6520 | 1.228600 | 1 | 0 | 0 | 4 | | 96.0263 | 1.036300 | 2 | 3 | 0 | 0 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 98.8790 | 1.013900 | 2m | 1 | 1 | 4 | | 106.0623 | 0.964100 | 1 | 2 | 0 | 4 | | 118.2628 | 0.897400 | 1 | 2 | 2 | 0 | |
| 98.8790 | 1.013900 | m | 3 | 0 | 1 | | 107.5746 | 0.954700 | 2 | 2 | 1 | 3 | | | | | | | | |
| 103.1389 | 0.983300 | <1 | 0 | 0 | 5 | | 110.5164 | 0.937390 | <1 | 1 | 0 | 5 | | | | | | | | |

**04-017-0477** Jun 9, 2020 2:39 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Mg0.18 Mn2.82 O4
**Empirical Formula:** Mg0.18 Mn2.82 O4 **Weight %:** Mg1.96 Mn69.38 O28.66 **Atomic %:** Mg2.57 Mn40.29 O57.14
**Compound Name:** Magnesium Manganese Oxide **Mineral Name:** Hausmannite, magnesian, syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 2.64 **I/Ic - ND:** 0.93

**SYS:** Tetragonal **SPGR:** I41/amd (141)
**Author's Cell [ AuthCell a:** 5.7550(3) Å **AuthCell c:** 9.4365(8) Å **AuthCell Vol:** 312.54 Å³ **AuthCell Z:** 4.00
**AuthCell MolVol:** 78.14 ] **Author's Cell Axial Ratio [ c/a:** 1.640 ]
**Density [ Dcalc:** 4.746 g/cm³ **Dstruc:** 4.75 g/cm³ ] **SS/FOM:** F(30) = 703.9(0.0013, 33)
**Temp:** 296.0 K (Author provided temperature) **R-factor:** 0.0268

**Space Group:** I41/amd (141) **Molecular Weight:** 223.30
**Crystal Data [ XtlCell a:** 5.755 Å **XtlCell b:** 5.755 Å **XtlCell c:** 9.436 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 312.54 Å³ **XtlCell Z:** 4.00 ]
**Crystal Data Axial Ratio [ c/a:** 1.640 **a/b:** 1.000 **c/b:** 1.640 ]
**Reduced Cell [ RedCell a:** 5.755 Å **RedCell b:** 5.755 Å **RedCell c:** 6.231 Å **RedCell α:** 117.50°
**RedCell β:** 117.50° **RedCell γ:** 90.00° **RedCell Vol:** 156.27 Å³ ]

**ADP:** U **Origin:** O2 **Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 5 | -y+1/4,x+3/4,z+1/4 | 9 | -x+1/2,y,-z+1/2 | 13 | y+1/4,x+3/4,-z+1/4 |
| 2 | -x,-y,-z | 6 | y+3/4,-x+1/4,-z+3/4 | 10 | x+1/2,-y,z+1/2 | 14 | -y+3/4,-x+1/4,z+3/4 |
| 3 | -x+1/2,-y,z+1/2 | 7 | y+1/4,-x+1/4,z+3/4 | 11 | x,-y,-z | 15 | -y+1/4,-x+1/4,-z+3/4 |
| 4 | x+1/2,y,-z+1/2 | 8 | -y+3/4,x+3/4,-z+1/4 | 12 | -x,y,z | 16 | y+3/4,x+3/4,z+1/4 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Mn | 1 | 4a | -4m2 | 0.0 | 0.25 | 0.875 | 0.83 | 0.00581 | |
| Mg | 2 | 4a | -4m2 | 0.0 | 0.25 | 0.875 | 0.17 | 0.00581 | |
| Mn | 3 | 8d | .2/m. | 0.0 | 0.5 | 0.5 | 1.0 | 0.00392 | |
| O | 4 | 16h | .m. | 0.0 | 0.47266 | 0.25827 | 1.0 | 0.00528 | |

**Anisotropic Displacement Parameters:**

| Atom | Num | Uani11 | Uani22 | Uani33 | Uani12 | Uani13 | Uani23 |
|---|---|---|---|---|---|---|---|
| Mn | 1 | 0.00572 | 0.00572 | 0.006 | 0.0 | 0.0 | 0.0 |
| Mg | 2 | 0.00572 | 0.00572 | 0.006 | 0.0 | 0.0 | 0.0 |
| Mn | 3 | 0.00337 | 0.00247 | 0.00593 | 0.0 | 0.0 | -6.5E-4 |
| O | 4 | 0.00425 | 0.00411 | 0.00749 | 0.0 | 0.0 | 2.8E-4 |

**Subfile(s):** Inorganic, Mineral Related (Mineral , Synthetic)
**LPF Prototype Structure [Formula Order]:** Cd Mn2 O4,tI28,141
**LPF Prototype Structure [Alpha Order]:** Cd Mn2 O4,tI28,141 **Pearson Symbol:** tI28.00
**Cross-Ref PDF #'s:** 01-079-6005 (Related Phase) **Entry Date:** 09/01/2013

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Crystal chemistry of the MgAl2O4-MgMn2O4-MnMn2O4 system: Analysis of structural distortion in spinel- and hausmannite-type structures". Bosi F., Halenius U., Skogby H. Am. Mineral. 95, 602 (2010). |

**Database Comments:** LPF Collection Code: 1224723. Sample Preparation: STARTING MATERIALS: MgO,MnO,Mn2O3. COMPOUND PREPARATION: heated at 1473 K for 24 h, cooled to 1073 K at a rate of 4 K h-1, cooled to rt, flux dissolved in HCl solution. CRUCIBLE: platinum crucible.ATMOSPHERE: air.SOLVENT: Na2B4O7 flux. Calculated Pattern Original Remarks: LPF Editor Comment: editor took fixed coordinates from the literature. Temperature of Data Collection: 296 K. Unit Cell Data Source: Single Crystal.

**d-Spacings (87) - Mg0.18 Mn2.82 O4 - 04-017-0477 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.0392 | 4.913360 | 335 | 1 | 0 | 1 | | 45.4992 | 1.991910 | 7 | 2 | 1 | 3 | | 60.8106 | 1.521950 | 12 | 2 | 1 | 5 | |
| 28.9506 | 3.081580 | 334 | 1 | 1 | 2 | | 48.3782 | 1.879880 | 1 | 3 | 0 | 1 | | 63.3461 | 1.467000 | 21 | 1 | 1 | 6 | |
| 31.0538 | 2.877500 | 140 | 2 | 0 | 0 | | 49.9493 | 1.824370 | 54 | 2 | 0 | 4 | | 64.7396 | 1.438750 | 193 | 4 | 0 | 0 | |
| 32.4099 | **2.760130** | 765 | 1 | 0 | 3 | | 50.8748 | 1.793330 | 223 | 1 | 0 | 5 | | 65.5256 | 1.423380 | 15 | 3 | 2 | 3 | |
| 36.1449 | **2.483020** | 999 | 2 | 1 | 1 | | 53.9562 | 1.697960 | 83 | 3 | 1 | 2 | | 67.8559 | 1.380060 | 34m | 2 | 0 | 6 | |
| 36.5460 | 2.456680 | 155 | 2 | 0 | 2 | | 56.1097 | 1.637790 | 78 | 3 | 0 | 3 | | 67.8559 | 1.380060 | m | 4 | 1 | 1 | |
| 38.1144 | 2.359120 | 214 | 0 | 0 | 4 | | 58.6079 | 1.573790 | 289 | 3 | 2 | 1 | | 69.8559 | 1.345360 | 46 | 3 | 0 | 5 | |
| 44.4905 | 2.034700 | 248 | 2 | 2 | 0 | | 59.9901 | **1.540790** | 525 | 2 | 2 | 4 | | 71.8693 | 1.312540 | 1 | 1 | 0 | 7 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 72.4361 | 1.303660 | 13 | 3 | 3 | 2 | | 98.0195 | 1.020480 | 21 | 2 | 2 | 8 | | 118.8371 | 0.894731 | 5 | 5 | 4 | 1 | |
| 73.5356 | 1.286860 | 11 | 4 | 2 | 0 | | 98.4260 | 1.017350 | 42m | 4 | 4 | 0 | | 119.1089 | 0.893481 | 1 | 6 | 2 | 2 | |
| 74.2783 | 1.275820 | 88 | 4 | 1 | 3 | | 98.4260 | 1.017350 | m | 5 | 1 | 4 | | 120.2033 | 0.888534 | 2 | 6 | 0 | 4 | |
| 76.6963 | 1.241510 | 43 | 4 | 2 | 2 | | 99.1480 | 1.011870 | 1 | 5 | 2 | 3 | | 123.0381 | 0.876338 | 33 | 3 | 2 | 9 | |
| 77.6715 | 1.228340 | 49 | 4 | 0 | 4 | | 101.3222 | 0.995953 | 21 | 4 | 2 | 6 | | 124.7125 | 0.869538 | 6 | 4 | 2 | 8 | |
| 78.4008 | 1.218730 | 13 | 3 | 2 | 5 | | 102.1908 | 0.989832 | 1 | 3 | 1 | 8 | | 126.0811 | 0.864194 | 32 | 5 | 4 | 3 | |
| 80.3356 | 1.194180 | 47 | 2 | 1 | 7 | | 103.2314 | 0.982671 | 50 | 4 | 3 | 5 | | 128.7291 | 0.854381 | 31 | 6 | 3 | 1 | |
| 80.6791 | 1.189960 | 21 | 3 | 1 | 6 | | 104.9850 | 0.971014 | 32 | 2 | 1 | 9 | | 130.2696 | 0.848981 | 108m | 1 | 0 | 11 | |
| 81.5398 | 1.179560 | 38 | 0 | 0 | 8 | | 105.7534 | 0.966064 | 9 | 5 | 3 | 2 | | 130.2696 | 0.848981 | m | 6 | 2 | 4 | |
| 84.7822 | 1.142530 | 6 | 5 | 0 | 1 | | 106.8489 | 0.959167 | 3 | 6 | 0 | 0 | | 131.2111 | 0.845789 | 2 | 6 | 1 | 5 | |
| 85.9750 | 1.129710 | 17 | 4 | 2 | 4 | | 109.8163 | 0.941396 | 26 | 6 | 1 | 1 | | 133.7908 | 0.837452 | 15m | 3 | 1 | 10 | |
| 86.6890 | 1.122230 | 59 | 4 | 1 | 5 | | 110.0692 | 0.939941 | 11 | 6 | 0 | 2 | | 133.7908 | 0.837452 | m | 5 | 2 | 7 | |
| 88.5926 | 1.102970 | 1 | 3 | 0 | 7 | | 111.0849 | 0.934187 | 16 | 4 | 4 | 4 | | 134.2615 | 0.835994 | 6 | 5 | 3 | 6 | |
| 89.1327 | 1.097680 | 14 | 5 | 1 | 2 | | 111.8514 | 0.929940 | 1 | 5 | 2 | 5 | | 137.0750 | 0.827673 | 3 | 6 | 3 | 3 | |
| 89.7819 | 1.091420 | 7 | 2 | 0 | 8 | | 113.8458 | 0.919258 | 4 | 1 | 1 | 10 | | 140.3172 | 0.818893 | 9m | 6 | 0 | 6 | |
| 90.8973 | 1.080910 | 58 | 4 | 3 | 3 | | 114.2866 | 0.916967 | 6 | 5 | 1 | 6 | | 140.3172 | 0.818893 | m | 7 | 0 | 1 | |
| 93.0019 | 1.061890 | 26m | 4 | 0 | 6 | | 115.2229 | 0.912184 | 59 | 4 | 0 | 8 | | 141.6684 | 0.815480 | 1 | 5 | 1 | 8 | |
| 93.0019 | 1.061890 | m | 5 | 2 | 1 | | 115.6687 | 0.909945 | 17m | 5 | 3 | 4 | | 142.3364 | 0.813845 | 1 | 2 | 1 | 11 | |
| 96.6180 | 1.031520 | 4 | 1 | 0 | 9 | | 115.6687 | 0.909945 | m | 6 | 2 | 0 | | 143.3359 | 0.811462 | 34 | 5 | 4 | 5 | |
| 96.8206 | 1.029900 | 37 | 3 | 2 | 7 | | 116.4627 | 0.906019 | 1 | 6 | 1 | 3 | | 147.6466 | 0.802035 | 9 | 7 | 1 | 2 | |
| 97.1618 | 1.027190 | 7 | 3 | 3 | 6 | | 118.4202 | 0.896665 | 8 | 2 | 0 | 10 | | 149.6682 | 0.798075 | 4 | 6 | 4 | 0 | |

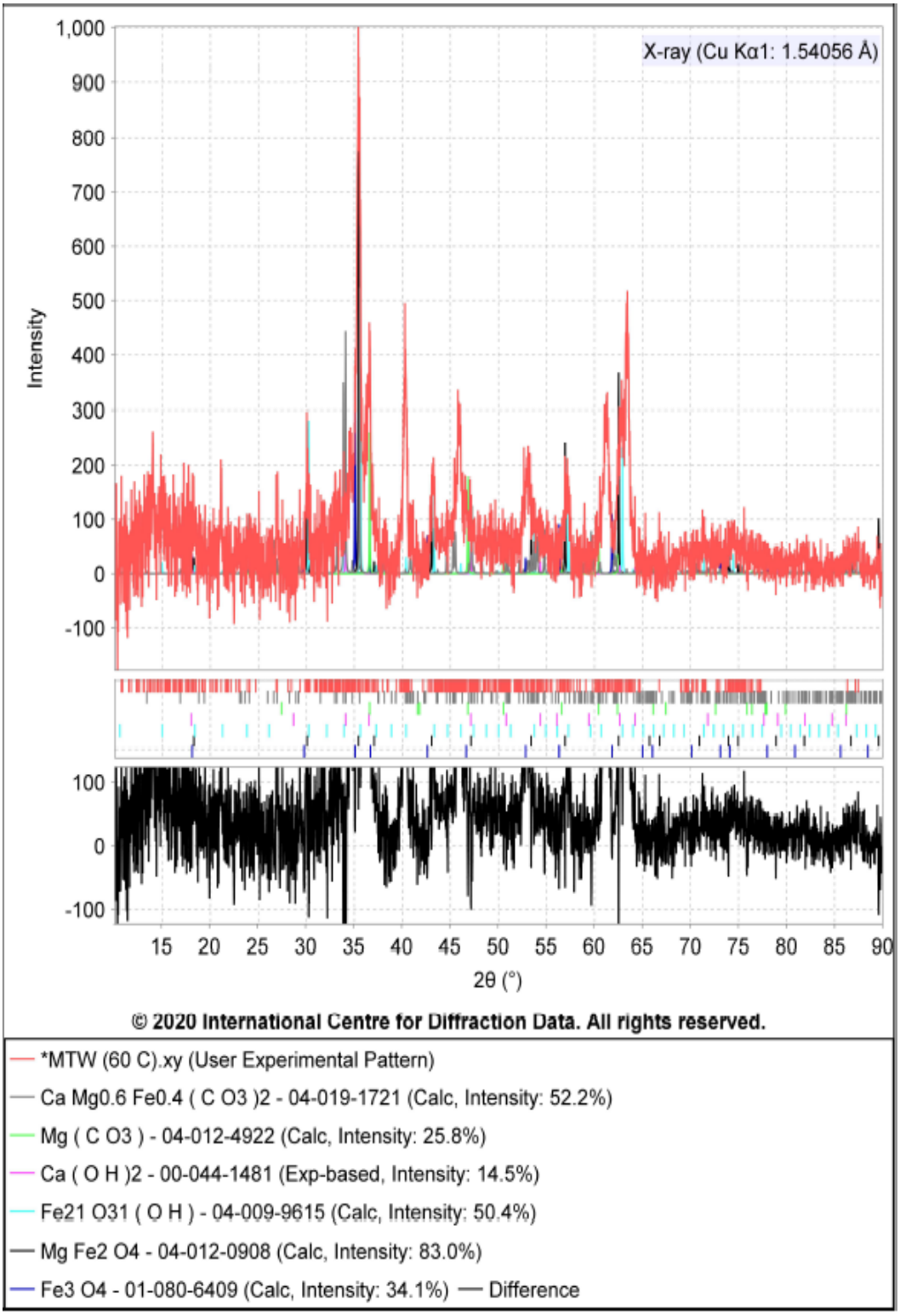


**Figure E.2 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) tank at 60 °C from experiment with a tank with 70.4 in$^2$ of exposed iron**

# SIeve+ Report

## Experiment

**Search Line:** 2.541329 Å **D1 Range:** 2.531 Å - 2.552 Å
**Search Line:** 1.466467 Å **D1 Range:** 1.463 Å - 1.470 Å
**Search Line:** 1.462872 Å **D1 Range:** 1.460 Å - 1.466 Å
**Search Line:** 1.468115 Å **D1 Range:** 1.465 Å - 1.471 Å
**Search Line:** 2.236972 Å **D1 Range:** 2.229 Å - 2.245 Å
**Search Line:** 2.232486 Å **D1 Range:** 2.225 Å - 2.240 Å
**Search Line:** 1.511506 Å **D1 Range:** 1.508 Å - 1.515 Å
**Search Line:** 2.464816 Å **D1 Range:** 2.455 Å - 2.475 Å
**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (6)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 04-019-1721 | I | Calcium Magnesium Iron Carbonate | 0.522 | 20.088 | 0.8 | 53 |
| 2 | true | 04-012-4922 | I | Magnesium Carbonate | 0.258 | 9.928 | *1.82 | 11 |
| 3 | true | 00-044-1481 | S | Calcium Hydroxide | 0.145 | 5.564 | *3.61 | 3 |
| 4 | true | 04-009-9615 | I | Iron Oxide Hydroxide | 0.504 | 19.397 | 3.58 | 11 |
| 5 | true | 04-012-0908 | S | Magnesium Iron Oxide | 0.830 | 31.921 | *4.21 | 16 |
| 6 | true | 01-080-6409 | S | Iron Oxide | 0.341 | 13.102 | *5.16 | 5 |

**04-019-1721** Jun 23, 2020 12:45 PM (fal-sharji2)

**Status** Primary **QM:** Indexed **Pressure/Temperature:** Pressure (Non-ambient)
**Chemical Formula:** Ca Mg0.6 Fe0.4 ( C O3 )2 **Empirical Formula:** C2 Ca Fe0.4 Mg0.6 O6
**Weight %:** C12.19 Ca20.34 Fe11.34 Mg7.40 O48.72 **Atomic %:** C20.00 Ca10.00 Fe4.00 Mg6.00 O60.00
**ANX:** ABC2X6 **Compound Name:** Calcium Magnesium Iron Carbonate **Mineral Name:** Dolomite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 0.8 **I/Ic - ND:** 0.36

**SYS:** Triclinic (Anorthic) **SPGR:** P-1 (2)
**Author's Cell [ AuthCell a:** 4.7407(10) Å **AuthCell b:** 5.3885(10) Å **AuthCell c:** 6.743(1) Å
**AuthCell α:** 101.42(1)° **AuthCell β:** 89.27(1)° **AuthCell γ:** 95.72(1)° **AuthCell Vol:** 168.00 Å³
**AuthCell Z:** 2.00 **AuthCell MolVol:** 84.00 **]** **Author's Cell Axial Ratio [ c/a:** 1.422 **a/b:** 0.880 **c/b:** 1.251 **]**
**Density [ Dcalc:** 3.895 g/cm³ **Dstruc:** 3.89 g/cm³ **]** **SS/FOM:** F(30) = 498.5(0.0017, 35)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.0582

**Space Group:** P-1 (2) **Molecular Weight:** 197.02
**Crystal Data [ XtlCell a:** 5.389 Å **XtlCell b:** 6.743 Å **XtlCell c:** 4.741 Å **XtlCell α:** 90.73° **XtlCell β:** 95.72°
**XtlCell γ:** 78.58° **XtlCell Vol:** 168.00 Å³ **XtlCell Z:** 2.00 **]**
**Crystal Data Axial Ratio [ c/a:** 0.880 **a/b:** 0.799 **c/b:** 0.703 **]**
**Reduced Cell [ RedCell a:** 4.741 Å **RedCell b:** 5.389 Å **RedCell c:** 6.743 Å **RedCell α:** 78.58°
**RedCell β:** 89.27° **RedCell γ:** 84.28° **RedCell Vol:** 168.00 Å³ **]**

**ADP:** U **Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator |
|---|---|---|---|
| 1 | x,y,z | 2 | -x,-y,-z |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Mg | 1 | 2i | 1 | -0.2 | 0.7473 | -0.2016 | 0.6 | 0.0167 | |
| Fe | 2 | 2i | 1 | -0.2 | 0.7473 | -0.2016 | 0.4 | 0.0167 | |
| Ca | 3 | 2i | 1 | -0.2418 | 0.7926 | 0.3039 | 1.0 | 0.0167 | |
| C | 4 | 2i | 1 | 0.3 | 0.73 | -0.486 | 1.0 | 0.013 | |
| C | 5 | 2i | 1 | 0.262 | 0.74 | -0.014 | 1.0 | 0.018 | |
| O | 6 | 2i | 1 | 0.143 | 0.586 | -0.147 | 1.0 | 0.0143 | |
| O | 7 | 2i | 1 | -0.129 | 0.1226 | -0.123 | 1.0 | 0.0206 | |
| O | 8 | 2i | 1 | 0.546 | 0.742 | 0.026 | 1.0 | 0.0201 | |
| O | 9 | 2i | 1 | 0.493 | 0.863 | -0.372 | 1.0 | 0.0139 | |
| O | 10 | 2i | 1 | 0.349 | 0.5819 | -0.638 | 1.0 | 0.019 | |
| O | 11 | 2i | 1 | 0.041 | 0.791 | -0.447 | 1.0 | 0.0169 | |

**Subfile(s):** Inorganic, Mineral Related (Mineral , Natural) **Former PDF's #:** 01-081-9916
**LPF Prototype Structure [Formula Order]:** Ca ( Mg0.6 Fe0.4 ) [ C O3 ]2,aP20,2
**LPF Prototype Structure [Alpha Order]:** C2 Ca Fe0.4 Mg0.6 O6,aP20,2
**Mineral Classification:** Calcite (Supergroup), dolomite (Group) **Pearson Symbol:** aP20.00 **Entry Date:** 09/01/2015

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Structures of dolomite at ultrahigh pressure and their influence on the deep carbon cycle". Merlini M., Crichton W.A., Hanfland M., Gemmi M., Muller H., Kupenko I., Dubrovinsky L.S. Proc. Natl. Acad. Sci. U. S. A. 109, 13509,13514 (2012). |

**Database Comments:** ANX: ABC2X6. LPF Collection Code: 1229824. Polymorphism/Phase Transition: High pressure phase 1. Pressure of Datacollection: 34.4 GPa. Calculated Pattern Original Remarks: LPF Editor Comment: unit for isotropic displacement parameters omitted, assumed to be angstrom2. Sample Source or Locality: France, Vizille, Vaulnaveys, Chachatier. Minor Warning: Minor warning from the LPF Editor exist. LPF Editor Comment: editor assigned an approximate value to the Fe/Mg ratio of site Mg,Fe based on the nominal composition. Unit Cell Data Source: Single Crystal.

**d-Spacings (199) - Ca Mg0.6 Fe0.4 ( C O3 )2 - 04-019-1721 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 13.3854 | 6.609330 | 7 | 0 | 0 | 1 | | 25.9738 | 3.427610 | 28 | 1 | -1 | 1 | | 33.1844 | 2.697460 | 207 | 1 | 0 | 2 | |
| 16.8550 | 5.255810 | 15 | 0 | 1 | 0 | | 26.5916 | 3.349360 | 123 | 1 | 1 | 0 | | 33.8537 | **2.645640** | 720 | 1 | -1 | 2 | |
| 18.7970 | 4.716970 | 7 | 1 | 0 | 0 | | 26.9579 | 3.304670 | 54 | 0 | 0 | 2 | | 34.0891 | **2.627910** | 879m | 0 | 2 | 0 | |
| 19.3719 | 4.578260 | 3 | 0 | -1 | 1 | | 28.2235 | 3.159300 | 1 | -1 | -1 | 1 | | 34.0891 | **2.627910** | m | 0 | -2 | 1 | |
| 23.0670 | 3.852540 | 5 | -1 | 0 | 1 | | 28.9077 | 3.086060 | 55 | 0 | -1 | 2 | | 34.7786 | 2.577370 | 48 | 0 | 1 | 2 | |
| 23.2261 | 3.826500 | 19 | 1 | 0 | 1 | | 29.1829 | 3.057580 | 30 | -1 | 1 | 1 | | 35.5439 | **2.523610** | 999 | -1 | -1 | 2 | |
| 23.5994 | 3.766820 | 21 | 0 | 1 | 1 | | 31.4605 | 2.841220 | 2 | 1 | 1 | 1 | | 37.4570 | 2.399000 | 44 | -1 | 2 | 0 | |
| 24.0491 | 3.697390 | 216 | -1 | 1 | 0 | | 32.9551 | 2.715700 | 28 | -1 | 0 | 2 | | 37.5222 | 2.394980 | 40 | 1 | -2 | 1 | |

**04-019-1721** Jun 23, 2020 12:45 PM (fal-sharji2)

| 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|
| 38.1249 | 2.358490 | 153 | 2 | 0 | 0 | |
| 38.8667 | 2.315170 | 82 | -1 | 1 | 2 | |
| 39.3269 | 2.289130 | 78m | 0 | 2 | 1 | |
| 39.3269 | 2.289130 | m | 0 | -2 | 2 | |
| 40.2985 | 2.236150 | 14 | -2 | 1 | 0 | |
| 40.4835 | 2.226360 | 2 | -2 | 0 | 1 | |
| 40.7602 | 2.211880 | 53 | 1 | 1 | 2 | |
| 40.8997 | 2.204660 | 63m | 0 | 0 | 3 | |
| 40.8997 | 2.204660 | m | 1 | 2 | 0 | |
| 41.1419 | 2.192240 | 13 | 0 | -1 | 3 | |
| 41.5879 | 2.169750 | 43 | 2 | -1 | 1 | |
| 42.2539 | 2.137080 | 75 | -1 | 2 | 1 | |
| 42.4306 | 2.128590 | 98 | 1 | -2 | 2 | |
| 43.6888 | 2.070160 | 12 | -2 | 1 | 1 | |
| 44.5886 | 2.030450 | 82 | -2 | -1 | 1 | |
| 44.9599 | 2.014540 | 6 | 1 | -1 | 3 | |
| 45.2659 | 2.001630 | 105 | -1 | 0 | 3 | |
| 45.4825 | 1.992600 | 164m | 1 | 0 | 3 | |
| 45.4825 | 1.992600 | m | 1 | 2 | 1 | |
| 46.2195 | 1.962530 | 2 | -1 | -1 | 3 | |
| 46.9243 | 1.934680 | 38 | 2 | 1 | 1 | |
| 47.1416 | 1.926270 | 245 | -2 | 0 | 2 | |
| 47.2454 | 1.922280 | 241 | 2 | -1 | 2 | |
| 47.4820 | 1.913250 | 27 | 2 | 0 | 2 | |
| 48.2818 | 1.883410 | 76m | 0 | 2 | 2 | |
| 48.2818 | 1.883410 | m | 0 | -2 | 3 | |
| 49.3415 | 1.845410 | 99 | 2 | -2 | 1 | |
| 49.8139 | 1.829010 | 9 | -2 | -1 | 2 | |
| 50.7872 | 1.796220 | 57 | -1 | 2 | 2 | |
| 51.0098 | 1.788900 | 74m | 1 | -2 | 3 | |
| 51.0098 | 1.788900 | m | -2 | 1 | 2 | |
| 52.1660 | 1.751940 | 44 | 0 | 3 | 0 | |
| 52.5860 | 1.738930 | 13 | 1 | 1 | 3 | |
| 53.0354 | 1.725250 | 46 | 1 | -3 | 1 | |
| 53.1520 | 1.721740 | 47 | -2 | 2 | 1 | |
| 53.4174 | 1.713810 | 67 | 2 | -2 | 2 | |
| 53.6961 | 1.705570 | 118 | 1 | 2 | 2 | |
| 53.9490 | 1.698170 | 118 | -1 | 3 | 0 | |
| 54.0650 | 1.694800 | 129m | 0 | -3 | 2 | |
| 54.0650 | 1.694800 | m | 2 | 1 | 2 | |
| 54.7998 | 1.673800 | 166m | 0 | -1 | 4 | |
| 54.7998 | 1.673800 | m | 2 | 2 | 0 | |
| 55.9573 | 1.641890 | 80 | 1 | -3 | 2 | |
| 56.2582 | 1.633820 | 4 | 2 | -1 | 3 | |
| 56.9286 | 1.616160 | 19m | 0 | 3 | 1 | |
| 56.9286 | 1.616160 | m | -1 | -3 | 1 | |
| 57.3907 | 1.604240 | 3 | 2 | 0 | 3 | |
| 57.8879 | 1.591640 | 57m | 1 | 3 | 0 | |
| 57.8879 | 1.591640 | m | 1 | -1 | 4 | |
| 58.3695 | 1.579650 | 89m | -2 | -1 | 3 | |
| 58.3695 | 1.579650 | m | -2 | -2 | 2 | |
| 58.6681 | 1.572320 | 29 | 3 | 0 | 0 | |
| 58.9492 | 1.565490 | 37 | -1 | -1 | 4 | |
| 59.0553 | 1.562930 | 44 | -1 | 0 | 4 | |
| 59.3467 | 1.555950 | 40 | 1 | 0 | 4 | |
| 59.6644 | 1.548420 | 157m | -1 | -3 | 2 | |
| 59.6644 | 1.548420 | m | -3 | 1 | 0 | |
| 59.8941 | 1.543030 | 56m | 0 | 2 | 3 | |
| 59.8941 | 1.543030 | m | 0 | -2 | 4 | |
| 60.3652 | 1.532110 | 10 | -3 | 0 | 1 | |
| 60.5100 | 1.528790 | 40 | -2 | 2 | 2 | |
| 60.5809 | 1.527170 | 42m | 0 | -3 | 3 | |
| 60.5809 | 1.527170 | m | 3 | 0 | 1 | |
| 61.2528 | 1.512020 | 1 | -2 | 1 | 3 | |
| 61.9719 | 1.496190 | 51 | -1 | 2 | 3 | |
| 62.0719 | 1.494020 | 95m | 0 | 1 | 4 | |
| 62.0719 | 1.494020 | m | 2 | -3 | 1 | |
| 62.1949 | 1.491360 | 69 | -3 | 1 | 1 | |
| 62.2859 | 1.489400 | 58m | 1 | -2 | 4 | |
| 62.2859 | 1.489400 | m | 1 | -3 | 3 | |
| 62.8084 | 1.478260 | 5 | -2 | 3 | 0 | |
| 63.3476 | 1.466970 | 14 | 3 | 1 | 0 | |
| 64.1155 | 1.451240 | 9m | 2 | 1 | 3 | |
| 64.1155 | 1.451240 | m | -3 | -1 | 1 | |
| 64.4392 | 1.444730 | 32 | -1 | -2 | 4 | |
| 64.7113 | 1.439310 | 16m | 2 | -3 | 2 | |
| 64.7113 | 1.439310 | m | -1 | 1 | 4 | |
| 64.9341 | 1.434910 | 12 | 0 | 3 | 2 | |
| 65.1283 | 1.431100 | 15 | 3 | -1 | 2 | |
| 65.3721 | 1.426350 | 2 | -2 | -2 | 3 | |
| 65.5049 | 1.423780 | 1 | -3 | 0 | 2 | |
| 65.9167 | 1.415880 | 34 | 3 | 0 | 2 | |
| 66.2146 | 1.410230 | 20m | 1 | 1 | 4 | |
| 66.2146 | 1.410230 | m | 3 | -2 | 1 | |
| 66.4294 | 1.406190 | 10 | -1 | 3 | 2 | |
| 67.0225 | 1.395180 | 3 | -2 | 3 | 1 | |
| 67.8079 | 1.380920 | 17 | 2 | -1 | 4 | |
| 68.0930 | 1.375830 | 38 | -3 | 1 | 2 | |
| 68.2714 | 1.372670 | 22 | -3 | -1 | 2 | |
| 69.0494 | 1.359090 | 9 | -2 | -3 | 1 | |
| 69.1214 | 1.357850 | 10 | -2 | 0 | 4 | |
| 69.6838 | 1.348260 | 9m | 2 | 0 | 4 | |
| 69.6838 | 1.348260 | m | 3 | -2 | 2 | |
| 69.9333 | 1.344060 | 10 | 2 | 3 | 0 | |
| 70.0719 | 1.341740 | 47m | 0 | -3 | 4 | |
| 70.0719 | 1.341740 | m | 0 | -4 | 1 | |
| 70.6831 | 1.331630 | 32m | 2 | -3 | 3 | |
| 70.6831 | 1.331630 | m | -2 | 2 | 3 | |
| 71.1186 | 1.324540 | 7 | 1 | -4 | 1 | |
| 71.2252 | 1.322820 | 6m | 0 | 0 | 5 | |
| 71.2252 | 1.322820 | m | 2 | -2 | 4 | |
| 71.4768 | 1.318780 | 7 | -2 | -3 | 2 | |
| 71.7802 | 1.313950 | 19m | 0 | 4 | 0 | |
| 71.7802 | 1.313950 | m | 0 | -4 | 2 | |
| 71.9637 | 1.311050 | 18 | 3 | 1 | 2 | |
| 72.6090 | 1.300980 | 2 | 1 | -1 | 5 | |
| 72.8057 | 1.297950 | 4m | 1 | -4 | 2 | |
| 72.8057 | 1.297950 | m | 3 | -1 | 3 | |
| 73.0684 | 1.293930 | 14m | 3 | 2 | 0 | |
| 73.0684 | 1.293930 | m | -3 | -2 | 1 | |
| 73.4140 | 1.288690 | 8m | 0 | 2 | 4 | |
| 73.4140 | 1.288690 | m | -1 | -1 | 5 | |
| 73.8370 | 1.282350 | 11 | -2 | 1 | 4 | |
| 74.0782 | 1.278770 | 3 | 2 | 3 | 1 | |
| 74.3689 | 1.274490 | 10m | -1 | 0 | 5 | |
| 74.3689 | 1.274490 | m | -2 | 3 | 2 | |
| 74.8567 | 1.267390 | 1 | -1 | -3 | 4 | |
| 75.3284 | 1.260620 | 25m | -1 | 2 | 4 | |
| 75.3284 | 1.260620 | m | -2 | -2 | 4 | |
| 75.5940 | 1.256850 | 8m | 0 | 3 | 3 | |
| 75.5940 | 1.256850 | m | -1 | -4 | 1 | |
| 76.3049 | 1.246900 | 1 | 3 | -2 | 3 | |
| 76.6036 | 1.242780 | 23m | 0 | -4 | 3 | |
| 76.6036 | 1.242780 | m | 2 | 1 | 4 | |
| 76.9734 | 1.237730 | 7m | -1 | 3 | 3 | |
| 76.9734 | 1.237730 | m | -3 | 1 | 3 | |
| 77.0862 | 1.236200 | 3 | -2 | -3 | 3 | |
| 77.2097 | 1.234530 | 3m | 1 | 4 | 0 | |
| 77.2097 | 1.234530 | m | -1 | -4 | 2 | |
| 77.3635 | 1.232460 | 4 | -3 | 3 | 0 | |
| 77.6108 | 1.229150 | 8m | 1 | -4 | 3 | |
| 77.6108 | 1.229150 | m | -1 | -2 | 5 | |
| 77.8213 | 1.226350 | 14m | 0 | 1 | 5 | |
| 77.8213 | 1.226350 | m | 1 | 2 | 4 | |
| 78.4031 | 1.218700 | 7 | 2 | -4 | 1 | |
| 79.1707 | 1.208800 | 3 | 3 | -3 | 2 | |
| 79.6259 | 1.203030 | 2 | 2 | -3 | 4 | |
| 79.9073 | 1.199500 | 9 | -2 | 4 | 0 | |
| 80.0685 | 1.197490 | 16 | 2 | -4 | 2 | |
| 80.2555 | 1.195170 | 4 | -1 | 1 | 5 | |
| 80.5688 | 1.191310 | 4 | 1 | 3 | 3 | |
| 80.8718 | 1.187610 | 5 | 3 | 1 | 3 | |
| 81.3027 | 1.182400 | 16m | 2 | 3 | 2 | |
| 81.3027 | 1.182400 | m | -3 | 3 | 1 | |
| 81.5667 | 1.179240 | 11m | 2 | -1 | 5 | |
| 81.5667 | 1.179240 | m | 4 | 0 | 0 | |
| 81.8562 | 1.175800 | 6m | -1 | -4 | 3 | |
| 81.8562 | 1.175800 | m | -4 | 1 | 0 | |
| 81.9738 | 1.174410 | 5 | 1 | 4 | 1 | |
| 82.1327 | 1.172540 | 1 | 0 | -3 | 5 | |
| 82.3737 | 1.169720 | 5 | -3 | -2 | 3 | |
| 82.8040 | 1.164730 | 20m | 3 | 2 | 2 | |
| 82.8040 | 1.164730 | m | 4 | -1 | 1 | |
| 83.0110 | 1.162350 | 5 | -4 | 0 | 1 | |
| 83.2034 | 1.160150 | 11m | 3 | -1 | 4 | |
| 83.2034 | 1.160150 | m | 4 | 0 | 1 | |
| 83.4286 | 1.157590 | 5 | -2 | 2 | 4 | |
| 83.5117 | 1.156650 | 6 | -2 | 0 | 5 | |
| 83.7255 | 1.154240 | 1 | 1 | -3 | 5 | |
| 84.0714 | 1.150370 | 2m | 2 | 0 | 5 | |
| 84.0714 | 1.150370 | m | 2 | -2 | 5 | |
| 84.5959 | 1.144570 | 52m | 0 | -4 | 4 | |
| 84.5959 | 1.144570 | m | -2 | 3 | 3 | |
| 84.7264 | 1.143140 | 22m | 3 | -3 | 3 | |
| 84.7264 | 1.143140 | m | -3 | 0 | 4 | |
| 85.3171 | 1.136730 | 3 | -1 | 4 | 2 | |
| 85.4800 | 1.134980 | 7 | 3 | 0 | 4 | |
| 85.6062 | 1.133630 | 5 | 1 | -4 | 4 | |
| 85.7262 | 1.132350 | 7m | -2 | -3 | 4 | |
| 85.7262 | 1.132350 | m | -3 | -1 | 4 | |
| 85.8721 | 1.130800 | 6 | 3 | -2 | 4 | |
| 86.2302 | 1.127020 | 21 | 4 | 1 | 0 | |
| 86.5514 | 1.123660 | 5 | 0 | -1 | 6 | |
| 86.8881 | 1.120170 | 4m | 4 | -1 | 2 | |
| 86.8881 | 1.120170 | m | -4 | -1 | 1 | |

**04-012-4922** Jun 23, 2020 12:45 PM (fal-sharji2)

**Status** Alternate **QM:** Indexed **Pressure/Temperature:** Pressure (Non-ambient) **Chemical Formula:** Mg ( C O3 )
**Empirical Formula:** C Mg O3 **Weight %:** C14.25 Mg28.83 O56.93 **Atomic %:** C20.00 Mg20.00 O60.00
**ANX:** ABX3 **Compound Name:** Magnesium Carbonate **Mineral Name:** Magnesite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.36 **I/Ic - ND:** 1.1

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.3401(3) Å **AuthCell c:** 12.9538(22) Å **AuthCell Vol:** 211.31 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 35.22 **] Author's Cell Axial Ratio [ c/a:** 2.985 **]**
**Density [ Dcalc:** 3.975 g/cm³ **Dstruc:** 3.97 g/cm³ **] SS/FOM:** F(30) = 309.2(0.0031, 31)
**Temp:** 293.0 K (Author provided temperature)

**Space Group:** R-3c (167) **Molecular Weight:** 84.31
**Crystal Data [ XtlCell a:** 4.340 Å **XtlCell b:** 4.340 Å **XtlCell c:** 12.954 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 211.31 Å³ **XtlCell Z:** 6.00 **]**
**Crystal Data Axial Ratio [ c/a:** 2.985 **a/b:** 1.000 **c/b:** 2.985 **]**
**Reduced Cell [ RedCell a:** 4.340 Å **RedCell b:** 4.340 Å **RedCell c:** 4.992 Å **RedCell α:** 64.24°
**RedCell β:** 64.23° **RedCell γ:** 60.00° **RedCell Vol:** 70.44 Å³ **]**

**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | IDP | AET |
|---|---|---|---|---|---|---|---|---|---|
| O | 1 | 18e | .2 | 0.2967 | 0.0 | 0.25 | 1.0 | | |
| Mg | 2 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | | |
| C | 3 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | | |

**Subfile(s):** Inorganic, Mineral Related (Mineral , Natural) **Former PDF's #:** 01-070-8519
**LPF Prototype Structure [Formula Order]:** Ca ( C O3 ),hR30,167
**LPF Prototype Structure [Alpha Order]:** C Ca O3,hR30,167 **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 01-080-0101 (Alternate), 01-083-1761 (Alternate), 01-086-0175 (Alternate), ✓ 04-012-4916 (Alternate), ✓ 04-012-4917 (Alternate), ✓ 04-012-4918 (Alternate), ✓ 04-012-4919 (Alternate), ✓ 04-012-4920 (Alternate), ✓ 04-012-4921 (Alternate), ✓ 04-012-4923 (Alternate), ✓ 04-012-4924 (Alternate), ✓ 04-012-4925 (Alternate), ✓ 04-012-4926 (Alternate), ✓ 04-013-2017 (Alternate), ✓ 04-013-2018 (Alternate), ✓ 04-013-2019 (Alternate), ✓ 04-013-2020 (Alternate), ✓ 04-013-2021 (Alternate), ✓ 04-014-4830 (Primary), ✓ 04-014-4846 (Alternate)

**Entry Date:** 09/01/2009 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Structural refinements of magnesite at very high pressure". Fiquet G., Guyot F., Kunz M., Matas J., Andrault D., Hanfland M. Am. Mineral. 87, 1261,1265 (2002). |

**Database Comments:** ANX: ABX3. In Situ Condition: Powdered samples were placed in diamond anvil without pressure transmitting medium. Powdered platinum was used as pressure calibrant. At each pressure samples were annealed by heating with laser and allowed to cool before diffraction data was collected. LPF Collection Code: 1811867. Sample Preparation: Compound Preparation: annealed by local heating at 2000-2500 K by focused infrared laser beam at each pressure step. CRUCIBLE: diamond anvil pressure cell. Pressure of Datacollection: 60.2 GPa. Calculated Pattern Original Remarks: LPF Editor Comment: editor took fixed coordinates from the literature. Temperature of Data Collection: 293 K. Minor Warning: No R factors reported/abstracted. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (48) - Mg ( C O3 ) - 04-012-4922 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 27.4125 | 3.250890 | 61 | 0 | 1 | 2 | | 66.1125 | 1.412160 | 24 | 2 | 1 | 1 | | 90.4572 | 1.085020 | 7 | 2 | 2 | 0 | |
| 36.5966 | **2.453400** | 999 | 1 | 0 | 4 | | 67.4353 | 1.387640 | 60 | 1 | 2 | 2 | | 90.6055 | 1.083630 | 7 | 0 | 3 | 6 | |
| 41.5819 | 2.170050 | 67 | 1 | 1 | 0 | | 72.6103 | 1.300960 | 77 | 2 | 1 | 4 | | 91.0516 | 1.079480 | 30 | 0 | 0 | 12 | |
| 41.8053 | 2.158970 | 114 | 0 | 0 | 6 | | 75.8759 | 1.252880 | 159 | 3 | 0 | 0 | | 92.3255 | 1.067890 | 32 | 1 | 2 | 8 | |
| 46.8146 | **1.938960** | 658 | 1 | 1 | 3 | | 76.3953 | 1.245650 | 13 | 1 | 2 | 5 | | 92.4744 | 1.066560 | 14 | 0 | 2 | 10 | |
| 50.5263 | 1.804880 | 131 | 2 | 0 | 2 | | 77.7949 | 1.226700 | 23 | 2 | 0 | 8 | | 94.1069 | 1.052310 | 19 | 2 | 2 | 3 | |
| 56.5738 | 1.625450 | 76 | 0 | 2 | 4 | | 77.9467 | 1.224690 | 7 | 1 | 0 | 10 | | 95.6838 | 1.039100 | 2 | 1 | 3 | 1 | |
| 60.4345 | **1.530520** | 251 | 1 | 1 | 6 | | 79.9105 | 1.199460 | 56 | 1 | 1 | 9 | | 96.9072 | 1.029210 | 1 | 3 | 1 | 2 | |
| 62.3930 | 1.487100 | 129 | 0 | 1 | 8 | | 86.2445 | 1.126870 | 7 | 2 | 1 | 7 | | 101.8363 | 0.992314 | 50 | 1 | 3 | 4 | |




**04-012-4922** Jun 23, 2020 12:45 PM (fal-sharji2)

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 105.2219 | 0.969478 | 24 | 2 | 2 | 6 | | 117.2008 | 0.902438 | 28 | 4 | 0 | 4 | | 136.2260 | 0.830114 | 4 | 2 | 0 | 14 | |
| 105.6845 | 0.966504 | 8m | 1 | 1 | 12 | | 118.0394 | 0.898449 | 1 | 0 | 1 | 14 | | 139.8134 | 0.820202 | 9 | 4 | 1 | 0 | |
| 105.6845 | 0.966504 | m | 3 | 1 | 5 | | 122.9950 | 0.876517 | 34 | 3 | 1 | 8 | | 140.7438 | 0.817800 | 63 | 0 | 3 | 12 | |
| 107.1675 | 0.957196 | 10 | 2 | 1 | 10 | | 125.5062 | 0.866416 | 10 | 2 | 2 | 9 | | 141.5477 | 0.815779 | 3 | 2 | 1 | 13 | |
| 111.8543 | 0.929924 | 1 | 0 | 4 | 2 | | 127.0869 | 0.860386 | 4 | 3 | 2 | 1 | | 142.8026 | 0.812724 | 23 | 0 | 4 | 8 | |
| 116.0074 | 0.908261 | 1 | 1 | 3 | 7 | | 128.6264 | 0.854749 | 13 | 2 | 3 | 2 | | 145.8526 | 0.805793 | 13 | 4 | 1 | 3 | |
| 116.3387 | 0.906627 | 3 | 1 | 2 | 11 | | 135.1620 | 0.833258 | 7 | 3 | 2 | 4 | | 147.4752 | 0.802384 | 12 | 1 | 1 | 15 | |

**00-044-1481** Jun 23, 2020 12:44 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca ( O H )2
**Empirical Formula:** Ca H2 O2 **Weight %:** Ca54.09 H2.72 O43.19 **Atomic %:** Ca20.00 H40.00 O40.00
**Compound Name:** Calcium Hydroxide **Mineral Name:** Portlandite, syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **Filter:** Graph Mono **d-Spacing:** Diff. **Cutoff:** 15.00
**Intensity:** Diffractometer **I/Ic:** 2.9

**SYS:** Hexagonal **SPGR:** P-3m1 (164)
**Author's Cell [ AuthCell a:** 3.5899(4) Å **AuthCell c:** 4.916(3) Å **AuthCell Vol:** 54.87 Å³ **AuthCell Z:** 1.00
**AuthCell MolVol:** 54.87 ] **Author's Cell Axial Ratio [ c/a:** 1.369 ] **Density [ Dcalc:** 2.242 g/cm³ ]
**SS/FOM:** F(25) = 51.7(0.0167, 29) **Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **Color:** White

**Space Group:** P-3m1 (164) **Molecular Weight:** 74.09
**Crystal Data [ XtlCell a:** 3.590 Å **XtlCell b:** 3.590 Å **XtlCell c:** 4.916 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 54.87 Å³ **XtlCell Z:** 1.00 ]
**Crystal Data Axial Ratio [ c/a:** 1.369 **a/b:** 1.000 **c/b:** 1.369 ]
**Reduced Cell [ RedCell a:** 3.590 Å **RedCell b:** 3.590 Å **RedCell c:** 4.916 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 120.00° **RedCell Vol:** 54.87 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-006-9147** **ADP:** U
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z | 9 | x,x-y,z | 11 | -x+y,y,z |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z | 10 | -x,-x+y,-z | 12 | x-y,-y,-z |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 1a | -3m. | 0.0 | 0.0 | 0.0 | 1.0 | 0.01194 | |
| O | 2 | 2d | 3m. | 0.33333 | 0.66666 | 0.234 | 1.0 | 0.01203 | |
| H | 3 | 2d | 3m. | 0.33333 | 0.66666 | 0.4256 | 1.0 | 0.04203 | |

**Anisotropic Displacement Parameters:**

| Atom | Num | Uani11 | Uani22 | Uani33 | Uani12 | Uani13 | Uani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.0083 | 0.0083 | 0.0193 | 0.0042 | 0.0 | 0.0 |
| O | 2 | 0.0106 | 0.0106 | 0.0149 | 0.0053 | 0.0 | 0.0 |
| H | 3 | 0.0528 | 0.0528 | 0.0205 | 0.0264 | 0.0 | 0.0 |

**Subfile(s):** Cement and Hydration Product, Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic), Pharmaceutical (Excipient)

**Mineral Classification:** Brucite (Group), hydroxide (Subgroup) **Pearson Symbol:** hP5.00
**Pearson Symbol w/o H:** hP3

**Cross-Ref PDF #'s:** ✓ 04-006-9147 (Alternate), ✓ 04-006-9148 (Alternate), ✓ 04-006-9149 (Alternate), ✓ 04-006-9150 (Alternate), ✓ 04-006-9151 (Alternate), ✓ 04-006-9152 (Alternate), ✓ 04-007-5231 (Alternate), ✓ 04-008-0220 (Alternate), ✓ 04-010-3117 (Primary)

**CAS Number - PR:** 1305-62-0 **Entry Date:** 09/01/1994

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA. ICDD Grant-in-Aid (1992). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Optical Data | | Winchell, A., Winchell, H. Microscopic Character of Artificial Inorg. Solid Sub. 69 (1964). |

**Database Comments:** Additional Patterns: Validated by a calculated pattern. Color: White. General Comments: Average relative standard deviation in intensity of the ten strongest reflections for three specimen mounts = 2.2%. Astringent. Sample Source or Locality: Sample obtained from Sigma Chemical Co. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (2θ) - Ca ( O H )2 - 00-044-1481 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.0073 | **4.922000** | 72 | 0 | 0 | 1 | | 56.0907 | 1.638300 | 1 | 0 | 0 | 3 | | 79.0924 | 1.209800 | 2 | 1 | 1 | 3 | |
| 28.6709 | 3.111000 | 27 | 1 | 0 | 0 | | 59.4244 | 1.554100 | 3 | 2 | 0 | 0 | | 81.9069 | 1.175200 | 2 | 2 | 1 | 0 | |
| 34.1013 | **2.627000** | 100 | 1 | 0 | 1 | | 62.6319 | 1.482000 | 9 | 2 | 0 | 1 | | 84.7484 | 1.142900 | 5m | 1 | 0 | 4 | |
| 36.5257 | 2.458000 | 1 | 0 | 0 | 2 | | 64.2314 | 1.448900 | 7m | 1 | 0 | 3 | | 84.7484 | 1.142900 | m | 2 | 1 | 1 | |
| 47.1200 | 1.927100 | 30 | 1 | 0 | 2 | | 64.2314 | 1.448900 | m | 1 | 1 | 2 | | 86.1940 | 1.127400 | 2 | 2 | 0 | 3 | |
| 50.8120 | **1.795400** | 31 | 1 | 1 | 0 | | 71.8086 | 1.313500 | 6 | 2 | 0 | 2 | | 93.2060 | 1.060100 | 3 | 2 | 1 | 2 | |
| 54.3565 | 1.686400 | 14 | 1 | 1 | 1 | | 77.6520 | 1.228600 | 1 | 0 | 0 | 4 | | 96.0263 | 1.036300 | 2 | 3 | 0 | 0 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 98.8790 | 1.013900 | 2m | 1 | 1 | 4 | | 106.0623 | 0.964100 | 1 | 2 | 0 | 4 | | 118.2628 | 0.897400 | 1 | 2 | 2 | 0 | |
| 98.8790 | 1.013900 | m | 3 | 0 | 1 | | 107.5746 | 0.954700 | 2 | 2 | 1 | 3 | | | | | | | | |
| 103.1389 | 0.983300 | <1 | 0 | 0 | 5 | | 110.5164 | 0.937390 | <1 | 1 | 0 | 5 | | | | | | | | |

**04-009-9615** Jun 23, 2020 12:44 PM (fal-sharji2)

**Status** Primary **QM:** Indexed **Pressure/Temperature:** Ambient **Chemical Formula:** Fe21 O31 ( O H )
**Empirical Formula:** Fe21 H O32 **Weight %:** Fe69.57 H0.06 O30.37 **Atomic %:** Fe38.89 H1.85 O59.26
**ANX:** A21X32 **Compound Name:** Iron Oxide Hydroxide **Mineral Name:** Maghemite, syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 3.58 **I/Ic - ND:** 1.33

**SYS:** Cubic **SPGR:** P-43m (215)
**Author's Cell [ AuthCell a:** 8.35 Å **AuthCell Vol:** 582.18 Å³ **AuthCell Z:** 1.00 **AuthCell MolVol:** 582.18 **]**
**Density [ Dcalc:** 4.808 g/cm³ **Dstruc:** 4.81 g/cm³ **]** **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor)

**Space Group:** P-43m (215) **Molecular Weight:** 1685.78
**Crystal Data [ XtlCell a:** 8.350 Å **XtlCell b:** 8.350 Å **XtlCell c:** 8.350 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 582.18 Å³ **XtlCell Z:** 1.00 **]**
**Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 **]**
**Reduced Cell [ RedCell a:** 8.350 Å **RedCell b:** 8.350 Å **RedCell c:** 8.350 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 90.00° **RedCell Vol:** 582.18 Å³ **]**

**Crystal (Symmetry Allowed):** Non-centrosymmetric - Piezo (2nd Harm.)

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 5 | y,x,z | 9 | y,-z,-x | 13 | -x,y,-z | 17 | -y,x,-z | 21 | -y,-z,x |
| 2 | z,x,y | 6 | z,y,x | 10 | x,-z,-y | 14 | -z,x,-y | 18 | -z,y,-x | 22 | -x,-z,y |
| 3 | y,z,x | 7 | x,-y,-z | 11 | y,-x,-z | 15 | -y,z,-x | 19 | -x,-y,z | 23 | -y,-x,z |
| 4 | x,z,y | 8 | z,-x,-y | 12 | z,-y,-x | 16 | -x,z,-y | 20 | -z,-x,y | 24 | -z,-y,x |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | IDP | AET |
|---|---|---|---|---|---|---|---|---|---|
| O | 1 | 12i | ..m | 0.125 | 0.125 | 0.375 | 1.0 | | 4-a |
| Fe | 2 | 12i | ..m | 0.125 | 0.125 | 0.625 | 1.0 | | 6-a |
| Fe | 3 | 3c | -42.m | 0.0 | 0.5 | 0.5 | 1.0 | | 4-a |
| Fe | 4 | 4e | .3m | 0.25 | 0.25 | 0.25 | 1.0 | | 4-a |
| H | 5 | 4e | .3m | 0.625 | 0.625 | 0.625 | 0.25 | | |
| O | 6 | 12i | ..m | 0.375 | 0.375 | -0.125 | 1.0 | | 3#a |
| O | 7 | 4e | .3m | -0.125 | -0.125 | -0.125 | 1.0 | | 4-a |
| Fe | 8 | 1b | -43m | 0.5 | 0.5 | 0.5 | 1.0 | | 4-a |
| Fe | 9 | 1a | -43m | 0.0 | 0.0 | 0.0 | 1.0 | | 4-a |
| O | 10 | 4e | .3m | 0.375 | 0.375 | 0.375 | 1.0 | | 2#b |

**Subfile(s):** Inorganic, Mineral Related (Mineral , Synthetic) **Former PDF's #:** 01-089-3850
**LPF Prototype Structure [Formula Order]:** Fe21 O31 [ O H ],cP53,215
**LPF Prototype Structure [Alpha Order]:** Fe21 H O32,cP53,215 **Pearson Symbol:** cP54.00
**Pearson Symbol w/o H:** cP53 **Entry Date:** 09/01/2006 **Last Modification Date:** 09/01/2011
**Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Ein Fehlstellenuberstruktur-Modell fur γ-Fe2O3". Sinha K.P., Sinha A.P.B. Z. Anorg. Allg. Chem. 293, 228 (1957). |

**Database Comments:** ANX: A21X32. LPF Collection Code: 1704332. Sample Preparation: STARTING MATERIAL:FeSO4,LiOH.Compound Formation:reacted, product filtered off, washed and oxidated at 383-393 K for 90 h in oxygen. Minor Warning: No e.s.d reported/abstracted on the cell dimension. No R factors reported/abstracted. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (93) - Fe21 O31 ( O H ) - 04-009-9615 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10.5860 | 8.350000 | 147 | 1 | 0 | 0 | | 43.3075 | 2.087500 | 157 | 4 | 0 | 0 | | 62.9113 | **1.476090** | 435 | 4 | 4 | 0 | |
| 14.9923 | 5.904340 | 40 | 1 | 1 | 0 | | 44.7111 | 2.025170 | 92 | 4 | 1 | 0 | | 64.0015 | 1.453550 | 12 | 5 | 2 | 2 | |
| 18.3882 | 4.820880 | 28 | 1 | 1 | 1 | | 46.0809 | 1.968110 | 33 | 4 | 1 | 1 | | 65.0818 | 1.432010 | 9 | 5 | 3 | 0 | |
| 21.2638 | 4.175000 | 9 | 2 | 0 | 0 | | 47.4197 | 1.915620 | 5 | 3 | 3 | 1 | | 66.1522 | 1.411410 | 3 | 5 | 3 | 1 | |
| 23.8083 | 3.734230 | 26 | 2 | 1 | 0 | | 48.7302 | 1.867120 | 3 | 4 | 2 | 0 | | 67.2140 | 1.391670 | 1 | 6 | 0 | 0 | |
| 26.1191 | 3.408870 | 102 | 2 | 1 | 1 | | 50.0152 | 1.822120 | 5 | 4 | 2 | 1 | | 68.2680 | 1.372730 | 1 | 6 | 1 | 0 | |
| 30.2493 | **2.952170** | 550 | 2 | 2 | 0 | | 51.2762 | 1.780230 | 12 | 3 | 3 | 2 | | 69.3138 | 1.354550 | 10 | 6 | 1 | 1 | |
| 32.1324 | 2.783330 | 142 | 3 | 0 | 0 | | 53.7346 | 1.704440 | 159 | 4 | 2 | 2 | | 71.3850 | 1.320250 | 50 | 6 | 2 | 0 | |
| 33.9216 | 2.640500 | 86 | 3 | 1 | 0 | | 54.9350 | 1.670000 | 13 | 5 | 0 | 0 | | 72.4110 | 1.304050 | 21 | 6 | 2 | 1 | |
| 35.6313 | **2.517620** | 999 | 3 | 1 | 1 | | 56.1179 | 1.637570 | 18 | 5 | 1 | 0 | | 73.4313 | 1.288430 | 1 | 5 | 4 | 1 | |
| 37.2726 | 2.410440 | 27 | 2 | 2 | 2 | | 57.2846 | 1.606960 | 245 | 5 | 1 | 1 | | 74.4461 | 1.273360 | 63 | 5 | 3 | 3 | |
| 38.8545 | 2.315870 | 6 | 3 | 2 | 0 | | 59.5738 | 1.550560 | 4 | 4 | 3 | 2 | | 75.4557 | 1.258810 | 13 | 6 | 2 | 2 | |
| 40.3837 | 2.231630 | 54 | 3 | 2 | 1 | | 60.6986 | 1.524490 | 12 | 5 | 2 | 1 | | 76.4612 | 1.244740 | 1 | 6 | 3 | 0 | |

**04-009-9615** Jun 23, 2020 12:44 PM (fal-sharji2)

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 77.4619 | 1.231140 | 4 | 6 | 3 | 1 | | 99.0524 | 1.012590 | 1 | 8 | 2 | 0 | | 120.9816 | 0.885098 | 6 | 7 | 6 | 2 | |
| 79.4524 | 1.205220 | 14 | 4 | 4 | 4 | | 100.0420 | 1.005220 | 1 | 8 | 2 | 1 | | 122.1260 | 0.880167 | 3 | 8 | 5 | 1 | |
| 80.4427 | 1.192860 | 7 | 6 | 3 | 2 | | 101.0336 | 0.998016 | 2 | 6 | 5 | 3 | | 123.2848 | 0.875318 | 27 | 9 | 3 | 1 | |
| 81.4303 | 1.180870 | 7 | 5 | 4 | 3 | | 103.0279 | 0.984057 | 20 | 8 | 2 | 2 | | 125.6505 | 0.865855 | 1 | 8 | 5 | 2 | |
| 82.4157 | 1.169230 | 1 | 5 | 5 | 1 | | 104.0308 | 0.977294 | 4 | 8 | 3 | 0 | | 126.8598 | 0.861237 | 2 | 9 | 3 | 2 | |
| 83.3978 | 1.157940 | 1 | 6 | 4 | 0 | | 105.0383 | 0.970668 | 5 | 8 | 3 | 1 | | 129.3385 | 0.852218 | 82 | 8 | 4 | 4 | |
| 84.3789 | 1.146960 | 1 | 6 | 4 | 1 | | 106.0505 | 0.964175 | 42 | 7 | 5 | 1 | | 130.6110 | 0.847814 | 3 | 9 | 4 | 0 | |
| 85.3580 | 1.136290 | 6 | 7 | 2 | 1 | | 107.0678 | 0.957811 | 5 | 6 | 6 | 2 | | 131.9084 | 0.843477 | 2 | 9 | 4 | 1 | |
| 87.3119 | 1.115820 | 45 | 6 | 4 | 2 | | 108.0908 | 0.951571 | 1 | 6 | 5 | 4 | | 133.2323 | 0.839207 | 1 | 7 | 7 | 1 | |
| 88.2887 | 1.105980 | 6 | 5 | 4 | 4 | | 109.1198 | 0.945451 | 1 | 7 | 5 | 2 | | 134.5860 | 0.835000 | 1 | 10 | 0 | 0 | |
| 89.2635 | 1.096410 | 2 | 7 | 3 | 0 | | 111.1975 | 0.933558 | 13 | 8 | 4 | 0 | | 135.9719 | 0.830856 | 1 | 9 | 4 | 2 | |
| 90.2385 | 1.087080 | 89 | 7 | 3 | 1 | | 112.2472 | 0.927778 | 6 | 8 | 4 | 1 | | 137.3935 | 0.826773 | 1 | 7 | 7 | 2 | |
| 92.1894 | 1.069110 | 1 | 6 | 5 | 0 | | 113.3049 | 0.922103 | 1 | 9 | 1 | 0 | | 140.3591 | 0.818785 | 24 | 10 | 2 | 0 | |
| 93.1660 | 1.060450 | 4 | 7 | 3 | 2 | | 114.3709 | 0.916532 | 1 | 7 | 5 | 3 | | 141.9131 | 0.814877 | 3 | 10 | 2 | 1 | |
| 95.1214 | 1.043750 | 40 | 8 | 0 | 0 | | 115.4461 | 0.911060 | 1 | 8 | 4 | 2 | | 143.5231 | 0.811024 | 1 | 9 | 5 | 0 | |
| 96.1013 | 1.035690 | 7 | 6 | 5 | 2 | | 116.5310 | 0.905685 | 1 | 9 | 2 | 0 | | 145.1968 | 0.807225 | 36 | 9 | 5 | 1 | |
| 97.0835 | 1.027810 | 5 | 7 | 4 | 1 | | 117.6262 | 0.900404 | 3 | 7 | 6 | 1 | | 146.9440 | 0.803479 | 5 | 10 | 2 | 2 | |
| 98.0661 | 1.020120 | 1 | 7 | 3 | 3 | | 119.8507 | 0.890113 | 10 | 6 | 6 | 4 | | 148.7771 | 0.799785 | 1 | 8 | 6 | 3 | |

**04-012-0908** Jun 23, 2020 12:43 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Temperature (Non-ambient) **Chemical Formula:** Mg Fe2 O4
**Empirical Formula:** Fe2 Mg O4 **Weight %:** Fe55.85 Mg12.15 O32.00 **Atomic %:** Fe28.57 Mg14.29 O57.14
**ANX:** A3X4 **Compound Name:** Magnesium Iron Oxide **Mineral Name:** Magnesioferrite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 4.2 **I/Ic - ND:** 1.82

**SYS:** Cubic **SPGR:** Fd-3m (227)
**Author's Cell [ AuthCell a:** 8.39704(5) Å **AuthCell Vol:** 592.08 Å³ **AuthCell Z:** 8.00 **AuthCell MolVol:** 74.01 **]**
**Density [ Dcalc:** 4.487 g/cm³ **Dstruc:** 4.49 g/cm³ **]** **SS/FOM:** F(30) = 999.9(0.0001, 30)
**Temp:** 301.0 K (Author provided temperature) **R-factor:** 0.011 **Color:** Brown

**Space Group:** Fd-3m (227) **Molecular Weight:** 200.00
**Crystal Data [ XtlCell a:** 8.397 Å **XtlCell b:** 8.397 Å **XtlCell c:** 8.397 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 592.08 Å³ **XtlCell Z:** 8.00 **]**
**Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 **]**
**Reduced Cell [ RedCell a:** 5.938 Å **RedCell b:** 5.938 Å **RedCell c:** 5.938 Å **RedCell α:** 60.00°
**RedCell β:** 60.00° **RedCell γ:** 60.00° **RedCell Vol:** 148.02 Å³ **]**

**ADP:** U **Origin:** O2 **Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 11 | z,-x+1/4,-y+1/4 | 21 | -y+1/4,z,-x+1/4 | 31 | -x+1/4,-z+1/4,y | 41 | z,y,x |
| 2 | -x,-y,-z | 12 | -z,x+3/4,y+3/4 | 22 | y+3/4,-z,x+3/4 | 32 | x+3/4,z+3/4,-y | 42 | -z,-y,-x |
| 3 | x,-y+1/4,-z+1/4 | 13 | -z+1/4,x,-y+1/4 | 23 | -y+1/4,-z+1/4,x | 33 | y,x,z | 43 | z,-y+1/4,-x+1/4 |
| 4 | -x,y+3/4,z+3/4 | 14 | z+3/4,-x,y+3/4 | 24 | y+3/4,z+3/4,-x | 34 | -y,-x,-z | 44 | -z,y+3/4,x+3/4 |
| 5 | -x+1/4,y,-z+1/4 | 15 | -z+1/4,-x+1/4,y | 25 | x,z,y | 35 | y,-x+1/4,-z+1/4 | 45 | -z+1/4,y,-x+1/4 |
| 6 | x+3/4,-y,z+3/4 | 16 | z+3/4,x+3/4,-y | 26 | -x,-z,-y | 36 | -y,x+3/4,z+3/4 | 46 | z+3/4,-y,x+3/4 |
| 7 | -x+1/4,-y+1/4,z | 17 | y,z,x | 27 | x,-z+1/4,-y+1/4 | 37 | -y+1/4,x,-z+1/4 | 47 | -z+1/4,-y+1/4,x |
| 8 | x+3/4,y+3/4,-z | 18 | -y,-z,-x | 28 | -x,z+3/4,y+3/4 | 38 | y+3/4,-x,z+3/4 | 48 | z+3/4,y+3/4,-x |
| 9 | z,x,y | 19 | y,-z+1/4,-x+1/4 | 29 | -x+1/4,z,-y+1/4 | 39 | -y+1/4,-x+1/4,z | | |
| 10 | -z,-x,-y | 20 | -y,z+3/4,x+3/4 | 30 | x+3/4,-z,y+3/4 | 40 | y+3/4,x+3/4,-z | | |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Fe | 1 | 8a | -43m | 0.125 | 0.125 | 0.125 | 0.841 | 0.0011 | |
| Mg | 2 | 8a | -43m | 0.125 | 0.125 | 0.125 | 0.159 | 0.0011 | |
| Fe | 3 | 16d | .-3m | 0.5 | 0.5 | 0.5 | 0.579 | 0.0022 | |
| Mg | 4 | 16d | .-3m | 0.5 | 0.5 | 0.5 | 0.421 | 0.0022 | |
| O | 5 | 32e | .3m | 0.2548 | 0.2548 | 0.2548 | 1.0 | 0.0052 | |

**Subfile(s):** Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural) **Former PDF's #:** 01-076-9733
**LPF Prototype Structure [Formula Order]:** Mg Al2 O4,cF56,227
**LPF Prototype Structure [Alpha Order]:** Al2 Mg O4,cF56,227 **Pearson Symbol:** cF56.00

**04-012-0908** Jun 23, 2020 12:43 PM (fal-sharji2)

**Cross-Ref PDF #'s:** 00-017-0464 (Primary), 00-017-0465 (Alternate), 00-036-0398 (Primary), 01-073-1960 (Alternate), 01-073-2410 (Alternate), 01-075-9708 (Alternate), 01-078-5428 (Alternate), 01-082-9881 (Alternate), 01-088-1935 (Alternate), 01-088-1936 (Alternate), 01-088-1937 (Alternate), 01-088-1938 (Alternate), 01-088-1939 (Alternate), 01-088-1940 (Alternate), 01-088-1941 (Alternate), 01-088-1942 (Alternate), 01-088-1943 (Alternate), 01-089-3084 (Alternate), 01-089-4924 (Alternate), 01-089-6187 (Alternate), 01-089-6188 (Alternate), 01-089-6189 (Alternate), ✓ 04-001-7921 (Alternate), ✓ 04-001-9288 (Alternate), ✓ 04-002-0587 (Alternate), ✓ 04-002-0619 (Alternate), ✓ 04-002-2458 (Alternate), ✓ 04-002-2459 (Alternate), ✓ 04-002-3054 (Alternate), ✓ 04-002-3768 (Alternate), ✓ 04-002-3769 (Alternate), ✓ 04-002-5223 (Alternate), ✓ 04-002-5328 (Alternate), ✓ 04-002-5461 (Alternate), ✓ 04-002-5666 (Alternate), ✓ 04-002-5894 (Alternate), ✓ 04-002-5904 (Alternate), ✓ 04-002-6403 (Alternate), ✓ 04-002-8191 (Alternate), ✓ 04-002-8204 (Alternate), ✓ 04-005-7127 (Alternate), ✓ 04-005-8346 (Alternate), ✓ 04-005-8349 (Alternate), ✓ 04-006-0223 (Alternate), ✓ 04-006-0426 (Alternate), ✓ 04-006-0427 (Alternate), ✓ 04-006-1839 (Alternate), ✓ 04-006-2461 (Alternate), ✓ 04-006-2469 (Alternate), ✓ 04-006-4005 (Alternate), ✓ 04-006-6673 (Alternate), ✓ 04-006-6676 (Alternate), ✓ 04-006-6677 (Alternate), ✓ 04-006-6682 (Alternate), ✓ 04-007-4190 (Alternate), ✓ 04-007-4269 (Alternate), ✓ 04-007-5629 (Alternate), ✓ 04-007-5630 (Alternate), ✓ 04-008-2382 (Alternate), ✓ 04-010-6157 (Primary), ✓ 04-011-9002 (Alternate), ✓ 04-011-9003 (Alternate), ✓ 04-012-0909 (Alternate), ✓ 04-012-0910 (Alternate), ✓ 04-012-0911 (Alternate), ✓ 04-012-0912 (Alternate), ✓ 04-012-0913 (Alternate), ✓ 04-012-0914 (Alternate), ✓ 04-012-0915 (Alternate), ✓ 04-012-0916 (Alternate), ✓ 04-012-0917 (Alternate), ✓ 04-012-0918 (Alternate), ✓ 04-012-0919 (Alternate), ✓ 04-012-0920 (Alternate), ✓ 04-012-0921 (Alternate), ✓ 04-012-0922 (Alternate), ✓ 04-012-0923 (Alternate), ✓ 04-012-0924 (Alternate), ✓ 04-012-0925 (Alternate), ✓ 04-012-0926 (Alternate), ✓ 04-012-0927 (Alternate), ✓ 04-012-0928 (Alternate), ✓ 04-012-0929 (Alternate), ✓ 04-012-0930 (Alternate), ✓ 04-012-0931 (Alternate), ✓ 04-012-0932 (Alternate), ✓ 04-012-0933 (Alternate), ✓ 04-012-0934 (Alternate), ✓ 04-012-0935 (Alternate), ✓ 04-012-0936 (Alternate), ✓ 04-012-0937 (Alternate), ✓ 04-012-0938 (Alternate), ✓ 04-012-0939 (Alternate), ✓ 04-012-0940 (Alternate), ✓ 04-012-0941 (Alternate), ✓ 04-012-0942 (Alternate), ✓ 04-012-0943 (Alternate), ✓ 04-012-0944 (Alternate), ✓ 04-012-0945 (Alternate), ✓ 04-012-0946 (Alternate), ✓ 04-012-0947 (Alternate), ✓ 04-012-0948 (Alternate), ✓ 04-012-0949 (Alternate), ✓ 04-012-0950 (Alternate), ✓ 04-012-0951 (Alternate), ✓ 04-012-1050 (Alternate), ✓ 04-012-1051 (Alternate), ✓ 04-012-1052 (Alternate), ✓ 04-012-1053 (Alternate), ✓ 04-012-1054 (Alternate), ✓ 04-012-1055 (Alternate), ✓ 04-012-1056 (Alternate), ✓ 04-012-1057 (Alternate), ✓ 04-012-1058 (Alternate), ✓ 04-012-1059 (Alternate), ✓ 04-012-1060 (Alternate), ✓ 04-012-1061 (Alternate), ✓ 04-012-1062 (Alternate), ✓ 04-012-1063 (Alternate), ✓ 04-012-1064 (Alternate), ✓ 04-012-1065 (Alternate), ✓ 04-012-1066 (Alternate), ✓ 04-012-1067 (Alternate), ✓ 04-012-1068 (Alternate), ✓ 04-012-1069 (Alternate), ✓ 04-012-1070 (Alternate), ✓ 04-012-1071 (Alternate), ✓ 04-012-1072 (Alternate), ✓ 04-012-1073 (Alternate), ✓ 04-012-1074 (Alternate), ✓ 04-012-1075 (Alternate), ✓ 04-012-1076 (Alternate), ✓ 04-012-1077 (Alternate), ✓ 04-012-1078 (Alternate), ✓ 04-012-1079 (Alternate), ✓ 04-012-1080 (Alternate), ✓ 04-012-1081 (Alternate), ✓ 04-014-3057 (Alternate), ✓ 04-014-3693 (Alternate), ✓ 04-014-3694 (Alternate), ✓ 04-014-3695 (Alternate), ✓ 04-014-3696 (Alternate), ✓ 04-014-3697 (Alternate), ✓ 04-014-3698 (Alternate), ✓ 04-014-3699 (Alternate), ✓ 04-014-3700 (Alternate), ✓ 04-014-3701 (Alternate), ✓ 04-014-3702 (Alternate), ✓ 04-014-3703 (Alternate), ✓ 04-014-3704 (Alternate), ✓ 04-014-3705 (Alternate), ✓ 04-014-3706 (Alternate), ✓ 04-014-3707 (Alternate), ✓ 04-014-3708 (Alternate), ✓ 04-014-3709 (Alternate), ✓ 04-014-3710 (Alternate), ✓ 04-014-3711 (Alternate), ✓ 04-014-3712 (Alternate), ✓ 04-014-3713 (Alternate), ✓ 04-014-3714 (Alternate), ✓ 04-014-3715 (Alternate), ✓ 04-014-3716 (Alternate), ✓ 04-014-3717 (Alternate), ✓ 04-014-3718 (Alternate), ✓ 04-014-3719 (Alternate), ✓ 04-014-3720 (Alternate), ✓ 04-014-3721 (Alternate), ✓ 04-014-3722 (Alternate), ✓ 04-014-3723 (Alternate), ✓ 04-014-3724 (Alternate), ✓ 04-014-3725 (Alternate), ✓ 04-014-3726 (Alternate), ✓ 04-014-3727 (Alternate), ✓ 04-014-3728 (Alternate), ✓ 04-014-3729 (Alternate), ✓ 04-014-3730 (Alternate), ✓ 04-014-3731 (Alternate), ✓ 04-014-3732 (Alternate), ✓ 04-014-3733 (Alternate), ✓ 04-014-3734 (Alternate), ✓ 04-015-7027 (Alternate)

**Entry Date:** 09/01/2009 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Cation ordering in magnesioferrite, MgFe2O4, to 982 °C using in situ synchrotron X-ray powder diffraction". Antao S.M., Hassan I., Parise J.B. Am. Mineral. 90, 219,228 (2005). |

**Database Comments:** ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 1601106. Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 K for 10 d, quenched in air. CRUCIBLE: sealed evacuated silica tube lined with silver foil. Temperature of Data Collection: 301 K. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (34) - Mg Fe2 O4 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.2844 | 4.848030 | 34 | 1 | 1 | 1 | | 73.9587 | 1.280540 | 79 | 5 | 3 | 3 | | 110.2654 | 0.938818 | 25 | 8 | 4 | 0 | |
| 30.0759 | **2.968800** | 346 | 2 | 2 | 0 | | 74.9599 | 1.265900 | 19 | 6 | 2 | 2 | | 113.3820 | 0.921695 | 1 | 9 | 1 | 1 | |
| 35.4251 | **2.531800** | 999 | 3 | 1 | 1 | | 78.9200 | 1.212010 | 23 | 4 | 4 | 4 | | 114.4369 | 0.916192 | 1 | 8 | 4 | 2 | |
| 37.0562 | 2.424020 | 27 | 2 | 2 | 2 | | 81.8545 | 1.175820 | 2 | 7 | 1 | 1 | | 118.7512 | 0.895128 | 10 | 6 | 6 | 4 | |
| 43.0527 | 2.099260 | 207 | 4 | 0 | 0 | | 86.7015 | 1.122100 | 40 | 6 | 4 | 2 | | 122.1067 | 0.880249 | 51 | 9 | 3 | 1 | |
| 47.1379 | 1.926410 | 1 | 3 | 3 | 1 | | 89.5961 | 1.093200 | 118 | 7 | 3 | 1 | | 127.9989 | 0.857019 | 112 | 8 | 4 | 4 | |
| 53.4097 | 1.714040 | 111 | 4 | 2 | 2 | | 94.4217 | 1.049630 | 47 | 8 | 0 | 0 | | 131.7695 | 0.843934 | 1 | 9 | 3 | 3 | |
| 56.9344 | 1.616010 | 303 | 5 | 1 | 1 | | 97.3303 | 1.025860 | 1 | 7 | 3 | 3 | | 138.6147 | 0.823398 | 28 | 10 | 2 | 0 | |
| 62.5192 | **1.484400** | 434 | 4 | 4 | 0 | | 98.3035 | 1.018290 | 1 | 6 | 4 | 4 | | 143.2036 | 0.811773 | 70 | 9 | 5 | 1 | |
| 65.7346 | 1.419360 | 3 | 5 | 3 | 1 | | 102.2239 | 0.989601 | 19 | 8 | 2 | 2 | | 144.8452 | 0.808006 | 10 | 10 | 2 | 2 | |
| 66.7879 | 1.399510 | 1 | 4 | 4 | 2 | | 105.2020 | 0.969607 | 66 | 7 | 5 | 1 | | | | | | | | |
| 70.9244 | 1.327690 | 38 | 6 | 2 | 0 | | 106.2036 | 0.963207 | 8 | 6 | 6 | 2 | | | | | | | | |

**01-080-6409** Jun 23, 2020 12:44 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Temperature (Non-ambient) **Chemical Formula:** Fe3 O4
**Empirical Formula:** Fe3 O4 **Weight %:** Fe72.36 O27.64 **Atomic %:** Fe42.86 O57.14 **ANX:** A3X4
**Compound Name:** Iron Oxide **Mineral Name:** Magnetite **Common Name:** Iron(II) diiron(III) tetraoxide

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 4.61 **I/Ic - ND:** 1.16

**SYS:** Cubic **SPGR:** Fd-3m (227)
**Author's Cell [ AuthCell a:** 8.4814(5) Å **AuthCell Vol:** 610.10 Å³ **AuthCell Z:** 8.00 **AuthCell MolVol:** 76.26 ]
**Density [ Dcalc:** 5.041 g/cm³ **Dstruc:** 5.04 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0001, 30)
**Temp:** 973.0 K (Author provided temperature) **R-factor:** 0.0219

**Space Group:** Fd-3m (227) **Molecular Weight:** 231.54
**Crystal Data [ XtlCell a:** 8.481 Å **XtlCell b:** 8.481 Å **XtlCell c:** 8.481 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 610.10 Å³ **XtlCell Z:** 8.00 ]
**Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 ]
**Reduced Cell [ RedCell a:** 5.997 Å **RedCell b:** 5.997 Å **RedCell c:** 5.997 Å **RedCell α:** 60.00°
**RedCell β:** 60.00° **RedCell γ:** 60.00° **RedCell Vol:** 152.53 Å³ ]

**Crystal (Symmetry Allowed):** Centrosymmetric

**Subfile(s):** Common Phase, Forensic, Inorganic, Metals & Alloys, Mineral Related (Mineral , Natural)
**Prototype Structure [Formula Order]:** Mg Al2 O4 **Prototype Structure [Alpha Order]:** Al2 Mg O4
**Pearson Symbol:** cF56.00

**Cross-Ref PDF #'s:**
00-001-1111 (Deleted), 00-002-1035 (Deleted), 00-003-0862 (Deleted), 00-007-0322 (Deleted), 00-011-0614 (Deleted), 00-019-0629 (Primary), 00-065-0731 (Primary), 01-071-4918 (Alternate), 01-072-2303 (Alternate), 01-074-1909 (Alternate), 01-074-1910 (Alternate), 01-075-0449 (Alternate), 01-075-1610 (Alternate), 01-075-9710 (Alternate), 01-076-1849 (Alternate), 01-076-5948 (Alternate), 01-078-6086 (Alternate), 01-080-6402 (Alternate), 01-080-6403 (Alternate), 01-080-6404 (Alternate), 01-080-6405 (Alternate), 01-080-6406 (Alternate), 01-080-6407 (Alternate), 01-080-6408 (Alternate), 01-080-6410 (Alternate), 01-080-7683 (Alternate), 01-087-2334 (Alternate), 01-088-0866 (Alternate), 01-089-3854 (Alternate), 01-089-4319 (Alternate), ✓ 03-065-3107 (Alternate), ✓ 04-001-7822 (Alternate), ✓ 04-001-7909 (Alternate), ✓ 04-001-9000 (Alternate), ✓ 04-001-9326 (Alternate), ✓ 04-002-0264 (Alternate), ✓ 04-002-0618 (Alternate), ✓ 04-002-0643 (Alternate), ✓ 04-002-1855 (Alternate), ✓ 04-002-2487 (Alternate), ✓ 04-002-2707 (Alternate), ✓ 04-002-2709 (Alternate), ✓ 04-002-2981 (Alternate), ✓ 04-002-3194 (Alternate), ✓ 04-002-3668 (Alternate), ✓ 04-002-5310 (Alternate), ✓ 04-002-5448 (Alternate), ✓ 04-002-5632 (Alternate), ✓ 04-002-5683 (Alternate), ✓ 04-002-5903 (Alternate), ✓ 04-002-6866 (Alternate), ✓ 04-002-6955 (Alternate), ✓ 04-002-8141 (Alternate), ✓ 04-002-8629 (Alternate), ✓ 04-002-9019 (Alternate), ✓ 04-002-9635 (Alternate), ✓ 04-003-1446 (Alternate), ✓ 04-004-2838 (Alternate), ✓ 04-005-4307 (Alternate), ✓ 04-005-4319 (Primary), ✓ 04-005-4404 (Alternate), ✓ 04-005-4551 (Alternate), ✓ 04-005-5733 (Alternate), ✓ 04-005-6268 (Alternate), ✓ 04-005-9786 (Alternate), ✓ 04-005-9788 (Alternate), ✓ 04-005-9815 (Alternate), ✓ 04-006-0225 (Alternate), ✓ 04-006-0424 (Alternate), ✓ 04-006-0425 (Alternate), ✓ 04-006-1668 (Alternate), ✓ 04-006-2406 (Alternate), ✓ 04-006-2467 (Alternate), ✓ 04-006-2752 (Alternate), ✓ 04-006-4615 (Alternate), ✓ 04-006-6497 (Alternate), ✓ 04-006-6550 (Alternate), ✓ 04-006-6692 (Alternate), ✓ 04-006-8076 (Alternate), ✓ 04-007-1427 (Alternate), ✓ 04-007-2718 (Alternate), ✓ 04-007-6010 (Alternate), ✓ 04-007-8567 (Alternate), ✓ 04-007-8976 (Alternate), ✓ 04-007-9093 (Alternate), ✓ 04-008-0315 (Alternate), ✓ 04-008-0777 (Alternate), ✓ 04-008-4423 (Alternate), ✓ 04-008-4511 (Alternate), ✓ 04-008-4512 (Alternate), ✓ 04-008-8145 (Alternate), ✓ 04-008-8146 (Alternate), ✓ 04-008-8147 (Alternate), ✓ 04-008-8148 (Alternate), ✓ 04-009-4225 (Alternate), ✓ 04-009-8417 (Alternate), ✓ 04-009-8418 (Alternate), ✓ 04-009-8419 (Alternate), ✓ 04-009-8420 (Alternate), ✓ 04-009-8421 (Alternate), ✓ 04-009-8422 (Alternate), ✓ 04-009-8423 (Alternate), ✓ 04-009-8424 (Alternate), ✓ 04-009-8425 (Alternate), ✓ 04-009-8426 (Alternate), ✓ 04-009-8427 (Alternate), ✓ 04-009-8428 (Alternate), ✓ 04-009-8429 (Alternate), ✓ 04-009-8430 (Alternate), ✓ 04-009-8431 (Alternate), ✓ 04-009-8432 (Alternate), ✓ 04-009-8433 (Alternate), ✓ 04-009-8434 (Alternate), ✓ 04-009-8435 (Alternate), ✓ 04-009-8436 (Alternate), ✓ 04-009-8437 (Alternate), ✓ 04-009-8438 (Alternate), ✓ 04-009-8439 (Alternate), ✓ 04-009-8440 (Alternate), ✓ 04-009-8441 (Alternate), ✓ 04-009-8442 (Alternate), ✓ 04-009-8443 (Alternate), ✓ 04-011-5952 (Alternate), ✓ 04-013-7099 (Alternate), ✓ 04-013-7100 (Alternate), ✓ 04-013-9806 (Alternate), ✓ 04-013-9807 (Alternate), ✓ 04-013-9808 (Alternate), ✓ 04-013-9809 (Alternate), ✓ 04-013-9810 (Alternate), ✓ 04-013-9811 (Alternate), ✓ 04-014-1396 (Alternate), ✓ 04-014-9664 (Alternate), ✓ 04-015-3100 (Alternate), ✓ 04-015-3101 (Alternate), ✓ 04-015-3102 (Alternate), ✓ 04-015-8200 (Alternate), ✓ 04-015-8203 (Alternate), ✓ 04-015-8204 (Alternate), ✓ 04-015-8207 (Alternate), ✓ 04-015-8209 (Alternate), ✓ 04-015-8211 (Alternate), ✓ 04-015-8213 (Alternate), ✓ 04-015-8214 (Alternate), ✓ 04-017-1024 (Alternate)

**Entry Date:** 09/01/2013

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Structure | | "Structure of magnetite (Fe3 O4) above the Curie temperature: a cation ordering study". Levy, D., Giustetto, R., Hoser, A. Phys. Chem. Miner. 39, 169 (2012). |




**01-080-6409** Jun 23, 2020 12:44 PM (fal-sharji2)

**Database Comments:** ANX: A3X4. Analysis: Fe3 O4. Formula from original source: Fe3 O4. ICSD Collection Code: 183976. Sample Source or Locality: Brosso mining area, Ivrea, Italy. Temperature of Data Collection: 973 K. Wyckoff Sequence: e d a (FD3-MZ). Unit Cell Data Source: Powder Diffraction.

**d-Spacings (34) - Fe3 O4 - 01-080-6409 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.1010 | 4.896740 | 104 | 1 | 1 | 1 | | 73.1032 | 1.293400 | 54 | 5 | 3 | 3 | | 108.6461 | 0.948249 | 12 | 8 | 4 | 0 | |
| 29.7697 | **2.998630** | 300 | 2 | 2 | 0 | | 74.0884 | 1.278620 | 22 | 6 | 2 | 2 | | 111.6669 | 0.930955 | 1 | 9 | 1 | 1 | |
| 35.0612 | **2.557240** | 999 | 3 | 1 | 1 | | 77.9854 | 1.224180 | 16 | 4 | 4 | 4 | | 112.6876 | 0.925397 | 1 | 8 | 4 | 2 | |
| 36.6745 | 2.448370 | 75 | 2 | 2 | 2 | | 80.8701 | 1.187630 | 3 | 5 | 5 | 1 | | 116.8524 | 0.904120 | 3 | 6 | 6 | 4 | |
| 42.6035 | 2.120350 | 199 | 4 | 0 | 0 | | 85.6305 | 1.133370 | 20 | 6 | 4 | 2 | | 120.0783 | 0.889092 | 21 | 9 | 3 | 1 | |
| 46.6410 | 1.945770 | 4 | 3 | 3 | 1 | | 88.4701 | 1.104180 | 67 | 7 | 3 | 1 | | 125.7088 | 0.865629 | 41 | 8 | 4 | 4 | |
| 52.8370 | 1.731260 | 80 | 4 | 2 | 2 | | 93.1980 | 1.060170 | 24 | 8 | 0 | 0 | | 129.2832 | 0.852413 | 1 | 9 | 3 | 3 | |
| 56.3171 | 1.632250 | 257 | 5 | 1 | 1 | | 96.0423 | 1.036170 | 1 | 7 | 3 | 3 | | 135.6954 | 0.831670 | 8 | 10 | 2 | 0 | |
| 61.8287 | **1.499310** | 321 | 4 | 4 | 0 | | 96.9940 | 1.028520 | 1 | 6 | 4 | 4 | | 139.9182 | 0.819928 | 24 | 9 | 5 | 1 | |
| 64.9997 | 1.433620 | 7 | 5 | 3 | 1 | | 100.8214 | 0.999543 | 8 | 8 | 2 | 2 | | 141.4095 | 0.816123 | 5 | 10 | 2 | 2 | |
| 66.0381 | 1.413570 | 1 | 4 | 4 | 2 | | 103.7236 | 0.979348 | 32 | 7 | 5 | 1 | | | | | | | | |
| 70.1145 | 1.341030 | 23 | 6 | 2 | 0 | | 104.6987 | 0.972883 | 6 | 6 | 6 | 2 | | | | | | | | |

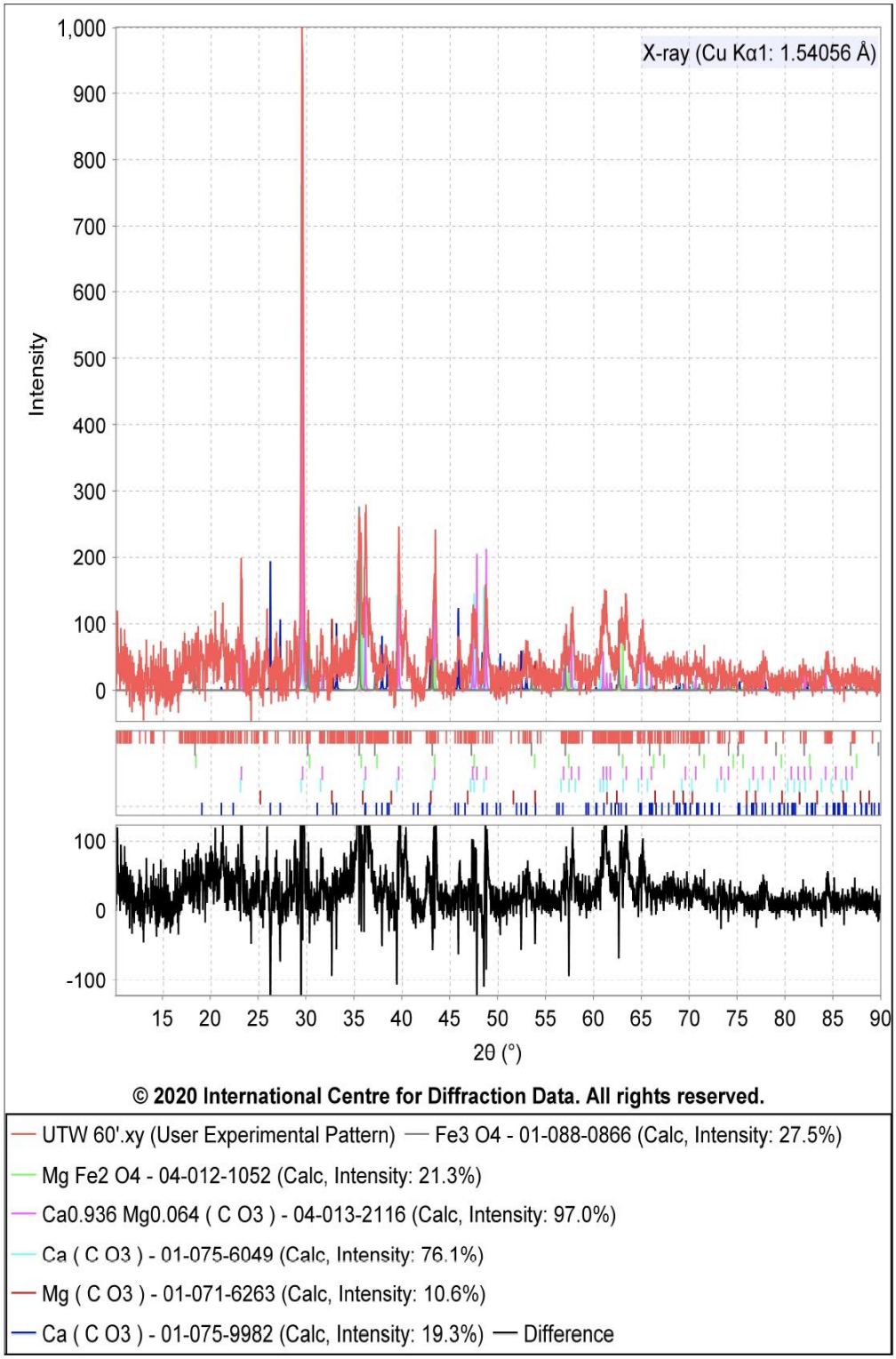


**Figure E.3 XRD patterns of substances precipitated from Untreated Water (UTW) tank at 60 °C from experiment with a tank with little exposure of iron.**

# SIeve+ Report

## Experiment

**Search Line:** 2.080316 Å **D1 Range:** 2.073 Å - 2.087 Å
**Search Line:** 1.514557 Å **D1 Range:** 1.511 Å - 1.518 Å
**Search Line:** 2.542048 Å **D1 Range:** 2.532 Å - 2.553 Å
**Search Line:** 2.264994 Å **D1 Range:** 2.257 Å - 2.273 Å
**Search Line:** 1.593774 Å **D1 Range:** 1.590 Å - 1.598 Å
**Search Line:** 3.441148 Å **D1 Range:** 3.422 Å - 3.461 Å
**Search Line:** 1.520713 Å **D1 Range:** 1.517 Å - 1.524 Å
**Search Line:** 1.467557 Å **D1 Range:** 1.464 Å - 1.471 Å
**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (6)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 01-088-0866 | S | Iron Oxide | 0.275 | 10.934 | *5.16 | 6 |
| 2 | true | 04-012-1052 | S | Magnesium Iron Oxide | 0.213 | 8.451 | *4.21 | 6 |
| 3 | true | 04-013-2116 | S | Calcium Magnesium Carbonate | 0.970 | 38.507 | 3.05 | 36 |
| 4 | true | 01-075-6049 | S | Calcium Carbonate | 0.761 | 30.213 | 3.2 | 27 |
| 5 | true | 01-071-6263 | S | Magnesium Carbonate | 0.106 | 4.218 | *1.85 | 6 |
| 6 | true | 01-075-9982 | S | Calcium Carbonate | 0.193 | 7.678 | 1.14 | 19 |

**01-088-0866** Jun 9, 2020 11:57 AM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Fe3 O4
**Empirical Formula:** Fe3 O4 **Weight %:** Fe72.36 O27.64 **Atomic %:** Fe42.86 O57.14 **ANX:** AB2X4
**Compound Name:** Iron Oxide **Mineral Name:** Magnetite **Common Name:** iron diiron(III) oxide

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 4.93 **I/Ic - ND:** 1.5

**SYS:** Cubic **SPGR:** Fd-3m (227)
**Author's Cell [ AuthCell a:** 8.3847(2) Å **AuthCell Vol:** 589.47 Å³ **AuthCell Z:** 8.00 **AuthCell MolVol:** 73.68 **]**
**Density [ Dcalc:** 5.218 g/cm³ **Dstruc:** 5.22 g/cm³ **]** **SS/FOM:** F(30) = 999.9(0.0001, 30)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.033

**Space Group:** Fd-3m (227) **Molecular Weight:** 231.54
**Crystal Data [ XtlCell a:** 8.385 Å **XtlCell b:** 8.385 Å **XtlCell c:** 8.385 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 589.47 Å³ **XtlCell Z:** 8.00 **]**
**Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 **]**
**Reduced Cell [ RedCell a:** 5.929 Å **RedCell b:** 5.929 Å **RedCell c:** 5.929 Å **RedCell α:** 60.00°
**RedCell β:** 60.00° **RedCell γ:** 60.00° **RedCell Vol:** 147.37 Å³ **]**

**Atomic parameters are cross-referenced from PDF entry 04-005-4319** **ADP:** B **Origin:** O2
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 11 | z,-x+1/4,-y+1/4 | 21 | -y+1/4,z,-x+1/4 | 31 | -x+1/4,-z+1/4,y | 41 | z,y,x |
| 2 | -x,-y,-z | 12 | -z,x+3/4,y+3/4 | 22 | y+3/4,-z,x+3/4 | 32 | x+3/4,z+3/4,-y | 42 | -z,-y,-x |
| 3 | x,-y+1/4,-z+1/4 | 13 | -z+1/4,x,-y+1/4 | 23 | -y+1/4,-z+1/4,x | 33 | y,x,z | 43 | z,-y+1/4,-x+1/4 |
| 4 | -x,y+3/4,z+3/4 | 14 | z+3/4,-x,y+3/4 | 24 | y+3/4,z+3/4,-x | 34 | -y,-x,-z | 44 | -z,y+3/4,x+3/4 |
| 5 | -x+1/4,y,-z+1/4 | 15 | -z+1/4,-x+1/4,y | 25 | x,z,y | 35 | y,-x+1/4,-z+1/4 | 45 | -z+1/4,y,-x+1/4 |
| 6 | x+3/4,-y,z+3/4 | 16 | z+3/4,x+3/4,-y | 26 | -x,-z,-y | 36 | -y,x+3/4,z+3/4 | 46 | z+3/4,-y,x+3/4 |
| 7 | -x+1/4,-y+1/4,z | 17 | y,z,x | 27 | x,-z+1/4,-y+1/4 | 37 | -y+1/4,x,-z+1/4 | 47 | -z+1/4,-y+1/4,x |
| 8 | x+3/4,y+3/4,-z | 18 | -y,-z,-x | 28 | -x,z+3/4,y+3/4 | 38 | y+3/4,-x,z+3/4 | 48 | z+3/4,y+3/4,-x |
| 9 | z,x,y | 19 | y,-z+1/4,-x+1/4 | 29 | -x+1/4,z,-y+1/4 | 39 | -y+1/4,-x+1/4,z | | |
| 10 | -z,-x,-y | 20 | -y,z+3/4,x+3/4 | 30 | x+3/4,-z,y+3/4 | 40 | y+3/4,x+3/4,-z | | |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Fe | 1 | 16d | .-3m | 0.5 | 0.5 | 0.5 | 1.0 | 0.47 | 6-a |
| Fe | 2 | 8a | -43m | 0.125 | 0.125 | 0.125 | 1.0 | 0.37 | 4-a |
| O | 3 | 32e | .3m | 0.2547 | 0.2547 | 0.2547 | 1.0 | 0.64 | 4-a |

**Subfile(s):** Common Phase, Forensic, Inorganic, Metals & Alloys, Micro & Mesoporous (Zeolite), Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Pigment/Dye

**Pearson Symbol:** cF56.00

**01-088-0866** Jun 9, 2020 11:57 AM (fal-sharji2)

**Cross-Ref PDF #'s:** 00-001-1111 (Deleted), 00-002-1035 (Deleted), 00-003-0862 (Deleted), 00-007-0322 (Deleted), 00-011-0614 (Deleted), 00-019-0629 (Primary), 00-065-0731 (Primary), 01-071-4918 (Alternate), 01-072-2303 (Alternate), 01-074-1909 (Alternate), 01-074-1910 (Alternate), 01-075-0449 (Alternate), 01-075-1610 (Alternate), 01-075-9710 (Alternate), 01-076-1849 (Alternate), 01-076-5948 (Alternate), 01-078-6086 (Alternate), 01-080-6402 (Alternate), 01-080-6403 (Alternate), 01-080-6404 (Alternate), 01-080-6405 (Alternate), 01-080-6406 (Alternate), 01-080-6407 (Alternate), 01-080-6408 (Alternate), 01-080-6409 (Alternate), 01-080-6410 (Alternate), 01-080-7683 (Alternate), 01-087-2334 (Alternate), 01-089-3854 (Alternate), 01-089-4319 (Alternate), ✓ 03-065-3107 (Alternate), ✓ 04-001-7822 (Alternate), ✓ 04-001-7909 (Alternate), ✓ 04-001-9000 (Alternate), ✓ 04-001-9326 (Alternate), ✓ 04-002-0264 (Alternate), ✓ 04-002-0618 (Alternate), ✓ 04-002-0643 (Alternate), ✓ 04-002-1855 (Alternate), ✓ 04-002-2487 (Alternate), ✓ 04-002-2707 (Alternate), ✓ 04-002-2709 (Alternate), ✓ 04-002-2981 (Alternate), ✓ 04-002-3194 (Alternate), ✓ 04-002-3668 (Alternate), ✓ 04-002-5310 (Alternate), ✓ 04-002-5448 (Alternate), ✓ 04-002-5632 (Alternate), ✓ 04-002-5683 (Alternate), ✓ 04-002-5903 (Alternate), ✓ 04-002-6866 (Alternate), ✓ 04-002-6955 (Alternate), ✓ 04-002-8141 (Alternate), ✓ 04-002-8629 (Alternate), ✓ 04-002-9019 (Alternate), ✓ 04-002-9635 (Alternate), ✓ 04-003-1446 (Alternate), ✓ 04-004-2838 (Alternate), ✓ 04-005-4307 (Alternate), ✓ 04-005-4319 (Primary), ✓ 04-005-4404 (Alternate), ✓ 04-005-4551 (Alternate), ✓ 04-005-5733 (Alternate), ✓ 04-005-6268 (Alternate), ✓ 04-005-9786 (Alternate), ✓ 04-005-9788 (Alternate), ✓ 04-005-9815 (Alternate), ✓ 04-006-0225 (Alternate), ✓ 04-006-0424 (Alternate), ✓ 04-006-0425 (Alternate), ✓ 04-006-1668 (Alternate), ✓ 04-006-2406 (Alternate), ✓ 04-006-2467 (Alternate), ✓ 04-006-2752 (Alternate), ✓ 04-006-4615 (Alternate), ✓ 04-006-6497 (Alternate), ✓ 04-006-6550 (Alternate), ✓ 04-006-6692 (Alternate), ✓ 04-006-8076 (Alternate), ✓ 04-007-1427 (Alternate), ✓ 04-007-2718 (Alternate), ✓ 04-007-6010 (Alternate), ✓ 04-007-8567 (Alternate), ✓ 04-007-8976 (Alternate), ✓ 04-007-9093 (Alternate), ✓ 04-008-0315 (Alternate), ✓ 04-008-0777 (Alternate), ✓ 04-008-4423 (Alternate), ✓ 04-008-4511 (Alternate), ✓ 04-008-4512 (Alternate), ✓ 04-008-8145 (Alternate), ✓ 04-008-8146 (Alternate), ✓ 04-008-8147 (Alternate), ✓ 04-008-8148 (Alternate), ✓ 04-009-4225 (Alternate), ✓ 04-009-8417 (Alternate), ✓ 04-009-8418 (Alternate), ✓ 04-009-8419 (Alternate), ✓ 04-009-8420 (Alternate), ✓ 04-009-8421 (Alternate), ✓ 04-009-8422 (Alternate), ✓ 04-009-8423 (Alternate), ✓ 04-009-8424 (Alternate), ✓ 04-009-8425 (Alternate), ✓ 04-009-8426 (Alternate), ✓ 04-009-8427 (Alternate), ✓ 04-009-8428 (Alternate), ✓ 04-009-8429 (Alternate), ✓ 04-009-8430 (Alternate), ✓ 04-009-8431 (Alternate), ✓ 04-009-8432 (Alternate), ✓ 04-009-8433 (Alternate), ✓ 04-009-8434 (Alternate), ✓ 04-009-8435 (Alternate), ✓ 04-009-8436 (Alternate), ✓ 04-009-8437 (Alternate), ✓ 04-009-8438 (Alternate), ✓ 04-009-8439 (Alternate), ✓ 04-009-8440 (Alternate), ✓ 04-009-8441 (Alternate), ✓ 04-009-8442 (Alternate), ✓ 04-009-8443 (Alternate), ✓ 04-011-5952 (Alternate), ✓ 04-013-7099 (Alternate), ✓ 04-013-7100 (Alternate), ✓ 04-013-9806 (Alternate), ✓ 04-013-9807 (Alternate), ✓ 04-013-9808 (Alternate), ✓ 04-013-9809 (Alternate), ✓ 04-013-9810 (Alternate), ✓ 04-013-9811 (Alternate), ✓ 04-014-1396 (Alternate), ✓ 04-014-9664 (Alternate), ✓ 04-015-3100 (Alternate), ✓ 04-015-3101 (Alternate), ✓ 04-015-3102 (Alternate), ✓ 04-015-8200 (Alternate), ✓ 04-015-8203 (Alternate), ✓ 04-015-8204 (Alternate), ✓ 04-015-8207 (Alternate), ✓ 04-015-8209 (Alternate), ✓ 04-015-8211 (Alternate), ✓ 04-015-8213 (Alternate), ✓ 04-015-8214 (Alternate), ✓ 04-017-1024 (Alternate)

**Entry Date:** 09/01/2000 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "Donathite discredited : a mixture of two spinels". Burns, P.C., Hawthorne, F.C., Libowitzky, E., Bordes, N., Ewing, R.C. Neues Jahrb. Mineral., Monatsh. 1997, 163 (1997). |

**Database Comments:** ANX: AB2X4. Analysis: Fe3 O4. Formula from original source: Fe3 O4. ICSD Collection Code: 85177. Calculated Pattern Original Remarks: Cr-content not given in paper. Sample Source or Locality: Specimen from Ramberget, Hestmona, Norway. Wyckoff Sequence: e d a(FD3-MZ). Unit Cell Data Source: Powder Diffraction.

**d-Spacings (34) - Fe3 O4 - 01-088-0866 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.3115 | 4.840910 | 109 | 1 | 1 | 1 | | 74.0863 | 1.278650 | 67 | 5 | 3 | 3 | | 110.5079 | 0.937438 | 18 | 8 | 4 | 0 | |
| 30.1211 | **2.964440** | 301 | 2 | 2 | 0 | | 75.0893 | 1.264040 | 24 | 6 | 2 | 2 | | 113.6392 | 0.920340 | 1 | 9 | 1 | 1 | |
| 35.4790 | **2.528080** | 999 | 3 | 1 | 1 | | 79.0588 | 1.210230 | 20 | 4 | 4 | 4 | | 114.6991 | 0.914846 | 1 | 8 | 4 | 2 | |
| 37.1128 | 2.420450 | 73 | 2 | 2 | 2 | | 82.0010 | 1.174090 | 4 | 5 | 5 | 1 | | 119.0368 | 0.893812 | 6 | 6 | 6 | 4 | |
| 43.1194 | 2.096170 | 206 | 4 | 0 | 0 | | 86.8609 | 1.120450 | 30 | 6 | 4 | 2 | | 122.4124 | 0.878955 | 39 | 9 | 3 | 1 | |
| 47.2115 | 1.923580 | 2 | 3 | 3 | 1 | | 89.7641 | 1.091590 | 90 | 7 | 3 | 1 | | 128.3456 | 0.855760 | 76 | 8 | 4 | 4 | |
| 53.4946 | 1.711520 | 88 | 4 | 2 | 2 | | 94.6038 | 1.048090 | 36 | 8 | 0 | 0 | | 132.1476 | 0.842694 | 1 | 9 | 3 | 3 | |
| 57.0257 | 1.613640 | 291 | 5 | 1 | 1 | | 97.5225 | 1.024350 | 1 | 7 | 3 | 3 | | 139.0638 | 0.822187 | 18 | 8 | 6 | 2 | |
| 62.6216 | **1.482220** | 368 | 4 | 4 | 0 | | 98.4992 | 1.016790 | 1 | 6 | 4 | 4 | | 143.7141 | 0.810580 | 50 | 9 | 5 | 1 | |
| 65.8438 | 1.417270 | 8 | 5 | 3 | 1 | | 102.4334 | 0.988146 | 14 | 8 | 2 | 2 | | 145.3818 | 0.806818 | 7 | 10 | 2 | 2 | |
| 66.8993 | 1.397450 | 1 | 4 | 4 | 2 | | 105.4228 | 0.968182 | 50 | 7 | 5 | 1 | | | | | | | | |
| 71.0445 | 1.325740 | 28 | 6 | 2 | 0 | | 106.4286 | 0.961791 | 8 | 6 | 6 | 2 | | | | | | | | |

**04-012-1052** Jun 9, 2020 11:58 AM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Pressure & Temperature (Non-ambient)
**Chemical Formula:** Mg Fe2 O4 **Empirical Formula:** Fe2 Mg O4 **Weight %:** Fe55.85 Mg12.15 O32.00
**Atomic %:** Fe28.57 Mg14.29 O57.14 **ANX:** A3X4 **Compound Name:** Magnesium Iron Oxide
**Mineral Name:** Magnesioferrite, Syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 4.06 **I/Ic - ND:** 1.5

**SYS:** Cubic **SPGR:** Fd-3m (227)
**Author's Cell [ AuthCell a:** 8.33588(8) Å **AuthCell Vol:** 579.23 Å³ **AuthCell Z:** 8.00 **AuthCell MolVol:** 72.40 **]**
**Density [ Dcalc:** 4.587 g/cm³ **Dstruc:** 4.59 g/cm³ **]** **SS/FOM:** F(30) = 999.9(0.0001, 30)
**Temp:** 885.0 K (Author provided temperature) **R-factor:** 0.082 **Color:** Brown

**Space Group:** Fd-3m (227) **Molecular Weight:** 200.00
**Crystal Data [ XtlCell a:** 8.336 Å **XtlCell b:** 8.336 Å **XtlCell c:** 8.336 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 579.23 Å³ **XtlCell Z:** 8.00 **]**
**Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 **]**
**Reduced Cell [ RedCell a:** 5.894 Å **RedCell b:** 5.894 Å **RedCell c:** 5.894 Å **RedCell α:** 60.00°
**RedCell β:** 60.00° **RedCell γ:** 60.00° **RedCell Vol:** 144.81 Å³ **]**

**ADP:** U **Origin:** O2 **Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 11 | z,-x+1/4,-y+1/4 | 21 | -y+1/4,z,-x+1/4 | 31 | -x+1/4,-z+1/4,y | 41 | z,y,x |
| 2 | -x,-y,-z | 12 | -z,x+3/4,y+3/4 | 22 | y+3/4,-z,x+3/4 | 32 | x+3/4,z+3/4,-y | 42 | -z,-y,-x |
| 3 | x,-y+1/4,-z+1/4 | 13 | -z+1/4,x,-y+1/4 | 23 | -y+1/4,-z+1/4,x | 33 | y,x,z | 43 | z,-y+1/4,-x+1/4 |
| 4 | -x,y+3/4,z+3/4 | 14 | z+3/4,-x,y+3/4 | 24 | y+3/4,z+3/4,-x | 34 | -y,-x,-z | 44 | -z,y+3/4,x+3/4 |
| 5 | -x+1/4,y,-z+1/4 | 15 | -z+1/4,-x+1/4,y | 25 | x,z,y | 35 | y,-x+1/4,-z+1/4 | 45 | -z+1/4,y,-x+1/4 |
| 6 | x+3/4,-y,z+3/4 | 16 | z+3/4,x+3/4,-y | 26 | -x,-z,-y | 36 | -y,x+3/4,z+3/4 | 46 | z+3/4,-y,x+3/4 |
| 7 | -x+1/4,-y+1/4,z | 17 | y,z,x | 27 | x,-z+1/4,-y+1/4 | 37 | -y+1/4,x,-z+1/4 | 47 | -z+1/4,-y+1/4,x |
| 8 | x+3/4,y+3/4,-z | 18 | -y,-z,-x | 28 | -x,z+3/4,y+3/4 | 38 | y+3/4,-x,z+3/4 | 48 | z+3/4,y+3/4,-x |
| 9 | z,x,y | 19 | y,-z+1/4,-x+1/4 | 29 | -x+1/4,z,-y+1/4 | 39 | -y+1/4,-x+1/4,z | | |
| 10 | -z,-x,-y | 20 | -y,z+3/4,x+3/4 | 30 | x+3/4,-z,y+3/4 | 40 | y+3/4,x+3/4,-z | | |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Fe | 1 | 8a | -43m | 0.125 | 0.125 | 0.125 | 0.918 | 0.0099 | |
| Mg | 2 | 8a | -43m | 0.125 | 0.125 | 0.125 | 0.082 | 0.0099 | |
| Fe | 3 | 16d | .-3m | 0.5 | 0.5 | 0.5 | 0.541 | 0.0044 | |
| Mg | 4 | 16d | .-3m | 0.5 | 0.5 | 0.5 | 0.459 | 0.0044 | |
| O | 5 | 32e | .3m | 0.2573 | 0.2573 | 0.2573 | 1.0 | 0.0078 | |

**Subfile(s):** Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic)
**LPF Prototype Structure [Formula Order]:** Mg Al2 O4,cF56,227
**LPF Prototype Structure [Alpha Order]:** Al2 Mg O4,cF56,227 **Pearson Symbol:** cF56.00

**04-012-1052** Jun 9, 2020 11:58 AM (fal-sharji2)

**Cross-Ref PDF #'s:** 00-017-0464 (Primary), 00-036-0398 (Primary), 01-073-1960 (Alternate), 01-073-2410 (Alternate), 01-075-9708 (Alternate), 01-078-5428 (Alternate), 01-082-9881 (Alternate), 01-088-1935 (Alternate), 01-088-1936 (Alternate), 01-088-1937 (Alternate), 01-088-1938 (Alternate), 01-088-1939 (Alternate), 01-088-1940 (Alternate), 01-088-1941 (Alternate), 01-088-1942 (Alternate), 01-088-1943 (Alternate), 01-089-3084 (Alternate), 01-089-4924 (Alternate), 01-089-6187 (Alternate), 01-089-6188 (Alternate), 01-089-6189 (Alternate), ✓ 04-001-7921 (Alternate), ✓ 04-001-9288 (Alternate), ✓ 04-002-0587 (Alternate), ✓ 04-002-0619 (Alternate), ✓ 04-002-2458 (Alternate), ✓ 04-002-2459 (Alternate), ✓ 04-002-3054 (Alternate), ✓ 04-002-3768 (Alternate), ✓ 04-002-3769 (Alternate), ✓ 04-002-5223 (Alternate), ✓ 04-002-5328 (Alternate), ✓ 04-002-5461 (Alternate), ✓ 04-002-5666 (Alternate), ✓ 04-002-5894 (Alternate), ✓ 04-002-5904 (Alternate), ✓ 04-002-6403 (Alternate), ✓ 04-002-8191 (Alternate), ✓ 04-002-8204 (Alternate), ✓ 04-005-7127 (Alternate), ✓ 04-005-8346 (Alternate), ✓ 04-005-8349 (Alternate), ✓ 04-006-0223 (Alternate), ✓ 04-006-0426 (Alternate), ✓ 04-006-0427 (Alternate), ✓ 04-006-1839 (Alternate), ✓ 04-006-2461 (Alternate), ✓ 04-006-2469 (Alternate), ✓ 04-006-4005 (Alternate), ✓ 04-006-6673 (Alternate), ✓ 04-006-6676 (Alternate), ✓ 04-006-6677 (Alternate), ✓ 04-006-6682 (Alternate), ✓ 04-007-4190 (Alternate), ✓ 04-007-4269 (Alternate), ✓ 04-007-5629 (Alternate), ✓ 04-007-5630 (Alternate), ✓ 04-008-2382 (Alternate), ✓ 04-010-6157 (Primary), ✓ 04-011-9002 (Alternate), ✓ 04-011-9003 (Alternate), ✓ 04-012-0908 (Alternate), ✓ 04-012-0909 (Alternate), ✓ 04-012-0910 (Alternate), ✓ 04-012-0911 (Alternate), ✓ 04-012-0912 (Alternate), ✓ 04-012-0913 (Alternate), ✓ 04-012-0914 (Alternate), ✓ 04-012-0915 (Alternate), ✓ 04-012-0916 (Alternate), ✓ 04-012-0917 (Alternate), ✓ 04-012-0918 (Alternate), ✓ 04-012-0919 (Alternate), ✓ 04-012-0920 (Alternate), ✓ 04-012-0921 (Alternate), ✓ 04-012-0922 (Alternate), ✓ 04-012-0923 (Alternate), ✓ 04-012-0924 (Alternate), ✓ 04-012-0925 (Alternate), ✓ 04-012-0926 (Alternate), ✓ 04-012-0927 (Alternate), ✓ 04-012-0928 (Alternate), ✓ 04-012-0929 (Alternate), ✓ 04-012-0930 (Alternate), ✓ 04-012-0931 (Alternate), ✓ 04-012-0932 (Alternate), ✓ 04-012-0933 (Alternate), ✓ 04-012-0934 (Alternate), ✓ 04-012-0935 (Alternate), ✓ 04-012-0936 (Alternate), ✓ 04-012-0937 (Alternate), ✓ 04-012-0938 (Alternate), ✓ 04-012-0939 (Alternate), ✓ 04-012-0940 (Alternate), ✓ 04-012-0941 (Alternate), ✓ 04-012-0942 (Alternate), ✓ 04-012-0943 (Alternate), ✓ 04-012-0944 (Alternate), ✓ 04-012-0945 (Alternate), ✓ 04-012-0946 (Alternate), ✓ 04-012-0947 (Alternate), ✓ 04-012-0948 (Alternate), ✓ 04-012-0949 (Alternate), ✓ 04-012-0950 (Alternate), ✓ 04-012-0951 (Alternate), ✓ 04-012-1050 (Alternate), ✓ 04-012-1051 (Alternate), ✓ 04-012-1053 (Alternate), ✓ 04-012-1054 (Alternate), ✓ 04-012-1055 (Alternate), ✓ 04-012-1056 (Alternate), ✓ 04-012-1057 (Alternate), ✓ 04-012-1058 (Alternate), ✓ 04-012-1059 (Alternate), ✓ 04-012-1060 (Alternate), ✓ 04-012-1061 (Alternate), ✓ 04-012-1062 (Alternate), ✓ 04-012-1063 (Alternate), ✓ 04-012-1064 (Alternate), ✓ 04-012-1065 (Alternate), ✓ 04-012-1066 (Alternate), ✓ 04-012-1067 (Alternate), ✓ 04-012-1068 (Alternate), ✓ 04-012-1069 (Alternate), ✓ 04-012-1070 (Alternate), ✓ 04-012-1071 (Alternate), ✓ 04-012-1072 (Alternate), ✓ 04-012-1073 (Alternate), ✓ 04-012-1074 (Alternate), ✓ 04-012-1075 (Alternate), ✓ 04-012-1076 (Alternate), ✓ 04-012-1077 (Alternate), ✓ 04-012-1078 (Alternate), ✓ 04-012-1079 (Alternate), ✓ 04-012-1080 (Alternate), ✓ 04-012-1081 (Alternate), ✓ 04-014-3057 (Alternate), ✓ 04-014-3693 (Alternate), ✓ 04-014-3694 (Alternate), ✓ 04-014-3695 (Alternate), ✓ 04-014-3696 (Alternate), ✓ 04-014-3697 (Alternate), ✓ 04-014-3698 (Alternate), ✓ 04-014-3699 (Alternate), ✓ 04-014-3700 (Alternate), ✓ 04-014-3701 (Alternate), ✓ 04-014-3702 (Alternate), ✓ 04-014-3703 (Alternate), ✓ 04-014-3704 (Alternate), ✓ 04-014-3705 (Alternate), ✓ 04-014-3706 (Alternate), ✓ 04-014-3707 (Alternate), ✓ 04-014-3708 (Alternate), ✓ 04-014-3709 (Alternate), ✓ 04-014-3710 (Alternate), ✓ 04-014-3711 (Alternate), ✓ 04-014-3712 (Alternate), ✓ 04-014-3713 (Alternate), ✓ 04-014-3714 (Alternate), ✓ 04-014-3715 (Alternate), ✓ 04-014-3716 (Alternate), ✓ 04-014-3717 (Alternate), ✓ 04-014-3718 (Alternate), ✓ 04-014-3719 (Alternate), ✓ 04-014-3720 (Alternate), ✓ 04-014-3721 (Alternate), ✓ 04-014-3722 (Alternate), ✓ 04-014-3723 (Alternate), ✓ 04-014-3724 (Alternate), ✓ 04-014-3725 (Alternate), ✓ 04-014-3726 (Alternate), ✓ 04-014-3727 (Alternate), ✓ 04-014-3728 (Alternate), ✓ 04-014-3729 (Alternate), ✓ 04-014-3730 (Alternate), ✓ 04-014-3731 (Alternate), ✓ 04-014-3732 (Alternate), ✓ 04-014-3733 (Alternate), ✓ 04-014-3734 (Alternate), ✓ 04-015-7027 (Alternate)

**Entry Date:** 09/01/2009 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Effects of high pressure and high temperature on cation ordering in magnesioferrite, MgFe2O4, using in situ synchrotron X-ray powder diffraction up to1430 K and 6 GPa". Antao S.M., Hassan I., Crichton W.A., Parise J.B. Am. Mineral. 90, 1500,1505 (2005). |

**Database Comments:** ANX: A3X4. Color: brown. In Situ Condition: In gold capsule (crimped closed). LPF Collection Code: 1601263. Sample Preparation: Compound Preparation: solid-state reaction. Sample dried at 423 K for 1 d. Pressure of Datacollection: 6 GPa. Temperature of Data Collection: 885 K. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (34) - Mg Fe2 O4 - 04-012-1052 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.4197 | 4.812720 | 31 | 1 | 1 | 1 | | 74.5934 | 1.271210 | 71 | 5 | 3 | 3 | | 111.4814 | 0.931980 | 24 | 8 | 4 | 0 | |
| 30.3018 | **2.947180** | 383 | 2 | 2 | 0 | | 75.6060 | 1.256680 | 17 | 6 | 2 | 2 | | 114.6725 | 0.914982 | 2 | 9 | 1 | 1 | |
| 35.6938 | **2.513360** | 999 | 3 | 1 | 1 | | 79.6140 | 1.203180 | 22 | 4 | 4 | 4 | | 115.7541 | 0.909519 | 1 | 8 | 4 | 2 | |
| 37.3382 | 2.406360 | 24 | 2 | 2 | 2 | | 82.5852 | 1.167260 | 3 | 7 | 1 | 1 | | 120.1867 | 0.888608 | 7 | 6 | 6 | 4 | |
| 43.3845 | 2.083970 | 194 | 4 | 0 | 0 | | 87.4976 | 1.113930 | 35 | 6 | 4 | 2 | | 123.6454 | 0.873838 | 44 | 9 | 3 | 1 | |
| 47.5049 | 1.912380 | 1 | 3 | 3 | 1 | | 90.4338 | 1.085240 | 100 | 7 | 3 | 1 | | 129.7501 | 0.850777 | 92 | 8 | 4 | 4 | |
| 53.8332 | 1.701550 | 109 | 4 | 2 | 2 | | 95.3333 | 1.041990 | 41 | 8 | 0 | 0 | | 133.6832 | 0.837788 | 1 | 9 | 3 | 3 | |
| 57.3907 | 1.604240 | 305 | 5 | 1 | 1 | | 98.2905 | 1.018390 | 1 | 7 | 3 | 3 | | 140.9014 | 0.817400 | 19 | 8 | 6 | 2 | |
| 63.0302 | **1.473590** | 409 | 4 | 4 | 0 | | 99.2811 | 1.010870 | 1 | 6 | 4 | 4 | | 145.8216 | 0.805860 | 58 | 9 | 5 | 1 | |
| 66.2788 | 1.409020 | 4 | 5 | 3 | 1 | | 103.2723 | 0.982393 | 16 | 8 | 2 | 2 | | 147.6047 | 0.802120 | 9 | 10 | 2 | 2 | |
| 67.3434 | 1.389310 | 1 | 4 | 4 | 2 | | 106.3086 | 0.962545 | 57 | 7 | 5 | 1 | | | | | | | | |
| 71.5243 | 1.318020 | 34 | 6 | 2 | 0 | | 107.3309 | 0.956191 | 8 | 6 | 6 | 2 | | | | | | | | |

**04-013-2116** Jun 9, 2020 12:03 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca0.936 Mg0.064 ( C O3 )
**Empirical Formula:** C Ca0.936 Mg0.064 O3 **Weight %:** C12.12 Ca37.86 Mg1.57 O48.44
**Atomic %:** C20.00 Ca18.72 Mg1.28 O60.00 **ANX:** ABX3 **Compound Name:** Calcium Magnesium Carbonate
**Mineral Name:** Calcite, magnesian

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 3.05 **I/Ic - ND:** 0.88

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.9673(3) Å **AuthCell c:** 16.9631(7) Å **AuthCell Vol:** 362.47 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 60.41 ] **Author's Cell Axial Ratio [ c/a:** 3.415 ]
**Density [ Dcalc:** 2.723 g/cm³ **Dstruc:** 2.72 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 297.0 K (Author provided temperature) **R-factor:** 0.023

**Space Group:** R-3c (167) **Molecular Weight:** 99.08
**Crystal Data [ XtlCell a:** 4.967 Å **XtlCell b:** 4.967 Å **XtlCell c:** 16.963 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 362.47 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.415 **a/b:** 1.000 **c/b:** 3.415 ]
**Reduced Cell [ RedCell a:** 4.967 Å **RedCell b:** 4.967 Å **RedCell c:** 6.340 Å **RedCell α:** 66.94°
**RedCell β:** 66.94° **RedCell γ:** 60.00° **RedCell Vol:** 120.82 Å³ ]

**ADP:** U **Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3. | 0.0 | 0.0 | 0.0 | 0.936 | 0.01473 | |
| Mg | 2 | 6b | -3. | 0.0 | 0.0 | 0.0 | 0.064 | 0.01473 | |
| C | 3 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | 0.01426 | |
| O | 4 | 18e | .2 | 0.2575 | 0.0 | 0.25 | 1.0 | 0.02852 | |

**Anisotropic Displacement Parameters:**

| Atom | Num | Uani11 | Uani22 | Uani33 | Uani12 | Uani13 | Uani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.0151 | 0.0151 | 0.014 | 0.00755 | 0.0 | 0.0 |
| Mg | 2 | 0.0151 | 0.0151 | 0.014 | 0.00755 | 0.0 | 0.0 |
| C | 3 | 0.0128 | 0.0128 | 0.0172 | 0.00642 | 0.0 | 0.0 |
| O | 4 | 0.0161 | 0.0336 | 0.0306 | 0.00849 | -0.018 | -0.0089 |

**Subfile(s):** Inorganic, Mineral Related (Mineral , Natural) **Former PDF's #:** 01-086-2335
**LPF Prototype Structure [Formula Order]:** Ca ( C O3 ),hR30,167
**LPF Prototype Structure [Alpha Order]:** C Ca O3,hR30,167
**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00
**Cross-Ref PDF #'s:** 01-089-1304 (Related Phase), 01-089-1305 (Related Phase) **Entry Date:** 09/01/2010
**Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Single-crystal X-ray structure refinements of two biogenic magnesian calcite crystals". Paquette J., Reeder R.J. Am. Mineral. 75, 1151,1158 (1990). |

**Database Comments:** ANX: ABX3. LPF Collection Code: 1213141. Calculated Pattern Original Remarks: same sample studied in Am. Mineral. (1983) 68, 1183. same sample studied in Am. Mineral. (1985) 70, 581. Temperature of Data Collection: 297 K. Unit Cell Data Source: Single Crystal.

**d-Spacings (77) - Ca0.936 Mg0.064 ( C O3 ) - 04-013-2116 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.1645 | 3.836550 | 89 | 0 | 1 | 2 | | 48.7639 | **1.865910** | 193 | 1 | 1 | 6 | | 64.9834 | 1.433940 | 56 | 3 | 0 | 0 | |
| 29.5539 | **3.020030** | 999 | 1 | 0 | 4 | | 56.8384 | 1.618510 | 29 | 2 | 1 | 1 | | 66.0371 | 1.413590 | 30 | 0 | 0 | 12 | |
| 31.6208 | 2.827180 | 20 | 0 | 0 | 6 | | 57.6812 | 1.596850 | 85 | 1 | 2 | 2 | | 69.5704 | 1.350180 | 9 | 2 | 1 | 7 | |
| 36.1354 | 2.483650 | 143 | 1 | 1 | 0 | | 58.4344 | 1.578050 | 11 | 1 | 0 | 10 | | 70.6641 | 1.331940 | 18 | 0 | 2 | 10 | |
| 39.6004 | 2.273950 | 181 | 1 | 1 | 3 | | 60.9781 | 1.518170 | 53 | 2 | 1 | 4 | | 73.3101 | 1.290260 | 27 | 1 | 2 | 8 | |
| 43.3640 | 2.084910 | 148 | 2 | 0 | 2 | | 61.3431 | 1.510010 | 22 | 2 | 0 | 8 | | 74.0728 | 1.278850 | 6 | 3 | 0 | 6 | |
| 47.3501 | 1.918270 | 67 | 0 | 2 | 4 | | 61.7328 | 1.501410 | 22 | 1 | 1 | 9 | | 76.6736 | 1.241820 | 11 | 2 | 2 | 0 | |
| 47.7829 | **1.901900** | 188 | 0 | 1 | 8 | | 63.3828 | 1.466240 | 17 | 1 | 2 | 5 | | 77.6565 | 1.228540 | 19 | 1 | 1 | 12 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 78.8492 | 1.212920 | 1 | 2 | 2 | 3 | | 102.8556 | 0.985236 | 2 | 3 | 2 | 1 | | 121.9071 | 0.881099 | 7m | 1 | 1 | 18 | |
| 80.6619 | 1.190170 | 1 | 1 | 3 | 1 | | 103.5836 | 0.980289 | 9 | 2 | 3 | 2 | | 121.9071 | 0.881099 | m | 1 | 3 | 13 | |
| 81.3802 | 1.181470 | 5 | 3 | 1 | 2 | | 104.2421 | 0.975891 | 3 | 1 | 3 | 10 | | 128.2879 | 0.855969 | 2 | 5 | 0 | 2 | |
| 82.0256 | 1.173800 | 20 | 2 | 1 | 10 | | 104.9024 | 0.971552 | 8 | 1 | 2 | 14 | | 129.1066 | 0.853037 | 6 | 3 | 2 | 10 | |
| 82.6706 | 1.166270 | 3 | 0 | 1 | 14 | | 106.5202 | 0.961217 | 8 | 3 | 2 | 4 | | 129.9353 | 0.850134 | 2m | 1 | 2 | 17 | |
| 84.2379 | 1.148520 | 36 | 1 | 3 | 4 | | 106.8537 | 0.959137 | 14 | 0 | 4 | 8 | | 129.9353 | 0.850134 | m | 3 | 1 | 14 | |
| 85.2939 | 1.136980 | 16 | 2 | 2 | 6 | | 108.1942 | 0.950949 | 4 | 0 | 2 | 16 | | 131.3977 | 0.843184 | 5 | 0 | 5 | 4 | |
| 86.3723 | 1.125530 | 1 | 3 | 1 | 5 | | 108.7518 | 0.947622 | 2 | 2 | 3 | 5 | | 132.8953 | 0.840279 | 1 | 4 | 1 | 9 | |
| 87.0123 | 1.118890 | 4 | 1 | 2 | 11 | | 109.4280 | 0.943648 | 1 | 3 | 1 | 11 | | 134.2180 | 0.836128 | 1 | 2 | 2 | 15 | |
| 92.0460 | 1.070400 | 1 | 1 | 3 | 7 | | 109.6438 | 0.942394 | 1 | 0 | 0 | 18 | | 135.5383 | 0.832135 | 6 | 0 | 1 | 20 | |
| 92.4352 | 1.066910 | 1 | 0 | 4 | 2 | | 110.2807 | 0.938731 | 14 | 4 | 1 | 0 | | 135.8378 | 0.831250 | 1 | 2 | 3 | 11 | |
| 93.7158 | 1.055670 | 7 | 2 | 0 | 14 | | 111.3060 | 0.932954 | 8 | 2 | 2 | 12 | | 137.0012 | 0.827883 | 3 | 3 | 3 | 0 | |
| 95.2778 | 1.042450 | 20 | 4 | 0 | 4 | | 112.5652 | 0.926056 | 1 | 4 | 1 | 3 | | 140.2177 | 0.819150 | 1 | 3 | 3 | 3 | |
| 95.5986 | 1.039800 | 24 | 3 | 1 | 8 | | 114.8627 | 0.914011 | 2 | 3 | 2 | 7 | | 143.0935 | 0.812033 | 1 | 2 | 4 | 1 | |
| 96.8846 | 1.029390 | 12m | 1 | 0 | 16 | | 116.0013 | 0.908291 | 1 | 4 | 0 | 10 | | 144.2906 | 0.809256 | 5 | 4 | 2 | 2 | |
| 96.8846 | 1.029390 | m | 1 | 1 | 15 | | 118.8360 | 0.894736 | 6 | 2 | 3 | 8 | | 146.5426 | 0.804320 | 1 | 0 | 4 | 14 | |
| 98.3856 | 1.017660 | 2 | 2 | 1 | 13 | | 119.6750 | 0.890905 | 6 | 1 | 4 | 6 | | 149.4824 | 0.798427 | 6 | 2 | 4 | 4 | |
| 99.8440 | 1.006680 | 21 | 0 | 3 | 12 | | 120.3057 | 0.888078 | 7 | 2 | 1 | 16 | | | | | | | | |

**01-075-6049** Jun 9, 2020 12:04 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca ( C O3 )
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Calcite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 3.2 **I/Ic - ND:** 0.89

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.988(1) Å **AuthCell c:** 17.061(1) Å **AuthCell Vol:** 367.61 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 61.27 ] **Author's Cell Axial Ratio [ c/a:** 3.420 ]
**Density [ Dcalc:** 2.713 g/cm³ **Dstruc:** 2.71 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 297.0 K (Author provided temperature) **R-factor:** 0.022

**Space Group:** R-3c (167) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 4.988 Å **XtlCell b:** 4.988 Å **XtlCell c:** 17.061 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 367.61 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.420 **a/b:** 1.000 **c/b:** 3.420 ]
**Reduced Cell [ RedCell a:** 4.988 Å **RedCell b:** 4.988 Å **RedCell c:** 6.375 Å **RedCell α:** 66.97°
**RedCell β:** 66.97° **RedCell γ:** 60.00° **RedCell Vol:** 122.54 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-007-8659**
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | IDP | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | | 6-a |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | | 3#b |
| O | 3 | 18e | .2 | 0.2593 | 0.0 | 0.25 | 1.0 | | 1#a |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 00-001-0837 (Deleted), 00-002-0623 (Deleted), 00-002-0629 (Deleted), 00-003-0569 (Deleted), 00-003-0596 (Deleted), 00-003-0670 (Deleted), 00-004-0636 (Deleted), 00-004-0637 (Deleted), 00-005-0586 (Primary), 00-024-0027 (Deleted), 00-047-1743 (Primary), 01-071-3699 (Alternate), 01-072-1937 (Alternate), 01-072-4582 (Alternate), 01-078-3262 (Alternate), 01-078-4614 (Alternate), 01-078-4615 (Alternate), 01-080-2791 (Alternate), 01-080-2792 (Alternate), 01-080-2793 (Alternate), 01-080-2794 (Alternate), 01-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 01-080-2799 (Alternate), 01-080-2800 (Alternate), 01-080-2801 (Alternate), 01-080-2802 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2806 (Alternate), 01-080-2807 (Alternate), 01-080-2808 (Alternate), 01-080-2809 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-9775 (Alternate), 01-080-9776 (Alternate), 01-083-0577 (Alternate), 01-083-0578 (Alternate), 01-085-0849 (Alternate), 01-086-2334 (Alternate), 01-086-2339 (Alternate), 01-086-2340 (Alternate), 01-086-2341 (Alternate), 01-086-2342 (Alternate), 01-086-2343 (Alternate), ✓ 04-001-7249 (Alternate), ✓ 04-002-9082 (Alternate), ✓ 04-006-6528 (Alternate), ✓ 04-007-0049 (Alternate), ✓ 04-007-2808 (Alternate), ✓ 04-007-4388 (Alternate), ✓ 04-007-8659 (Primary), ✓ 04-008-0198 (Alternate), ✓ 04-008-0212 (Alternate), ✓ 04-008-0213 (Alternate), ✓ 04-008-0788 (Alternate), ✓ 04-012-8072 (Alternate), ✓ 04-016-9713 (Alternate)

**Entry Date:** 09/01/2008 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Additional Reference | | Markgraf, S.A., Reeder, R.J. Golden Book of Phase Transitions, Wroclaw 1, 1 (2002). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "High-temperature structure refinements of calcite and magnesite". Markgraf, S.A., Reeder, R.J. Am. Mineral. 70, 590 (1985). |




**01-075-6049** Jun 9, 2020 12:04 PM (fal-sharji2)

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca (C O3). ICSD Collection Code: 40543. Calculated Pattern Original Remarks: Stable up to 1260 K (2nd ref., Tomaszewski), above R3-m, m.p. 1520 K. Sample Source or Locality: Specimen from Guam. Temperature of Data Collection: 297 K. Wyckoff Sequence: e b a(R3-CH). Unit Cell Data Source: Single Crystal.

**d-Spacings (78) - Ca ( C O3 ) - 01-075-6049 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.0594 | 3.853790 | 96 | 0 | 1 | 2 | | 80.9689 | 1.186430 | 5 | 3 | 1 | 2 | | 109.6009 | 0.942643 | 17 | 4 | 1 | 0 | |
| 29.4042 | **3.035070** | 999 | 1 | 0 | 4 | | 81.5373 | 1.179590 | 22 | 2 | 1 | 10 | | 110.4984 | 0.937492 | 9 | 2 | 2 | 12 | |
| 31.4346 | 2.843500 | 19 | 0 | 0 | 6 | | 82.1055 | 1.172860 | 3 | 0 | 1 | 14 | | 111.8486 | 0.929955 | 1 | 4 | 1 | 3 | |
| 35.9803 | 2.494000 | 146 | 1 | 1 | 0 | | 83.7967 | 1.153440 | 41 | 1 | 3 | 4 | | 114.0818 | 0.918028 | 2 | 3 | 2 | 7 | |
| 39.4185 | 2.284020 | 183 | 1 | 1 | 3 | | 84.8299 | 1.142010 | 18 | 2 | 2 | 6 | | 115.1617 | 0.912493 | 1 | 4 | 0 | 10 | |
| 43.1706 | 2.093800 | 157 | 2 | 0 | 2 | | 85.9079 | 1.130420 | 1 | 3 | 1 | 5 | | 117.9818 | 0.898720 | 7 | 2 | 3 | 8 | |
| 47.1252 | 1.926900 | 67 | 0 | 2 | 4 | | 86.4709 | 1.124500 | 4 | 1 | 2 | 11 | | 118.8310 | 0.894759 | 7 | 1 | 4 | 6 | |
| 47.5076 | **1.912280** | 194 | 0 | 1 | 8 | | 91.5171 | 1.075200 | 1 | 1 | 3 | 7 | | 119.2626 | 0.892778 | 8 | 2 | 1 | 16 | |
| 48.5128 | **1.874980** | 201 | 1 | 1 | 6 | | 91.9375 | 1.071380 | 1 | 0 | 4 | 2 | | 120.7744 | 0.886006 | 8 | 1 | 1 | 18 | |
| 56.5803 | 1.625280 | 33 | 2 | 1 | 1 | | 93.0622 | 1.061360 | 8 | 2 | 0 | 14 | | 127.3113 | 0.859550 | 2 | 5 | 0 | 2 | |
| 57.4158 | 1.603600 | 93 | 1 | 2 | 2 | | 94.7450 | 1.046900 | 24 | 4 | 0 | 4 | | 128.0214 | 0.856937 | 7 | 3 | 2 | 10 | |
| 58.0805 | 1.586820 | 11 | 1 | 0 | 10 | | 95.0279 | 1.044530 | 28 | 3 | 1 | 8 | | 128.5609 | 0.854984 | 2 | 1 | 2 | 17 | |
| 60.6846 | 1.524810 | 53 | 2 | 1 | 4 | | 96.1567 | 1.035240 | 13m | 1 | 0 | 16 | | 128.7386 | 0.854347 | 2 | 3 | 1 | 14 | |
| 61.0066 | 1.517530 | 23 | 2 | 0 | 8 | | 96.1567 | 1.035240 | m | 1 | 1 | 15 | | 130.9248 | 0.846751 | 6 | 0 | 5 | 4 | |
| 61.3800 | 1.509190 | 24 | 1 | 1 | 9 | | 97.7080 | 1.022900 | 2 | 2 | 1 | 13 | | 131.7349 | 0.844048 | 1 | 4 | 1 | 9 | |
| 63.0684 | 1.472790 | 20 | 1 | 2 | 5 | | 99.1719 | 1.011690 | 23 | 0 | 3 | 12 | | 132.8750 | 0.840344 | 1 | 2 | 2 | 15 | |
| 64.6811 | 1.439910 | 60 | 3 | 0 | 0 | | 102.2604 | 0.989347 | 3 | 3 | 2 | 1 | | 133.9722 | 0.836888 | 7 | 0 | 1 | 20 | |
| 65.6102 | 1.421750 | 32 | 0 | 0 | 12 | | 102.9784 | 0.984395 | 11 | 2 | 3 | 2 | | 134.5529 | 0.835101 | 1 | 2 | 3 | 11 | |
| 69.2017 | 1.356470 | 11 | 2 | 1 | 7 | | 103.5560 | 0.980475 | 3 | 1 | 3 | 10 | | 135.8096 | 0.831333 | 4 | 3 | 3 | 0 | |
| 70.2484 | 1.338800 | 19 | 0 | 2 | 10 | | 104.1349 | 0.976602 | 9 | 1 | 2 | 14 | | 138.9133 | 0.822591 | 1 | 3 | 3 | 3 | |
| 72.9068 | 1.296400 | 28 | 1 | 2 | 8 | | 105.8730 | 0.965302 | 9 | 3 | 2 | 4 | | 141.6927 | 0.815420 | 1 | 2 | 4 | 1 | |
| 73.6863 | 1.284600 | 6 | 3 | 0 | 6 | | 106.1654 | 0.963448 | 17 | 0 | 4 | 8 | | 142.8378 | 0.812640 | 7 | 4 | 2 | 2 | |
| 76.2977 | 1.247000 | 12 | 2 | 2 | 0 | | 107.3394 | 0.956139 | 5 | 0 | 2 | 16 | | 144.7406 | 0.808240 | 1 | 0 | 4 | 14 | |
| 77.1638 | 1.235150 | 20 | 1 | 1 | 12 | | 108.0712 | 0.951689 | 2 | 2 | 3 | 5 | | 147.7630 | 0.801799 | 7 | 2 | 4 | 4 | |
| 78.4523 | 1.218060 | 1 | 2 | 2 | 3 | | 108.6635 | 0.948146 | 1m | 0 | 0 | 18 | | 148.2937 | 0.800736 | 6 | 5 | 0 | 8 | |
| 80.2579 | 1.195140 | 1 | 1 | 3 | 1 | | 108.6635 | 0.948146 | m | 3 | 1 | 11 | | 149.7446 | 0.797931 | 7 | 3 | 3 | 6 | |

**01-071-6263** Jun 9, 2020 12:05 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Mg ( C O3 )
**Empirical Formula:** C Mg O3 **Weight %:** C14.25 Mg28.83 O56.93 **Atomic %:** C20.00 Mg20.00 O60.00
**ANX:** ABX3 **Compound Name:** Magnesium Carbonate **Mineral Name:** Magnesite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.83 **I/Ic - ND:** 1.08

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.6339(4) Å **AuthCell c:** 15.0177(9) Å **AuthCell Vol:** 279.27 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 46.54 ] **Author's Cell Axial Ratio [ c/a:** 3.241 ]
**Density [ Dcalc:** 3.008 g/cm³ **Dstruc:** 3.01 g/cm³ ] **SS/FOM:** F(30) = 731.0(0.0011, 36)
**Temp:** 297.0 K (Author provided temperature) **R-factor:** 0.035

**Space Group:** R-3c (167) **Molecular Weight:** 84.31
**Crystal Data [ XtlCell a:** 4.634 Å **XtlCell b:** 4.634 Å **XtlCell c:** 15.018 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 279.27 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.241 **a/b:** 1.000 **c/b:** 3.241 ]
**Reduced Cell [ RedCell a:** 4.634 Å **RedCell b:** 4.634 Å **RedCell c:** 5.676 Å **RedCell α:** 65.91°
**RedCell β:** 65.91° **RedCell γ:** 60.00° **RedCell Vol:** 93.09 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-009-2317** **ADP:** B
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| O | 1 | 18e | .2 | 0.2775 | 0.0 | 0.25 | 1.0 | 0.36879 | 1#a |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | 0.34715 | 3#b |
| Mg | 3 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | 0.35475 | 6-a |

**Anisotropic Displacement Parameters:**

| Atom | Num | Bani11 | Bani22 | Bani33 | Bani12 | Bani13 | Bani23 |
|---|---|---|---|---|---|---|---|
| O | 1 | 0.469464 | 0.646158 | 0.0496549 | 0.323079 | -0.0386154 | -0.0772308 |
| C | 2 | 0.506867 | 0.506867 | 0.0277294 | 0.253433 | 0.0 | 0.0 |
| Mg | 3 | 0.51525 | 0.51525 | 0.034178 | 0.257947 | 0.0 | 0.0 |

**Subfile(s):** Cement and Hydration Product, Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural)
**Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 00-002-0875 (Deleted), 00-003-0773 (Deleted), 00-003-0788 (Deleted), 00-008-0479 (Primary), 00-036-0383 (Primary), 01-071-1534 (Alternate), 01-071-3698 (Alternate), 01-080-0042 (Alternate), 01-086-2344 (Alternate), ✓ 04-009-2317 (Primary), ✓ 04-010-3138 (Alternate), ✓ 04-012-1188 (Alternate), ✓ 04-012-1189 (Alternate)

**Entry Date:** 09/01/2005 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "The equation of state and high pressure behavior of magnesite". Ross, N.L., Reeder, R.J. Am. Mineral. 82, 682 (1997). |

**Database Comments:** ANX: ABX3. Analysis: C1 Mg1 O3. Formula from original source: Mg (C O3). ICSD Collection Code: 77481. Sample Source or Locality: Specimen from British Museum of Natural History (BM1984,547). Temperature of Data Collection: 297 K. Wyckoff Sequence: e b a(R3-CH). Unit Cell Data Source: Single Crystal.

**d-Spacings (59) - Mg ( C O3 ) - 01-071-6263 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 25.1404 | 3.539310 | 7 | 0 | 1 | 2 | | 62.4084 | 1.486770 | 71 | 1 | 2 | 2 | | 81.5198 | 1.179800 | 29m | 1 | 2 | 8 | |
| 32.6343 | **2.741660** | 999 | 1 | 0 | 4 | | 66.4204 | 1.406360 | 60m | 1 | 0 | 10 | | 81.5198 | 1.179800 | m | 3 | 0 | 6 | |
| 35.8472 | 2.502950 | 131 | 0 | 0 | 6 | | 66.4204 | 1.406360 | m | 2 | 1 | 4 | | 83.3502 | 1.158480 | 7 | 2 | 2 | 0 | |
| 38.8356 | 2.316950 | 62 | 1 | 1 | 0 | | 68.3757 | 1.370830 | 19 | 2 | 0 | 8 | | 86.0753 | 1.128650 | 9 | 2 | 2 | 3 | |
| 42.9799 | **2.102650** | 501 | 1 | 1 | 3 | | 69.3443 | 1.354030 | 88m | 1 | 1 | 9 | | 87.8886 | 1.109980 | 1 | 1 | 3 | 1 | |
| 46.8258 | 1.938520 | 130 | 2 | 0 | 2 | | 69.3443 | 1.354030 | m | 1 | 2 | 5 | | 88.7806 | 1.101120 | 10m | 1 | 1 | 12 | |
| 51.6050 | 1.769660 | 51 | 0 | 2 | 4 | | 70.3153 | 1.337690 | 119 | 3 | 0 | 0 | | 88.7806 | 1.101120 | m | 3 | 1 | 2 | |
| 53.8763 | **1.700290** | 400m | 0 | 1 | 8 | | 75.9765 | 1.251470 | 43 | 0 | 0 | 12 | | 92.4117 | 1.067120 | 72m | 1 | 3 | 4 | |
| 53.8763 | **1.700290** | m | 1 | 1 | 6 | | 76.9153 | 1.238520 | 17 | 2 | 1 | 7 | | 92.4117 | 1.067120 | m | 2 | 1 | 10 | |
| 61.3832 | 1.509120 | 46 | 2 | 1 | 1 | | 79.6823 | 1.202320 | 17 | 0 | 2 | 10 | | 94.2217 | 1.051330 | 22 | 2 | 2 | 6 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 95.1310 | 1.043670 | 1 | 3 | 1 | 5 | | 113.8860 | 0.919048 | m | 3 | 2 | 1 | | 129.9324 | 0.850144 | m | 2 | 2 | 12 | |
| 96.0251 | 1.036310 | 1 | 0 | 1 | 14 | | 114.8870 | 0.913887 | 80 | 3 | 0 | 12 | | 131.1335 | 0.846049 | 6 | 3 | 2 | 7 | |
| 98.7683 | 1.014740 | 7 | 1 | 2 | 11 | | 118.9589 | 0.894170 | 6m | 1 | 3 | 10 | | 134.8381 | 0.834234 | 2m | 0 | 0 | 18 | |
| 101.5363 | 0.994432 | 2 | 0 | 4 | 2 | | 118.9589 | 0.894170 | m | 3 | 2 | 4 | | 134.8381 | 0.834234 | m | 4 | 0 | 10 | |
| 102.4572 | 0.987981 | 1 | 1 | 3 | 7 | | 121.0434 | 0.884828 | 30 | 0 | 4 | 8 | | 137.4543 | 0.826602 | 14m | 1 | 4 | 6 | |
| 105.2558 | 0.969259 | 37 | 4 | 0 | 4 | | 122.1092 | 0.880238 | 7 | 2 | 3 | 5 | | 137.4543 | 0.826602 | m | 2 | 3 | 8 | |
| 107.1357 | 0.957392 | 39 | 3 | 1 | 8 | | 123.1862 | 0.875725 | 22m | 1 | 2 | 14 | | 147.8984 | 0.801526 | 1 | 1 | 3 | 13 | |
| 108.0833 | 0.951616 | 4 | 2 | 2 | 9 | | 123.1862 | 0.875725 | m | 4 | 1 | 0 | | 149.6285 | 0.798150 | 12m | 2 | 1 | 16 | |
| 109.0271 | 0.945996 | 6 | 2 | 0 | 14 | | 126.4923 | 0.862625 | 4 | 1 | 4 | 3 | | 149.6285 | 0.798150 | m | 5 | 0 | 2 | |
| 113.8860 | 0.919048 | 24m | 1 | 1 | 15 | | 129.9324 | 0.850144 | 10m | 0 | 2 | 16 | | | | | | | | |

**01-075-9982** Jun 9, 2020 12:05 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca ( C O3 )
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Aragonite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.14 **I/Ic - ND:** 0.58

**SYS:** Orthorhombic **SPGR:** Pmcn (62)
**Author's Cell [ AuthCell a:** 4.96524(6) Å **AuthCell b:** 7.96358(10) Å **AuthCell c:** 5.74840(5) Å
**AuthCell Vol:** 227.30 Å³ **AuthCell Z:** 4.00 **AuthCell MolVol:** 56.83 ]
**Author's Cell Axial Ratio [ c/a:** 1.158 **a/b:** 0.623 **c/b:** 0.722 ]
**Density [ Dcalc:** 2.925 g/cm³ **Dstruc:** 2.92 g/cm³ ] **SS/FOM:** F(30) = 146.3(0.0062, 33)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.035

**Space Group:** Pnam (62) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 5.748 Å **XtlCell b:** 7.964 Å **XtlCell c:** 4.965 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 227.30 Å³ **XtlCell Z:** 4.00 ]
**Crystal Data Axial Ratio [ c/a:** 0.864 **a/b:** 0.722 **c/b:** 0.623 ]
**Reduced Cell [ RedCell a:** 4.965 Å **RedCell b:** 5.748 Å **RedCell c:** 7.964 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 90.00° **RedCell Vol:** 227.30 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-008-5421** **ADP:** B
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -x+1/2,-y+1/2,z+1/2 | 5 | x+1/2,-y,-z | 7 | -x,y+1/2,-z+1/2 |
| 2 | -x,-y,-z | 4 | x+1/2,y+1/2,-z+1/2 | 6 | -x+1/2,y,z | 8 | x,-y+1/2,z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 4c | m.. | 0.25 | 0.41508 | 0.24046 | 1.0 | 0.61095 | 9-a |
| C | 2 | 4c | m.. | 0.25 | 0.76211 | 0.08518 | 1.0 | 0.43867 | 3#a |
| O | 3 | 4c | m.. | 0.25 | 0.92224 | 0.09557 | 1.0 | 0.77616 | 1#a |
| O | 4 | 8d | 1 | 0.47347 | 0.68065 | 0.08726 | 1.0 | 0.70856 | 1#a |

**Anisotropic Displacement Parameters:**

| Atom | Num | Bani11 | Bani22 | Bani33 | Bani12 | Bani13 | Bani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.665479 | 0.670266 | 0.497141 | 0.0 | 0.0 | 0.0201231 |
| C | 2 | 0.442997 | 0.573788 | 0.299269 | 0.0 | 0.0 | 0.0073175 |
| O | 3 | 1.13407 | 0.540783 | 0.653666 | 0.0 | 0.0 | -0.05854 |
| O | 4 | 0.509938 | 0.926694 | 0.689106 | 0.180227 | -0.0136696 | 0.0841512 |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**Mineral Classification:** Aragonite (Group), carbonate (Subgroup) **Pearson Symbol:** oP20.00

**Cross-Ref PDF #'s:** 00-001-0628 (Deleted), 00-003-0405 (Deleted), 00-003-0425 (Deleted), 00-003-1067 (Deleted), 00-005-0453 (Alternate), 00-041-1475 (Primary), ✓ 00-061-0390 (Primary), 01-071-2392 (Alternate), 01-071-2396 (Alternate), 01-071-3700 (Alternate), 01-071-4891 (Alternate), 01-075-9983 (Alternate), 01-075-9984 (Alternate), 01-075-9985 (Alternate), 01-075-9986 (Alternate), 01-075-9987 (Alternate), 01-076-0606 (Alternate), 01-078-4337 (Alternate), 01-078-4338 (Alternate), 01-078-4339 (Alternate), 01-080-2768 (Alternate), 01-080-2769 (Alternate), 01-080-2770 (Alternate), 01-080-2771 (Alternate), 01-080-2772 (Alternate), 01-080-2773 (Alternate), 01-080-2774 (Alternate), 01-080-2775 (Alternate), 01-080-2789 (Alternate), 01-080-2790 (Alternate), ✓ 04-006-5441 (Alternate), ✓ 04-006-5444 (Alternate), ✓ 04-006-6531 (Alternate), ✓ 04-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate), ✓ 04-014-1837 (Alternate), ✓ 04-015-4109 (Alternate), ✓ 04-017-9180 (Alternate)

**Entry Date:** 09/01/2009 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "Atomic structure of biogenic aragonite". Pokroy, B., Fieramosca, J.S., von Dreele, R.B., Fitch, A.N., Caspi, E.N., Zolotoyabko, E. Chem. Mater. 19, 3244 (2007). |

**01-075-9982** Jun 9, 2020 12:05 PM (fal-sharji2

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca (C O3). ICSD Collection Code: 157992. Calculated Pattern Original Remarks: Sample from mollusk shell `Acanthocardia tuberculata`. Sample Source or Locality: biogenic, from Acantochardia tuberculata. Wyckoff Sequence: d c3 (PMCN). Unit Cell Data Source: Powder Diffraction.

**d-Spacings (198) - Ca ( C O3 ) - 01-075-9982 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 19.0249 | 4.660960 | 2 | 0 | 1 | 1 | | 76.5331 | 1.243750 | m | 3 | 4 | 1 | | 106.7505 | 0.959779 | 19 | 1 | 7 | 3 | |
| 21.0679 | 4.213370 | 18 | 1 | 1 | 0 | | 76.7109 | 1.241310 | 55 | 4 | 0 | 0 | | 107.0264 | 0.958067 | 23 | 0 | 0 | 6 | |
| 22.3085 | 3.981790 | 8 | 0 | 2 | 0 | | 77.0036 | 1.237320 | 86 | 3 | 1 | 3 | | 107.8887 | 0.952791 | 1 | 3 | 4 | 4 | |
| 26.2019 | **3.398280** | 999 | 1 | 1 | 1 | | 77.9437 | 1.224730 | 58m | 0 | 5 | 3 | | 108.1511 | 0.951208 | 1 | 0 | 1 | 6 | |
| 27.2218 | **3.273230** | 544 | 0 | 2 | 1 | | 77.9437 | 1.224730 | m | 1 | 3 | 4 | | 109.9345 | 0.940715 | 2m | 0 | 8 | 2 | |
| 31.0903 | 2.874200 | 45 | 0 | 0 | 2 | | 78.6950 | 1.214910 | 12 | 2 | 5 | 2 | | 109.9345 | 0.940715 | m | 1 | 0 | 6 | |
| 32.7426 | 2.732840 | 86 | 1 | 2 | 1 | | 79.3459 | 1.206570 | 56 | 2 | 4 | 3 | | 110.3028 | 0.938605 | 10 | 5 | 0 | 2 | |
| 33.1080 | 2.703510 | 510 | 0 | 1 | 2 | | 79.4706 | 1.204990 | 21 | 0 | 6 | 2 | | 110.4690 | 0.937659 | 13m | 3 | 1 | 5 | |
| 36.0775 | 2.487500 | 322m | 1 | 0 | 2 | | 80.2846 | 1.194810 | 3 | 3 | 2 | 3 | | 110.4690 | 0.937659 | m | 3 | 7 | 0 | |
| 36.0775 | 2.487500 | m | 2 | 0 | 0 | | 80.7421 | 1.189190 | 44 | 1 | 5 | 3 | | 111.3110 | 0.932926 | 13 | 4 | 1 | 4 | |
| 37.2800 | 2.409980 | 129 | 0 | 3 | 1 | | 82.3077 | 1.170490 | 57m | 1 | 6 | 2 | | 111.4502 | 0.932153 | 21m | 0 | 2 | 6 | |
| 37.8604 | 2.374360 | 407 | 1 | 1 | 2 | | 82.3077 | 1.170490 | m | 2 | 6 | 0 | | 111.4502 | 0.932153 | m | 5 | 1 | 2 | |
| 38.4212 | 2.340980 | 241 | 1 | 3 | 0 | | 82.7598 | 1.165240 | 5 | 0 | 4 | 4 | | 111.8229 | 0.930096 | 10 | 5 | 3 | 0 | |
| 38.6012 | 2.330480 | 190 | 0 | 2 | 2 | | 83.1596 | 1.160650 | 28 | 4 | 2 | 1 | | 112.7045 | 0.925306 | 5 | 3 | 7 | 1 | |
| 41.1627 | 2.191180 | 125 | 2 | 1 | 1 | | 84.3798 | 1.146950 | 1m | 2 | 6 | 1 | | 112.9362 | 0.924064 | 8m | 2 | 4 | 5 | |
| 41.6213 | 2.168090 | 5 | 1 | 3 | 1 | | 84.3798 | 1.146950 | m | 3 | 5 | 0 | | 112.9362 | 0.924064 | m | 2 | 8 | 0 | |
| 42.8936 | 2.106680 | 193m | 1 | 2 | 2 | | 85.0542 | 1.139570 | 7 | 4 | 0 | 2 | | 114.0574 | 0.918155 | 1m | 3 | 2 | 5 | |
| 42.8936 | 2.106680 | m | 2 | 2 | 0 | | 85.2104 | 1.137880 | 3 | 0 | 1 | 5 | | 114.0574 | 0.918155 | m | 5 | 3 | 1 | |
| 45.5238 | 1.990890 | 35 | 0 | 4 | 0 | | 85.5323 | 1.134420 | 2 | 1 | 4 | 4 | | 114.4380 | 0.916186 | 12m | 1 | 2 | 6 | |
| 45.8366 | **1.978030** | 648 | 2 | 2 | 1 | | 85.6877 | 1.132760 | 4 | 3 | 3 | 3 | | 114.4380 | 0.916186 | m | 1 | 5 | 5 | |
| 46.5318 | 1.950080 | 5 | 0 | 3 | 2 | | 86.1294 | 1.128080 | 14 | 4 | 1 | 2 | | 114.8072 | 0.914294 | 9 | 4 | 2 | 4 | |
| 48.3405 | 1.881260 | 290m | 0 | 4 | 1 | | 86.3828 | 1.125420 | 24m | 2 | 3 | 4 | | 115.2132 | 0.912233 | 9 | 2 | 8 | 1 | |
| 48.3405 | 1.881260 | m | 2 | 0 | 2 | | 86.3828 | 1.125420 | m | 3 | 5 | 1 | | 115.6329 | 0.910124 | 1 | 2 | 7 | 3 | |
| 48.8461 | 1.862960 | 6 | 0 | 1 | 3 | | 87.2933 | 1.116010 | 1 | 0 | 7 | 1 | | 116.1508 | 0.907552 | 3 | 2 | 6 | 4 | |
| 49.8261 | 1.828590 | 22 | 2 | 1 | 2 | | 87.9732 | 1.109130 | 25m | 1 | 1 | 5 | | 116.3436 | 0.906603 | 8 | 4 | 6 | 0 | |
| 50.2220 | 1.815100 | 259 | 1 | 3 | 2 | | 87.9732 | 1.109130 | m | 1 | 7 | 0 | | 117.4657 | 0.901169 | 3 | 0 | 3 | 6 | |
| 51.9340 | 1.759220 | 32 | 1 | 4 | 1 | | 88.4317 | 1.104560 | 11m | 0 | 2 | 5 | | 118.3968 | 0.896774 | 9 | 3 | 5 | 4 | |
| 52.4141 | 1.744230 | 298 | 1 | 1 | 3 | | 88.4317 | 1.104560 | m | 4 | 3 | 1 | | 119.0352 | 0.893819 | 9 | 2 | 0 | 6 | |
| 52.9042 | 1.729220 | 84 | 2 | 3 | 1 | | 89.0556 | 1.098430 | 1 | 2 | 5 | 3 | | 119.5850 | 0.891312 | 7 | 3 | 7 | 2 | |
| 52.9904 | 1.726610 | 139 | 0 | 2 | 3 | | 89.3482 | 1.095590 | 14 | 4 | 2 | 2 | | 119.9598 | 0.889623 | 1 | 3 | 3 | 5 | |
| 53.9157 | 1.699140 | 20 | 2 | 2 | 2 | | 90.0527 | 1.088840 | 6 | 1 | 7 | 1 | | 120.2689 | 0.888242 | 2 | 2 | 1 | 6 | |
| 56.1537 | 1.636610 | 22 | 0 | 4 | 2 | | 90.5617 | 1.084040 | 7 | 2 | 6 | 2 | | 120.6207 | 0.886683 | 17 | 1 | 3 | 6 | |
| 56.3709 | 1.630820 | 9 | 1 | 2 | 3 | | 91.1902 | 1.078200 | 1 | 1 | 2 | 5 | | 121.0232 | 0.884916 | 16 | 5 | 3 | 2 | |
| 56.7642 | 1.620450 | 17 | 3 | 1 | 0 | | 91.5182 | 1.075190 | 10 | 3 | 1 | 4 | | 121.3823 | 0.883355 | 1 | 0 | 8 | 3 | |
| 59.1910 | 1.559670 | 57 | 3 | 1 | 1 | | 92.5587 | 1.065810 | 10m | 1 | 6 | 3 | | 122.2571 | 0.879611 | 3 | 2 | 8 | 2 | |
| 59.4640 | 1.553160 | 10m | 0 | 3 | 3 | | 92.5587 | 1.065810 | m | 3 | 5 | 2 | | 122.6554 | 0.877934 | 8m | 1 | 7 | 4 | |
| 59.4640 | 1.553160 | m | 2 | 4 | 0 | | 93.1980 | 1.060170 | 1 | 3 | 4 | 3 | | 122.6554 | 0.877934 | m | 5 | 4 | 1 | |
| 60.2445 | 1.534890 | 18m | 0 | 5 | 1 | | 93.4698 | 1.057800 | 1 | 0 | 7 | 2 | | 123.0418 | 0.876323 | 15 | 5 | 1 | 3 | |
| 60.2445 | 1.534890 | m | 2 | 3 | 2 | | 93.8132 | 1.054830 | 13m | 0 | 3 | 5 | | 123.4734 | 0.874542 | 1 | 0 | 9 | 1 | |
| 61.0480 | 1.516600 | 1 | 1 | 5 | 0 | | 93.8132 | 1.054830 | m | 2 | 4 | 4 | | 124.0692 | 0.872116 | 10m | 2 | 2 | 6 | |
| 61.8246 | 1.499400 | 47 | 2 | 4 | 1 | | 93.9866 | 1.053340 | 4 | 4 | 4 | 0 | | 124.0692 | 0.872116 | m | 4 | 5 | 3 | |
| 62.2543 | 1.490080 | 2 | 2 | 1 | 3 | | 94.7141 | 1.047160 | 1m | 3 | 2 | 4 | | 124.3170 | 0.871118 | 3 | 1 | 9 | 0 | |
| 62.5962 | 1.482760 | 1 | 1 | 3 | 3 | | 94.7141 | 1.047160 | m | 4 | 3 | 2 | | 124.6721 | 0.869699 | 1 | 1 | 8 | 3 | |
| 62.8681 | 1.477000 | 30 | 3 | 2 | 1 | | 95.1923 | 1.043160 | 9 | 1 | 5 | 4 | | 125.9726 | 0.864611 | 11 | 4 | 6 | 2 | |
| 63.3741 | 1.466420 | 44 | 1 | 5 | 1 | | 96.0521 | 1.036090 | 32 | 4 | 4 | 1 | | 126.3130 | 0.863307 | 3 | 0 | 4 | 6 | |
| 64.8230 | 1.437100 | 3 | 0 | 0 | 4 | | 96.2592 | 1.034410 | 23m | 1 | 7 | 2 | | 126.9691 | 0.860827 | 1m | 1 | 9 | 1 | |
| 64.9661 | 1.434280 | 5 | 3 | 0 | 2 | | 96.2592 | 1.034410 | m | 2 | 1 | 5 | | 126.9691 | 0.860827 | m | 5 | 2 | 3 | |
| 66.0018 | 1.414260 | 40 | 0 | 1 | 4 | | 98.2060 | 1.019040 | 1 | 3 | 6 | 1 | | 128.2823 | 0.855989 | 1 | 1 | 6 | 5 | |
| 66.1437 | 1.411570 | 29 | 3 | 1 | 2 | | 98.3556 | 1.017890 | 2 | 2 | 7 | 1 | | 129.0776 | 0.853140 | 2 | 3 | 4 | 5 | |
| 66.5219 | 1.404460 | 28 | 3 | 3 | 0 | | 99.5072 | 1.009180 | 30 | 2 | 2 | 5 | | 130.0984 | 0.849570 | 5 | 4 | 4 | 4 | |
| 67.8346 | 1.380440 | 2m | 0 | 4 | 3 | | 99.6820 | 1.007880 | 24 | 4 | 2 | 3 | | 130.8250 | 0.847088 | 5 | 2 | 3 | 6 | |
| 67.8346 | 1.380440 | m | 1 | 0 | 4 | | 100.1482 | 1.004440 | 28 | 3 | 3 | 4 | | 131.2455 | 0.845674 | 1 | 0 | 9 | 2 | |
| 68.6271 | 1.366420 | 26 | 2 | 4 | 2 | | 100.9151 | 0.998868 | 4 | 2 | 6 | 3 | | 131.8092 | 0.843803 | 1 | 3 | 8 | 1 | |
| 68.9874 | 1.360160 | 50 | 1 | 1 | 4 | | 101.3716 | 0.995601 | 14m | 0 | 4 | 5 | | 132.3202 | 0.842132 | 14m | 3 | 7 | 3 | |
| 69.4780 | 1.351750 | 19 | 0 | 2 | 4 | | 101.3716 | 0.995601 | m | 0 | 8 | 0 | | 132.3202 | 0.842132 | m | 5 | 5 | 0 | |
| 69.6165 | 1.349400 | 6 | 3 | 2 | 2 | | 102.3080 | 0.989016 | 6 | 4 | 4 | 2 | | 133.1560 | 0.839449 | 5 | 2 | 7 | 4 | |
| 70.0971 | 1.341320 | 20 | 1 | 5 | 2 | | 102.9554 | 0.984552 | 12 | 3 | 5 | 3 | | 133.3642 | 0.838790 | 3 | 4 | 1 | 5 | |
| 70.7753 | 1.330120 | 5 | 1 | 4 | 3 | | 103.5861 | 0.980272 | 10m | 0 | 8 | 1 | | 134.0228 | 0.836731 | 2 | 5 | 3 | 3 | |
| 70.9508 | 1.327260 | 12 | 0 | 6 | 0 | | 103.5861 | 0.980272 | m | 2 | 5 | 4 | | 135.0252 | 0.833669 | 13m | 1 | 9 | 2 | |
| 71.5870 | 1.317020 | 1 | 2 | 3 | 3 | | 104.3710 | 0.975038 | 8 | 0 | 6 | 4 | | 135.0252 | 0.833669 | m | 5 | 5 | 1 | |
| 72.3159 | 1.305530 | 6 | 2 | 5 | 1 | | 104.5050 | 0.974155 | 10 | 3 | 6 | 2 | | 135.5023 | 0.832242 | 4 | 2 | 8 | 3 | |
| 72.3962 | 1.304280 | 5 | 1 | 2 | 4 | | 104.6579 | 0.973150 | 6 | 2 | 7 | 2 | | 136.2954 | 0.829912 | 1 | 4 | 7 | 1 | |
| 73.1137 | 1.293240 | 1 | 0 | 6 | 1 | | 104.9489 | 0.971249 | 18m | 2 | 3 | 5 | | 136.5533 | 0.829166 | 1 | 3 | 0 | 6 | |
| 75.2415 | 1.261860 | 58 | 3 | 3 | 2 | | 104.9489 | 0.971249 | m | 5 | 1 | 1 | | 137.1219 | 0.827540 | 6 | 6 | 0 | 0 | |
| 75.9751 | 1.251490 | 1 | 1 | 6 | 1 | | 105.8926 | 0.965177 | 2 | 4 | 5 | 1 | | 137.9677 | 0.825171 | 13m | 3 | 1 | 6 | |
| 76.5331 | 1.243750 | 32m | 2 | 0 | 4 | | 106.3549 | 0.962254 | 2 | 1 | 8 | 1 | | 137.9677 | 0.825171 | m | 4 | 2 | 5 | |

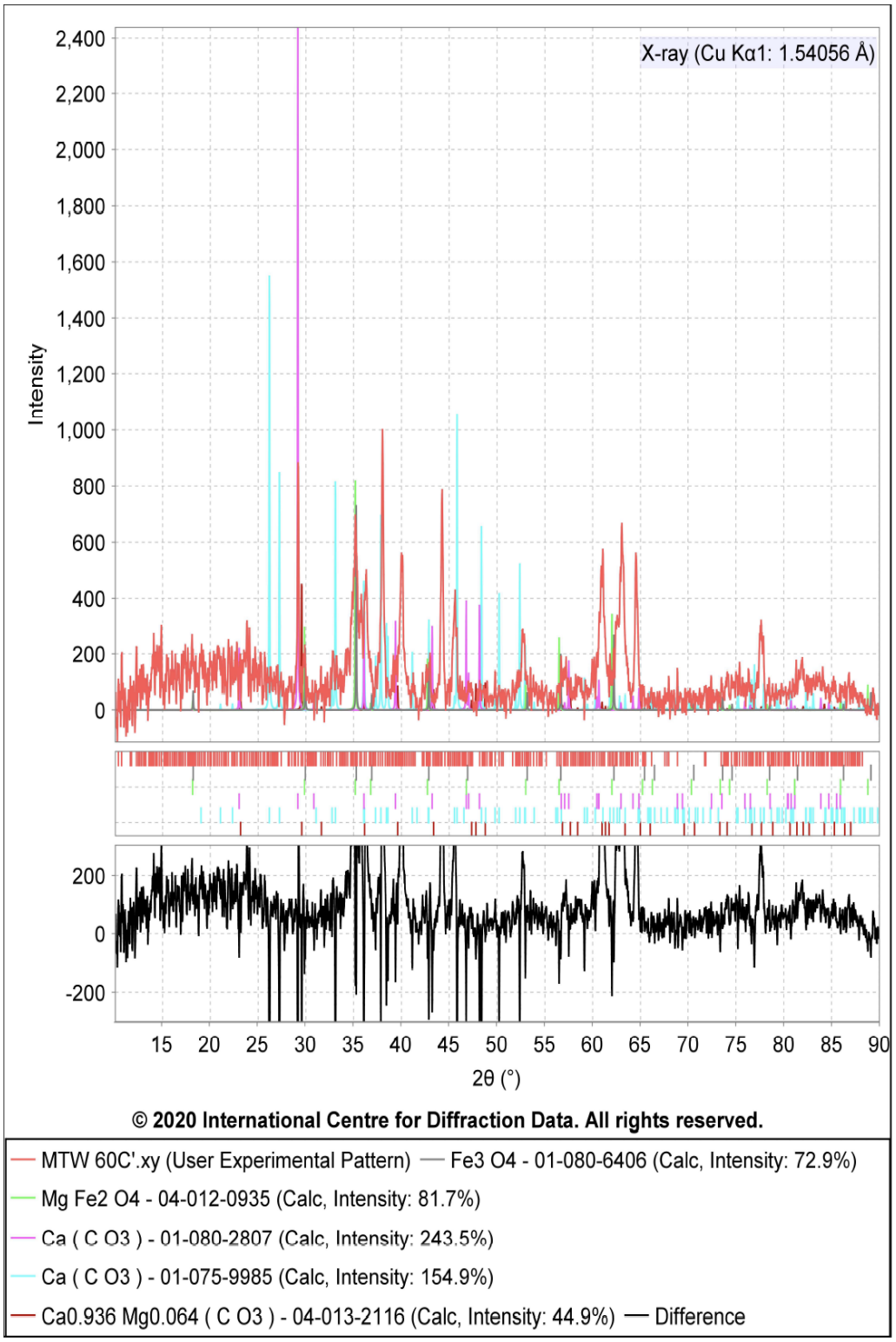


**Figure E.4 XRD patterns of substances precipitated from Magnetically treated Water (MTW) tank at 60 °C from experiment with a tank with little exposure of iron.**

# SIeve+ Report

## Experiment

| | | | |
|---|---|---|---|
| **Search Line:** | 2.365239 Å | **D1 Range:** | 2.356 Å - 2.374 Å |
| **Search Line:** | 2.045914 Å | **D1 Range:** | 2.039 Å - 2.053 Å |
| **Search Line:** | 1.473345 Å | **D1 Range:** | 1.470 Å - 1.476 Å |
| **Search Line:** | 1.516107 Å | **D1 Range:** | 1.513 Å - 1.519 Å |
| **Search Line:** | 1.443179 Å | **D1 Range:** | 1.440 Å - 1.446 Å |
| **Search Line:** | 2.253650 Å | **D1 Range:** | 2.246 Å - 2.262 Å |
| **Search Line:** | 2.245449 Å | **D1 Range:** | 2.237 Å - 2.253 Å |
| **Search Line:** | 1.469431 Å | **D1 Range:** | 1.466 Å - 1.473 Å |

**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (5)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 01-080-6406 | S | Iron Oxide | 0.729 | 12.193 | *5.16 | 5 |
| 2 | true | 04-012-0935 | S | Magnesium Iron Oxide | 0.817 | 13.665 | *4.21 | 7 |
| 3 | true | 01-080-2807 | S | Calcium Carbonate | 2.435 | 40.727 | 2.93 | 31 |
| 4 | true | 01-075-9985 | S | Calcium Carbonate | 1.549 | 25.908 | 1.14 | 51 |
| 5 | true | 04-013-2116 | S | Calcium Magnesium Carbonate | 0.449 | 7.507 | 3.05 | 6 |

**01-080-6406** Jun 9, 2020 12:22 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Temperature (Non-ambient) **Chemical Formula:** Fe3 O4
**Empirical Formula:** Fe3 O4 **Weight %:** Fe72.36 O27.64 **Atomic %:** Fe42.86 O57.14 **ANX:** A3X4
**Compound Name:** Iron Oxide **Mineral Name:** Magnetite **Common Name:** Iron(II) diiron(III) tetraoxide

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 4.8 **I/Ic - ND:** 1.31

**SYS:** Cubic **SPGR:** Fd-3m (227)
**Author's Cell [ AuthCell a:** 8.4324(5) Å **AuthCell Vol:** 599.59 Å³ **AuthCell Z:** 8.00 **AuthCell MolVol:** 74.95 **]**
**Density [ Dcalc:** 5.13 g/cm³ **Dstruc:** 5.13 g/cm³ **]** **SS/FOM:** F(30) = 999.9(0.0001, 30)
**Temp:** 673.0 K (Author provided temperature) **R-factor:** 0.026

**Space Group:** Fd-3m (227) **Molecular Weight:** 231.54
**Crystal Data [ XtlCell a:** 8.432 Å **XtlCell b:** 8.432 Å **XtlCell c:** 8.432 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 599.59 Å³ **XtlCell Z:** 8.00 **]**
**Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 **]**
**Reduced Cell [ RedCell a:** 5.963 Å **RedCell b:** 5.963 Å **RedCell c:** 5.963 Å **RedCell α:** 60.00°
**RedCell β:** 60.00° **RedCell γ:** 60.00° **RedCell Vol:** 149.90 Å³ **]**

**Crystal (Symmetry Allowed):** Centrosymmetric

**Subfile(s):** Common Phase, Forensic, Inorganic, Metals & Alloys, Micro & Mesoporous, Mineral Related (Mineral , Natural)
**Prototype Structure [Formula Order]:** Mg Al2 O4 **Prototype Structure [Alpha Order]:** Al2 Mg O4
**Pearson Symbol:** cF56.00

**Cross-Ref PDF #'s:**
00-001-1111 (Deleted), 00-002-1035 (Deleted), 00-003-0862 (Deleted), 00-007-0322 (Deleted), 00-011-0614 (Deleted), 00-019-0629 (Primary), 00-065-0731 (Primary), 01-071-4918 (Alternate), 01-072-2303 (Alternate), 01-074-1909 (Alternate), 01-074-1910 (Alternate), 01-075-0449 (Alternate), 01-075-1610 (Alternate), 01-075-9710 (Alternate), 01-076-1849 (Alternate), 01-076-5948 (Alternate), 01-078-6086 (Alternate), 01-080-6402 (Alternate), 01-080-6403 (Alternate), 01-080-6404 (Alternate), 01-080-6405 (Alternate), 01-080-6407 (Alternate), 01-080-6408 (Alternate), 01-080-6409 (Alternate), 01-080-6410 (Alternate), 01-080-7683 (Alternate), 01-087-2334 (Alternate), 01-088-0866 (Alternate), 01-089-3854 (Alternate), 01-089-4319 (Alternate), ✓ 03-065-3107 (Alternate), ✓ 04-001-7822 (Alternate), ✓ 04-001-7909 (Alternate), ✓ 04-001-9000 (Alternate), ✓ 04-001-9326 (Alternate), ✓ 04-002-0264 (Alternate), ✓ 04-002-0618 (Alternate), ✓ 04-002-0643 (Alternate), ✓ 04-002-1855 (Alternate), ✓ 04-002-2487 (Alternate), ✓ 04-002-2707 (Alternate), ✓ 04-002-2709 (Alternate), ✓ 04-002-2981 (Alternate), ✓ 04-002-3194 (Alternate), ✓ 04-002-3668 (Alternate), ✓ 04-002-5310 (Alternate), ✓ 04-002-5448 (Alternate), ✓ 04-002-5632 (Alternate), ✓ 04-002-5683 (Alternate), ✓ 04-002-5903 (Alternate), ✓ 04-002-6866 (Alternate), ✓ 04-002-6955 (Alternate), ✓ 04-002-8141 (Alternate), ✓ 04-002-8629 (Alternate), ✓ 04-002-9019 (Alternate), ✓ 04-002-9635 (Alternate), ✓ 04-003-1446 (Alternate), ✓ 04-004-2838 (Alternate), ✓ 04-005-4307 (Alternate), ✓ 04-005-4319 (Primary), ✓ 04-005-4404 (Alternate), ✓ 04-005-4551 (Alternate), ✓ 04-005-5733 (Alternate), ✓ 04-005-6268 (Alternate), ✓ 04-005-9786 (Alternate), ✓ 04-005-9788 (Alternate), ✓ 04-005-9815 (Alternate), ✓ 04-006-0225 (Alternate), ✓ 04-006-0424 (Alternate), ✓ 04-006-0425 (Alternate), ✓ 04-006-1668 (Alternate), ✓ 04-006-2406 (Alternate), ✓ 04-006-2467 (Alternate), ✓ 04-006-2752 (Alternate), ✓ 04-006-4615 (Alternate), ✓ 04-006-6497 (Alternate), ✓ 04-006-6550 (Alternate), ✓ 04-006-6692 (Alternate), ✓ 04-006-8076 (Alternate), ✓ 04-007-1427 (Alternate), ✓ 04-007-2718 (Alternate), ✓ 04-007-6010 (Alternate), ✓ 04-007-8567 (Alternate), ✓ 04-007-8976 (Alternate), ✓ 04-007-9093 (Alternate), ✓ 04-008-0315 (Alternate), ✓ 04-008-0777 (Alternate), ✓ 04-008-4423 (Alternate), ✓ 04-008-4511 (Alternate), ✓ 04-008-4512 (Alternate), ✓ 04-008-8145 (Alternate), ✓ 04-008-8146 (Alternate), ✓ 04-008-8147 (Alternate), ✓ 04-008-8148 (Alternate), ✓ 04-009-4225 (Alternate), ✓ 04-009-8417 (Alternate), ✓ 04-009-8418 (Alternate), ✓ 04-009-8419 (Alternate), ✓ 04-009-8420 (Alternate), ✓ 04-009-8421 (Alternate), ✓ 04-009-8422 (Alternate), ✓ 04-009-8423 (Alternate), ✓ 04-009-8424 (Alternate), ✓ 04-009-8425 (Alternate), ✓ 04-009-8426 (Alternate), ✓ 04-009-8427 (Alternate), ✓ 04-009-8428 (Alternate), ✓ 04-009-8429 (Alternate), ✓ 04-009-8430 (Alternate), ✓ 04-009-8431 (Alternate), ✓ 04-009-8432 (Alternate), ✓ 04-009-8433 (Alternate), ✓ 04-009-8434 (Alternate), ✓ 04-009-8435 (Alternate), ✓ 04-009-8436 (Alternate), ✓ 04-009-8437 (Alternate), ✓ 04-009-8438 (Alternate), ✓ 04-009-8439 (Alternate), ✓ 04-009-8440 (Alternate), ✓ 04-009-8441 (Alternate), ✓ 04-009-8442 (Alternate), ✓ 04-009-8443 (Alternate), ✓ 04-011-5952 (Alternate), ✓ 04-013-7099 (Alternate), ✓ 04-013-7100 (Alternate), ✓ 04-013-9806 (Alternate), ✓ 04-013-9807 (Alternate), ✓ 04-013-9808 (Alternate), ✓ 04-013-9809 (Alternate), ✓ 04-013-9810 (Alternate), ✓ 04-013-9811 (Alternate), ✓ 04-014-1396 (Alternate), ✓ 04-014-9664 (Alternate), ✓ 04-015-3100 (Alternate), ✓ 04-015-3101 (Alternate), ✓ 04-015-3102 (Alternate), ✓ 04-015-8200 (Alternate), ✓ 04-015-8203 (Alternate), ✓ 04-015-8204 (Alternate), ✓ 04-015-8207 (Alternate), ✓ 04-015-8209 (Alternate), ✓ 04-015-8211 (Alternate), ✓ 04-015-8213 (Alternate), ✓ 04-015-8214 (Alternate), ✓ 04-017-1024 (Alternate)

**Entry Date:** 09/01/2013

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Structure | | "Structure of magnetite (Fe3 O4) above the Curie temperature: a cation ordering study". Levy, D., Giustetto, R., Hoser, A. Phys. Chem. Miner. 39, 169 (2012). |




**01-080-6406** Jun 9, 2020 12:22 PM (fal-sharji2)

**Database Comments:** ANX: A3X4. Analysis: Fe3 O4. Formula from original source: Fe3 O4. ICSD Collection Code: 183973. Sample Source or Locality: Brosso mining area, Ivrea,Italy. Structures: Magnetic structure also determined. Temperature of Data Collection: 673 K. Wyckoff Sequence: e d a (FD3-MZ). Unit Cell Data Source: Powder Diffraction.

**d-Spacings (34) - Fe3 O4 - 01-080-6406 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.2070 | 4.868450 | 96 | 1 | 1 | 1 | | 73.5975 | 1.285930 | 60 | 5 | 3 | 3 | | 109.5788 | 0.942771 | 15 | 8 | 4 | 0 | |
| 29.9468 | **2.981300** | 295 | 2 | 2 | 0 | | 74.5920 | 1.271230 | 24 | 6 | 2 | 2 | | 112.6543 | 0.925576 | 1 | 9 | 1 | 1 | |
| 35.2717 | **2.542460** | 999 | 3 | 1 | 1 | | 78.5253 | 1.217110 | 18 | 4 | 4 | 4 | | 113.6945 | 0.920050 | 1 | 8 | 4 | 2 | |
| 36.8953 | 2.434220 | 75 | 2 | 2 | 2 | | 81.4386 | 1.180770 | 3 | 5 | 5 | 1 | | 117.9443 | 0.898897 | 4 | 6 | 6 | 4 | |
| 42.8633 | 2.108100 | 201 | 4 | 0 | 0 | | 86.2483 | 1.126830 | 24 | 6 | 4 | 2 | | 121.2437 | 0.883956 | 27 | 9 | 3 | 1 | |
| 46.9282 | 1.934530 | 4 | 3 | 3 | 1 | | 89.1203 | 1.097800 | 78 | 7 | 3 | 1 | | 127.0222 | 0.860628 | 54 | 8 | 4 | 4 | |
| 53.1680 | 1.721260 | 83 | 4 | 2 | 2 | | 93.9039 | 1.054050 | 29 | 8 | 0 | 0 | | 130.7070 | 0.847488 | 1 | 9 | 3 | 3 | |
| 56.6738 | 1.622820 | 264 | 5 | 1 | 1 | | 96.7855 | 1.030180 | 1 | 7 | 3 | 3 | | 137.3608 | 0.826865 | 11 | 10 | 2 | 0 | |
| 62.2278 | **1.490650** | 341 | 4 | 4 | 0 | | 97.7491 | 1.022580 | 1 | 6 | 4 | 4 | | 141.7855 | 0.815191 | 32 | 9 | 5 | 1 | |
| 65.4243 | 1.425340 | 7 | 5 | 3 | 1 | | 101.6301 | 0.993768 | 10 | 8 | 2 | 2 | | 143.3589 | 0.811408 | 6 | 10 | 2 | 2 | |
| 66.4716 | 1.405400 | 1 | 4 | 4 | 2 | | 104.5757 | 0.973690 | 39 | 7 | 5 | 1 | | | | | | | | |
| 70.5825 | 1.333280 | 25 | 6 | 2 | 0 | | 105.5659 | 0.967263 | 7 | 6 | 6 | 2 | | | | | | | | |

**04-012-0935** Jun 9, 2020 12:22 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Temperature (Non-ambient) **Chemical Formula:** Mg Fe2 O4
**Empirical Formula:** Fe2 Mg O4 **Weight %:** Fe55.85 Mg12.15 O32.00 **Atomic %:** Fe28.57 Mg14.29 O57.14
**ANX:** A3X4 **Compound Name:** Magnesium Iron Oxide **Mineral Name:** Magnesioferrite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 4.01 **I/Ic - ND:** 1.38

**SYS:** Cubic **SPGR:** Fd-3m (227)
**Author's Cell [ AuthCell a:** 8.45708(4) Å **AuthCell Vol:** 604.87 Å³ **AuthCell Z:** 8.00 **AuthCell MolVol:** 75.61 ]
**Density [ Dcalc:** 4.392 g/cm³ **Dstruc:** 4.39 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0001, 30)
**Temp:** 1026.0 K (Author provided temperature) **R-factor:** 0.012 **Color:** Brown

**Space Group:** Fd-3m (227) **Molecular Weight:** 200.00
**Crystal Data [ XtlCell a:** 8.457 Å **XtlCell b:** 8.457 Å **XtlCell c:** 8.457 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 604.87 Å³ **XtlCell Z:** 8.00 ]
**Crystal Data Axial Ratio [ a/b:** 1.000 **c/b:** 1.000 ]
**Reduced Cell [ RedCell a:** 5.980 Å **RedCell b:** 5.980 Å **RedCell c:** 5.980 Å **RedCell α:** 60.00°
**RedCell β:** 60.00° **RedCell γ:** 60.00° **RedCell Vol:** 151.22 Å³ ]

**ADP:** U **Origin:** O2 **Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 11 | z,-x+1/4,-y+1/4 | 21 | -y+1/4,z,-x+1/4 | 31 | -x+1/4,-z+1/4,y | 41 | z,y,x |
| 2 | -x,-y,-z | 12 | -z,x+3/4,y+3/4 | 22 | y+3/4,-z,x+3/4 | 32 | x+3/4,z+3/4,-y | 42 | -z,-y,-x |
| 3 | x,-y+1/4,-z+1/4 | 13 | -z+1/4,x,-y+1/4 | 23 | -y+1/4,-z+1/4,x | 33 | y,x,z | 43 | z,-y+1/4,-x+1/4 |
| 4 | -x,y+3/4,z+3/4 | 14 | z+3/4,-x,y+3/4 | 24 | y+3/4,z+3/4,-x | 34 | -y,-x,-z | 44 | -z,y+3/4,x+3/4 |
| 5 | -x+1/4,y,-z+1/4 | 15 | -z+1/4,-x+1/4,y | 25 | x,z,y | 35 | y,-x+1/4,-z+1/4 | 45 | -z+1/4,y,-x+1/4 |
| 6 | x+3/4,-y,z+3/4 | 16 | z+3/4,x+3/4,-y | 26 | -x,-z,-y | 36 | -y,x+3/4,z+3/4 | 46 | z+3/4,-y,x+3/4 |
| 7 | -x+1/4,-y+1/4,z | 17 | y,z,x | 27 | x,-z+1/4,-y+1/4 | 37 | -y+1/4,x,-z+1/4 | 47 | -z+1/4,-y+1/4,x |
| 8 | x+3/4,y+3/4,-z | 18 | -y,-z,-x | 28 | -x,z+3/4,y+3/4 | 38 | y+3/4,-x,z+3/4 | 48 | z+3/4,y+3/4,-x |
| 9 | z,x,y | 19 | y,-z+1/4,-x+1/4 | 29 | -x+1/4,z,-y+1/4 | 39 | -y+1/4,-x+1/4,z | | |
| 10 | -z,-x,-y | 20 | -y,z+3/4,x+3/4 | 30 | x+3/4,-z,y+3/4 | 40 | y+3/4,x+3/4,-z | | |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Fe | 1 | 8a | -43m | 0.125 | 0.125 | 0.125 | 0.826 | 0.0082 | |
| Mg | 2 | 8a | -43m | 0.125 | 0.125 | 0.125 | 0.174 | 0.0082 | |
| Fe | 3 | 16d | .-3m | 0.5 | 0.5 | 0.5 | 0.587 | 0.0108 | |
| Mg | 4 | 16d | .-3m | 0.5 | 0.5 | 0.5 | 0.413 | 0.0108 | |
| O | 5 | 32e | .3m | 0.2543 | 0.2543 | 0.2543 | 1.0 | 0.0151 | |

**Subfile(s):** Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural) **Former PDF's #:** 01-076-9752
**LPF Prototype Structure [Formula Order]:** Mg Al2 O4,cF56,227
**LPF Prototype Structure [Alpha Order]:** Al2 Mg O4,cF56,227 **Pearson Symbol:** cF56.00

**04-012-0935** Jun 9, 2020 12:22 PM (fal-sharji2)

**Cross-Ref PDF #'s:** 00-017-0464 (Primary), 00-036-0398 (Primary), 01-073-1960 (Alternate), 01-073-2410 (Alternate), 01-075-9708 (Alternate), 01-078-5428 (Alternate), 01-082-9881 (Alternate), 01-088-1935 (Alternate), 01-088-1936 (Alternate), 01-088-1937 (Alternate), 01-088-1938 (Alternate), 01-088-1939 (Alternate), 01-088-1940 (Alternate), 01-088-1941 (Alternate), 01-088-1942 (Alternate), 01-088-1943 (Alternate), 01-089-3084 (Alternate), 01-089-4924 (Alternate), 01-089-6187 (Alternate), 01-089-6188 (Alternate), 01-089-6189 (Alternate), ✓ 04-001-7921 (Alternate), ✓ 04-001-9288 (Alternate), ✓ 04-002-0587 (Alternate), ✓ 04-002-0619 (Alternate), ✓ 04-002-2458 (Alternate), ✓ 04-002-2459 (Alternate), ✓ 04-002-3054 (Alternate), ✓ 04-002-3768 (Alternate), ✓ 04-002-3769 (Alternate), ✓ 04-002-5223 (Alternate), ✓ 04-002-5328 (Alternate), ✓ 04-002-5461 (Alternate), ✓ 04-002-5666 (Alternate), ✓ 04-002-5894 (Alternate), ✓ 04-002-5904 (Alternate), ✓ 04-002-6403 (Alternate), ✓ 04-002-8191 (Alternate), ✓ 04-002-8204 (Alternate), ✓ 04-005-7127 (Alternate), ✓ 04-005-8346 (Alternate), ✓ 04-005-8349 (Alternate), ✓ 04-006-0223 (Alternate), ✓ 04-006-0426 (Alternate), ✓ 04-006-0427 (Alternate), ✓ 04-006-1839 (Alternate), ✓ 04-006-2461 (Alternate), ✓ 04-006-2469 (Alternate), ✓ 04-006-4005 (Alternate), ✓ 04-006-6673 (Alternate), ✓ 04-006-6676 (Alternate), ✓ 04-006-6677 (Alternate), ✓ 04-006-6682 (Alternate), ✓ 04-007-4190 (Alternate), ✓ 04-007-4269 (Alternate), ✓ 04-007-5629 (Alternate), ✓ 04-007-5630 (Alternate), ✓ 04-008-2382 (Alternate), ✓ 04-010-6157 (Primary), ✓ 04-011-9002 (Alternate), ✓ 04-011-9003 (Alternate), ✓ 04-012-0908 (Alternate), ✓ 04-012-0909 (Alternate), ✓ 04-012-0910 (Alternate), ✓ 04-012-0911 (Alternate), ✓ 04-012-0912 (Alternate), ✓ 04-012-0913 (Alternate), ✓ 04-012-0914 (Alternate), ✓ 04-012-0915 (Alternate), ✓ 04-012-0916 (Alternate), ✓ 04-012-0917 (Alternate), ✓ 04-012-0918 (Alternate), ✓ 04-012-0919 (Alternate), ✓ 04-012-0920 (Alternate), ✓ 04-012-0921 (Alternate), ✓ 04-012-0922 (Alternate), ✓ 04-012-0923 (Alternate), ✓ 04-012-0924 (Alternate), ✓ 04-012-0925 (Alternate), ✓ 04-012-0926 (Alternate), ✓ 04-012-0927 (Alternate), ✓ 04-012-0928 (Alternate), ✓ 04-012-0929 (Alternate), ✓ 04-012-0930 (Alternate), ✓ 04-012-0931 (Alternate), ✓ 04-012-0932 (Alternate), ✓ 04-012-0933 (Alternate), ✓ 04-012-0934 (Alternate), ✓ 04-012-0936 (Alternate), ✓ 04-012-0937 (Alternate), ✓ 04-012-0938 (Alternate), ✓ 04-012-0939 (Alternate), ✓ 04-012-0940 (Alternate), ✓ 04-012-0941 (Alternate), ✓ 04-012-0942 (Alternate), ✓ 04-012-0943 (Alternate), ✓ 04-012-0944 (Alternate), ✓ 04-012-0945 (Alternate), ✓ 04-012-0946 (Alternate), ✓ 04-012-0947 (Alternate), ✓ 04-012-0948 (Alternate), ✓ 04-012-0949 (Alternate), ✓ 04-012-0950 (Alternate), ✓ 04-012-0951 (Alternate), ✓ 04-012-1050 (Alternate), ✓ 04-012-1051 (Alternate), ✓ 04-012-1052 (Alternate), ✓ 04-012-1053 (Alternate), ✓ 04-012-1054 (Alternate), ✓ 04-012-1055 (Alternate), ✓ 04-012-1056 (Alternate), ✓ 04-012-1057 (Alternate), ✓ 04-012-1058 (Alternate), ✓ 04-012-1059 (Alternate), ✓ 04-012-1060 (Alternate), ✓ 04-012-1061 (Alternate), ✓ 04-012-1062 (Alternate), ✓ 04-012-1063 (Alternate), ✓ 04-012-1064 (Alternate), ✓ 04-012-1065 (Alternate), ✓ 04-012-1066 (Alternate), ✓ 04-012-1067 (Alternate), ✓ 04-012-1068 (Alternate), ✓ 04-012-1069 (Alternate), ✓ 04-012-1070 (Alternate), ✓ 04-012-1071 (Alternate), ✓ 04-012-1072 (Alternate), ✓ 04-012-1073 (Alternate), ✓ 04-012-1074 (Alternate), ✓ 04-012-1075 (Alternate), ✓ 04-012-1076 (Alternate), ✓ 04-012-1077 (Alternate), ✓ 04-012-1078 (Alternate), ✓ 04-012-1079 (Alternate), ✓ 04-012-1080 (Alternate), ✓ 04-012-1081 (Alternate), ✓ 04-014-3057 (Alternate), ✓ 04-014-3693 (Alternate), ✓ 04-014-3694 (Alternate), ✓ 04-014-3695 (Alternate), ✓ 04-014-3696 (Alternate), ✓ 04-014-3697 (Alternate), ✓ 04-014-3698 (Alternate), ✓ 04-014-3699 (Alternate), ✓ 04-014-3700 (Alternate), ✓ 04-014-3701 (Alternate), ✓ 04-014-3702 (Alternate), ✓ 04-014-3703 (Alternate), ✓ 04-014-3704 (Alternate), ✓ 04-014-3705 (Alternate), ✓ 04-014-3706 (Alternate), ✓ 04-014-3707 (Alternate), ✓ 04-014-3708 (Alternate), ✓ 04-014-3709 (Alternate), ✓ 04-014-3710 (Alternate), ✓ 04-014-3711 (Alternate), ✓ 04-014-3712 (Alternate), ✓ 04-014-3713 (Alternate), ✓ 04-014-3714 (Alternate), ✓ 04-014-3715 (Alternate), ✓ 04-014-3716 (Alternate), ✓ 04-014-3717 (Alternate), ✓ 04-014-3718 (Alternate), ✓ 04-014-3719 (Alternate), ✓ 04-014-3720 (Alternate), ✓ 04-014-3721 (Alternate), ✓ 04-014-3722 (Alternate), ✓ 04-014-3723 (Alternate), ✓ 04-014-3724 (Alternate), ✓ 04-014-3725 (Alternate), ✓ 04-014-3726 (Alternate), ✓ 04-014-3727 (Alternate), ✓ 04-014-3728 (Alternate), ✓ 04-014-3729 (Alternate), ✓ 04-014-3730 (Alternate), ✓ 04-014-3731 (Alternate), ✓ 04-014-3732 (Alternate), ✓ 04-014-3733 (Alternate), ✓ 04-014-3734 (Alternate), ✓ 04-015-7027 (Alternate)

**Entry Date:** 09/01/2009 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Cation ordering in magnesioferrite, MgFe2O4, to 982 °C using in situ synchrotron X-ray powder diffraction". Antao S.M., Hassan I., Parise J.B. Am. Mineral. 90, 219,228 (2005). |

**Database Comments:** ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 1601134. Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 K for 10 d, quenched in air. CRUCIBLE: sealed evacuated silica tube lined with silver foil. Temperature of Data Collection: 1026 K. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (34) - Mg Fe2 O4 - 04-012-0935 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.1535 | 4.882700 | 36 | 1 | 1 | 1 | | 73.3478 | 1.289690 | 69 | 5 | 3 | 3 | | 109.1064 | 0.945530 | 17 | 8 | 4 | 0 | |
| 29.8573 | **2.990030** | 345 | 2 | 2 | 0 | | 74.3375 | 1.274950 | 17 | 6 | 2 | 2 | | 112.1540 | 0.928285 | 1 | 9 | 1 | 1 | |
| 35.1653 | **2.549910** | 999 | 3 | 1 | 1 | | 78.2524 | 1.220670 | 19 | 4 | 4 | 4 | | 113.1842 | 0.922743 | 1 | 8 | 4 | 2 | |
| 36.7837 | 2.441350 | 28 | 2 | 2 | 2 | | 81.1508 | 1.184230 | 1 | 5 | 5 | 1 | | 117.3906 | 0.901528 | 7 | 6 | 6 | 4 | |
| 42.7320 | 2.114270 | 204 | 4 | 0 | 0 | | 85.9362 | 1.130120 | 33 | 6 | 4 | 2 | | 120.6524 | 0.886543 | 35 | 9 | 3 | 1 | |
| 46.7831 | 1.940190 | 1 | 3 | 3 | 1 | | 88.7908 | 1.101020 | 96 | 7 | 3 | 1 | | 126.3550 | 0.863147 | 75 | 8 | 4 | 4 | |
| 53.0010 | 1.726290 | 105 | 4 | 2 | 2 | | 93.5470 | 1.057130 | 37 | 8 | 0 | 0 | | 129.9829 | 0.849969 | 1 | 9 | 3 | 3 | |
| 56.4935 | 1.627570 | 280 | 5 | 1 | 1 | | 96.4090 | 1.033200 | 1 | 7 | 3 | 3 | | 136.5120 | 0.829285 | 19 | 10 | 2 | 0 | |
| 62.0262 | **1.495010** | 395 | 4 | 4 | 0 | | 97.3672 | 1.025570 | 1 | 6 | 4 | 4 | | 140.8316 | 0.817577 | 44 | 9 | 5 | 1 | |
| 65.2097 | 1.429510 | 3 | 5 | 3 | 1 | | 101.2208 | 0.996676 | 15 | 8 | 2 | 2 | | 142.3620 | 0.813783 | 6 | 10 | 2 | 2 | |
| 66.2528 | 1.409510 | 1 | 4 | 4 | 2 | | 104.1444 | 0.976539 | 50 | 7 | 5 | 1 | | | | | | | | |
| 70.3461 | 1.337180 | 34 | 6 | 2 | 0 | | 105.1267 | 0.970094 | 6 | 6 | 6 | 2 | | | | | | | | |

**01-080-2807** Jun 9, 2020 12:23 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Temperature (Non-ambient) **Chemical Formula:** Ca ( C O3 )
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Calcite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 2.93 **I/Ic - ND:** 0.79

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.9764(1) Å **AuthCell c:** 17.3886(5) Å **AuthCell Vol:** 372.93 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 62.16 ] **Author's Cell Axial Ratio [ c/a:** 3.494 ]
**Density [ Dcalc:** 2.674 g/cm³ **Dstruc:** 2.67 g/cm³ ] **SS/FOM:** F(30) = 272.6(0.0034, 32)
**Temp:** 893.0 K (Author provided temperature) **R-factor:** 0.0799

**Space Group:** R-3c (167) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 4.976 Å **XtlCell b:** 4.976 Å **XtlCell c:** 17.389 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 372.93 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.495 **a/b:** 1.000 **c/b:** 3.495 ]
**Reduced Cell [ RedCell a:** 4.976 Å **RedCell b:** 4.976 Å **RedCell c:** 6.469 Å **RedCell α:** 67.38°
**RedCell β:** 67.38° **RedCell γ:** 60.00° **RedCell Vol:** 124.31 Å³ ]

**Crystal (Symmetry Allowed):** Centrosymmetric

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 00-001-0837 (Deleted), 00-002-0623 (Deleted), 00-002-0629 (Deleted), 00-003-0569 (Deleted), 00-003-0596 (Deleted), 00-003-0670 (Deleted), 00-004-0636 (Deleted), 00-004-0637 (Deleted), 00-005-0586 (Primary), 00-024-0027 (Deleted), 00-047-1743 (Primary), 01-071-3699 (Alternate), 01-072-1937 (Alternate), 01-072-4582 (Alternate), 01-075-6049 (Alternate), 01-078-3262 (Alternate), 01-078-4614 (Alternate), 01-078-4615 (Alternate), 01-080-2791 (Alternate), 01-080-2792 (Alternate), 01-080-2793 (Alternate), 01-080-2794 (Alternate), 01-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 01-080-2799 (Alternate), 01-080-2800 (Alternate), 01-080-2801 (Alternate), 01-080-2802 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2806 (Alternate), 01-080-2808 (Alternate), 01-080-2809 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-9775 (Alternate), 01-080-9776 (Alternate), 01-083-0577 (Alternate), 01-083-0578 (Alternate), 01-085-0849 (Alternate), 01-086-2334 (Alternate), 01-086-2339 (Alternate), 01-086-2340 (Alternate), 01-086-2341 (Alternate), 01-086-2342 (Alternate), 01-086-2343 (Alternate), ✓ 04-001-7249 (Alternate), ✓ 04-002-9082 (Alternate), ✓ 04-006-6528 (Alternate), ✓ 04-007-0049 (Alternate), ✓ 04-007-2808 (Alternate), ✓ 04-007-4388 (Alternate), ✓ 04-007-8659 (Primary), ✓ 04-008-0198 (Alternate), ✓ 04-008-0212 (Alternate), ✓ 04-008-0213 (Alternate), ✓ 04-008-0788 (Alternate), ✓ 04-012-8072 (Alternate), ✓ 04-016-9713 (Alternate)

**Entry Date:** 09/01/2013

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Structure | | "Temperature dependence of the structural parameters in the transformation of aragonite to calcite, as determined from in situ synchrotron powder x-ray-diffraction data". Antao, S.M., Hassan, I. Can. Mineral. 48, 1225 (2010). |

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca (C O3). ICSD Collection Code: 169929. Sample Source or Locality: Cuenca, Spain. Temperature of Data Collection: 893 K. Wyckoff Sequence: e b a (R3-CH). Unit Cell Data Source: Powder Diffraction.

**d-Spacings (78) - Ca ( C O3 ) - 01-080-2807 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.0138 | 3.861330 | 91 | 0 | 1 | 2 | | 60.4449 | 1.530280 | 19 | 2 | 0 | 8 | | 78.5800 | 1.216400 | 1 | 2 | 2 | 3 | |
| 29.1537 | **3.060570** | 999 | 1 | 0 | 4 | | 60.6613 | 1.525340 | 45m | 1 | 1 | 9 | | 80.3932 | 1.193470 | 3m | 0 | 1 | 14 | |
| 30.8276 | 2.898100 | 15 | 0 | 0 | 6 | | 60.6613 | 1.525340 | m | 2 | 1 | 4 | | 80.3932 | 1.193470 | m | 1 | 3 | 1 | |
| 36.0670 | 2.488200 | 144 | 1 | 1 | 0 | | 62.9574 | 1.475120 | 9 | 1 | 2 | 5 | | 80.7757 | 1.188780 | 12 | 2 | 1 | 10 | |
| 39.3753 | 2.286430 | 129 | 1 | 1 | 3 | | 64.2240 | 1.449050 | 20 | 0 | 0 | 12 | | 81.1574 | 1.184150 | 5 | 3 | 1 | 2 | |
| 43.2192 | 2.091560 | 123 | 2 | 0 | 2 | | 64.8503 | 1.436560 | 31 | 3 | 0 | 0 | | 83.8788 | 1.152520 | 16 | 1 | 3 | 4 | |
| 46.7696 | **1.940720** | 160 | 0 | 1 | 8 | | 68.8713 | 1.362170 | 5 | 2 | 1 | 7 | | 84.7200 | 1.143210 | 10 | 2 | 2 | 6 | |
| 47.0276 | 1.930670 | 57 | 0 | 2 | 4 | | 69.3917 | 1.353220 | 13 | 0 | 2 | 10 | | 85.5332 | 1.134410 | 1 | 1 | 2 | 11 | |
| 48.1607 | **1.887860** | 157 | 1 | 1 | 6 | | 72.4470 | 1.303490 | 15 | 1 | 2 | 8 | | 91.4199 | 1.076090 | 3m | 1 | 3 | 7 | |
| 56.7123 | 1.621810 | 18 | 2 | 1 | 1 | | 73.5189 | 1.287110 | 7 | 3 | 0 | 6 | | 91.4199 | 1.076090 | m | 2 | 0 | 14 | |
| 57.0677 | 1.612550 | 10 | 1 | 0 | 10 | | 75.9258 | 1.252180 | 12 | 1 | 1 | 12 | | 92.1750 | 1.069240 | 1 | 0 | 4 | 2 | |
| 57.5158 | 1.601050 | 69 | 1 | 2 | 2 | | 76.5076 | 1.244100 | 6 | 2 | 2 | 0 | | 93.9330 | 1.053800 | 4 | 1 | 0 | 16 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 94.2851 | 1.050790 | 1 | 1 | 1 | 15 | | 108.1817 | 0.951024 | 1 | 2 | 3 | 5 | | 131.3038 | 0.845479 | 1m | 0 | 5 | 4 | |
| 94.6892 | 1.047370 | 9 | 3 | 1 | 8 | | 109.3798 | 0.943929 | 3 | 2 | 2 | 12 | | 131.3038 | 0.845479 | m | 1 | 4 | 9 | |
| 94.8784 | 1.045780 | 7m | 2 | 2 | 9 | | 109.9804 | 0.940451 | 4 | 4 | 1 | 0 | | 133.5348 | 0.838253 | 1 | 2 | 3 | 11 | |
| 94.8784 | 1.045780 | m | 4 | 0 | 4 | | 113.9679 | 0.918621 | 1 | 3 | 2 | 7 | | 136.4722 | 0.829400 | 1 | 3 | 3 | 0 | |
| 96.3433 | 1.033730 | 1 | 2 | 1 | 13 | | 114.5010 | 0.915862 | 1 | 4 | 0 | 10 | | 139.4960 | 0.821037 | 1 | 3 | 3 | 3 | |
| 98.0570 | 1.020190 | 7 | 0 | 3 | 12 | | 116.8679 | 0.904045 | 2 | 2 | 1 | 16 | | 142.3232 | 0.813877 | 1m | 0 | 4 | 14 | |
| 102.5011 | 0.987677 | 4m | 1 | 2 | 14 | | 117.5970 | 0.900543 | 3 | 1 | 1 | 18 | | 142.3232 | 0.813877 | m | 2 | 4 | 1 | |
| 102.5011 | 0.987677 | m | 3 | 2 | 1 | | 117.7163 | 0.899976 | 3 | 2 | 3 | 8 | | 143.5746 | 0.810904 | 2 | 4 | 2 | 2 | |
| 102.8875 | 0.985017 | 2 | 1 | 3 | 10 | | 118.8805 | 0.894531 | 3 | 1 | 4 | 6 | | 145.6303 | 0.806275 | 1 | 2 | 0 | 20 | |
| 103.2744 | 0.982379 | 4 | 2 | 3 | 2 | | 125.5524 | 0.866236 | 1 | 1 | 2 | 17 | | 146.6447 | 0.804105 | 2 | 1 | 3 | 16 | |
| 105.0859 | 0.970359 | 2 | 0 | 2 | 16 | | 126.8556 | 0.861253 | 1 | 3 | 1 | 14 | | 147.8428 | 0.801638 | 1 | 3 | 0 | 18 | |
| 105.8679 | 0.965334 | 4m | 0 | 0 | 18 | | 127.3283 | 0.859487 | 2 | 3 | 2 | 10 | | 148.0418 | 0.801238 | 1 | 5 | 0 | 8 | |
| 105.8679 | 0.965334 | m | 0 | 4 | 8 | | 127.8037 | 0.857733 | 1 | 5 | 0 | 2 | | 148.3997 | 0.800526 | 1 | 2 | 4 | 4 | |
| 106.0641 | 0.964089 | 3 | 3 | 2 | 4 | | 129.3266 | 0.852260 | 1 | 0 | 1 | 20 | | 149.7712 | 0.797881 | 1 | 2 | 1 | 19 | |

**01-075-9985** Jun 9, 2020 12:23 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca ( C O3 )
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Aragonite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.14 **I/Ic - ND:** 0.58

**SYS:** Orthorhombic **SPGR:** Pmcn (62)
**Author's Cell [ AuthCell a:** 4.96937(27) Å **AuthCell b:** 7.9591(4) Å **AuthCell c:** 5.75278(17) Å
**AuthCell Vol:** 227.53 Å³ **AuthCell Z:** 4.00 **AuthCell MolVol:** 56.88 ]
**Author's Cell Axial Ratio [ c/a:** 1.158 **a/b:** 0.624 **c/b:** 0.723 ]
**Density [ Dcalc:** 2.922 g/cm³ **Dstruc:** 2.92 g/cm³ ] **SS/FOM:** F(30) = 218.9(0.0042, 33)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.0231

**Space Group:** Pnam (62) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 5.753 Å **XtlCell b:** 7.959 Å **XtlCell c:** 4.969 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 227.53 Å³ **XtlCell Z:** 4.00 ]
**Crystal Data Axial Ratio [ c/a:** 0.864 **a/b:** 0.723 **c/b:** 0.624 ]
**Reduced Cell [ RedCell a:** 4.969 Å **RedCell b:** 5.753 Å **RedCell c:** 7.959 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 90.00° **RedCell Vol:** 227.53 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-008-5421** **ADP:** B
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -x+1/2,-y+1/2,z+1/2 | 5 | x+1/2,-y,-z | 7 | -x,y+1/2,-z+1/2 |
| 2 | -x,-y,-z | 4 | x+1/2,y+1/2,-z+1/2 | 6 | -x+1/2,y,z | 8 | x,-y+1/2,z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 4c | m.. | 0.25 | 0.41508 | 0.24046 | 1.0 | 0.61095 | 9-a |
| C | 2 | 4c | m.. | 0.25 | 0.76211 | 0.08518 | 1.0 | 0.43867 | 3#a |
| O | 3 | 4c | m.. | 0.25 | 0.92224 | 0.09557 | 1.0 | 0.77616 | 1#a |
| O | 4 | 8d | 1 | 0.47347 | 0.68065 | 0.08726 | 1.0 | 0.70856 | 1#a |

**Anisotropic Displacement Parameters:**

| Atom | Num | Bani11 | Bani22 | Bani33 | Bani12 | Bani13 | Bani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.665479 | 0.670266 | 0.497141 | 0.0 | 0.0 | 0.0201231 |
| C | 2 | 0.442997 | 0.573788 | 0.299269 | 0.0 | 0.0 | 0.0073175 |
| O | 3 | 1.13407 | 0.540783 | 0.653666 | 0.0 | 0.0 | -0.05854 |
| O | 4 | 0.509938 | 0.926694 | 0.689106 | 0.180227 | -0.0136696 | 0.0841512 |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**Mineral Classification:** Aragonite (Group), carbonate (Subgroup) **Pearson Symbol:** oP20.00

**Cross-Ref PDF #'s:** 00-001-0628 (Deleted), 00-003-0405 (Deleted), 00-003-0425 (Deleted), 00-003-1067 (Deleted), 00-005-0453 (Alternate), 00-041-1475 (Primary), ✓ 00-061-0390 (Primary), 01-071-2392 (Alternate), 01-071-2396 (Alternate), 01-071-3700 (Alternate), 01-071-4891 (Alternate), 01-075-9982 (Alternate), 01-075-9983 (Alternate), 01-075-9984 (Alternate), 01-075-9986 (Alternate), 01-075-9987 (Alternate), 01-076-0606 (Alternate), 01-078-4337 (Alternate), 01-078-4338 (Alternate), 01-078-4339 (Alternate), 01-080-2768 (Alternate), 01-080-2769 (Alternate), 01-080-2770 (Alternate), 01-080-2771 (Alternate), 01-080-2772 (Alternate), 01-080-2773 (Alternate), 01-080-2774 (Alternate), 01-080-2775 (Alternate), 01-080-2789 (Alternate), 01-080-2790 (Alternate), ✓ 04-006-5441 (Alternate), ✓ 04-006-5444 (Alternate), ✓ 04-006-6531 (Alternate), ✓ 04-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate), ✓ 04-014-1837 (Alternate), ✓ 04-015-4109 (Alternate), ✓ 04-017-9180 (Alternate)

**Entry Date:** 09/01/2009 **Last Modification Date:** 09/01/2015 **Last Modifications:** Update

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "Atomic structure of biogenic aragonite". Pokroy, B., Fieramosca, J.S., von Dreele, R.B., Fitch, A.N., Caspi, E.N., Zolotoyabko, E. Chem. Mater. 19, 3244 (2007). |

**01-075-9985** Jun 9, 2020 12:23 PM (fal-sharji2)

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca (C O3). ICSD Collection Code: 157995. General Comments: Biogenic. Calculated Pattern Original Remarks: Sample from mollusk shell `Strombus decorus persicus`. Sample Source or Locality: biogenic, from Strombus decorus persicus. Wyckoff Sequence: d c3 (PMCN). Unit Cell Data Source: Powder Diffraction.

**d-Spacings (199) - Ca ( C O3 ) - 01-075-9985 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 19.0190 | 4.662400 | 1 | 0 | 1 | 1 | | 76.6357 | 1.242340 | m | 4 | 0 | 0 | | 111.1798 | 0.933657 | 15 | 4 | 1 | 4 | |
| 21.0585 | 4.215220 | 11 | 1 | 1 | 0 | | 76.9337 | 1.238270 | 91 | 3 | 1 | 3 | | 111.3151 | 0.932903 | 20m | 0 | 5 | 5 | |
| 22.3212 | 3.979550 | 12 | 0 | 2 | 0 | | 77.8983 | 1.225330 | 53m | 0 | 5 | 3 | | 111.3151 | 0.932903 | m | 5 | 1 | 2 | |
| 26.1872 | **3.400160** | 999 | 1 | 1 | 1 | | 77.8983 | 1.225330 | m | 1 | 3 | 4 | | 111.7113 | 0.930710 | 11 | 5 | 3 | 0 | |
| 27.2256 | **3.272790** | 529 | 0 | 2 | 1 | | 78.6942 | 1.214920 | 9 | 2 | 5 | 2 | | 112.3708 | 0.927107 | 1 | 4 | 5 | 2 | |
| 31.0661 | 2.876390 | 40 | 0 | 0 | 2 | | 79.3184 | 1.206920 | 43 | 2 | 4 | 3 | | 112.8523 | 0.924513 | 6m | 1 | 8 | 2 | |
| 32.7373 | 2.733270 | 89 | 1 | 2 | 1 | | 79.5022 | 1.204590 | 10 | 0 | 6 | 2 | | 112.8523 | 0.924513 | m | 2 | 4 | 5 | |
| 33.0873 | 2.705150 | 520 | 0 | 1 | 2 | | 80.2192 | 1.195620 | 2 | 3 | 2 | 3 | | 113.9404 | 0.918764 | 1m | 3 | 2 | 5 | |
| 36.0484 | 2.489440 | 307 | 1 | 0 | 2 | | 80.7396 | 1.189220 | 38 | 1 | 5 | 3 | | 113.9404 | 0.918764 | m | 5 | 3 | 1 | |
| 36.1199 | 2.484680 | 236 | 2 | 0 | 0 | | 82.3334 | 1.170190 | 42m | 1 | 6 | 2 | | 114.3802 | 0.916484 | 10m | 1 | 2 | 6 | |
| 37.2928 | 2.409180 | 117 | 0 | 3 | 1 | | 82.3334 | 1.170190 | m | 2 | 6 | 0 | | 114.3802 | 0.916484 | m | 1 | 5 | 5 | |
| 37.8344 | 2.375930 | 417 | 1 | 1 | 2 | | 82.7286 | 1.165600 | 6 | 0 | 4 | 4 | | 114.6765 | 0.914962 | 10 | 4 | 2 | 4 | |
| 38.4315 | 2.340380 | 194 | 1 | 3 | 0 | | 83.0870 | 1.161480 | 32 | 4 | 2 | 1 | | 115.2748 | 0.911922 | 5 | 2 | 8 | 1 | |
| 38.5888 | 2.331200 | 171 | 0 | 2 | 2 | | 84.3065 | 1.147760 | 1 | 3 | 5 | 0 | | 115.6469 | 0.910054 | 1 | 2 | 7 | 3 | |
| 41.1319 | 2.192750 | 126 | 2 | 1 | 1 | | 84.4015 | 1.146710 | 1 | 2 | 6 | 1 | | 116.1228 | 0.907690 | 2 | 2 | 6 | 4 | |
| 41.6261 | 2.167850 | 7 | 1 | 3 | 1 | | 84.9677 | 1.140510 | 9 | 4 | 0 | 2 | | 116.3102 | 0.906767 | 6 | 4 | 6 | 0 | |
| 42.8737 | 2.107610 | 192m | 1 | 2 | 2 | | 85.1327 | 1.138720 | 3 | 0 | 1 | 5 | | 117.3509 | 0.901718 | 2 | 0 | 3 | 6 | |
| 42.8737 | 2.107610 | m | 2 | 2 | 0 | | 85.6287 | 1.133390 | 4 | 3 | 3 | 3 | | 118.3272 | 0.897099 | 6 | 3 | 5 | 4 | |
| 45.5506 | 1.989780 | 33 | 0 | 4 | 0 | | 86.0441 | 1.128980 | 16 | 4 | 1 | 2 | | 118.8855 | 0.894508 | 10 | 2 | 0 | 6 | |
| 45.8133 | **1.978980** | 630 | 2 | 2 | 1 | | 86.2454 | 1.126860 | 10 | 2 | 3 | 4 | | 119.5912 | 0.891284 | 4 | 3 | 7 | 2 | |
| 46.5296 | 1.950170 | 5 | 0 | 3 | 2 | | 86.3685 | 1.125570 | 17 | 3 | 5 | 1 | | 120.1186 | 0.888912 | 1 | 2 | 1 | 6 | |
| 48.3621 | 1.880470 | 387m | 0 | 4 | 1 | | 87.3492 | 1.115440 | 1 | 0 | 7 | 1 | | 120.4969 | 0.887230 | 16 | 1 | 3 | 6 | |
| 48.3621 | 1.880470 | m | 2 | 0 | 2 | | 87.8915 | 1.109950 | 23 | 1 | 1 | 5 | | 120.8877 | 0.885509 | 19m | 4 | 3 | 4 | |
| 48.8101 | 1.864250 | 6 | 0 | 1 | 3 | | 88.3581 | 1.105290 | 12 | 0 | 2 | 5 | | 120.8877 | 0.885509 | m | 5 | 3 | 2 | |
| 49.7874 | 1.829920 | 22 | 2 | 1 | 2 | | 89.2676 | 1.096370 | 15 | 4 | 2 | 2 | | 121.4397 | 0.883107 | 1 | 0 | 8 | 3 | |
| 50.2137 | 1.815380 | 244 | 1 | 3 | 2 | | 90.1033 | 1.088360 | 2 | 1 | 7 | 1 | | 122.4739 | 0.878696 | 5 | 5 | 4 | 1 | |
| 51.9486 | 1.758760 | 35 | 1 | 4 | 1 | | 90.3551 | 1.085980 | 1 | 3 | 0 | 4 | | 122.6606 | 0.877912 | 6 | 1 | 7 | 4 | |
| 52.3740 | 1.745470 | 303 | 1 | 1 | 3 | | 90.5734 | 1.083930 | 3 | 2 | 6 | 2 | | 122.8732 | 0.877024 | 20 | 5 | 1 | 3 | |
| 52.9610 | 1.727500 | 138m | 0 | 2 | 3 | | 91.1122 | 1.078920 | 1 | 1 | 2 | 5 | | 123.9169 | 0.872733 | 10m | 2 | 2 | 6 | |
| 52.9610 | 1.727500 | m | 2 | 3 | 1 | | 91.4286 | 1.076010 | 13 | 3 | 1 | 4 | | 123.9169 | 0.872733 | m | 4 | 5 | 3 | |
| 53.8835 | 1.700080 | 15 | 2 | 2 | 2 | | 92.5351 | 1.066020 | 8m | 1 | 6 | 3 | | 124.4300 | 0.870665 | 1 | 1 | 9 | 0 | |
| 56.1616 | 1.636400 | 20 | 0 | 4 | 2 | | 92.5351 | 1.066020 | m | 3 | 5 | 2 | | 124.8058 | 0.869168 | 1m | 0 | 6 | 5 | |
| 56.3370 | 1.631720 | 7 | 1 | 2 | 3 | | 93.1477 | 1.060610 | 1 | 3 | 4 | 3 | | 124.8058 | 0.869168 | m | 1 | 8 | 3 | |
| 56.7161 | 1.621710 | 16 | 3 | 1 | 0 | | 93.7644 | 1.055250 | 12m | 0 | 3 | 5 | | 125.9203 | 0.864812 | 7 | 4 | 6 | 2 | |
| 59.1410 | 1.560870 | 66 | 3 | 1 | 1 | | 93.7644 | 1.055250 | m | 2 | 4 | 4 | | 126.1973 | 0.863749 | 3 | 0 | 4 | 6 | |
| 59.4648 | 1.553140 | 11m | 0 | 3 | 3 | | 93.9318 | 1.053810 | 4 | 4 | 4 | 0 | | 126.7968 | 0.861474 | 1 | 5 | 2 | 3 | |
| 59.4648 | 1.553140 | m | 2 | 4 | 0 | | 94.6393 | 1.047790 | 1m | 3 | 2 | 4 | | 128.2321 | 0.856171 | 1 | 1 | 6 | 5 | |
| 60.2758 | 1.534170 | 23m | 0 | 5 | 1 | | 94.6393 | 1.047790 | m | 4 | 3 | 2 | | 128.9486 | 0.853598 | 1 | 3 | 4 | 5 | |
| 60.2758 | 1.534170 | m | 2 | 3 | 2 | | 95.1683 | 1.043360 | 6 | 1 | 5 | 4 | | 129.9627 | 0.850039 | 6m | 4 | 4 | 4 | |
| 61.0774 | 1.515940 | 1 | 1 | 5 | 0 | | 95.9943 | 1.036560 | 30 | 4 | 4 | 1 | | 129.9627 | 0.850039 | m | 5 | 4 | 2 | |
| 61.8223 | 1.499450 | 38 | 2 | 4 | 1 | | 96.1641 | 1.035180 | 18 | 2 | 1 | 5 | | 130.6663 | 0.847626 | 4 | 2 | 3 | 6 | |
| 62.2028 | 1.491190 | 3 | 2 | 1 | 3 | | 98.2047 | 1.019050 | 1 | 3 | 6 | 1 | | 131.3587 | 0.845296 | 1 | 0 | 9 | 2 | |
| 62.8235 | 1.477940 | 27 | 3 | 2 | 1 | | 98.3934 | 1.017600 | 2 | 2 | 7 | 1 | | 131.8536 | 0.843657 | 1 | 3 | 8 | 1 | |
| 63.3992 | 1.465900 | 30 | 1 | 5 | 1 | | 99.4134 | 1.009880 | 35 | 2 | 2 | 5 | | 132.3060 | 0.842178 | 9 | 3 | 7 | 3 | |
| 64.7678 | 1.438190 | 4 | 0 | 0 | 4 | | 99.5838 | 1.008610 | 28 | 4 | 2 | 3 | | 132.8878 | 0.840303 | 2 | 3 | 6 | 4 | |
| 64.9066 | 1.435450 | 7 | 3 | 0 | 2 | | 100.0665 | 1.005040 | 27 | 3 | 3 | 4 | | 133.1575 | 0.839444 | 5m | 2 | 7 | 4 | |
| 65.9487 | 1.415270 | 42 | 0 | 1 | 4 | | 100.9120 | 0.998890 | 5 | 2 | 6 | 3 | | 133.1575 | 0.839444 | m | 4 | 1 | 5 | |
| 66.0861 | 1.412660 | 35 | 3 | 1 | 2 | | 101.3115 | 0.996029 | 10 | 0 | 4 | 5 | | 133.8396 | 0.837300 | 1 | 5 | 3 | 3 | |
| 66.4892 | 1.405070 | 28 | 3 | 3 | 0 | | 101.4720 | 0.994888 | 3 | 0 | 8 | 0 | | 134.8708 | 0.834135 | 6 | 5 | 5 | 1 | |
| 67.1539 | 1.392770 | 1 | 0 | 5 | 2 | | 102.2399 | 0.989490 | 7 | 4 | 4 | 2 | | 135.1393 | 0.833326 | 4 | 1 | 9 | 2 | |
| 67.7755 | 1.381500 | 3m | 0 | 4 | 3 | | 102.9152 | 0.984827 | 12 | 3 | 5 | 3 | | 135.5461 | 0.832112 | 1 | 2 | 8 | 3 | |
| 67.7755 | 1.381500 | m | 1 | 0 | 4 | | 103.5468 | 0.980537 | 11m | 0 | 8 | 1 | | 136.3299 | 0.829812 | 2m | 3 | 0 | 6 | |
| 68.6151 | 1.366630 | 23 | 2 | 4 | 2 | | 103.5468 | 0.980537 | m | 2 | 5 | 4 | | 136.3299 | 0.829812 | m | 4 | 7 | 1 | |
| 68.9302 | 1.361150 | 51 | 1 | 1 | 4 | | 103.9227 | 0.978015 | 1 | 0 | 7 | 3 | | 136.8802 | 0.828228 | 8 | 6 | 0 | 0 | |
| 69.4293 | 1.352580 | 18 | 0 | 2 | 4 | | 104.3642 | 0.975083 | 5 | 0 | 6 | 4 | | 137.7490 | 0.825778 | 16m | 3 | 1 | 6 | |
| 69.5640 | 1.350290 | 5 | 3 | 2 | 2 | | 104.4943 | 0.974225 | 9 | 3 | 6 | 2 | | 137.7490 | 0.825778 | m | 4 | 2 | 5 | |
| 70.1109 | 1.341090 | 14 | 1 | 5 | 2 | | 104.8285 | 0.972034 | 21m | 2 | 3 | 5 | | 139.3903 | 0.821317 | 1 | 0 | 5 | 6 | |
| 70.7606 | 1.330360 | 4 | 1 | 4 | 3 | | 104.8285 | 0.972034 | m | 5 | 1 | 1 | | 139.7303 | 0.820420 | 1 | 2 | 6 | 5 | |
| 70.9964 | 1.326520 | 9 | 0 | 6 | 0 | | 105.8445 | 0.965483 | 3 | 4 | 5 | 1 | | 140.8702 | 0.817479 | 3m | 0 | 1 | 7 | |
| 71.5500 | 1.317610 | 1 | 2 | 3 | 3 | | 106.4273 | 0.961799 | 2 | 1 | 8 | 1 | | 140.8702 | 0.817479 | m | 5 | 0 | 4 | |
| 72.3435 | 1.305100 | 7m | 1 | 2 | 4 | | 106.7781 | 0.959607 | 16 | 1 | 7 | 3 | | 141.5159 | 0.815858 | 4m | 2 | 4 | 6 | |
| 72.3435 | 1.305100 | m | 2 | 5 | 1 | | 106.9085 | 0.958797 | 26 | 0 | 0 | 6 | | 141.5159 | 0.815858 | m | 6 | 1 | 1 | |
| 73.1558 | 1.292600 | 1 | 0 | 6 | 1 | | 107.8132 | 0.953249 | 1 | 3 | 4 | 4 | | 142.5401 | 0.813353 | 18 | 5 | 1 | 4 | |
| 75.1968 | 1.262500 | 58 | 3 | 3 | 2 | | 108.0339 | 0.951914 | 1 | 0 | 1 | 6 | | 142.8651 | 0.812575 | 13m | 3 | 2 | 6 | |
| 76.0123 | 1.250970 | 2 | 1 | 6 | 1 | | 109.8097 | 0.941434 | 2 | 1 | 0 | 6 | | 142.8651 | 0.812575 | m | 3 | 5 | 5 | |
| 76.4627 | 1.244720 | 36 | 2 | 0 | 4 | | 110.1673 | 0.939379 | 10 | 5 | 0 | 2 | | | | | | | | |
| 76.6357 | 1.242340 | 64m | 3 | 4 | 1 | | 110.3426 | 0.938378 | 14 | 3 | 1 | 5 | | | | | | | | |

**04-013-2116** Jun 9, 2020 12:23 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca0.936 Mg0.064 ( C O3 )
**Empirical Formula:** C Ca0.936 Mg0.064 O3 **Weight %:** C12.12 Ca37.86 Mg1.57 O48.44
**Atomic %:** C20.00 Ca18.72 Mg1.28 O60.00 **ANX:** ABX3 **Compound Name:** Calcium Magnesium Carbonate
**Mineral Name:** Calcite, magnesian

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 3.05 **I/Ic - ND:** 0.88

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.9673(3) Å **AuthCell c:** 16.9631(7) Å **AuthCell Vol:** 362.47 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 60.41 ] **Author's Cell Axial Ratio [ c/a:** 3.415 ]
**Density [ Dcalc:** 2.723 g/cm³ **Dstruc:** 2.72 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 297.0 K (Author provided temperature) **R-factor:** 0.023

**Space Group:** R-3c (167) **Molecular Weight:** 99.08
**Crystal Data [ XtlCell a:** 4.967 Å **XtlCell b:** 4.967 Å **XtlCell c:** 16.963 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 362.47 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.415 **a/b:** 1.000 **c/b:** 3.415 ]
**Reduced Cell [ RedCell a:** 4.967 Å **RedCell b:** 4.967 Å **RedCell c:** 6.340 Å **RedCell α:** 66.94°
**RedCell β:** 66.94° **RedCell γ:** 60.00° **RedCell Vol:** 120.82 Å³ ]

**ADP:** U **Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3. | 0.0 | 0.0 | 0.0 | 0.936 | 0.01473 | |
| Mg | 2 | 6b | -3. | 0.0 | 0.0 | 0.0 | 0.064 | 0.01473 | |
| C | 3 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | 0.01426 | |
| O | 4 | 18e | .2 | 0.2575 | 0.0 | 0.25 | 1.0 | 0.02852 | |

**Anisotropic Displacement Parameters:**

| Atom | Num | Uani11 | Uani22 | Uani33 | Uani12 | Uani13 | Uani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.0151 | 0.0151 | 0.014 | 0.00755 | 0.0 | 0.0 |
| Mg | 2 | 0.0151 | 0.0151 | 0.014 | 0.00755 | 0.0 | 0.0 |
| C | 3 | 0.0128 | 0.0128 | 0.0172 | 0.00642 | 0.0 | 0.0 |
| O | 4 | 0.0161 | 0.0336 | 0.0306 | 0.00849 | -0.018 | -0.0089 |

**Subfile(s):** Inorganic, Mineral Related (Mineral , Natural) **Former PDF's #:** 01-086-2335
**LPF Prototype Structure [Formula Order]:** Ca ( C O3 ),hR30,167
**LPF Prototype Structure [Alpha Order]:** C Ca O3,hR30,167
**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00
**Cross-Ref PDF #'s:** 01-089-1304 (Related Phase), 01-089-1305 (Related Phase) **Entry Date:** 09/01/2010
**Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Single-crystal X-ray structure refinements of two biogenic magnesian calcite crystals". Paquette J., Reeder R.J. Am. Mineral. 75, 1151,1158 (1990). |

**Database Comments:** ANX: ABX3. LPF Collection Code: 1213141. Calculated Pattern Original Remarks: same sample studied in Am. Mineral. (1983) 68, 1183. same sample studied in Am. Mineral. (1985) 70, 581. Temperature of Data Collection: 297 K. Unit Cell Data Source: Single Crystal.

**d-Spacings (77) - Ca0.936 Mg0.064 ( C O3 ) - 04-013-2116 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.1645 | 3.836550 | 89 | 0 | 1 | 2 | | 48.7639 | **1.865910** | 193 | 1 | 1 | 6 | | 64.9834 | 1.433940 | 56 | 3 | 0 | 0 | |
| 29.5539 | **3.020030** | 999 | 1 | 0 | 4 | | 56.8384 | 1.618510 | 29 | 2 | 1 | 1 | | 66.0371 | 1.413590 | 30 | 0 | 0 | 12 | |
| 31.6208 | 2.827180 | 20 | 0 | 0 | 6 | | 57.6812 | 1.596850 | 85 | 1 | 2 | 2 | | 69.5704 | 1.350180 | 9 | 2 | 1 | 7 | |
| 36.1354 | 2.483650 | 143 | 1 | 1 | 0 | | 58.4344 | 1.578050 | 11 | 1 | 0 | 10 | | 70.6641 | 1.331940 | 18 | 0 | 2 | 10 | |
| 39.6004 | 2.273950 | 181 | 1 | 1 | 3 | | 60.9781 | 1.518170 | 53 | 2 | 1 | 4 | | 73.3101 | 1.290260 | 27 | 1 | 2 | 8 | |
| 43.3640 | 2.084910 | 148 | 2 | 0 | 2 | | 61.3431 | 1.510010 | 22 | 2 | 0 | 8 | | 74.0728 | 1.278850 | 6 | 3 | 0 | 6 | |
| 47.3501 | 1.918270 | 67 | 0 | 2 | 4 | | 61.7328 | 1.501410 | 22 | 1 | 1 | 9 | | 76.6736 | 1.241820 | 11 | 2 | 2 | 0 | |
| 47.7829 | **1.901900** | 188 | 0 | 1 | 8 | | 63.3828 | 1.466240 | 17 | 1 | 2 | 5 | | 77.6565 | 1.228540 | 19 | 1 | 1 | 12 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 78.8492 | 1.212920 | 1 | 2 | 2 | 3 | | 102.8556 | 0.985236 | 2 | 3 | 2 | 1 | | 121.9071 | 0.881099 | 7m | 1 | 1 | 18 | |
| 80.6619 | 1.190170 | 1 | 1 | 3 | 1 | | 103.5836 | 0.980289 | 9 | 2 | 3 | 2 | | 121.9071 | 0.881099 | m | 1 | 3 | 13 | |
| 81.3802 | 1.181470 | 5 | 3 | 1 | 2 | | 104.2421 | 0.975891 | 3 | 1 | 3 | 10 | | 128.2879 | 0.855969 | 2 | 5 | 0 | 2 | |
| 82.0256 | 1.173800 | 20 | 2 | 1 | 10 | | 104.9024 | 0.971552 | 8 | 1 | 2 | 14 | | 129.1066 | 0.853037 | 6 | 3 | 2 | 10 | |
| 82.6706 | 1.166270 | 3 | 0 | 1 | 14 | | 106.5202 | 0.961217 | 8 | 3 | 2 | 4 | | 129.9353 | 0.850134 | 2m | 1 | 2 | 17 | |
| 84.2379 | 1.148520 | 36 | 1 | 3 | 4 | | 106.8537 | 0.959137 | 14 | 0 | 4 | 8 | | 129.9353 | 0.850134 | m | 3 | 1 | 14 | |
| 85.2939 | 1.136980 | 16 | 2 | 2 | 6 | | 108.1942 | 0.950949 | 4 | 0 | 2 | 16 | | 131.9977 | 0.843184 | 5 | 0 | 5 | 4 | |
| 86.3723 | 1.125530 | 1 | 3 | 1 | 5 | | 108.7518 | 0.947622 | 2 | 2 | 3 | 5 | | 132.8953 | 0.840279 | 1 | 4 | 1 | 9 | |
| 87.0123 | 1.118890 | 4 | 1 | 2 | 11 | | 109.4280 | 0.943648 | 1 | 3 | 1 | 11 | | 134.2180 | 0.836128 | 1 | 2 | 2 | 15 | |
| 92.0460 | 1.070400 | 1 | 1 | 3 | 7 | | 109.6438 | 0.942394 | 1 | 0 | 0 | 18 | | 135.5383 | 0.832135 | 6 | 0 | 1 | 20 | |
| 92.4352 | 1.066910 | 1 | 0 | 4 | 2 | | 110.2807 | 0.938731 | 14 | 4 | 1 | 0 | | 135.8378 | 0.831250 | 1 | 2 | 3 | 11 | |
| 93.7158 | 1.055670 | 7 | 2 | 0 | 14 | | 111.3060 | 0.932954 | 8 | 2 | 2 | 12 | | 137.0012 | 0.827883 | 3 | 3 | 3 | 0 | |
| 95.2778 | 1.042450 | 20 | 4 | 0 | 4 | | 112.5652 | 0.926056 | 1 | 4 | 1 | 3 | | 140.2177 | 0.819150 | 1 | 3 | 3 | 3 | |
| 95.5986 | 1.039800 | 24 | 3 | 1 | 8 | | 114.8627 | 0.914011 | 2 | 3 | 2 | 7 | | 143.0935 | 0.812033 | 1 | 2 | 4 | 1 | |
| 96.8846 | 1.029390 | 12m | 1 | 0 | 16 | | 116.0013 | 0.908291 | 1 | 4 | 0 | 10 | | 144.2906 | 0.809256 | 5 | 4 | 2 | 2 | |
| 96.8846 | 1.029390 | m | 1 | 1 | 15 | | 118.8360 | 0.894736 | 6 | 2 | 3 | 8 | | 146.5426 | 0.804320 | 1 | 0 | 4 | 14 | |
| 98.3856 | 1.017660 | 2 | 2 | 1 | 13 | | 119.6750 | 0.890905 | 6 | 1 | 4 | 6 | | 149.4824 | 0.798427 | 6 | 2 | 4 | 4 | |
| 99.8440 | 1.006680 | 21 | 0 | 3 | 12 | | 120.3057 | 0.888078 | 7 | 2 | 1 | 16 | | | | | | | | |

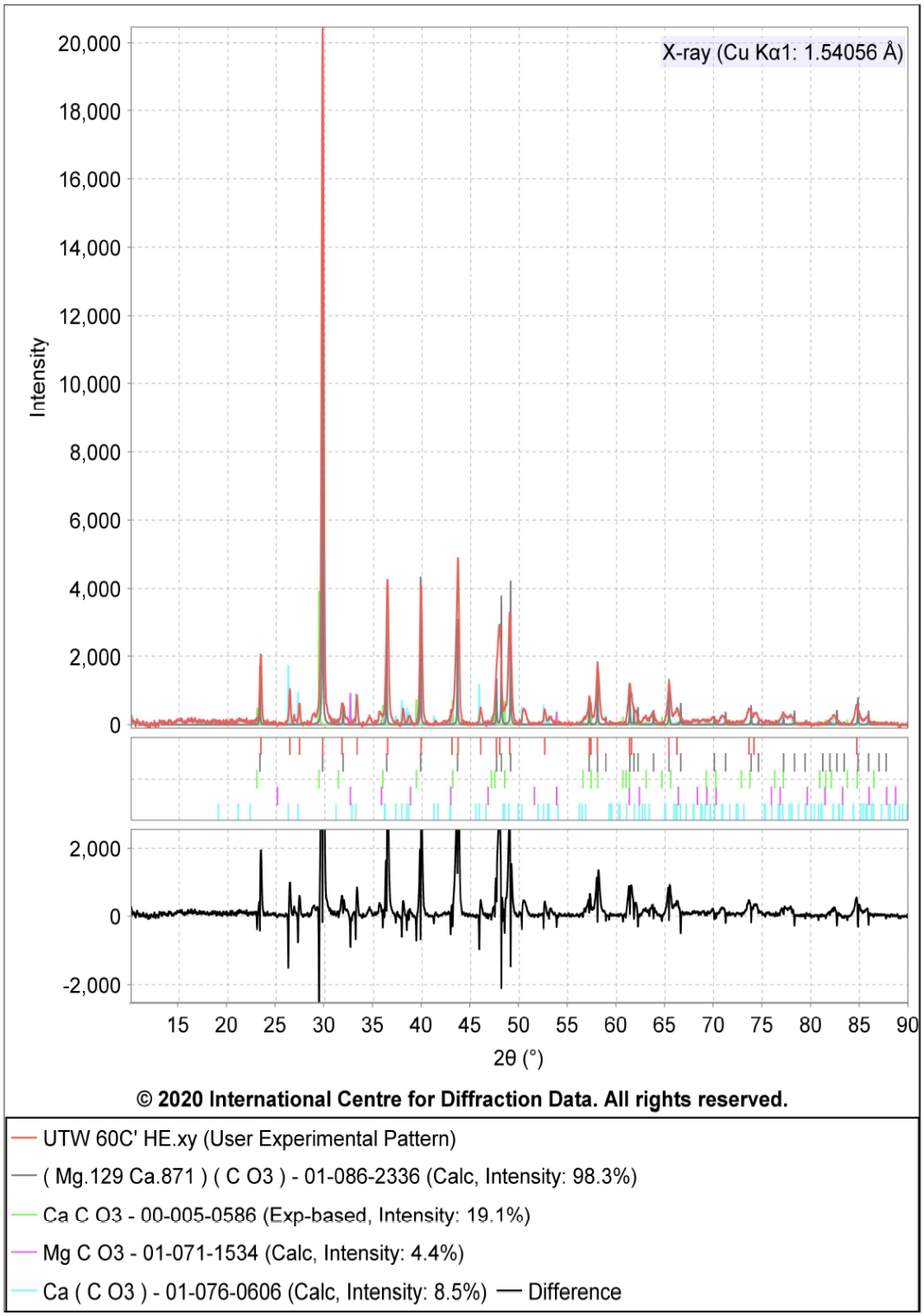


**Figure E.5 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 60 °C from experiment with a tank with little exposure of iron.**

# SIeve+ Report

## Experiment

**Search Line:** 1.893974 Å **D1 Range:** 1.888 Å - 1.900 Å
**Search Line:** 2.069972 Å **D1 Range:** 2.063 Å - 2.077 Å
**Search Line:** 2.463177 Å **D1 Range:** 2.453 Å - 2.473 Å
**Search Line:** 3.374027 Å **D1 Range:** 3.355 Å - 3.393 Å
**Search Line:** 1.505213 Å **D1 Range:** 1.502 Å - 1.509 Å
**Search Line:** 3.253189 Å **D1 Range:** 3.236 Å - 3.271 Å
**Search Line:** 1.970170 Å **D1 Range:** 1.964 Å - 1.976 Å
**Search Line:** 3.796134 Å **D1 Range:** 3.772 Å - 3.820 Å
**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (4)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 01-086-2336 | S | Magnesium Calcium Carbonate | 0.983 | 75.422 | 2.94 | 68 |
| 2 | true | 00-005-0586 | S | Calcium Carbonate | 0.191 | 14.662 | *3.23 | 12 |
| 3 | true | 01-071-1534 | S | Magnesium Carbonate | 0.044 | 3.386 | *1.85 | 5 |
| 4 | true | 01-076-0606 | S | Calcium Carbonate | 0.085 | 6.53 | 1.14 | 15 |

**01-086-2336** Jun 9, 2020 12:26 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** ( Mg.129 Ca.871 ) ( C O3 )
**Empirical Formula:** C Ca0.871 Mg0.129 O3 **Weight %:** C12.25 Ca35.60 Mg3.20 O48.95
**Atomic %:** C20.00 Ca17.42 Mg2.58 O60.00 **ANX:** ABX3 **Compound Name:** Magnesium Calcium Carbonate
**Mineral Name:** Calcite, magnesian

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 2.94 **I/Ic - ND:** 0.88

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.9382(4) Å **AuthCell c:** 16.832(1) Å **AuthCell Vol:** 355.47 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 59.25 ] **Author's Cell Axial Ratio [ c/a:** 3.409 ]
**Density [ Dcalc:** 2.748 g/cm³ **Dstruc:** 2.75 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.035

**Space Group:** R-3c (167) **Molecular Weight:** 98.05
**Crystal Data [ XtlCell a:** 4.938 Å **XtlCell b:** 4.938 Å **XtlCell c:** 16.832 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 355.47 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.409 **a/b:** 1.000 **c/b:** 3.409 ]
**Reduced Cell [ RedCell a:** 4.938 Å **RedCell b:** 4.938 Å **RedCell c:** 6.293 Å **RedCell α:** 66.90°
**RedCell β:** 66.90° **RedCell γ:** 60.00° **RedCell Vol:** 118.49 Å³ ]

**Crystal (Symmetry Allowed):** Centrosymmetric

**Subfile(s):** Inorganic, Mineral Related (Mineral , Natural) **Mineral Classification:** Calcite (Supergroup), calcite (Group)
**Pearson Symbol:** hR10.00 **Cross-Ref PDF #'s:** ✓ 04-008-8067 (Related Phase) **Entry Date:** 09/01/2000
**Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++ (1997). |
| Structure | | "Single-crystal X-ray structure refinements of two biogenetic magnesian calcite crystals". Paquette, J., Reeder, R.J. Am. Mineral. 75, 1151 (1990). |

**Database Comments:** ANX: ABX3. Analysis: C1 Ca0.871 Mg0.129 O3. Formula from original source: (Mg.129 Ca.871) (C O3). ICSD Collection Code: 40109. Sample Source or Locality: Specimen from the mouth of an echinoid. Wyckoff Sequence: e b a(R3-CH). Unit Cell Data Source: Single Crystal.

**d-Spacings (75) - ( Mg.129 Ca.871 ) ( C O3 ) - 01-086-2336 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.3120 | 3.812600 | 79 | 0 | 1 | 2 | | 81.2379 | 1.183180 | 1 | 1 | 3 | 1 | | 110.5044 | 0.937458 | 1 | 3 | 1 | 11 | |
| 29.7612 | **2.999470** | 999 | 1 | 0 | 4 | | 81.9654 | 1.174510 | 4 | 3 | 1 | 2 | | 111.2560 | 0.933232 | 13 | 4 | 1 | 0 | |
| 31.8737 | 2.805330 | 22 | 0 | 0 | 6 | | 82.7052 | 1.165870 | 18 | 2 | 1 | 10 | | 112.4410 | 0.926727 | 6 | 2 | 2 | 12 | |
| 36.3557 | 2.469100 | 133 | 1 | 1 | 0 | | 83.4436 | 1.157420 | 3 | 0 | 1 | 14 | | 113.5928 | 0.920584 | 1 | 1 | 4 | 3 | |
| 39.8562 | **2.259940** | 199 | 1 | 1 | 3 | | 84.8647 | 1.141630 | 34 | 1 | 3 | 4 | | 115.9767 | 0.908413 | 2 | 3 | 2 | 7 | |
| 43.6378 | 2.072460 | 142 | 2 | 0 | 2 | | 85.9504 | 1.129970 | 16 | 2 | 2 | 6 | | 117.1917 | 0.902482 | 1 | 4 | 0 | 10 | |
| 47.6658 | 1.906300 | 63 | 0 | 2 | 4 | | 87.0298 | 1.118710 | 1 | 3 | 1 | 5 | | 120.0551 | 0.889196 | 5 | 2 | 3 | 8 | |
| 48.1599 | 1.887890 | 178 | 0 | 1 | 8 | | 87.7644 | 1.111230 | 3 | 1 | 2 | 11 | | 120.8852 | 0.885520 | 4 | 1 | 4 | 6 | |
| 49.1133 | **1.853450** | 185 | 1 | 1 | 6 | | 92.7921 | 1.063740 | 1 | 1 | 3 | 7 | | 121.7645 | 0.881709 | 6 | 2 | 1 | 16 | |
| 57.2053 | 1.609000 | 32 | 2 | 1 | 1 | | 93.1455 | 1.060630 | 1 | 0 | 4 | 2 | | 123.4847 | 0.874496 | 5m | 1 | 1 | 18 | |
| 58.0576 | 1.587390 | 83 | 1 | 2 | 2 | | 94.6156 | 1.047990 | 6 | 2 | 0 | 14 | | 123.4847 | 0.874496 | m | 1 | 3 | 13 | |
| 58.9178 | 1.566250 | 10 | 1 | 0 | 10 | | 96.0349 | 1.036230 | 20 | 4 | 0 | 4 | | 129.7039 | 0.850938 | 1 | 5 | 0 | 2 | |
| 61.3926 | 1.508910 | 47 | 2 | 1 | 4 | | 96.4041 | 1.033240 | 21 | 3 | 1 | 8 | | 130.6637 | 0.847635 | 5 | 3 | 2 | 10 | |
| 61.8095 | 1.499730 | 21 | 2 | 0 | 8 | | 97.8815 | 1.021550 | 10m | 1 | 0 | 16 | | 131.6375 | 0.844370 | 2m | 1 | 2 | 17 | |
| 62.2194 | 1.490830 | 22 | 1 | 1 | 9 | | 97.8815 | 1.021550 | m | 1 | 1 | 15 | | 131.6375 | 0.844370 | m | 3 | 1 | 14 | |
| 63.8251 | 1.457140 | 18 | 1 | 2 | 5 | | 99.3252 | 1.010540 | 1 | 2 | 1 | 13 | | 133.5574 | 0.838182 | 5 | 0 | 5 | 4 | |
| 65.4139 | 1.425540 | 58 | 3 | 0 | 0 | | 100.7827 | 0.999822 | 19 | 0 | 3 | 12 | | 134.5719 | 0.835043 | 1 | 1 | 4 | 9 | |
| 66.6178 | 1.402670 | 27 | 0 | 0 | 12 | | 103.7072 | 0.979458 | 2 | 3 | 2 | 1 | | 136.1371 | 0.830373 | 1 | 2 | 2 | 15 | |
| 70.0875 | 1.341480 | 10 | 2 | 1 | 7 | | 104.4494 | 0.974521 | 9 | 2 | 3 | 2 | | 137.7547 | 0.825762 | 5m | 0 | 1 | 20 | |
| 71.2388 | 1.322600 | 16 | 0 | 2 | 10 | | 105.2078 | 0.969569 | 2 | 1 | 3 | 10 | | 137.7547 | 0.825762 | m | 2 | 3 | 11 | |
| 73.8733 | 1.281810 | 23 | 1 | 2 | 8 | | 105.9691 | 0.964691 | 7 | 1 | 2 | 14 | | 138.7494 | 0.823033 | 3 | 3 | 3 | 0 | |
| 74.6167 | 1.270870 | 4 | 3 | 0 | 6 | | 107.4448 | 0.955493 | 6 | 3 | 2 | 4 | | 142.1413 | 0.814319 | 1 | 3 | 3 | 3 | |
| 77.2082 | 1.234550 | 9 | 2 | 2 | 0 | | 107.8295 | 0.953150 | 13 | 0 | 4 | 8 | | 145.1751 | 0.807273 | 1 | 2 | 4 | 1 | |
| 78.3334 | 1.219610 | 17 | 1 | 1 | 12 | | 109.3768 | 0.943947 | 4 | 0 | 2 | 16 | | 146.4565 | 0.804502 | 5 | 4 | 2 | 2 | |
| 79.4137 | 1.205710 | 1 | 2 | 2 | 3 | | 109.7236 | 0.941932 | 2 | 2 | 3 | 5 | | 149.2118 | 0.798944 | 1 | 0 | 4 | 14 | |

**00-005-0586** Jun 9, 2020 12:27 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca C O3
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**Compound Name:** Calcium Carbonate **Mineral Name:** Calcite, syn

**Radiation:** CuKα1 **λ:** 1.5405 Å **Filter:** Ni Beta **Intensity:** Diffractometer **I/Ic:** 2

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.989 Å **AuthCell c:** 17.062 Å **AuthCell Vol:** 367.78 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 61.30 ] **Author's Cell Axial Ratio [ c/a:** 3.420 ]
**Density [ Dcalc:** 2.711 g/cm³ **Dmeas:** 2.71 g/cm³ ] **SS/FOM:** F(30) = 57.2(0.0159, 33)
**Temp:** 299.0 K (Author provided temperature) **Color:** Colorless

**Space Group:** R-3c (167) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 4.989 Å **XtlCell b:** 4.989 Å **XtlCell c:** 17.062 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 367.78 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.420 **a/b:** 1.000 **c/b:** 3.420 ]
**Reduced Cell [ RedCell a:** 4.989 Å **RedCell b:** 4.989 Å **RedCell c:** 6.375 Å **RedCell α:** 66.97°
**RedCell β:** 66.97° **RedCell γ:** 60.00° **RedCell Vol:** 122.59 Å³ ]

**εα:** =1.487 **πωβ:** =1.659 **Sign:** =-

**Atomic parameters are cross-referenced from PDF entry 04-012-8072** **ADP:** U
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | 0.01525 | |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | 0.02084 | |
| O | 3 | 18e | .2 | 0.25 | 0.0 | 0.25 | 1.0 | 0.02084 | |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Educational Pattern, Forensic, Inorganic, Mineral Related (Mineral , Synthetic), NBS Pattern, Pharmaceutical (Excipient), Pigment/Dye, Superconducting Material (Superconductor Related Materials)

**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 01-072-1937 (Alternate), 01-083-0577 (Alternate), 01-083-0578 (Alternate), ✓ 04-001-7249 (Alternate), ✓ 04-006-6528 (Alternate), ✓ 04-007-2808 (Alternate), ✓ 04-007-4388 (Alternate), ✓ 04-007-8659 (Primary), ✓ 04-008-0788 (Alternate), ✓ 04-012-0489 (Primary), ✓ 04-012-8072 (Alternate)

**CAS Number - PR:** 13397-26-7 **Entry Date:** 09/01/1955

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Swanson, Fuyat. Natl. Bur. Stand. (U. S. ), Circ. 539 II, 51 (1953). |
| Crystal Structure | | Crystal Structure Source: LPF |
| Optical Data | | Dana's System of Mineralogy, 7th Ed. II, 142. |

**Database Comments:** Additional Patterns: See PDF 01-072-1214 , 01-072-1937, 01-081-2027, 01-083-0577 and 01-083-0578. Analysis: Spectroscopic analysis: <0.1% Sr; <0.01% Ba; <0.001% Al, B, Cs, Cu, K, Mg, Na, Si, Sn; <0.0001% Ag, Cr, Fe, Li, Mn. Color: Colorless. General Comments: Additional weak reflections (indicated by brackets) were observed. Other form: aragonite. Pattern reviewed by Parks, J., McCarthy, G., North Dakota State Univ., Fargo, North Dakota, USA, ICDD Grant-in-Aid (1992). Agrees well with experimental and calculated patterns. Antacid. Sample Source or Locality: Sample from Mallinckrodt Chemical Works. Temperature of Data Collection: Pattern taken at 299 K. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (45) - Ca C O3 - 00-005-0586 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.0218 | 3.860000 | 12 | 0 | 1 | 2 | | 48.5122 | 1.875000 | 17 | 1 | 1 | 6 | | 64.6765 | 1.440000 | 5 | 3 | 0 | 0 | |
| 29.4049 | **3.035000** | 100 | 1 | 0 | 4 | | 56.5530 | 1.626000 | 4 | 2 | 1 | 1 | | 65.5972 | 1.422000 | 3 | 0 | 0 | 12 | |
| 31.4176 | 2.845000 | 3 | 0 | 0 | 6 | | 57.4001 | 1.604000 | 8 | 1 | 2 | 2 | | 69.2291 | 1.356000 | 1 | 2 | 1 | 7 | |
| 35.9654 | 2.495000 | 14 | 1 | 1 | 0 | | 58.0733 | 1.587000 | 2 | 1 | 0 | 10 | | 70.2364 | 1.339000 | 2 | 0 | 2 | 10 | |
| 39.4009 | **2.285000** | 18 | 1 | 1 | 3 | | 60.6762 | 1.525000 | 5 | 2 | 1 | 4 | | 72.8676 | 1.297000 | 2 | 1 | 2 | 8 | |
| 43.1447 | **2.095000** | 18 | 2 | 0 | 2 | | 60.9857 | 1.518000 | 4 | 2 | 0 | 8 | | 73.7264 | 1.284000 | 1 | 3 | 0 | 6 | |
| 47.1226 | 1.927000 | 5 | 0 | 2 | 4 | | 61.3435 | 1.510000 | 3 | 1 | 1 | 9 | | 76.2977 | 1.247000 | 1 | 2 | 2 | 0 | |
| 47.4886 | 1.913000 | 17 | 0 | 1 | 8 | | 63.0584 | 1.473000 | 2 | 1 | 2 | 5 | | 77.1749 | 1.235000 | 2 | 1 | 1 | 12 | |




**00-005-0586** Jun 9, 2020 12:27 PM (fal-sharji2)

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 80.9302 | 1.186900 | <1 | 3 | 1 | 2 | E | 94.6975 | 1.047300 | 3 | 4 | 0 | 4 | | 103.8950 | 0.978200 | 1 | 1 | 3 | 10 | |
| 81.5449 | 1.179500 | 3 | 2 | 1 | 10 | | 95.0075 | 1.044700 | 4 | 3 | 1 | 8 | | 104.1201 | 0.976700 | 3 | 1 | 2 | 14 | |
| 82.1106 | 1.172800 | <1 | 0 | 1 | 14 | E | 96.1617 | 1.035200 | 2 | 1 | 0 | 16 | | 105.8419 | 0.965500 | 2 | 3 | 2 | 4 | |
| 83.7646 | 1.153800 | 3 | 1 | 3 | 4 | | 97.6440 | 1.023400 | <1 | 2 | 1 | 13 | | 106.1414 | 0.963600 | 4 | 0 | 4 | 8 | |
| 84.7850 | 1.142500 | 1 | 2 | 2 | 6 | | 99.1573 | 1.011800 | 2 | 3 | 0 | 12 | | 107.3295 | 0.956200 | <1 | 0 | 2 | 16 | |
| 86.4804 | 1.124400 | <1 | 1 | 2 | 11 | | 102.2384 | 0.989500 | <1 | 3 | 2 | 1 | | 109.5566 | 0.942900 | 2 | 4 | 1 | 0 | |
| 93.0691 | 1.061300 | 1 | 2 | 0 | 14 | | 102.9484 | 0.984600 | 1 | 2 | 3 | 2 | | 110.4794 | 0.937600 | 2 | 2 | 2 | 12 | |

**01-071-1534** Jun 9, 2020 12:27 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Mg C O3
**Empirical Formula:** C Mg O3 **Weight %:** C14.25 Mg28.83 O56.93 **Atomic %:** C20.00 Mg20.00 O60.00
**ANX:** ABX3 **Compound Name:** Magnesium Carbonate **Mineral Name:** Magnesite, syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.83 **I/Ic - ND:** 1.08

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.637(1) Å **AuthCell c:** 15.023(3) Å **AuthCell Vol:** 279.74 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 46.62 ] **Author's Cell Axial Ratio [ c/a:** 3.240 ]
**Density [ Dcalc:** 3.003 g/cm³ ] **Dstruc:** 3 g/cm³ ] **SS/FOM:** F(30) = 599.5(0.0014, 36)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.037

**Space Group:** R-3c (167) **Molecular Weight:** 84.31
**Crystal Data [ XtlCell a:** 4.637 Å **XtlCell b:** 4.637 Å **XtlCell c:** 15.023 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 279.74 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.240 **a/b:** 1.000 **c/b:** 3.240 ]
**Reduced Cell [ RedCell a:** 4.637 Å **RedCell b:** 4.637 Å **RedCell c:** 5.678 Å **RedCell α:** 65.90°
**RedCell β:** 65.90° **RedCell γ:** 60.00° **RedCell Vol:** 93.25 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-009-2317** **ADP:** B
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| O | 1 | 18e | .2 | 0.2775 | 0.0 | 0.25 | 1.0 | 0.36879 | 1#a |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | 0.34715 | 3#b |
| Mg | 3 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | 0.35475 | 6-a |

**Anisotropic Displacement Parameters:**

| Atom | Num | Bani11 | Bani22 | Bani33 | Bani12 | Bani13 | Bani23 |
|---|---|---|---|---|---|---|---|
| O | 1 | 0.469464 | 0.646158 | 0.0496549 | 0.323079 | -0.0386154 | -0.0772308 |
| C | 2 | 0.506867 | 0.506867 | 0.0277294 | 0.253433 | 0.0 | 0.0 |
| Mg | 3 | 0.51525 | 0.51525 | 0.034178 | 0.257947 | 0.0 | 0.0 |

**Subfile(s):** Cement and Hydration Product, Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic)
**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 00-002-0875 (Deleted), 00-003-0773 (Deleted), 00-003-0788 (Deleted), 00-008-0479 (Primary), 00-036-0383 (Primary), 01-071-3698 (Alternate), 01-071-6263 (Alternate), 01-080-0042 (Alternate), 01-086-2344 (Alternate), ✓ 04-009-2317 (Primary), ✓ 04-010-3138 (Alternate), ✓ 04-012-1188 (Alternate), ✓ 04-012-1189 (Alternate)

**Entry Date:** 09/01/1998 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "The crystal structure of magnesite". Oh, K.D., Morikawa, H., Iwai, S.I., Aoki, H. Am. Mineral. 58, 1029 (1973). |

**Database Comments:** ANX: ABX3. Analysis: C1 Mg1 O3. Formula from original source: Mg (C O3). ICSD Collection Code: 10264. Wyckoff Sequence: e b a(R3-CH). Unit Cell Data Source: Single Crystal.

**d-Spacings (60) - Mg C O3 - 01-071-1534 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 25.1251 | 3.541430 | 5 | 0 | 1 | 2 | | 66.3734 | 1.407240 | 58m | 1 | 0 | 10 | | 83.2825 | 1.159250 | 8 | 2 | 2 | 0 | |
| 32.6175 | **2.743030** | 999 | 1 | 0 | 4 | | 66.3734 | 1.407240 | m | 2 | 1 | 4 | | 86.0062 | 1.129380 | 8 | 2 | 2 | 3 | |
| 35.8342 | 2.503830 | 123 | 0 | 0 | 6 | | 68.3365 | 1.371520 | 18 | 2 | 0 | 8 | | 87.8150 | 1.110720 | 1 | 1 | 3 | 1 | |
| 38.8086 | 2.318500 | 62 | 1 | 1 | 0 | | 69.3074 | 1.354660 | 83m | 1 | 1 | 9 | | 88.7338 | 1.101580 | 10m | 1 | 1 | 12 | |
| 42.9522 | **2.103940** | 480 | 1 | 1 | 3 | | 69.3074 | 1.354660 | m | 1 | 2 | 5 | | 88.7338 | 1.101580 | m | 3 | 1 | 2 | |
| 46.7938 | 1.939770 | 131 | 2 | 0 | 2 | | 70.2611 | 1.338590 | 114 | 3 | 0 | 0 | | 92.3345 | 1.067810 | 70m | 1 | 3 | 4 | |
| 51.5718 | 1.770720 | 49 | 0 | 2 | 4 | | 75.9444 | 1.251920 | 39 | 0 | 0 | 12 | | 92.3345 | 1.067810 | m | 2 | 1 | 10 | |
| 53.8459 | **1.701180** | 389m | 0 | 1 | 8 | | 76.8639 | 1.239220 | 16 | 2 | 1 | 7 | | 94.1467 | 1.051970 | 21 | 2 | 2 | 6 | |
| 53.8459 | **1.701180** | m | 1 | 1 | 6 | | 79.6378 | 1.202880 | 16 | 0 | 2 | 10 | | 95.0518 | 1.044330 | 1 | 3 | 1 | 5 | |
| 61.3377 | 1.510130 | 47 | 2 | 1 | 1 | | 81.4662 | 1.180440 | 28m | 1 | 2 | 8 | | 95.9772 | 1.036700 | 1 | 0 | 1 | 14 | |
| 62.3627 | 1.487750 | 70 | 1 | 2 | 2 | | 81.4662 | 1.180440 | m | 3 | 0 | 6 | | 98.7025 | 1.015240 | 6 | 1 | 2 | 11 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 101.4432 | 0.995092 | 2 | 0 | 4 | 2 | | 118.8323 | 0.894753 | 6m | 1 | 3 | 10 | | 129.8042 | 0.850589 | m | 2 | 2 | 12 | |
| 102.3714 | 0.988576 | 1 | 1 | 3 | 7 | | 118.8323 | 0.894753 | m | 3 | 2 | 4 | | 130.9773 | 0.846574 | 6 | 3 | 2 | 7 | |
| 105.1587 | 0.969887 | 36 | 4 | 0 | 4 | | 120.9221 | 0.885358 | 29 | 0 | 4 | 8 | | 134.6809 | 0.834711 | 2m | 0 | 0 | 18 | |
| 107.0447 | 0.957954 | 37 | 3 | 1 | 8 | | 121.9765 | 0.880803 | 7 | 2 | 3 | 5 | | 134.6809 | 0.834711 | m | 4 | 0 | 10 | |
| 107.9939 | 0.952155 | 4 | 2 | 2 | 9 | | 123.0447 | 0.876311 | 21m | 1 | 2 | 14 | | 137.2760 | 0.827104 | 13m | 2 | 3 | 8 | |
| 108.9592 | 0.946396 | 6 | 2 | 0 | 14 | | 123.0447 | 0.876311 | m | 4 | 1 | 0 | | 137.2760 | 0.827104 | m | 4 | 1 | 6 | |
| 113.8151 | 0.919418 | 21m | 1 | 1 | 15 | | 126.3427 | 0.863194 | 3m | 1 | 4 | 3 | | 147.6934 | 0.801940 | 1 | 1 | 3 | 13 | |
| 113.8151 | 0.919418 | m | 2 | 1 | 13 | | 126.3427 | 0.863194 | m | 3 | 1 | 11 | | 149.4430 | 0.798502 | 12m | 2 | 1 | 16 | |
| 114.7974 | 0.914344 | 73 | 0 | 3 | 12 | | 129.8042 | 0.850589 | 10m | 0 | 2 | 16 | | 149.4430 | 0.798502 | m | 5 | 0 | 2 | |

**01-076-0606** Jun 9, 2020 12:28 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca ( C O3 )
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Aragonite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.14 **I/Ic - ND:** 0.57

**SYS:** Orthorhombic **SPGR:** Pmcn (62)
**Author's Cell [ AuthCell a:** 4.9598(5) Å **AuthCell b:** 7.9641(9) Å **AuthCell c:** 5.7379(6) Å
**AuthCell Vol:** 226.65 Å³ **AuthCell Z:** 4.00 **AuthCell MolVol:** 56.66 **]**
**Author's Cell Axial Ratio [ c/a:** 1.157 **a/b:** 0.623 **c/b:** 0.720 **]**
**Density [ Dcalc:** 2.933 g/cm³ **Dstruc:** 2.93 g/cm³ **]** **SS/FOM:** F(30) = 306.0(0.0031, 32)
**Temp:** 298.0 K (Author provided temperature) **R-factor:** 0.03

**Space Group:** Pnam (62) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 5.738 Å **XtlCell b:** 7.964 Å **XtlCell c:** 4.960 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 226.65 Å³ **XtlCell Z:** 4.00 **]**
**Crystal Data Axial Ratio [ c/a:** 0.864 **a/b:** 0.720 **c/b:** 0.623 **]**
**Reduced Cell [ RedCell a:** 4.960 Å **RedCell b:** 5.738 Å **RedCell c:** 7.964 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 90.00° **RedCell Vol:** 226.65 Å³ **]**

**Atomic parameters are cross-referenced from PDF entry 04-008-5421** **ADP:** B
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -x+1/2,-y+1/2,z+1/2 | 5 | x+1/2,-y,-z | 7 | -x,y+1/2,-z+1/2 |
| 2 | -x,-y,-z | 4 | x+1/2,y+1/2,-z+1/2 | 6 | -x+1/2,y,z | 8 | x,-y+1/2,z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 4c | m.. | 0.25 | 0.41508 | 0.24046 | 1.0 | 0.61095 | 9-a |
| C | 2 | 4c | m.. | 0.25 | 0.76211 | 0.08518 | 1.0 | 0.43867 | 3#a |
| O | 3 | 4c | m.. | 0.25 | 0.92224 | 0.09557 | 1.0 | 0.77616 | 1#a |
| O | 4 | 8d | 1 | 0.47347 | 0.68065 | 0.08726 | 1.0 | 0.70856 | 1#a |

**Anisotropic Displacement Parameters:**

| Atom | Num | Bani11 | Bani22 | Bani33 | Bani12 | Bani13 | Bani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.665479 | 0.670266 | 0.497141 | 0.0 | 0.0 | 0.0201231 |
| C | 2 | 0.442997 | 0.573788 | 0.299269 | 0.0 | 0.0 | 0.0073175 |
| O | 3 | 1.13407 | 0.540783 | 0.653666 | 0.0 | 0.0 | -0.05854 |
| O | 4 | 0.509938 | 0.926694 | 0.689106 | 0.180227 | -0.0136696 | 0.0841512 |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**LPF Prototype Structure [Formula Order]:** Ca [ C O3 ],oP20,62
**LPF Prototype Structure [Alpha Order]:** C Ca O3,oP20,62
**Mineral Classification:** Aragonite (Group), carbonate (Subgroup) **Pearson Symbol:** oP20.00

**Cross-Ref PDF #'s:** 00-001-0628 (Deleted), 00-003-0405 (Deleted), 00-003-0425 (Deleted), 00-003-1067 (Deleted), 00-005-0453 (Alternate), 00-041-1475 (Primary), ✓ 00-061-0390 (Primary), 01-071-2392 (Alternate), 01-071-2396 (Alternate), 01-071-3700 (Alternate), 01-071-4891 (Alternate), 01-075-9982 (Alternate), 01-075-9983 (Alternate), 01-075-9984 (Alternate), 01-075-9985 (Alternate), 01-075-9986 (Alternate), 01-075-9987 (Alternate), 01-078-4337 (Alternate), 01-078-4338 (Alternate), 01-078-4339 (Alternate), 01-080-2768 (Alternate), 01-080-2769 (Alternate), 01-080-2770 (Alternate), 01-080-2771 (Alternate), 01-080-2772 (Alternate), 01-080-2773 (Alternate), 01-080-2774 (Alternate), 01-080-2775 (Alternate), 01-080-2789 (Alternate), 01-080-2790 (Alternate), ✓ 04-006-5441 (Alternate), ✓ 04-006-5444 (Alternate), ✓ 04-006-6531 (Alternate), ✓ 04-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate), ✓ 04-014-1837 (Alternate), ✓ 04-015-4109 (Alternate), ✓ 04-017-9180 (Alternate)

**CAS Number - PR:** 14791-73-2 **Entry Date:** 09/01/1998 **Last Modification Date:** 09/01/2011
**Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++ (2004). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "Refinement of the crystal structure of the aragonite phase of Ca C O3". Dickens, B., Bowen, J.S. J. Res. Natl. Bur. Stand., Sect. A 75, 27 (1971). |

**01-076-0606** Jun 9, 2020 12:28 PM (fal-sharji2)

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca C O3. ICSD Collection Code: 34308. Sample Source or Locality: Specimen from National Museum of Natural History, Smithsonian Institution, Washington, D.C., USA, sample No. 75538. Temperature of Data Collection: 298 K. Wyckoff Sequence: d c3(PMCN). Unit Cell Data Source: Single Crystal.

**d-Spacings (199) - Ca ( C O3 ) - 01-076-0606 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|
| 19.0476 | 4.655460 | 2 | 0 | 1 | 1 | |
| 21.0843 | 4.210120 | 16 | 1 | 1 | 0 | |
| 22.3070 | 3.982050 | 6 | 0 | 2 | 0 | |
| 26.2324 | **3.394400** | 999 | 1 | 1 | 1 | |
| 27.2371 | **3.271430** | 562 | 0 | 2 | 1 | |
| 31.1487 | 2.868950 | 47 | 0 | 0 | 2 | |
| 32.7667 | 2.730880 | 80 | 1 | 2 | 1 | |
| 33.1629 | 2.699160 | 504 | 0 | 1 | 2 | |
| 36.1390 | 2.483410 | 341m | 1 | 0 | 2 | |
| 36.1390 | 2.483410 | m | 2 | 0 | 0 | |
| 37.2904 | 2.409330 | 134 | 0 | 3 | 1 | |
| 37.9191 | 2.370820 | 404 | 1 | 1 | 2 | |
| 38.4291 | 2.340520 | 256 | 1 | 3 | 0 | |
| 38.6486 | 2.327730 | 191 | 0 | 2 | 2 | |
| 41.2106 | 2.188740 | 129 | 2 | 1 | 1 | |
| 41.6400 | 2.167160 | 5 | 1 | 3 | 1 | |
| 42.9282 | 2.105060 | 196m | 1 | 2 | 2 | |
| 42.9282 | 2.105060 | m | 2 | 2 | 0 | |
| 45.5204 | 1.991030 | 36 | 0 | 4 | 0 | |
| 45.8799 | **1.976260** | 665 | 2 | 2 | 1 | |
| 46.5718 | 1.948500 | 5 | 0 | 3 | 2 | |
| 48.3476 | 1.881000 | 268 | 0 | 4 | 1 | |
| 48.4808 | 1.876140 | 204 | 2 | 0 | 2 | |
| 48.9360 | 1.859750 | 4 | 0 | 1 | 3 | |
| 49.8970 | 1.826160 | 22 | 2 | 1 | 2 | |
| 50.2673 | 1.813570 | 271 | 1 | 3 | 2 | |
| 51.9482 | 1.758770 | 30 | 1 | 4 | 1 | |
| 52.5071 | 1.741360 | 298 | 1 | 1 | 3 | |
| 52.9425 | 1.728060 | 69 | 2 | 3 | 1 | |
| 53.0746 | 1.724070 | 135 | 0 | 2 | 3 | |
| 53.9824 | 1.697200 | 22 | 2 | 2 | 2 | |
| 56.1870 | 1.635720 | 24 | 0 | 4 | 2 | |
| 56.4588 | 1.628490 | 9 | 1 | 2 | 3 | |
| 56.8289 | 1.618760 | 18 | 3 | 1 | 0 | |
| 59.2633 | 1.557940 | 58 | 3 | 1 | 1 | |
| 59.4893 | 1.552560 | 11m | 0 | 3 | 3 | |
| 59.4893 | 1.552560 | m | 2 | 4 | 0 | |
| 60.2493 | 1.534780 | 16 | 0 | 5 | 1 | |
| 61.0507 | 1.516540 | 1 | 1 | 5 | 0 | |
| 61.8580 | 1.498670 | 54 | 2 | 4 | 1 | |
| 62.3580 | 1.487850 | 1 | 2 | 1 | 3 | |
| 62.6781 | 1.481020 | 1 | 1 | 3 | 3 | |
| 62.9369 | 1.475550 | 29 | 3 | 2 | 1 | |
| 63.3852 | 1.466190 | 54 | 1 | 5 | 1 | |
| 64.9564 | 1.434470 | 3 | 0 | 0 | 4 | |
| 65.0593 | 1.432450 | 5 | 3 | 0 | 2 | |
| 65.9319 | 1.415590 | 5 | 2 | 2 | 3 | |
| 66.1336 | 1.411760 | 41 | 0 | 1 | 4 | |
| 66.2363 | 1.409820 | 32 | 3 | 1 | 2 | |
| 66.5803 | 1.403370 | 32 | 3 | 3 | 0 | |
| 67.9711 | 1.378000 | 2m | 0 | 4 | 3 | |
| 67.9711 | 1.378000 | m | 1 | 0 | 4 | |
| 68.6832 | 1.365440 | 29 | 2 | 4 | 2 | |
| 69.1232 | 1.357820 | 50 | 1 | 1 | 4 | |
| 69.6058 | 1.349580 | 19 | 0 | 2 | 4 | |
| 70.1318 | 1.340740 | 22 | 1 | 5 | 2 | |
| 70.9453 | 1.327350 | 15 | 0 | 6 | 0 | |
| 71.6832 | 1.315490 | 1 | 2 | 3 | 3 | |
| 72.3461 | 1.305060 | 5 | 2 | 5 | 1 | |
| 72.5282 | 1.302230 | 3 | 1 | 2 | 4 | |
| 73.1164 | 1.293200 | 1 | 0 | 6 | 1 | |
| 75.3277 | 1.260630 | 61 | 3 | 3 | 2 | |
| 75.9844 | 1.251360 | 1 | 1 | 6 | 1 | |
| 76.6817 | 1.241710 | 34m | 2 | 0 | 4 | |
| 76.6817 | 1.241710 | m | 3 | 4 | 1 | |
| 76.8104 | 1.239950 | 57 | 4 | 0 | 0 | |
| 77.1290 | 1.235620 | 87 | 3 | 1 | 3 | |
| 78.0719 | 1.223040 | 61m | 0 | 5 | 3 | |
| 78.0719 | 1.223040 | m | 1 | 3 | 4 | |
| 78.7469 | 1.214240 | 13 | 2 | 5 | 2 | |
| 79.4374 | 1.205410 | 66m | 0 | 6 | 2 | |
| 79.4374 | 1.205410 | m | 2 | 4 | 3 | |
| 80.4086 | 1.193280 | 3 | 3 | 2 | 3 | |
| 80.8134 | 1.188320 | 48 | 1 | 5 | 3 | |
| 81.0531 | 1.185410 | 5 | 2 | 2 | 4 | |
| 82.3274 | 1.170260 | 63m | 1 | 6 | 2 | |
| 82.3274 | 1.170260 | m | 2 | 6 | 0 | |
| 82.8786 | 1.163870 | 5m | 0 | 4 | 4 | |
| 82.8786 | 1.163870 | m | 3 | 4 | 2 | |
| 83.2640 | 1.159460 | 30 | 4 | 2 | 1 | |
| 84.4061 | 1.146660 | 1m | 2 | 6 | 1 | |
| 84.4061 | 1.146660 | m | 3 | 5 | 0 | |
| 85.1817 | 1.138190 | 7 | 4 | 0 | 2 | |
| 85.3989 | 1.135850 | 2 | 0 | 1 | 5 | |
| 85.6568 | 1.133090 | 2 | 1 | 4 | 4 | |
| 85.8090 | 1.131470 | 4 | 3 | 3 | 3 | |
| 86.2559 | 1.126750 | 15 | 4 | 1 | 2 | |
| 86.4412 | 1.124810 | 31m | 2 | 3 | 4 | |
| 86.4412 | 1.124810 | m | 3 | 5 | 1 | |
| 87.2943 | 1.116000 | 1 | 0 | 7 | 1 | |
| 87.9932 | 1.108930 | 4 | 1 | 7 | 0 | |
| 88.1672 | 1.107190 | 25 | 1 | 1 | 5 | |
| 88.6200 | 1.102700 | 13m | 0 | 2 | 5 | |
| 88.6200 | 1.102700 | m | 4 | 3 | 1 | |
| 89.1450 | 1.097560 | 1 | 2 | 5 | 3 | |
| 89.4746 | 1.094370 | 14 | 4 | 2 | 2 | |
| 90.0590 | 1.088780 | 9 | 1 | 7 | 1 | |
| 90.6108 | 1.083580 | 11m | 2 | 6 | 2 | |
| 90.6108 | 1.083580 | m | 3 | 0 | 4 | |
| 91.3838 | 1.076420 | 1 | 1 | 2 | 5 | |
| 91.6937 | 1.073590 | 10 | 3 | 1 | 4 | |
| 92.6397 | 1.065090 | 12m | 1 | 6 | 3 | |
| 92.6397 | 1.065090 | m | 3 | 5 | 2 | |
| 93.3182 | 1.059120 | 1 | 3 | 4 | 3 | |
| 93.4929 | 1.057600 | 1 | 0 | 7 | 2 | |
| 93.9563 | 1.053600 | 13m | 0 | 3 | 5 | |
| 93.9563 | 1.053600 | m | 2 | 4 | 4 | |
| 94.8403 | 1.046100 | 1m | 3 | 2 | 4 | |
| 94.8403 | 1.046100 | m | 4 | 3 | 2 | |
| 95.3164 | 1.042130 | 10 | 1 | 5 | 4 | |
| 96.1543 | 1.035260 | 35m | 1 | 7 | 2 | |
| 96.1543 | 1.035260 | m | 4 | 4 | 1 | |
| 96.4736 | 1.032680 | 16 | 2 | 1 | 5 | |
| 98.3804 | 1.017700 | 2 | 2 | 7 | 1 | |
| 99.7224 | 1.007580 | 32 | 2 | 2 | 5 | |
| 99.8494 | 1.006640 | 27 | 4 | 2 | 3 | |
| 100.3244 | 1.003150 | 29 | 3 | 3 | 4 | |
| 101.0037 | 0.998231 | 4 | 2 | 6 | 3 | |
| 101.3840 | 0.995513 | 4 | 0 | 8 | 0 | |
| 101.5617 | 0.994252 | 12 | 0 | 4 | 5 | |
| 102.4357 | 0.988130 | 7 | 4 | 4 | 2 | |
| 103.0774 | 0.983719 | 15m | 3 | 5 | 3 | |
| 103.0774 | 0.983719 | m | 5 | 1 | 0 | |
| 103.4990 | 0.980859 | 10 | 0 | 8 | 1 | |
| 103.7316 | 0.979294 | 7 | 2 | 5 | 4 | |
| 104.4904 | 0.974251 | 11m | 0 | 6 | 4 | |
| 104.4904 | 0.974251 | m | 1 | 4 | 5 | |
| 104.5872 | 0.973614 | 11 | 3 | 6 | 2 | |
| 105.1133 | 0.970181 | 17m | 2 | 3 | 5 | |
| 105.1133 | 0.970181 | m | 5 | 1 | 1 | |
| 105.9975 | 0.964511 | 2 | 4 | 5 | 1 | |
| 106.3597 | 0.962224 | 2 | 1 | 8 | 1 | |
| 106.8204 | 0.959344 | 21 | 1 | 7 | 3 | |
| 107.3104 | 0.956317 | 22m | 0 | 0 | 6 | |
| 107.3104 | 0.956317 | m | 1 | 6 | 4 | |
| 108.0705 | 0.951693 | 2 | 3 | 4 | 4 | |
| 108.4368 | 0.949496 | 1m | 0 | 1 | 6 | |
| 108.4368 | 0.949496 | m | 5 | 2 | 1 | |
| 109.9717 | 0.940501 | 1 | 0 | 8 | 2 | |
| 110.4965 | 0.937503 | 10m | 3 | 7 | 0 | |
| 110.4965 | 0.937503 | m | 5 | 0 | 2 | |
| 110.7283 | 0.936191 | 13 | 3 | 1 | 5 | |
| 111.6453 | 0.931074 | 22m | 0 | 5 | 5 | |
| 111.6453 | 0.931074 | m | 5 | 1 | 2 | |
| 111.9847 | 0.929209 | 11m | 0 | 2 | 6 | |
| 111.9847 | 0.929209 | m | 5 | 3 | 0 | |
| 112.7645 | 0.924984 | 7 | 3 | 7 | 1 | |
| 113.1648 | 0.922846 | 9 | 2 | 4 | 5 | |
| 114.2302 | 0.917259 | 2m | 3 | 2 | 5 | |
| 114.2302 | 0.917259 | m | 5 | 3 | 1 | |
| 114.6481 | 0.915107 | 13 | 1 | 5 | 5 | |
| 115.0462 | 0.913078 | 10 | 4 | 2 | 4 | |
| 115.2383 | 0.912106 | 13m | 2 | 8 | 1 | |
| 115.2383 | 0.912106 | m | 5 | 2 | 2 | |
| 115.7275 | 0.909652 | 1 | 2 | 7 | 3 | |
| 116.4459 | 0.906101 | 10 | 4 | 6 | 0 | |
| 117.7705 | 0.899719 | 2 | 0 | 3 | 6 | |
| 118.5919 | 0.895866 | 10 | 3 | 5 | 4 | |
| 119.3738 | 0.892271 | 9 | 2 | 0 | 6 | |
| 119.6744 | 0.890908 | 8m | 0 | 7 | 4 | |
| 119.6744 | 0.890908 | m | 3 | 7 | 2 | |
| 120.2392 | 0.888374 | 1 | 3 | 3 | 5 | |
| 120.6116 | 0.886723 | 2 | 2 | 1 | 6 | |
| 120.9420 | 0.885271 | 19 | 1 | 3 | 6 | |
| 121.2338 | 0.883999 | 18m | 4 | 3 | 4 | |
| 121.2338 | 0.883999 | m | 5 | 3 | 2 | |
| 122.3108 | 0.879384 | 4 | 2 | 8 | 2 | |
| 122.7979 | 0.877338 | 10m | 1 | 7 | 4 | |
| 122.7979 | 0.877338 | m | 5 | 4 | 1 | |
| 123.3035 | 0.875241 | 16 | 5 | 1 | 3 | |
| 124.4260 | 0.870681 | 11m | 2 | 2 | 6 | |
| 124.4260 | 0.870681 | m | 4 | 5 | 3 | |
| 124.7511 | 0.869385 | 1 | 1 | 8 | 3 | |
| 125.0720 | 0.868116 | 1 | 0 | 6 | 5 | |
| 126.1234 | 0.864032 | 14 | 4 | 6 | 2 | |
| 126.6479 | 0.862036 | 2 | 0 | 4 | 6 | |
| 127.2433 | 0.859803 | 1 | 5 | 2 | 3 | |
| 128.5242 | 0.855116 | 1 | 1 | 6 | 5 | |
| 129.3883 | 0.852043 | 1 | 3 | 4 | 5 | |
| 130.3804 | 0.848601 | 5m | 4 | 4 | 4 | |
| 130.3804 | 0.848601 | m | 5 | 4 | 2 | |
| 131.2150 | 0.845776 | 4m | 0 | 9 | 2 | |
| 131.2150 | 0.845776 | m | 2 | 3 | 6 | |
| 131.8804 | 0.843569 | 1 | 3 | 8 | 1 | |
| 132.4764 | 0.841626 | 16m | 3 | 7 | 3 | |
| 132.4764 | 0.841626 | m | 5 | 5 | 0 | |
| 133.3452 | 0.838850 | 5m | 2 | 7 | 4 | |
| 133.3452 | 0.838850 | m | 3 | 6 | 4 | |
| 133.7578 | 0.837555 | 2 | 4 | 1 | 5 | |
| 134.3266 | 0.835794 | 2 | 5 | 3 | 3 | |
| 135.0605 | 0.833563 | 13m | 1 | 9 | 2 | |
| 135.0605 | 0.833563 | m | 5 | 5 | 1 | |
| 135.6210 | 0.831890 | 7 | 2 | 8 | 3 | |
| 136.4369 | 0.829502 | 1 | 4 | 7 | 1 | |
| 137.0293 | 0.827803 | 1 | 3 | 0 | 6 | |
| 137.4433 | 0.826633 | 6 | 6 | 0 | 0 | |
| 138.3947 | 0.823997 | 12 | 4 | 2 | 5 | |
| 139.9316 | 0.819893 | 1m | 0 | 5 | 6 | |
| 139.9316 | 0.819893 | m | 2 | 6 | 5 | |

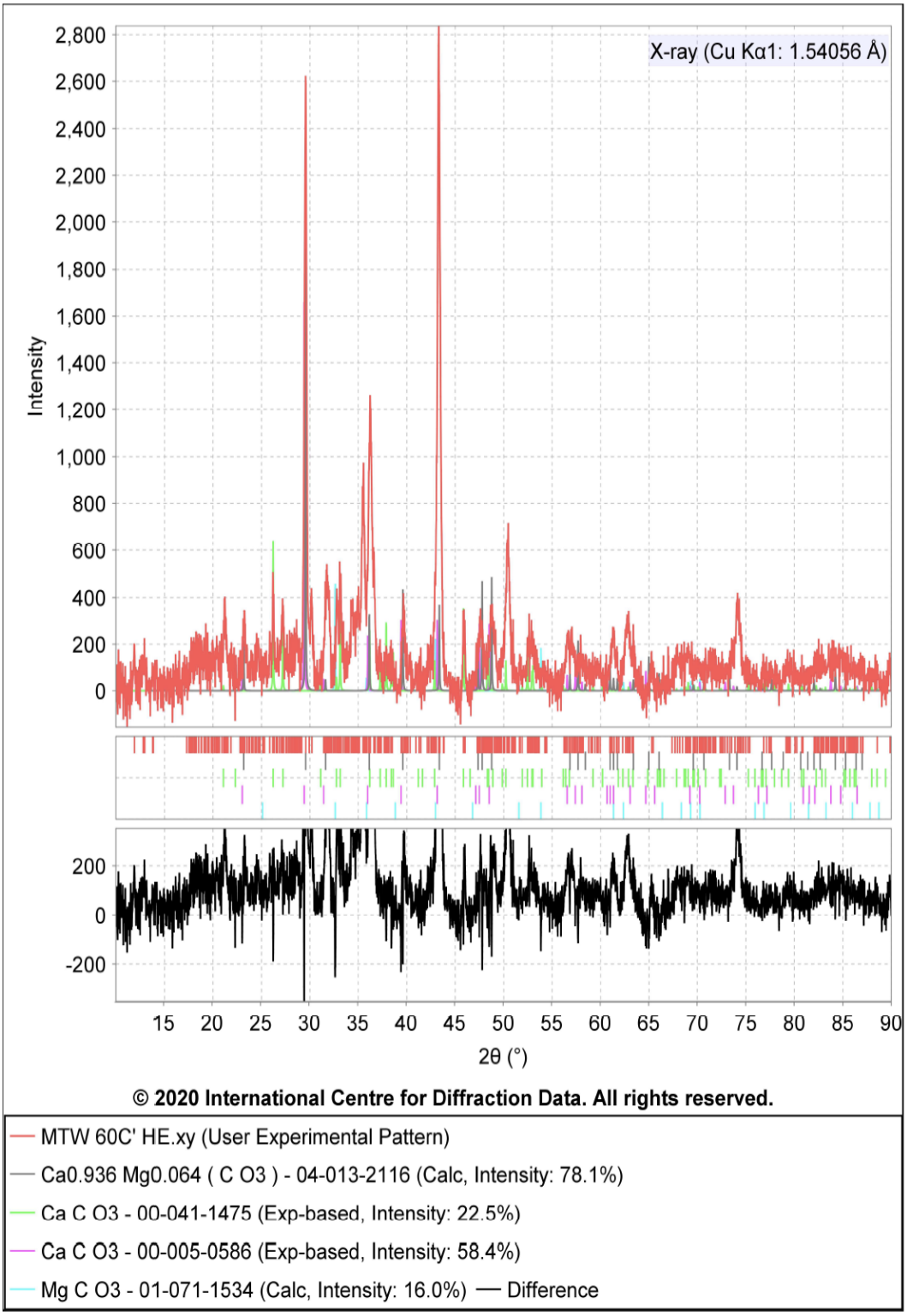


**Figure E.6 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 60 °C from experiment with a tank with little exposure of iron.**

# SIeve+ Report

## Experiment

**Search Line:** 2.087679 Å **D1 Range:** 2.081 Å - 2.095 Å
**Search Line:** 2.082635 Å **D1 Range:** 2.076 Å - 2.089 Å
**Search Line:** 2.476839 Å **D1 Range:** 2.467 Å - 2.487 Å
**Search Line:** 2.527288 Å **D1 Range:** 2.517 Å - 2.538 Å
**Search Line:** 2.516984 Å **D1 Range:** 2.507 Å - 2.527 Å
**Search Line:** 1.810385 Å **D1 Range:** 1.805 Å - 1.815 Å
**Search Line:** 2.486714 Å **D1 Range:** 2.477 Å - 2.497 Å
**Search Line:** 2.452726 Å **D1 Range:** 2.443 Å - 2.462 Å
**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (4)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 04-013-2116 | S | Calcium Magnesium Carbonate | 0.781 | 44.629 | 3.05 | 36 |
| 2 | true | 00-041-1475 | S | Calcium Carbonate | 0.225 | 12.876 | *1.14 | 27 |
| 3 | true | 00-005-0586 | S | Calcium Carbonate | 0.584 | 33.353 | *3.23 | 25 |
| 4 | true | 01-071-1534 | S | Magnesium Carbonate | 0.160 | 9.142 | *1.85 | 12 |

**04-013-2116** Jun 9, 2020 12:34 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca0.936 Mg0.064 ( C O3 )
**Empirical Formula:** C Ca0.936 Mg0.064 O3 **Weight %:** C12.12 Ca37.86 Mg1.57 O48.44
**Atomic %:** C20.00 Ca18.72 Mg1.28 O60.00 **ANX:** ABX3 **Compound Name:** Calcium Magnesium Carbonate
**Mineral Name:** Calcite, magnesian

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 3.05 **I/Ic - ND:** 0.88

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.9673(3) Å **AuthCell c:** 16.9631(7) Å **AuthCell Vol:** 362.47 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 60.41 ] **Author's Cell Axial Ratio [ c/a:** 3.415 ]
**Density [ Dcalc:** 2.723 g/cm³ **Dstruc:** 2.72 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 297.0 K (Author provided temperature) **R-factor:** 0.023

**Space Group:** R-3c (167) **Molecular Weight:** 99.08
**Crystal Data [ XtlCell a:** 4.967 Å **XtlCell b:** 4.967 Å **XtlCell c:** 16.963 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 362.47 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.415 **a/b:** 1.000 **c/b:** 3.415 ]
**Reduced Cell [ RedCell a:** 4.967 Å **RedCell b:** 4.967 Å **RedCell c:** 6.340 Å **RedCell α:** 66.94°
**RedCell β:** 66.94° **RedCell γ:** 60.00° **RedCell Vol:** 120.82 Å³ ]

**ADP:** U **Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3. | 0.0 | 0.0 | 0.0 | 0.936 | 0.01473 | |
| Mg | 2 | 6b | -3. | 0.0 | 0.0 | 0.0 | 0.064 | 0.01473 | |
| C | 3 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | 0.01426 | |
| O | 4 | 18e | .2 | 0.2575 | 0.0 | 0.25 | 1.0 | 0.02852 | |

**Anisotropic Displacement Parameters:**

| Atom | Num | Uani11 | Uani22 | Uani33 | Uani12 | Uani13 | Uani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.0151 | 0.0151 | 0.014 | 0.00755 | 0.0 | 0.0 |
| Mg | 2 | 0.0151 | 0.0151 | 0.014 | 0.00755 | 0.0 | 0.0 |
| C | 3 | 0.0128 | 0.0128 | 0.0172 | 0.00642 | 0.0 | 0.0 |
| O | 4 | 0.0161 | 0.0336 | 0.0306 | 0.00849 | -0.018 | -0.0089 |

**Subfile(s):** Inorganic, Mineral Related (Mineral , Natural) **Former PDF's #:** 01-086-2335
**LPF Prototype Structure [Formula Order]:** Ca ( C O3 ),hR30,167
**LPF Prototype Structure [Alpha Order]:** C Ca O3,hR30,167
**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00
**Cross-Ref PDF #'s:** 01-089-1304 (Related Phase), 01-089-1305 (Related Phase) **Entry Date:** 09/01/2010
**Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from LPF using POWD-12++. |
| Structure | | "Single-crystal X-ray structure refinements of two biogenic magnesian calcite crystals". Paquette J., Reeder R.J. Am. Mineral. 75, 1151,1158 (1990). |

**Database Comments:** ANX: ABX3. LPF Collection Code: 1213141. Calculated Pattern Original Remarks: same sample studied in Am. Mineral. (1983) 68, 1183. same sample studied in Am. Mineral. (1985) 70, 581. Temperature of Data Collection: 297 K. Unit Cell Data Source: Single Crystal.

**d-Spacings (77) - Ca0.936 Mg0.064 ( C O3 ) - 04-013-2116 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.1645 | 3.836550 | 89 | 0 | 1 | 2 | | 48.7639 | **1.865910** | 193 | 1 | 1 | 6 | | 64.9834 | 1.433940 | 56 | 3 | 0 | 0 | |
| 29.5539 | **3.020030** | 999 | 1 | 0 | 4 | | 56.8384 | 1.618510 | 29 | 2 | 1 | 1 | | 66.0371 | 1.413590 | 30 | 0 | 0 | 12 | |
| 31.6208 | 2.827180 | 20 | 0 | 0 | 6 | | 57.6812 | 1.596850 | 85 | 1 | 2 | 2 | | 69.5704 | 1.350180 | 9 | 2 | 1 | 7 | |
| 36.1354 | 2.483650 | 143 | 1 | 1 | 0 | | 58.4344 | 1.578050 | 11 | 1 | 0 | 10 | | 70.6641 | 1.331940 | 18 | 0 | 2 | 10 | |
| 39.6004 | 2.273950 | 181 | 1 | 1 | 3 | | 60.9781 | 1.518170 | 53 | 2 | 1 | 4 | | 73.3101 | 1.290260 | 27 | 1 | 2 | 8 | |
| 43.3640 | 2.084910 | 148 | 2 | 0 | 2 | | 61.3431 | 1.510010 | 22 | 2 | 0 | 8 | | 74.0728 | 1.278850 | 6 | 3 | 0 | 6 | |
| 47.3501 | 1.918270 | 67 | 0 | 2 | 4 | | 61.7328 | 1.501410 | 22 | 1 | 1 | 9 | | 76.6736 | 1.241820 | 11 | 2 | 2 | 0 | |
| 47.7829 | **1.901900** | 188 | 0 | 1 | 8 | | 63.3828 | 1.466240 | 17 | 1 | 2 | 5 | | 77.6565 | 1.228540 | 19 | 1 | 1 | 12 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 78.8492 | 1.212920 | 1 | 2 | 2 | 3 | | 102.8556 | 0.985236 | 2 | 3 | 2 | 1 | | 121.9071 | 0.881099 | 7m | 1 | 1 | 18 | |
| 80.6619 | 1.190170 | 1 | 1 | 3 | 1 | | 103.5836 | 0.980289 | 9 | 2 | 3 | 2 | | 121.9071 | 0.881099 | m | 1 | 3 | 13 | |
| 81.3802 | 1.181470 | 5 | 3 | 1 | 2 | | 104.2421 | 0.975891 | 3 | 1 | 3 | 10 | | 128.2879 | 0.855969 | 2 | 5 | 0 | 2 | |
| 82.0256 | 1.173800 | 20 | 2 | 1 | 10 | | 104.9024 | 0.971552 | 8 | 1 | 2 | 14 | | 129.1066 | 0.853037 | 6 | 3 | 2 | 10 | |
| 82.6706 | 1.166270 | 3 | 0 | 1 | 14 | | 106.5202 | 0.961217 | 8 | 3 | 2 | 4 | | 129.9353 | 0.850134 | 2m | 1 | 2 | 17 | |
| 84.2379 | 1.148520 | 36 | 1 | 3 | 4 | | 106.8537 | 0.959137 | 14 | 0 | 4 | 8 | | 129.9353 | 0.850134 | m | 3 | 1 | 14 | |
| 85.2939 | 1.136980 | 16 | 2 | 2 | 6 | | 108.1942 | 0.950949 | 4 | 0 | 2 | 16 | | 131.9977 | 0.843184 | 5 | 0 | 5 | 4 | |
| 86.3723 | 1.125530 | 1 | 3 | 1 | 5 | | 108.7518 | 0.947622 | 2 | 2 | 3 | 5 | | 132.8953 | 0.840279 | 1 | 4 | 1 | 9 | |
| 87.0123 | 1.118890 | 4 | 1 | 2 | 11 | | 109.4280 | 0.943648 | 1 | 3 | 1 | 11 | | 134.2180 | 0.836128 | 1 | 2 | 2 | 15 | |
| 92.0460 | 1.070400 | 1 | 1 | 3 | 7 | | 109.6438 | 0.942394 | 1 | 0 | 0 | 18 | | 135.5383 | 0.832135 | 6 | 0 | 1 | 20 | |
| 92.4352 | 1.066910 | 1 | 0 | 4 | 2 | | 110.2807 | 0.938731 | 14 | 4 | 1 | 0 | | 135.8378 | 0.831250 | 1 | 2 | 3 | 11 | |
| 93.7158 | 1.055670 | 7 | 2 | 0 | 14 | | 111.3060 | 0.932954 | 8 | 2 | 2 | 12 | | 137.0012 | 0.827883 | 3 | 3 | 3 | 0 | |
| 95.2778 | 1.042450 | 20 | 4 | 0 | 4 | | 112.5652 | 0.926056 | 1 | 4 | 1 | 3 | | 140.2177 | 0.819150 | 1 | 3 | 3 | 3 | |
| 95.5986 | 1.039800 | 24 | 3 | 1 | 8 | | 114.8627 | 0.914011 | 2 | 3 | 2 | 7 | | 143.0935 | 0.812033 | 1 | 2 | 4 | 1 | |
| 96.8846 | 1.029390 | 12m | 1 | 0 | 16 | | 116.0013 | 0.908291 | 1 | 4 | 0 | 10 | | 144.2906 | 0.809256 | 5 | 4 | 2 | 2 | |
| 96.8846 | 1.029390 | m | 1 | 1 | 15 | | 118.8360 | 0.894736 | 6 | 2 | 3 | 8 | | 146.5426 | 0.804320 | 1 | 0 | 4 | 14 | |
| 98.3856 | 1.017660 | 2 | 2 | 1 | 13 | | 119.6750 | 0.890905 | 6 | 1 | 4 | 6 | | 149.4824 | 0.798427 | 6 | 2 | 4 | 4 | |
| 99.8440 | 1.006680 | 21 | 0 | 3 | 12 | | 120.3057 | 0.888078 | 7 | 2 | 1 | 16 | | | | | | | | |

**00-005-0586** Jun 9, 2020 12:39 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca C O3
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**Compound Name:** Calcium Carbonate **Mineral Name:** Calcite, syn

**Radiation:** CuKα1 **λ:** 1.5405 Å **Filter:** Ni Beta **Intensity:** Diffractometer **I/Ic:** 2

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.989 Å **AuthCell c:** 17.062 Å **AuthCell Vol:** 367.78 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 61.30 ] **Author's Cell Axial Ratio [ c/a:** 3.420 ]
**Density [ Dcalc:** 2.711 g/cm³ **Dmeas:** 2.71 g/cm³ ] **SS/FOM:** F(30) = 57.2(0.0159, 33)
**Temp:** 299.0 K (Author provided temperature) **Color:** Colorless

**Space Group:** R-3c (167) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 4.989 Å **XtlCell b:** 4.989 Å **XtlCell c:** 17.062 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 367.78 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.420 **a/b:** 1.000 **c/b:** 3.420 ]
**Reduced Cell [ RedCell a:** 4.989 Å **RedCell b:** 4.989 Å **RedCell c:** 6.375 Å **RedCell α:** 66.97°
**RedCell β:** 66.97° **RedCell γ:** 60.00° **RedCell Vol:** 122.59 Å³ ]

**εα:** =1.487 **πωβ:** =1.659 **Sign:** =-

**Atomic parameters are cross-referenced from PDF entry 04-012-8072** **ADP:** U
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3 | 0.0 | 0.0 | 0.0 | 1.0 | 0.01525 | |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | 0.02084 | |
| O | 3 | 18e | .2 | 0.25 | 0.0 | 0.25 | 1.0 | 0.02084 | |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Educational Pattern, Forensic, Inorganic, Mineral Related (Mineral , Synthetic), NBS Pattern, Pharmaceutical (Excipient), Pigment/Dye, Superconducting Material (Superconductor Related Materials)

**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 01-072-1937 (Alternate), 01-083-0577 (Alternate), 01-083-0578 (Alternate), ✓ 04-001-7249 (Alternate), ✓ 04-006-6528 (Alternate), ✓ 04-007-2808 (Alternate), ✓ 04-007-4388 (Alternate), ✓ 04-007-8659 (Primary), ✓ 04-008-0788 (Alternate), ✓ 04-012-0489 (Primary), ✓ 04-012-8072 (Alternate)

**CAS Number - PR:** 13397-26-7 **Entry Date:** 09/01/1955

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Swanson, Fuyat. Natl. Bur. Stand. (U. S. ), Circ. 539 II, 51 (1953). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Optical Data | | Dana's System of Mineralogy, 7th Ed. II, 142. |

**Database Comments:** Additional Patterns: See PDF 01-072-1214 , 01-072-1937, 01-081-2027, 01-083-0577 and 01-083-0578. Analysis: Spectroscopic analysis: <0.1% Sr; <0.01% Ba; <0.001% Al, B, Cs, Cu, K, Mg, Na, Si, Sn; <0.0001% Ag, Cr, Fe, Li, Mn. Color: Colorless. General Comments: Additional weak reflections (indicated by brackets) were observed. Other form: aragonite. Pattern reviewed by Parks, J., McCarthy, G., North Dakota State Univ., Fargo, North Dakota, USA, ICDD Grant-in-Aid (1992). Agrees well with experimental and calculated patterns. Antacid. Sample Source or Locality: Sample from Mallinckrodt Chemical Works. Temperature of Data Collection: Pattern taken at 299 K. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (45) - Ca C O3 - 00-005-0586 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.0218 | 3.860000 | 12 | 0 | 1 | 2 | | 48.5122 | 1.875000 | 17 | 1 | 1 | 6 | | 64.6765 | 1.440000 | 5 | 3 | 0 | 0 | |
| 29.4049 | **3.035000** | 100 | 1 | 0 | 4 | | 56.5530 | 1.626000 | 4 | 2 | 1 | 1 | | 65.5972 | 1.422000 | 3 | 0 | 0 | 12 | |
| 31.4176 | 2.845000 | 3 | 0 | 0 | 6 | | 57.4001 | 1.604000 | 8 | 1 | 2 | 2 | | 69.2291 | 1.356000 | 1 | 2 | 1 | 7 | |
| 35.9654 | 2.495000 | 14 | 1 | 1 | 0 | | 58.0733 | 1.587000 | 2 | 1 | 0 | 10 | | 70.2364 | 1.339000 | 2 | 0 | 2 | 10 | |
| 39.4009 | **2.285000** | 18 | 1 | 1 | 3 | | 60.6762 | 1.525000 | 5 | 2 | 1 | 4 | | 72.8676 | 1.297000 | 2 | 1 | 2 | 8 | |
| 43.1447 | **2.095000** | 18 | 2 | 0 | 2 | | 60.9857 | 1.518000 | 4 | 2 | 0 | 8 | | 73.7264 | 1.284000 | 1 | 3 | 0 | 6 | |
| 47.1226 | 1.927000 | 5 | 0 | 2 | 4 | | 61.3435 | 1.510000 | 3 | 1 | 1 | 9 | | 76.2977 | 1.247000 | 1 | 2 | 2 | 0 | |
| 47.4886 | 1.913000 | 17 | 0 | 1 | 8 | | 63.0584 | 1.473000 | 2 | 1 | 2 | 5 | | 77.1749 | 1.235000 | 2 | 1 | 1 | 12 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 80.9302 | 1.186900 | <1 | 3 | 1 | 2 | E | 94.6975 | 1.047300 | 3 | 4 | 0 | 4 | | 103.8950 | 0.978200 | 1 | 1 | 3 | 10 | |
| 81.5449 | 1.179500 | 3 | 2 | 1 | 10 | | 95.0075 | 1.044700 | 4 | 3 | 1 | 8 | | 104.1201 | 0.976700 | 3 | 1 | 2 | 14 | |
| 82.1106 | 1.172800 | <1 | 0 | 1 | 14 | E | 96.1617 | 1.035200 | 2 | 1 | 0 | 16 | | 105.8419 | 0.965500 | 2 | 3 | 2 | 4 | |
| 83.7646 | 1.153800 | 3 | 1 | 3 | 4 | | 97.6440 | 1.023400 | <1 | 2 | 1 | 13 | | 106.1414 | 0.963600 | 4 | 0 | 4 | 8 | |
| 84.7850 | 1.142500 | 1 | 2 | 2 | 6 | | 99.1573 | 1.011800 | 2 | 3 | 0 | 12 | | 107.3295 | 0.956200 | <1 | 0 | 2 | 16 | |
| 86.4804 | 1.124400 | <1 | 1 | 2 | 11 | | 102.2384 | 0.989500 | <1 | 3 | 2 | 1 | | 109.5566 | 0.942900 | 2 | 4 | 1 | 0 | |
| 93.0691 | 1.061300 | 1 | 2 | 0 | 14 | | 102.9484 | 0.984600 | 1 | 2 | 3 | 2 | | 110.4794 | 0.937600 | 2 | 2 | 2 | 12 | |

**00-041-1475** Jun 9, 2020 12:34 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca C O3
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**Compound Name:** Calcium Carbonate **Mineral Name:** Aragonite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Diff. **Intensity:** Diffractometer **I/Ic:** 1

**SYS:** Orthorhombic **SPGR:** Pmcn (62)
**Author's Cell [ AuthCell a:** 4.9623(3) Å **AuthCell b:** 7.968(1) Å **AuthCell c:** 5.7439(3) Å
**AuthCell Vol:** 227.11 Å³ **AuthCell Z:** 4.00 **AuthCell MolVol:** 56.78 ]
**Author's Cell Axial Ratio [ c/a:** 1.158 **a/b:** 0.623 **c/b:** 0.721 ]
**Density [ Dcalc:** 2.927 g/cm³ **Dmeas:** 2.95 g/cm³ ] **SS/FOM:** F(30) = 220.6(0.0040, 34)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **Color:** Colorless

**Space Group:** Pnam (62) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 5.744 Å **XtlCell b:** 7.968 Å **XtlCell c:** 4.962 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 227.11 Å³ **XtlCell Z:** 4.00 ]
**Crystal Data Axial Ratio [ c/a:** 0.864 **a/b:** 0.721 **c/b:** 0.623 ]
**Reduced Cell [ RedCell a:** 4.962 Å **RedCell b:** 5.744 Å **RedCell c:** 7.968 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 90.00° **RedCell Vol:** 227.11 Å³ ]

**εα:** =1.5300 **πωβ:** =1.6810 **εγ:** =1.6854 **Sign:** =- **2V:** =18(calc.)°

**Atomic parameters are cross-referenced from PDF entry 04-012-0488** **ADP:** U
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -x+1/2,-y+1/2,z+1/2 | 5 | x+1/2,-y,-z | 7 | -x,y+1/2,-z+1/2 |
| 2 | -x,-y,-z | 4 | x+1/2,y+1/2,-z+1/2 | 6 | -x+1/2,y,z | 8 | x,-y+1/2,z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 4c | m.. | 0.25 | 0.41502 | 0.75985 | 1.0 | | |
| C | 2 | 4c | m.. | 0.25 | 0.76194 | -0.0824 | 1.0 | | |
| O | 3 | 4c | m.. | 0.25 | 0.92238 | -0.09453 | 1.0 | | |
| O | 4 | 8d | 1 | 0.47499 | 0.68012 | -0.08725 | 1.0 | | |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Educational Pattern, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material (Superconductor Related Materials)

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**LPF Prototype Structure [Formula Order]:** Ca [ C O3 ],oP20,62
**LPF Prototype Structure [Alpha Order]:** C Ca O3,oP20,62
**Mineral Classification:** Aragonite (Group), carbonate (Subgroup) **Pearson Symbol:** oP20.00
**Cross-Ref PDF #'s:** 00-005-0453 (Alternate), 01-071-2392 (Alternate), 01-076-0606 (Alternate), ✓ 04-006-5441 (Alternate), ✓ 04-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate)
**CAS Number - PR:** 14791-73-2 **Entry Date:** 09/01/1991

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Keller, L., Rask, J., Buseck, P., Arizona State Univ., Tempe, AZ, USA. ICDD Grant-in-Aid (1989). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Optical Data | | Dana's System of Mineralogy, 7th Ed. II, 182 (1951). |
| Structure | | Jarosch, D., Heger, G. Tschermaks Mineral. Petrogr. Mitt. 35, 127 (1986). |

**Database Comments:** Additional Patterns: To replace 00-005-0453 and validated by calculated pattern 00-024-0025. See PDF 01-071-2392 and 01-076-0606. Analysis: Microprobe analyses (wt.%): major Ca, and trace Sr(<<1). Color: Colorless. General Comments: Antacid. Optical Data Specimen location: Optical data on specimen from Bilin, Bohemia, Czechoslovakia. Sample Source or Locality: Specimen from Sefrou, Morocco. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (82) - Ca C O3 - 00-041-1475 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 21.0748 | 4.212000 | 3 | 1 | 1 | 0 | | 27.2153 | 3.274000 | 50 | 0 | 2 | 1 | | 33.1270 | **2.702000** | 60 | 0 | 1 | 2 | |
| 22.2959 | 3.984000 | 1 | 0 | 2 | 0 | | 31.1148 | 2.872000 | 6 | 0 | 0 | 2 | | 36.1753 | 2.481000 | 40 | 2 | 0 | 0 | |
| 26.2120 | **3.397000** | 100 | 1 | 1 | 1 | | 32.7406 | 2.733000 | 9 | 1 | 2 | 1 | | 37.2636 | 2.411000 | 14 | 0 | 3 | 1 | |




**00-041-1475** Jun 9, 2020 12:34 PM (fal-sharji2)

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 37.8829 | 2.373000 | 45 | 1 | 1 | 2 | | 62.2998 | 1.489100 | 1 | 2 | 1 | 3 | | 77.9611 | 1.224500 | 3m | 0 | 5 | 3 | |
| 38.4039 | 2.342000 | 25 | 1 | 3 | 0 | | 62.8965 | 1.476400 | 2 | 3 | 2 | 1 | | 77.9611 | 1.224500 | m | 1 | 3 | 4 | |
| 38.6095 | 2.330000 | 25 | 0 | 2 | 2 | | 63.3365 | 1.467200 | 4 | 1 | 5 | 1 | | 78.6958 | 1.214900 | 2 | 2 | 5 | 2 | |
| 41.1858 | 2.190000 | 12 | 2 | 1 | 1 | | 64.8787 | 1.436000 | 1 | 0 | 0 | 4 | | 79.3988 | 1.205900 | 4m | 0 | 6 | 2 | |
| 41.6231 | 2.168000 | 2 | 1 | 3 | 1 | | 65.8737 | 1.416700 | 1 | 2 | 2 | 3 | | 79.3988 | 1.205900 | m | 2 | 4 | 3 | |
| 42.8654 | 2.108000 | 20m | 1 | 2 | 2 | | 66.0576 | 1.413200 | 3 | 0 | 1 | 4 | | 80.7577 | 1.189000 | 3 | 1 | 5 | 3 | |
| 42.8654 | 2.108000 | m | 2 | 2 | 0 | | 66.1897 | 1.410700 | 4 | 3 | 1 | 2 | | 80.9714 | 1.186400 | 2 | 2 | 2 | 4 | |
| 45.8520 | **1.977400** | 55 | 2 | 2 | 1 | | 66.5465 | 1.404000 | 3 | 3 | 3 | 0 | | 82.2556 | 1.171100 | 3m | 1 | 6 | 2 | |
| 46.5339 | 1.950000 | 1 | 0 | 3 | 2 | | 67.8369 | 1.380400 | <1 | 0 | 4 | 3 | | 82.2556 | 1.171100 | m | 2 | 6 | 0 | |
| 48.3175 | 1.882100 | 25 | 0 | 4 | 1 | | 68.6339 | 1.366300 | 2 | 2 | 4 | 2 | | 82.8500 | 1.164200 | 1m | 0 | 4 | 4 | |
| 48.4435 | 1.877500 | 25 | 2 | 0 | 2 | | 68.7716 | 1.363900 | 2 | 3 | 3 | 1 | | 82.8500 | 1.164200 | m | 3 | 4 | 2 | |
| 48.8842 | 1.861600 | 2 | 0 | 1 | 3 | | 69.0430 | 1.359200 | 5 | 1 | 1 | 4 | | 83.2166 | 1.160000 | 2 | 4 | 2 | 1 | |
| 49.8579 | 1.827500 | 4 | 2 | 1 | 2 | | 69.5398 | 1.350700 | 2 | 0 | 2 | 4 | | 85.1161 | 1.138900 | 1 | 4 | 0 | 2 | |
| 50.2279 | 1.814900 | 20 | 1 | 3 | 2 | | 69.6578 | 1.348700 | 3 | 3 | 2 | 2 | | 85.2920 | 1.137000 | <1 | 0 | 1 | 5 | |
| 51.9156 | 1.759800 | 3 | 1 | 4 | 1 | | 70.0803 | 1.341600 | 2 | 1 | 5 | 2 | | 85.7309 | 1.132300 | 1 | 3 | 3 | 3 | |
| 52.4539 | 1.743000 | 25 | 1 | 1 | 3 | | 70.8439 | 1.329000 | 1m | 0 | 6 | 0 | | 86.1940 | 1.127400 | 1 | 4 | 1 | 2 | |
| 52.9114 | 1.729000 | 12 | 2 | 3 | 1 | | 70.8439 | 1.329000 | m | 1 | 4 | 3 | | 86.3656 | 1.125600 | 2m | 2 | 3 | 4 | |
| 53.0205 | 1.725700 | 16 | 0 | 2 | 3 | | 72.2986 | 1.305800 | 1 | 2 | 5 | 1 | | 86.3656 | 1.125600 | m | 3 | 5 | 1 | |
| 53.9411 | 1.698400 | 2 | 2 | 2 | 2 | | 72.4464 | 1.303500 | 1 | 1 | 2 | 4 | | 87.9962 | 1.108900 | 2m | 1 | 1 | 5 | |
| 56.1429 | 1.636900 | 3 | 0 | 4 | 2 | | 75.2667 | 1.261500 | 5 | 3 | 3 | 2 | | 87.9962 | 1.108900 | m | 1 | 7 | 0 | |
| 56.4018 | 1.630000 | 1 | 1 | 2 | 3 | | 75.9315 | 1.252100 | 1 | 1 | 6 | 1 | | 88.5389 | 1.103500 | 1m | 0 | 2 | 5 | |
| 56.7891 | 1.619800 | 2 | 3 | 1 | 0 | | 76.6095 | 1.242700 | 3m | 2 | 0 | 4 | | 88.5389 | 1.103500 | m | 4 | 3 | 1 | |
| 59.2273 | 1.558800 | 4 | 3 | 1 | 1 | | 76.6095 | 1.242700 | m | 3 | 4 | 1 | | 89.4092 | 1.095000 | <1 | 4 | 2 | 2 | |
| 60.2095 | 1.535700 | 2 | 0 | 5 | 1 | | 76.7628 | 1.240600 | 4 | 4 | 0 | 0 | | | | | | | | |
| 61.8292 | 1.499300 | 4 | 2 | 4 | 1 | | 77.0640 | 1.236500 | 6 | 3 | 1 | 3 | | | | | | | | |

**01-071-1534** Jun 9, 2020 12:39 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Mg C O3
**Empirical Formula:** C Mg O3 **Weight %:** C14.25 Mg28.83 O56.93 **Atomic %:** C20.00 Mg20.00 O60.00
**ANX:** ABX3 **Compound Name:** Magnesium Carbonate **Mineral Name:** Magnesite, syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.83 **I/Ic - ND:** 1.08

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.637(1) Å **AuthCell c:** 15.023(3) Å **AuthCell Vol:** 279.74 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 46.62 ] **Author's Cell Axial Ratio [ c/a:** 3.240 ]
**Density [ Dcalc:** 3.003 g/cm³ **Dstruc:** 3 g/cm³ ] **SS/FOM:** F(30) = 599.5(0.0014, 36)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.037

**Space Group:** R-3c (167) **Molecular Weight:** 84.31
**Crystal Data [ XtlCell a:** 4.637 Å **XtlCell b:** 4.637 Å **XtlCell c:** 15.023 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 279.74 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.240 **a/b:** 1.000 **c/b:** 3.240 ]
**Reduced Cell [ RedCell a:** 4.637 Å **RedCell b:** 4.637 Å **RedCell c:** 5.678 Å **RedCell α:** 65.90°
**RedCell β:** 65.90° **RedCell γ:** 60.00° **RedCell Vol:** 93.25 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-009-2317** **ADP:** B
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| O | 1 | 18e | .2 | 0.2775 | 0.0 | 0.25 | 1.0 | 0.36879 | 1#a |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | 0.34715 | 3#b |
| Mg | 3 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | 0.35475 | 6-a |

**Anisotropic Displacement Parameters:**

| Atom | Num | Bani11 | Bani22 | Bani33 | Bani12 | Bani13 | Bani23 |
|---|---|---|---|---|---|---|---|
| O | 1 | 0.469464 | 0.646158 | 0.0496549 | 0.323079 | -0.0386154 | -0.0772308 |
| C | 2 | 0.506867 | 0.506867 | 0.0277294 | 0.253433 | 0.0 | 0.0 |
| Mg | 3 | 0.51525 | 0.51525 | 0.034178 | 0.257947 | 0.0 | 0.0 |

**Subfile(s):** Cement and Hydration Product, Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic)
**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 00-002-0875 (Deleted), 00-003-0773 (Deleted), 00-003-0788 (Deleted), 00-008-0479 (Primary), 00-036-0383 (Primary), 01-071-3698 (Alternate), 01-071-6263 (Alternate), 01-080-0042 (Alternate), 01-086-2344 (Alternate), ✓ 04-009-2317 (Primary), ✓ 04-010-3138 (Alternate), ✓ 04-012-1188 (Alternate), ✓ 04-012-1189 (Alternate)

**Entry Date:** 09/01/1998 **Last Modification Date:** 09/01/2011 **Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "The crystal structure of magnesite". Oh, K.D., Morikawa, H., Iwai, S.I., Aoki, H. Am. Mineral. 58, 1029 (1973). |

**Database Comments:** ANX: ABX3. Analysis: C1 Mg1 O3. Formula from original source: Mg (C O3). ICSD Collection Code: 10264. Wyckoff Sequence: e b a(R3-CH). Unit Cell Data Source: Single Crystal.

**d-Spacings (60) - Mg C O3 - 01-071-1534 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 25.1251 | 3.541430 | 5 | 0 | 1 | 2 | | 66.3734 | 1.407240 | 58m | 1 | 0 | 10 | | 83.2825 | 1.159250 | 8 | 2 | 2 | 0 | |
| 32.6175 | **2.743030** | 999 | 1 | 0 | 4 | | 66.3734 | 1.407240 | m | 2 | 1 | 4 | | 86.0062 | 1.129380 | 8 | 2 | 2 | 3 | |
| 35.8342 | 2.503830 | 123 | 0 | 0 | 6 | | 68.3365 | 1.371520 | 18 | 2 | 0 | 8 | | 87.8150 | 1.110720 | 1 | 1 | 3 | 1 | |
| 38.8086 | 2.318500 | 62 | 1 | 1 | 0 | | 69.3074 | 1.354660 | 83m | 1 | 1 | 9 | | 88.7338 | 1.101580 | 10m | 1 | 1 | 12 | |
| 42.9522 | **2.103940** | 480 | 1 | 1 | 3 | | 69.3074 | 1.354660 | m | 1 | 2 | 5 | | 88.7338 | 1.101580 | m | 3 | 1 | 2 | |
| 46.7938 | 1.939770 | 131 | 2 | 0 | 2 | | 70.2611 | 1.338590 | 114 | 3 | 0 | 0 | | 92.3345 | 1.067810 | 70m | 1 | 3 | 4 | |
| 51.5718 | 1.770720 | 49 | 0 | 2 | 4 | | 75.9444 | 1.251920 | 39 | 0 | 0 | 12 | | 92.3345 | 1.067810 | m | 2 | 1 | 10 | |
| 53.8459 | **1.701180** | 389m | 0 | 1 | 8 | | 76.8639 | 1.239220 | 16 | 2 | 1 | 7 | | 94.1467 | 1.051970 | 21 | 2 | 2 | 6 | |
| 53.8459 | **1.701180** | m | 1 | 1 | 6 | | 79.6378 | 1.202880 | 16 | 0 | 2 | 10 | | 95.0518 | 1.044330 | 1 | 3 | 1 | 5 | |
| 61.3377 | 1.510130 | 47 | 2 | 1 | 1 | | 81.4662 | 1.180440 | 28m | 1 | 2 | 8 | | 95.9772 | 1.036700 | 1 | 0 | 1 | 14 | |
| 62.3627 | 1.487750 | 70 | 1 | 2 | 2 | | 81.4662 | 1.180440 | m | 3 | 0 | 6 | | 98.7025 | 1.015240 | 6 | 1 | 2 | 11 | |






| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 101.4432 | 0.995092 | 2 | 0 | 4 | 2 | | 118.8323 | 0.894753 | 6m | 1 | 3 | 10 | | 129.8042 | 0.850589 | m | 2 | 2 | 12 | |
| 102.3714 | 0.988576 | 1 | 1 | 3 | 7 | | 118.8323 | 0.894753 | m | 3 | 2 | 4 | | 130.9773 | 0.846574 | 6 | 3 | 2 | 7 | |
| 105.1587 | 0.969887 | 36 | 4 | 0 | 4 | | 120.9221 | 0.885358 | 29 | 0 | 4 | 8 | | 134.6809 | 0.834711 | 2m | 0 | 0 | 18 | |
| 107.0447 | 0.957954 | 37 | 3 | 1 | 8 | | 121.9765 | 0.880803 | 7 | 2 | 3 | 5 | | 134.6809 | 0.834711 | m | 4 | 0 | 10 | |
| 107.9939 | 0.952155 | 4 | 2 | 2 | 9 | | 123.0447 | 0.876311 | 21m | 1 | 2 | 14 | | 137.2760 | 0.827104 | 13m | 2 | 3 | 8 | |
| 108.9592 | 0.946396 | 6 | 2 | 0 | 14 | | 123.0447 | 0.876311 | m | 4 | 1 | 0 | | 137.2760 | 0.827104 | m | 4 | 1 | 6 | |
| 113.8151 | 0.919418 | 21m | 1 | 1 | 15 | | 126.3427 | 0.863194 | 3m | 1 | 4 | 3 | | 147.6934 | 0.801940 | 1 | 1 | 3 | 13 | |
| 113.8151 | 0.919418 | m | 2 | 1 | 13 | | 126.3427 | 0.863194 | m | 3 | 1 | 11 | | 149.4430 | 0.798502 | 12m | 2 | 1 | 16 | |
| 114.7974 | 0.914344 | 73 | 0 | 3 | 12 | | 129.8042 | 0.850589 | 10m | 0 | 2 | 16 | | 149.4430 | 0.798502 | m | 5 | 0 | 2 | |

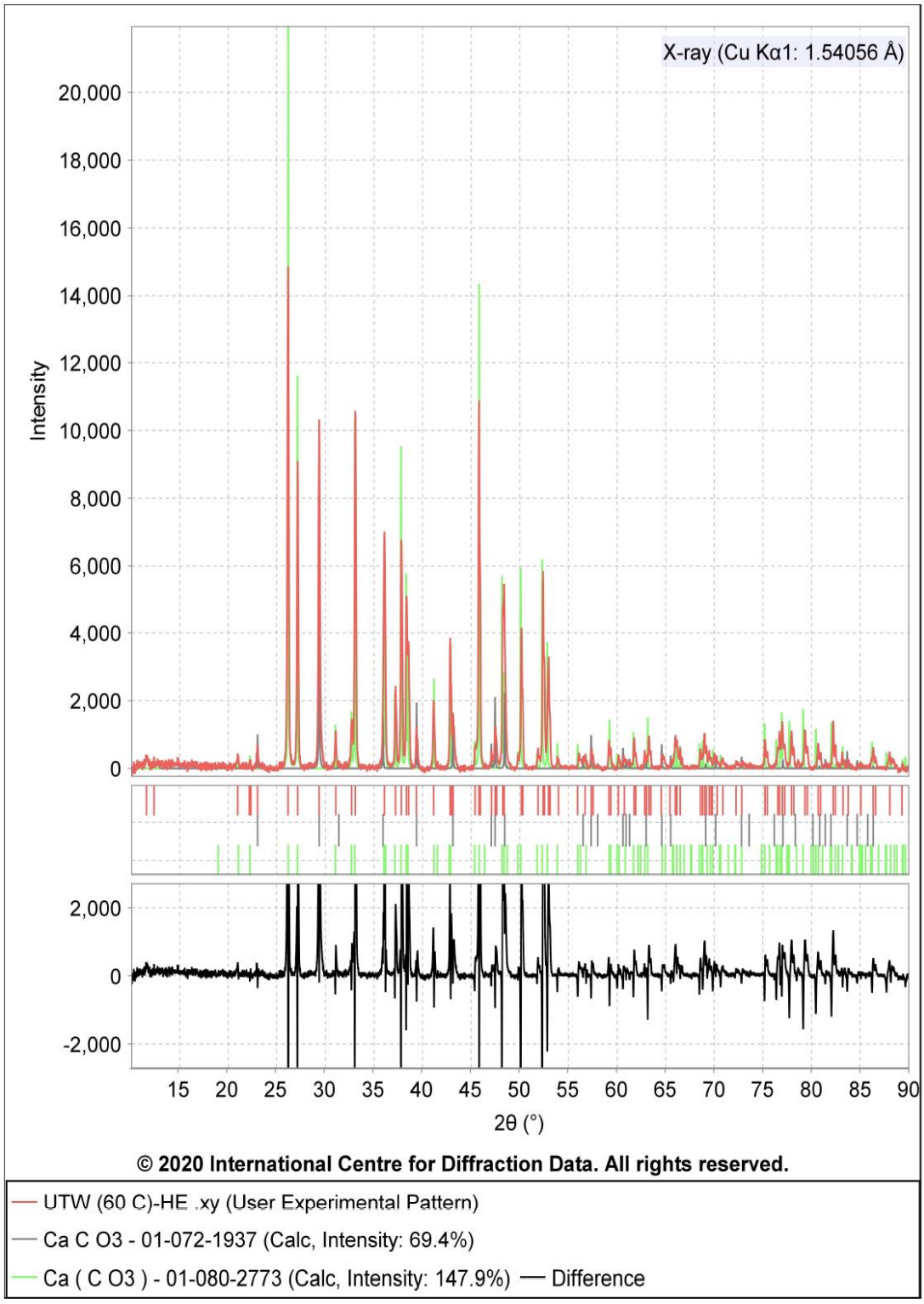


**Figure E.7 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 60 °C from accelerated scale simulation study**

# SIeve+ Report

## Experiment

**Search Line:** 1.974036 Å **D1 Range:** 1.968 Å - 1.980 Å
**Search Line:** 1.740186 Å **D1 Range:** 1.736 Å - 1.745 Å
**Search Line:** 2.487231 Å **D1 Range:** 2.477 Å - 2.497 Å
**Search Line:** 2.706595 Å **D1 Range:** 2.695 Å - 2.719 Å
**Search Line:** 2.103234 Å **D1 Range:** 2.096 Å - 2.110 Å
**Search Line:** 3.039483 Å **D1 Range:** 3.024 Å - 3.055 Å
**Search Line:** 1.811916 Å **D1 Range:** 1.807 Å - 1.817 Å
**Search Line:** 1.879290 Å **D1 Range:** 1.874 Å - 1.885 Å
**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (2)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 01-072-1937 | S | Calcium Carbonate | 0.694 | 31.937 | 3.23 | 14 |
| 2 | true | 01-080-2773 | S | Calcium Carbonate | 1.479 | 68.063 | *1.14 | 86 |

**01-080-2773** Jun 9, 2020 1:46 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Temperature (Non-ambient) **Chemical Formula:** Ca ( C O3 )
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Aragonite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.19 **I/Ic - ND:** 0.52

**SYS:** Orthorhombic **SPGR:** Pmcn (62)
**Author's Cell [ AuthCell a:** 4.9605(4) Å **AuthCell b:** 7.9925(6) Å **AuthCell c:** 5.7629(5) Å
**AuthCell Vol:** 228.48 Å$^3$ **AuthCell Z:** 4.00 **AuthCell MolVol:** 57.12 ]
**Author's Cell Axial Ratio [ c/a:** 1.162 **a/b:** 0.621 **c/b:** 0.721 ]
**Density [ Dcalc:** 2.91 g/cm$^3$ **Dstruc:** 2.91 g/cm$^3$ ] **SS/FOM:** F(30) = 999.9(0.0001, 32)
**Temp:** 408.0 K (Author provided temperature) **R-factor:** 0.0329

**Space Group:** Pnam (62) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 5.763 Å **XtlCell b:** 7.992 Å **XtlCell c:** 4.960 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 228.48 Å$^3$ **XtlCell Z:** 4.00 ]
**Crystal Data Axial Ratio [ c/a:** 0.861 **a/b:** 0.721 **c/b:** 0.621 ]
**Reduced Cell [ RedCell a:** 4.960 Å **RedCell b:** 5.763 Å **RedCell c:** 7.992 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 90.00° **RedCell Vol:** 228.48 Å$^3$ ]

**Atomic parameters are cross-referenced from PDF entry 04-008-5421** **ADP:** B
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -x+1/2,-y+1/2,z+1/2 | 5 | x+1/2,-y,-z | 7 | -x,y+1/2,-z+1/2 |
| 2 | -x,-y,-z | 4 | x+1/2,y+1/2,-z+1/2 | 6 | -x+1/2,y,z | 8 | x,-y+1/2,z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 4c | m.. | 0.25 | 0.41508 | 0.24046 | 1.0 | 0.61095 | 9-a |
| C | 2 | 4c | m.. | 0.25 | 0.76211 | 0.08518 | 1.0 | 0.43867 | 3#a |
| O | 3 | 4c | m.. | 0.25 | 0.92224 | 0.09557 | 1.0 | 0.77616 | 1#a |
| O | 4 | 8d | 1 | 0.47347 | 0.68065 | 0.08726 | 1.0 | 0.70856 | 1#a |

**Anisotropic Displacement Parameters:**

| Atom | Num | Bani11 | Bani22 | Bani33 | Bani12 | Bani13 | Bani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.665479 | 0.670266 | 0.497141 | 0.0 | 0.0 | 0.0201231 |
| C | 2 | 0.442997 | 0.573788 | 0.299269 | 0.0 | 0.0 | 0.0073175 |
| O | 3 | 1.13407 | 0.540783 | 0.653666 | 0.0 | 0.0 | -0.05854 |
| O | 4 | 0.509938 | 0.926694 | 0.689106 | 0.180227 | -0.0136696 | 0.0841512 |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**Mineral Classification:** Aragonite (Group), carbonate (Subgroup) **Pearson Symbol:** oP20.00

**Cross-Ref PDF #'s:** 00-001-0628 (Deleted), 00-003-0405 (Deleted), 00-003-0425 (Deleted), 00-003-1067 (Deleted), 00-005-0453 (Alternate), 00-041-1475 (Primary), ✓ 00-061-0390 (Primary), 01-071-2392 (Alternate), 01-071-2396 (Alternate), 01-071-3700 (Alternate), 01-071-4891 (Alternate), 01-075-9982 (Alternate), 01-075-9983 (Alternate), 01-075-9984 (Alternate), 01-075-9985 (Alternate), 01-075-9986 (Alternate), 01-075-9987 (Alternate), 01-076-0606 (Alternate), 01-078-4337 (Alternate), 01-078-4338 (Alternate), 01-078-4339 (Alternate), 01-080-2768 (Alternate), 01-080-2769 (Alternate), 01-080-2770 (Alternate), 01-080-2771 (Alternate), 01-080-2772 (Alternate), 01-080-2774 (Alternate), 01-080-2775 (Alternate), 01-080-2789 (Alternate), 01-080-2790 (Alternate), ✓ 04-006-5441 (Alternate), ✓ 04-006-5444 (Alternate), ✓ 04-006-6531 (Alternate), ✓ 04-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate), ✓ 04-014-1837 (Alternate), ✓ 04-015-4109 (Alternate), ✓ 04-017-9180 (Alternate)

**Entry Date:** 09/01/2013

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "Temperature dependence of the structural parameters in the transformation of aragonite to calcite, as determined from in situ synchrotron powder x-ray-diffraction data". Antao, S.M., Hassan, I. Can. Mineral. 48, 1225 (2010). |

**01-080-2773** Jun 9, 2020 1:46 PM (fal-sharji2)

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca (C O3). ICSD Collection Code: 169895. Sample Source or Locality: Cuenca,Spain. Temperature of Data Collection: 408 K. Wyckoff Sequence: d c3 (PMCN). Unit Cell Data Source: Powder Diffraction.

**d-Spacings (198) - Ca ( C O3 ) - 01-080-2773 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.9693 | 4.674490 | 4 | 0 | 1 | 1 | | 77.7084 | 1.227850 | m | 1 | 3 | 4 | | 108.4014 | 0.949707 | 1 | 5 | 2 | 1 | |
| 21.0610 | 4.214730 | 16 | 1 | 1 | 0 | | 78.4768 | 1.217740 | 8 | 2 | 5 | 2 | | 109.3790 | 0.943934 | 1 | 0 | 8 | 2 | |
| 22.2267 | 3.996250 | 16 | 0 | 2 | 0 | | 79.1464 | 1.209110 | 73m | 0 | 6 | 2 | | 109.5447 | 0.942969 | 1 | 1 | 0 | 6 | |
| 26.1729 | **3.401980** | 999 | 1 | 1 | 1 | | 79.1464 | 1.209110 | m | 2 | 4 | 3 | | 110.0783 | 0.939889 | 6 | 4 | 0 | 4 | |
| 27.1313 | **3.283940** | 525 | 0 | 2 | 1 | | 80.4573 | 1.192680 | 50 | 1 | 5 | 3 | | 110.2355 | 0.938989 | 12m | 3 | 1 | 5 | |
| 31.0102 | 2.881450 | 56 | 0 | 0 | 2 | | 80.7298 | 1.189340 | 3 | 2 | 2 | 4 | | 110.2355 | 0.938989 | m | 3 | 7 | 0 | |
| 32.6759 | 2.738260 | 79 | 1 | 2 | 1 | | 81.1359 | 1.184410 | 1 | 4 | 2 | 0 | | 110.3993 | 0.938055 | 4 | 5 | 0 | 2 | |
| 33.0180 | 2.710670 | 494 | 0 | 1 | 2 | | 82.0477 | 1.173540 | 56 | 2 | 6 | 0 | | 110.6782 | 0.936474 | 2 | 1 | 1 | 6 | |
| 36.0163 | 2.491590 | 184 | 1 | 0 | 2 | | 82.4681 | 1.168620 | 5 | 0 | 4 | 4 | | 110.9580 | 0.934898 | 3 | 0 | 5 | 5 | |
| 36.1866 | 2.480250 | 171 | 2 | 0 | 0 | | 83.2026 | 1.160160 | 27 | 4 | 2 | 1 | | 111.2157 | 0.933457 | 4m | 0 | 2 | 6 | |
| 37.1477 | 2.418260 | 96 | 0 | 3 | 1 | | 84.1100 | 1.149940 | 1m | 2 | 6 | 1 | | 111.2157 | 0.933457 | m | 4 | 1 | 4 | |
| 37.7888 | 2.378690 | 423 | 1 | 1 | 2 | | 84.1100 | 1.149940 | m | 3 | 5 | 0 | | 111.5392 | 0.931660 | 9 | 5 | 1 | 2 | |
| 38.3175 | 2.347080 | 275 | 1 | 3 | 0 | | 85.0967 | 1.139110 | 8 | 4 | 0 | 2 | | 111.8900 | 0.929728 | 10 | 5 | 3 | 0 | |
| 38.4851 | 2.337240 | 167 | 0 | 2 | 2 | | 85.5725 | 1.133990 | 3 | 3 | 3 | 3 | | 112.3339 | 0.927307 | 9m | 1 | 8 | 2 | |
| 41.1674 | 2.190940 | 116 | 2 | 1 | 1 | | 86.2254 | 1.127070 | 33m | 3 | 5 | 1 | | 112.3339 | 0.927307 | m | 3 | 7 | 1 | |
| 41.5087 | 2.173710 | 6 | 1 | 3 | 1 | | 86.2254 | 1.127070 | m | 4 | 1 | 2 | | 112.5444 | 0.926168 | 12m | 2 | 4 | 5 | |
| 42.8790 | 2.107360 | 175 | 2 | 2 | 0 | | 86.9036 | 1.120010 | 1 | 0 | 7 | 1 | | 112.5444 | 0.926168 | m | 2 | 8 | 0 | |
| 45.3499 | 1.998120 | 35 | 0 | 4 | 0 | | 87.7119 | 1.111760 | 20m | 1 | 1 | 5 | | 112.9799 | 0.923831 | 4 | 4 | 4 | 3 | |
| 45.8084 | **1.979180** | 626 | 2 | 2 | 1 | | 87.7119 | 1.111760 | m | 1 | 7 | 0 | | 113.9483 | 0.918723 | 14 | 1 | 5 | 5 | |
| 46.3788 | 1.956160 | 4 | 0 | 3 | 2 | | 88.1421 | 1.107440 | 14 | 0 | 2 | 5 | | 114.6784 | 0.914952 | 23m | 2 | 8 | 1 | |
| 48.1605 | 1.887870 | 266 | 0 | 4 | 1 | | 88.5399 | 1.103490 | 2 | 4 | 3 | 1 | | 114.6784 | 0.914952 | m | 4 | 2 | 4 | |
| 48.3809 | 1.879780 | 134 | 2 | 0 | 2 | | 88.7908 | 1.101020 | 1 | 2 | 5 | 3 | | 115.6804 | 0.909887 | 8 | 2 | 6 | 4 | |
| 48.7119 | 1.867780 | 4 | 0 | 1 | 3 | | 89.3606 | 1.095470 | 10m | 0 | 6 | 3 | | 116.1267 | 0.907671 | 10 | 4 | 6 | 0 | |
| 49.7895 | 1.829850 | 22 | 2 | 1 | 2 | | 89.3606 | 1.095470 | m | 4 | 2 | 2 | | 116.9687 | 0.903557 | 1 | 0 | 3 | 6 | |
| 50.0842 | 1.819770 | 260 | 1 | 3 | 2 | | 89.6680 | 1.092510 | 13 | 1 | 7 | 1 | | 118.0432 | 0.898431 | 5 | 3 | 5 | 4 | |
| 51.7699 | 1.764410 | 19 | 1 | 4 | 1 | | 90.2618 | 1.086860 | 15m | 2 | 6 | 2 | | 118.6343 | 0.895669 | 8 | 2 | 0 | 6 | |
| 52.2934 | 1.747970 | 267 | 1 | 1 | 3 | | 90.2618 | 1.086860 | m | 3 | 0 | 4 | | 119.1565 | 0.893263 | 9 | 3 | 7 | 2 | |
| 52.8347 | 1.731330 | 161m | 0 | 2 | 3 | | 90.9059 | 1.080830 | 1 | 1 | 2 | 5 | | 120.1146 | 0.888930 | 15 | 1 | 3 | 6 | |
| 52.8347 | 1.731330 | m | 2 | 3 | 1 | | 91.3926 | 1.076340 | 5 | 3 | 1 | 4 | | 120.6951 | 0.886355 | 4m | 0 | 8 | 3 | |
| 53.8524 | 1.700990 | 31 | 2 | 2 | 2 | | 92.0693 | 1.070190 | 1 | 0 | 5 | 4 | | 120.6951 | 0.886355 | m | 4 | 3 | 4 | |
| 55.9543 | 1.641970 | 30 | 0 | 4 | 2 | | 92.3703 | 1.067490 | 9 | 3 | 5 | 2 | | 121.0475 | 0.884810 | 15 | 5 | 3 | 2 | |
| 56.2278 | 1.634630 | 1 | 1 | 2 | 3 | | 93.0474 | 1.061490 | 1m | 0 | 7 | 2 | | 121.6492 | 0.882204 | 4 | 2 | 8 | 2 | |
| 56.8116 | 1.619210 | 17 | 3 | 1 | 0 | | 93.0474 | 1.061490 | m | 3 | 4 | 3 | | 122.0166 | 0.880632 | 6 | 1 | 7 | 4 | |
| 59.2253 | 1.558850 | 62m | 0 | 3 | 3 | | 93.5447 | 1.057150 | 8m | 0 | 3 | 5 | | 122.5876 | 0.878218 | 2m | 0 | 9 | 1 | |
| 59.2253 | 1.558850 | m | 3 | 1 | 1 | | 93.5447 | 1.057150 | m | 2 | 4 | 4 | | 122.5876 | 0.878218 | m | 5 | 4 | 1 | |
| 59.3446 | 1.556000 | 22 | 2 | 4 | 0 | | 93.9469 | 1.053680 | 4 | 4 | 4 | 0 | | 123.0789 | 0.876169 | 13 | 5 | 1 | 3 | |
| 60.0094 | 1.540340 | 18 | 0 | 5 | 1 | | 94.8379 | 1.046120 | 6 | 1 | 5 | 4 | | 123.6092 | 0.873986 | 11m | 1 | 9 | 0 | |
| 60.1991 | 1.535940 | 9 | 2 | 3 | 2 | | 95.8192 | 1.037990 | 13 | 1 | 7 | 2 | | 123.6092 | 0.873986 | m | 2 | 2 | 6 | |
| 60.8327 | 1.521450 | 2 | 1 | 5 | 0 | | 96.0017 | 1.036500 | 32m | 2 | 1 | 5 | | 125.6817 | 0.865734 | 15m | 0 | 4 | 6 | |
| 61.6963 | 1.502210 | 46 | 2 | 4 | 1 | | 96.0017 | 1.036500 | m | 4 | 4 | 1 | | 125.6817 | 0.865734 | m | 4 | 6 | 2 | |
| 62.8747 | 1.476860 | 20 | 3 | 2 | 1 | | 97.9833 | 1.020760 | 3m | 2 | 7 | 1 | | 127.6078 | 0.858453 | 1 | 1 | 6 | 5 | |
| 63.1516 | 1.471050 | 63 | 1 | 5 | 1 | | 97.9833 | 1.020760 | m | 3 | 6 | 1 | | 128.6476 | 0.854673 | 1 | 3 | 4 | 5 | |
| 64.6403 | 1.440720 | 4 | 0 | 0 | 4 | | 99.2345 | 1.011220 | 21 | 2 | 2 | 5 | | 129.8309 | 0.850496 | 4 | 4 | 4 | 4 | |
| 64.9727 | 1.434150 | 1 | 3 | 0 | 2 | | 99.6416 | 1.008180 | 19 | 4 | 2 | 3 | | 130.2710 | 0.848976 | 2m | 0 | 9 | 2 | |
| 65.8124 | 1.417870 | 19m | 0 | 1 | 4 | | 99.9578 | 1.005840 | 29 | 3 | 3 | 4 | | 130.2710 | 0.848976 | m | 2 | 3 | 6 | |
| 65.8124 | 1.417870 | m | 2 | 2 | 3 | | 100.5579 | 1.001450 | 4 | 2 | 6 | 3 | | 131.1970 | 0.845836 | 1 | 3 | 8 | 1 | |
| 66.1421 | 1.411600 | 32 | 3 | 1 | 2 | | 100.9818 | 0.998388 | 9m | 0 | 4 | 5 | | 131.7477 | 0.844006 | 16 | 3 | 7 | 3 | |
| 66.4978 | 1.404910 | 29 | 3 | 3 | 0 | | 100.9818 | 0.998388 | m | 0 | 8 | 0 | | 132.4417 | 0.841738 | 3m | 2 | 7 | 4 | |
| 67.6615 | 1.383550 | 5m | 0 | 4 | 3 | | 102.2252 | 0.989592 | 7 | 4 | 4 | 2 | | 132.4417 | 0.841738 | m | 3 | 6 | 4 | |
| 67.6615 | 1.383550 | m | 1 | 0 | 4 | | 102.7101 | 0.986235 | 15 | 3 | 5 | 3 | | 133.1144 | 0.839581 | 1 | 4 | 1 | 5 | |
| 68.4723 | 1.369130 | 30 | 2 | 4 | 2 | | 102.9806 | 0.984380 | 12m | 0 | 8 | 1 | | 134.0942 | 0.836510 | 16m | 1 | 9 | 2 | |
| 68.8073 | 1.363280 | 35 | 1 | 1 | 4 | | 102.9806 | 0.984380 | m | 5 | 1 | 0 | | 134.0942 | 0.836510 | m | 5 | 3 | 3 | |
| 69.2677 | 1.355340 | 17 | 0 | 2 | 4 | | 103.2387 | 0.982621 | 3 | 2 | 5 | 4 | | 134.6980 | 0.834659 | 10 | 2 | 8 | 3 | |
| 69.5899 | 1.349850 | 3 | 3 | 2 | 2 | | 103.9130 | 0.978080 | 12m | 0 | 6 | 4 | | 134.8923 | 0.834070 | 10 | 5 | 5 | 1 | |
| 69.8523 | 1.345420 | 23 | 1 | 5 | 2 | | 103.9130 | 0.978080 | m | 1 | 4 | 5 | | 135.8551 | 0.831199 | 1 | 4 | 7 | 1 | |
| 70.6556 | 1.332080 | 16 | 0 | 6 | 0 | | 104.2451 | 0.975871 | 8m | 2 | 7 | 2 | | 136.0830 | 0.830531 | 1 | 3 | 0 | 6 | |
| 71.4380 | 1.319400 | 1 | 2 | 3 | 3 | | 104.2451 | 0.975871 | m | 3 | 6 | 2 | | 137.4016 | 0.826750 | 6 | 6 | 0 | 0 | |
| 72.1240 | 1.308530 | 4m | 1 | 2 | 4 | | 104.6767 | 0.973027 | 3 | 2 | 3 | 5 | | 137.6621 | 0.826020 | 16m | 3 | 1 | 6 | |
| 72.1240 | 1.308530 | m | 2 | 5 | 1 | | 105.0668 | 0.970483 | 14m | 4 | 3 | 3 | | 137.6621 | 0.826020 | m | 4 | 2 | 5 | |
| 72.8116 | 1.297860 | 2 | 0 | 6 | 1 | | 105.0668 | 0.970483 | m | 5 | 1 | 1 | | 139.0191 | 0.822307 | 1 | 2 | 6 | 5 | |
| 75.1758 | 1.262800 | 57 | 3 | 3 | 2 | | 105.7684 | 0.965968 | 2m | 1 | 8 | 1 | | 139.5161 | 0.820984 | 1m | 0 | 8 | 4 | |
| 75.6825 | 1.255600 | 1 | 1 | 6 | 1 | | 105.7684 | 0.965968 | m | 4 | 5 | 1 | | 139.5161 | 0.820984 | m | 4 | 6 | 3 | |
| 76.3844 | 1.245800 | 36 | 2 | 0 | 4 | | 106.2631 | 0.962832 | 20 | 1 | 7 | 3 | | 139.9823 | 0.819761 | 1 | 3 | 8 | 2 | |
| 76.7979 | 1.240120 | 43 | 4 | 0 | 0 | | 106.6376 | 0.960483 | 12 | 0 | 0 | 6 | | 140.2997 | 0.818938 | 1 | 0 | 1 | 7 | |
| 76.9491 | 1.238060 | 70 | 3 | 1 | 3 | | 107.6348 | 0.954333 | 1 | 3 | 4 | 4 | | 140.9357 | 0.817313 | 4m | 2 | 4 | 6 | |
| 77.7084 | 1.227850 | 58m | 0 | 5 | 3 | | 107.7517 | 0.953622 | 1 | 0 | 1 | 6 | | 140.9357 | 0.817313 | m | 5 | 0 | 4 | |

**01-072-1937** Jun 9, 2020 1:46 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca C O3
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Calcite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 3.23 **I/Ic - ND:** 0.89

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.994(2) Å **AuthCell c:** 17.081(5) Å **AuthCell Vol:** 368.93 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 61.49 ] **Author's Cell Axial Ratio [ c/a:** 3.420 ]
**Density [ Dcalc:** 2.703 g/cm³ **Dstruc:** 2.7 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.019

**Space Group:** R-3c (167) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 4.994 Å **XtlCell b:** 4.994 Å **XtlCell c:** 17.081 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 368.93 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.420 **a/b:** 1.000 **c/b:** 3.420 ]
**Reduced Cell [ RedCell a:** 4.994 Å **RedCell b:** 4.994 Å **RedCell c:** 6.382 Å **RedCell α:** 66.97°
**RedCell β:** 66.97° **RedCell γ:** 60.00° **RedCell Vol:** 122.97 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-007-8659**
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | IDP | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | | 6-a |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | | 3#b |
| O | 3 | 18e | .2 | 0.2593 | 0.0 | 0.25 | 1.0 | | 1#a |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Pigment/Dye, Superconducting Material

**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 00-001-0837 (Deleted), 00-002-0623 (Deleted), 00-002-0629 (Deleted), 00-003-0569 (Deleted), 00-003-0596 (Deleted), 00-003-0670 (Deleted), 00-004-0636 (Deleted), 00-004-0637 (Deleted), 00-005-0586 (Primary), 00-024-0027 (Deleted), 00-047-1743 (Primary), 01-071-3699 (Alternate), 01-072-4582 (Alternate), 01-075-6049 (Alternate), 01-078-3262 (Alternate), 01-078-4614 (Alternate), 01-078-4615 (Alternate), 01-080-2791 (Alternate), 01-080-2792 (Alternate), 01-080-2793 (Alternate), 01-080-2794 (Alternate), 01-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 01-080-2799 (Alternate), 01-080-2800 (Alternate), 01-080-2801 (Alternate), 01-080-2802 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2806 (Alternate), 01-080-2807 (Alternate), 01-080-2808 (Alternate), 01-080-2809 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-9775 (Alternate), 01-080-9776 (Alternate), 01-083-0577 (Alternate), 01-083-0578 (Alternate), 01-085-0849 (Alternate), 01-086-2334 (Alternate), 01-086-2339 (Alternate), 01-086-2340 (Alternate), 01-086-2341 (Alternate), 01-086-2342 (Alternate), 01-086-2343 (Alternate), ✓ 04-001-7249 (Alternate), ✓ 04-002-9082 (Alternate), ✓ 04-006-6528 (Alternate), ✓ 04-007-0049 (Alternate), ✓ 04-007-2808 (Alternate), ✓ 04-007-4388 (Alternate), ✓ 04-007-8659 (Primary), ✓ 04-008-0198 (Alternate), ✓ 04-008-0212 (Alternate), ✓ 04-008-0213 (Alternate), ✓ 04-008-0788 (Alternate), ✓ 04-012-0489 (Primary), ✓ 04-012-8072 (Alternate), ✓ 04-016-9713 (Alternate)

**CAS Number - PR:** 13397-26-7 **Entry Date:** 09/01/1998 **Last Modification Date:** 09/01/2011
**Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++ (2004). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "The isomorphous series calcite - otavite". Borodin, V.L., Lutin, V.I., Ilyukhin, V.V., Belov, N.V. Dokl. Akad. Nauk SSSR 245, 1099 (1979). |

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca (C O3). ICSD Collection Code: 20179. Sample Source or Locality: Specimen unknown. Wyckoff Sequence: e b a(R3-CH). Unit Cell Data Source: Single Crystal.




**01-072-1937** Jun 9, 2020 1:46 PM (fal-sharji2)

**d-Spacings (78) - Ca C O3 - 01-072-1937 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.0315 | 3.858400 | 95 | 0 | 1 | 2 | | 80.8512 | 1.187860 | 5 | 3 | 1 | 2 | | 109.4059 | 0.943777 | 18 | 4 | 1 | 0 | |
| 29.3686 | **3.038670** | 999 | 1 | 0 | 4 | | 81.4203 | 1.180990 | 24 | 2 | 1 | 10 | | 110.3023 | 0.938608 | 10 | 2 | 2 | 12 | |
| 31.3969 | 2.846830 | 19 | 0 | 0 | 6 | | 81.9883 | 1.174240 | 3 | 0 | 1 | 14 | | 111.6455 | 0.931073 | 1 | 4 | 1 | 3 | |
| 35.9356 | 2.497000 | 144 | 1 | 1 | 0 | | 83.6739 | 1.154820 | 43 | 1 | 3 | 4 | | 113.8704 | 0.919129 | 2 | 3 | 2 | 7 | |
| 39.3693 | 2.286760 | 183 | 1 | 1 | 3 | | 84.7045 | 1.143380 | 20 | 2 | 2 | 6 | | 114.9470 | 0.913582 | 1 | 4 | 0 | 10 | |
| 43.1163 | 2.096310 | 155 | 2 | 0 | 2 | | 85.7798 | 1.131780 | 1 | 3 | 1 | 5 | | 117.7542 | 0.899796 | 8 | 2 | 3 | 8 | |
| 47.0656 | 1.929200 | 68 | 0 | 2 | 4 | | 86.3436 | 1.125830 | 4 | 1 | 2 | 11 | | 118.5992 | 0.895832 | 8 | 1 | 4 | 6 | |
| 47.4483 | **1.914530** | 196 | 0 | 1 | 8 | | 91.3762 | 1.076490 | 1 | 1 | 3 | 7 | | 119.0322 | 0.893833 | 9 | 2 | 1 | 16 | |
| 48.4512 | **1.877220** | 205 | 1 | 1 | 6 | | 91.7950 | 1.072670 | 1 | 0 | 4 | 2 | | 120.5380 | 0.887048 | 9 | 1 | 1 | 18 | |
| 56.5060 | 1.627240 | 33 | 2 | 1 | 1 | | 92.9201 | 1.062610 | 8 | 2 | 0 | 14 | | 127.0340 | 0.860584 | 2 | 5 | 0 | 2 | |
| 57.3403 | 1.605530 | 94 | 1 | 2 | 2 | | 94.5955 | 1.048160 | 26 | 4 | 0 | 4 | | 127.7415 | 0.857961 | 8 | 3 | 2 | 10 | |
| 58.0056 | 1.588690 | 11 | 1 | 0 | 10 | | 94.8784 | 1.045780 | 30 | 3 | 1 | 8 | | 128.2812 | 0.855993 | 2 | 1 | 2 | 17 | |
| 60.6042 | 1.526640 | 55 | 2 | 1 | 4 | | 96.0079 | 1.036450 | 14m | 1 | 0 | 16 | | 128.4559 | 0.855362 | 3 | 3 | 1 | 14 | |
| 60.9262 | 1.519340 | 24 | 2 | 0 | 8 | | 96.0079 | 1.036450 | m | 1 | 1 | 15 | | 130.6242 | 0.847769 | 7 | 0 | 5 | 4 | |
| 61.2995 | 1.510980 | 25 | 1 | 1 | 9 | | 97.5532 | 1.024110 | 2 | 2 | 1 | 13 | | 131.4301 | 0.845058 | 1 | 4 | 1 | 9 | |
| 62.9845 | 1.474550 | 20 | 1 | 2 | 5 | | 99.0126 | 1.012890 | 26 | 0 | 3 | 12 | | 132.5646 | 0.841341 | 1 | 2 | 2 | 15 | |
| 64.5940 | 1.441640 | 62 | 3 | 0 | 0 | | 102.0898 | 0.990537 | 3 | 3 | 2 | 1 | | 133.6570 | 0.837870 | 8 | 0 | 1 | 20 | |
| 65.5236 | 1.423420 | 34 | 0 | 0 | 12 | | 102.8057 | 0.985578 | 12 | 2 | 3 | 2 | | 134.2277 | 0.836098 | 1 | 2 | 3 | 11 | |
| 69.1075 | 1.358090 | 11 | 2 | 1 | 7 | | 103.3829 | 0.981644 | 4 | 1 | 3 | 10 | | 135.4717 | 0.832333 | 4 | 3 | 3 | 0 | |
| 70.1529 | 1.340390 | 20 | 0 | 2 | 10 | | 103.9614 | 0.977757 | 10 | 1 | 2 | 14 | | 138.5477 | 0.823580 | 1 | 3 | 3 | 3 | |
| 72.8057 | 1.297950 | 29 | 1 | 2 | 8 | | 105.6912 | 0.966461 | 10 | 3 | 2 | 4 | | 141.2982 | 0.816401 | 1 | 2 | 4 | 1 | |
| 73.5842 | 1.286130 | 7 | 3 | 0 | 6 | | 105.9833 | 0.964601 | 18 | 0 | 4 | 8 | | 142.4302 | 0.813618 | 8 | 4 | 2 | 2 | |
| 76.1896 | 1.248500 | 12 | 2 | 2 | 0 | | 107.1563 | 0.957265 | 5 | 0 | 2 | 16 | | 144.3148 | 0.809201 | 1 | 0 | 4 | 14 | |
| 77.0567 | 1.236600 | 21 | 1 | 1 | 12 | | 107.8820 | 0.952832 | 2 | 2 | 3 | 5 | | 147.2902 | 0.802763 | 8 | 2 | 4 | 4 | |
| 78.3403 | 1.219520 | 1 | 2 | 2 | 3 | | 108.4736 | 0.949276 | 1m | 0 | 0 | 18 | | 147.8140 | 0.801696 | 6 | 5 | 0 | 8 | |
| 80.1425 | 1.196570 | 1 | 1 | 3 | 1 | | 108.4736 | 0.949276 | m | 3 | 1 | 11 | | 149.2409 | 0.798888 | 8 | 3 | 3 | 6 | |

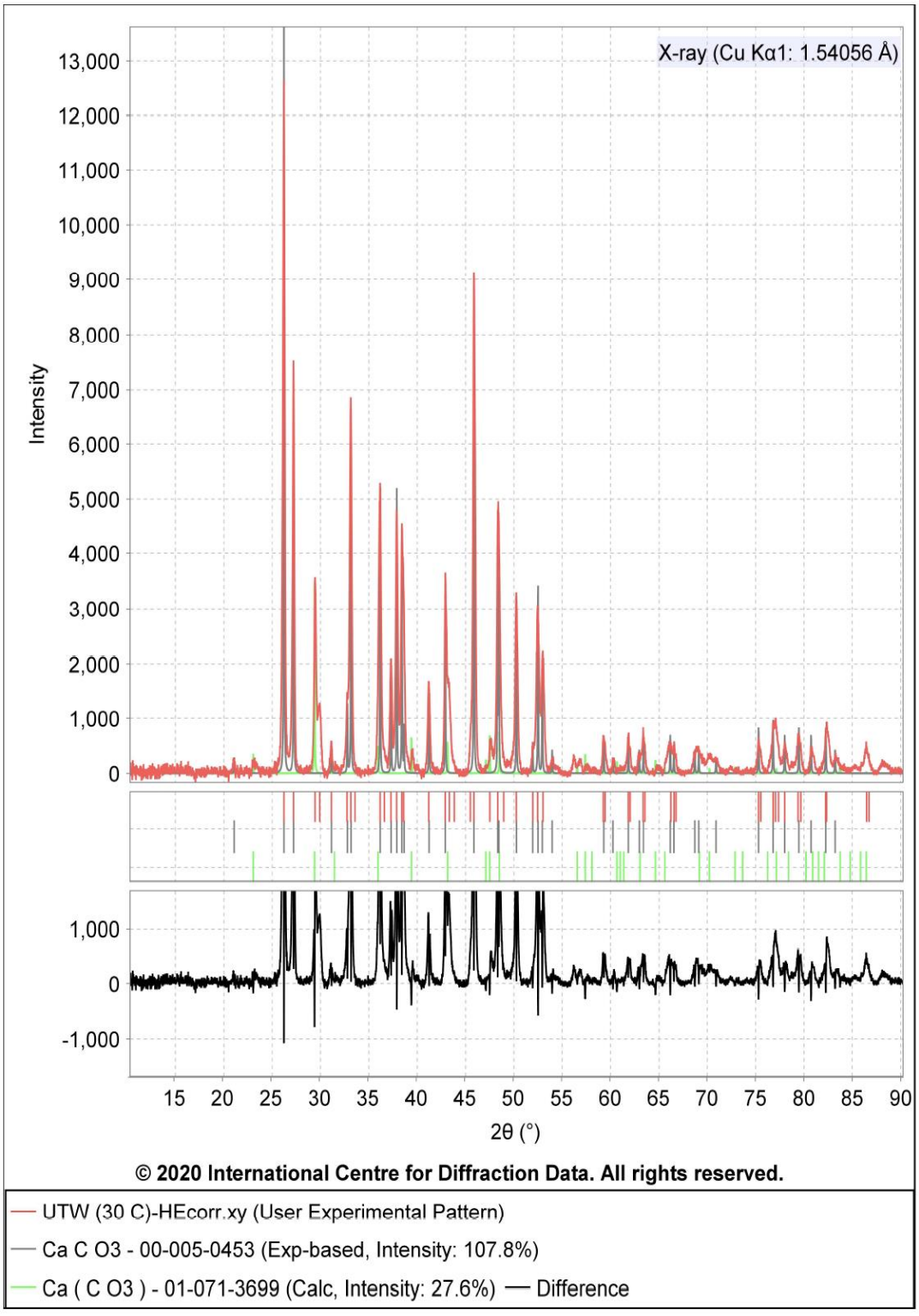


**Figure E.8 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 30 °C from accelerated scale simulation study**

# SIeve+ Report

## Experiment

**Search Line:** 2.330781 Å **D1 Range:** 2.322 Å - 2.339 Å
**Search Line:** 2.086682 Å **D1 Range:** 2.080 Å - 2.094 Å
**Search Line:** 2.983988 Å **D1 Range:** 2.969 Å - 2.999 Å
**Search Line:** 1.170193 Å **D1 Range:** 1.168 Å - 1.172 Å
**Search Line:** 1.236700 Å **D1 Range:** 1.235 Å - 1.239 Å
**Search Line:** 2.481368 Å **D1 Range:** 2.471 Å - 2.491 Å
**Search Line:** 1.992372 Å **D1 Range:** 1.986 Å - 1.999 Å
**Search Line:** 1.553837 Å **D1 Range:** 1.550 Å - 1.557 Å
**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (2)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 00-005-0453 | I | Calcium Carbonate | 1.078 | 79.593 | *1.14 | 92 |
| 2 | true | 01-071-3699 | S | Calcium Carbonate | 0.276 | 20.407 | 3.23 | 8 |

**00-005-0453** Jun 9, 2020 2:05 PM (fal-sharji2)

**Status** Alternate **QM:** Indexed **Pressure/Temperature:** Ambient **Chemical Formula:** Ca C O3
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**Compound Name:** Calcium Carbonate **Mineral Name:** Aragonite, syn

**Radiation:** CuKα1 **λ:** 1.5405 Å **Filter:** Ni Beta **Intensity:** Diffractometer

**SYS:** Orthorhombic **SPGR:** Pmcn (62)
**Author's Cell [ AuthCell a:** 4.959 Å **AuthCell b:** 7.968 Å **AuthCell c:** 5.741 Å **AuthCell Vol:** 226.85 Å³
**AuthCell Z:** 4.00 **AuthCell MolVol:** 56.71 ] **Author's Cell Axial Ratio [ c/a:** 1.158 **a/b:** 0.622 **c/b:** 0.721 ]
**Density [ Dcalc:** 2.931 g/cm³ **Dmeas:** 2.947 g/cm³ ] **SS/FOM:** F(30) = 28.7(0.0180, 58)
**Temp:** 299.0 K (Author provided temperature) **Color:** Colorless

**Space Group:** Pnam (62) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 5.741 Å **XtlCell b:** 7.968 Å **XtlCell c:** 4.959 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 226.85 Å³ **XtlCell Z:** 4.00 ]
**Crystal Data Axial Ratio [ c/a:** 0.864 **a/b:** 0.721 **c/b:** 0.622 ]
**Reduced Cell [ RedCell a:** 4.959 Å **RedCell b:** 5.741 Å **RedCell c:** 7.968 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 90.00° **RedCell Vol:** 226.85 Å³ ]

**εα:** =1.530 **πωβ:** =1.6810 **εγ:** =1.6854 **Sign:** =- **2V:** =18°

**Atomic parameters are cross-referenced from PDF entry 04-008-5421** **ADP:** B
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -x+1/2,-y+1/2,z+1/2 | 5 | x+1/2,-y,-z | 7 | -x,y+1/2,-z+1/2 |
| 2 | -x,-y,-z | 4 | x+1/2,y+1/2,-z+1/2 | 6 | -x+1/2,y,z | 8 | x,-y+1/2,z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 4c | m.. | 0.25 | 0.41508 | 0.24046 | 1.0 | 0.61095 | 9-a |
| C | 2 | 4c | m.. | 0.25 | 0.76211 | 0.08518 | 1.0 | 0.43867 | 3#a |
| O | 3 | 4c | m.. | 0.25 | 0.92224 | 0.09557 | 1.0 | 0.77616 | 1#a |
| O | 4 | 8d | 1 | 0.47347 | 0.68065 | 0.08726 | 1.0 | 0.70856 | 1#a |

**Anisotropic Displacement Parameters:**

| Atom | Num | Bani11 | Bani22 | Bani33 | Bani12 | Bani13 | Bani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.665479 | 0.670266 | 0.497141 | 0.0 | 0.0 | 0.0201231 |
| C | 2 | 0.442997 | 0.573788 | 0.299269 | 0.0 | 0.0 | 0.0073175 |
| O | 3 | 1.13407 | 0.540783 | 0.653666 | 0.0 | 0.0 | -0.05854 |
| O | 4 | 0.509938 | 0.926694 | 0.689106 | 0.180227 | -0.0136696 | 0.0841512 |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic), NBS Pattern, Pharmaceutical (Excipient), Superconducting Material

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**LPF Prototype Structure [Formula Order]:** Ca [ C O3 ],oP20,62
**LPF Prototype Structure [Alpha Order]:** C Ca O3,oP20,62 **Mineral Classification:** Aragonite (Group), Class Member
**Pearson Symbol:** oP20.00

**Cross-Ref PDF #'s:** 00-001-0628 (Deleted), 00-003-0405 (Deleted), 00-003-0425 (Deleted), 00-003-1067 (Deleted), 00-041-1475 (Primary), ✓ 00-061-0390 (Primary), 01-071-2392 (Alternate), 01-071-2396 (Alternate), 01-071-3700 (Alternate), 01-071-4891 (Alternate), 01-075-9982 (Alternate), 01-075-9983 (Alternate), 01-075-9984 (Alternate), 01-075-9985 (Alternate), 01-075-9986 (Alternate), 01-075-9987 (Alternate), 01-076-0606 (Alternate), 01-078-4337 (Alternate), 01-078-4338 (Alternate), 01-078-4339 (Alternate), 01-080-2768 (Alternate), 01-080-2769 (Alternate), 01-080-2770 (Alternate), 01-080-2771 (Alternate), 01-080-2772 (Alternate), 01-080-2773 (Alternate), 01-080-2774 (Alternate), 01-080-2775 (Alternate), 01-080-2789 (Alternate), 01-080-2790 (Alternate), ✓ 04-006-5441 (Alternate), ✓ 04-006-5444 (Alternate), ✓ 04-006-6531 (Alternate), ✓ 04-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate), ✓ 04-014-1837 (Alternate), ✓ 04-015-4109 (Alternate), ✓ 04-017-9180 (Alternate)

**CAS Number - PR:** 14791-73-2 **Entry Date:** 09/01/1955

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Swanson, Fuyat. Natl. Bur. Stand. (U. S. ), Circ. 539 3, 53 (1954). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Optical Data | | Winchell. Elements of Optical Mineralogy (1951). |

**00-005-0453** Jun 9, 2020 2:05 PM (fal-sharji2)

**Database Comments:** Additional Patterns: See PDF 00-041-1475. Analysis: Spectroscopic analysis: <0.1% Al, Ba, Cu, Fe, Mg, Ni, Pb; <0.001% Ag, Mn, Sn. Color: Colorless. General Comments: Validated by calculated data 00-024-0025. Antacid. Polymorphism/Phase Transition: Other polymorph: calcite (rhombohedral). Sample Preparation: Solutions of potassium carbonate and calcium chloride were heated to boiling and poured quickly together into a third beaker. The resulting mixture was digested until precipitation was complete and then filtered. Sample Source or Locality: Sample prepared at NBS. Temperature of Data Collection: Pattern taken at 299 K. Warning: Not enough reflections above the intensity cut off to meet higher quality mark criteria. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (38) - Ca C O3 - 00-005-0453 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 21.0748 | 4.212000 | 2 | 1 | 1 | 0 | | 45.8618 | **1.977000** | 65 | 2 | 2 | 1 | | 66.1738 | 1.411000 | 5 | 3 | 1 | 2 | |
| 26.2198 | **3.396000** | 100 | 1 | 1 | 1 | | 48.3202 | 1.882000 | 32 | 0 | 4 | 1 | | 66.5465 | 1.404000 | 3 | 3 | 3 | 0 | |
| 27.2238 | **3.273000** | 52 | 0 | 2 | 1 | | 48.4572 | 1.877000 | 25 | 2 | 0 | 2 | | 68.7085 | 1.365000 | 3 | 2 | 4 | 2 | |
| 31.1259 | 2.871000 | 4 | 0 | 0 | 2 | | 50.2546 | 1.814000 | 23 | 1 | 3 | 2 | | 69.1127 | 1.358000 | 3 | 1 | 1 | 4 | |
| 32.7776 | 2.730000 | 9 | 1 | 2 | 1 | | 51.9409 | 1.759000 | 4 | 1 | 4 | 1 | | 70.9053 | 1.328000 | 2 | 0 | 6 | 0 | |
| 33.1522 | 2.700000 | 46 | 0 | 1 | 2 | | 52.4863 | 1.742000 | 25 | 1 | 1 | 3 | | 75.3018 | 1.261000 | 6 | 3 | 3 | 2 | |
| 36.1753 | 2.481000 | 33 | 2 | 0 | 0 | | 52.9444 | 1.728000 | 15 | 2 | 3 | 1 | | 76.8067 | 1.240000 | 7 | 4 | 0 | 0 | |
| 37.2957 | 2.409000 | 14 | 0 | 3 | 1 | | 53.9549 | 1.698000 | 3 | 2 | 2 | 2 | | 77.9990 | 1.224000 | 5 | 1 | 3 | 4 | |
| 37.8995 | 2.372000 | 38 | 1 | 1 | 2 | | 59.3027 | 1.557000 | 4 | 3 | 1 | 1 | | 79.4698 | 1.205000 | 6 | 0 | 6 | 2 | |
| 38.4209 | 2.341000 | 31 | 1 | 3 | 0 | | 60.2398 | 1.535000 | 2 | 0 | 5 | 1 | | 80.7413 | 1.189200 | 5 | 1 | 5 | 3 | |
| 38.6439 | 2.328000 | 6 | 0 | 2 | 2 | | 61.8429 | 1.499000 | 4 | 2 | 4 | 1 | | 82.2470 | 1.171200 | 6 | 1 | 6 | 2 | |
| 41.2252 | 2.188000 | 11 | 2 | 1 | 1 | | 62.9631 | 1.475000 | 3 | 3 | 2 | 1 | | 83.2254 | 1.159900 | 3 | 4 | 2 | 1 | |
| 42.9081 | 2.106000 | 23 | 2 | 2 | 0 | | 63.3944 | 1.466000 | 5 | 1 | 5 | 1 | | | | | | | | |

**01-071-3699** Jun 9, 2020 2:05 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca ( C O3 )
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Calcite, syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 3.23 **I/Ic - ND:** 0.9

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.991(2) Å **AuthCell c:** 17.062(2) Å **AuthCell Vol:** 368.07 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 61.34 ] **Author's Cell Axial Ratio [ c/a:** 3.419 ]
**Density [ Dcalc:** 2.709 g/cm³ **Dstruc:** 2.71 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.017

**Space Group:** R-3c (167) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 4.991 Å **XtlCell b:** 4.991 Å **XtlCell c:** 17.062 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 368.07 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.419 **a/b:** 1.000 **c/b:** 3.419 ]
**Reduced Cell [ RedCell a:** 4.991 Å **RedCell b:** 4.991 Å **RedCell c:** 6.376 Å **RedCell α:** 66.96°
**RedCell β:** 66.96° **RedCell γ:** 60.00° **RedCell Vol:** 122.69 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-007-8659**
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | IDP | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | | 6-a |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | | 3#b |
| O | 3 | 18e | .2 | 0.2593 | 0.0 | 0.25 | 1.0 | | 1#a |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic), Pharmaceutical (Excipient), Pigment/Dye, Superconducting Material

**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 00-001-0837 (Deleted), 00-002-0623 (Deleted), 00-002-0629 (Deleted), 00-003-0569 (Deleted), 00-003-0596 (Deleted), 00-003-0670 (Deleted), 00-004-0636 (Deleted), 00-004-0637 (Deleted), 00-005-0586 (Primary), 00-024-0027 (Deleted), 00-047-1743 (Primary), 01-072-1937 (Alternate), 01-072-4582 (Alternate), 01-075-6049 (Alternate), 01-078-3262 (Alternate), 01-078-4614 (Alternate), 01-078-4615 (Alternate), 01-080-2791 (Alternate), 01-080-2792 (Alternate), 01-080-2793 (Alternate), 01-080-2794 (Alternate), 01-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 01-080-2799 (Alternate), 01-080-2800 (Alternate), 01-080-2801 (Alternate), 01-080-2802 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2806 (Alternate), 01-080-2807 (Alternate), 01-080-2808 (Alternate), 01-080-2809 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-9775 (Alternate), 01-080-9776 (Alternate), 01-083-0577 (Alternate), 01-083-0578 (Alternate), 01-085-0849 (Alternate), 01-086-2334 (Alternate), 01-086-2339 (Alternate), 01-086-2340 (Alternate), 01-086-2341 (Alternate), 01-086-2342 (Alternate), 01-086-2343 (Alternate), ✓ 04-001-7249 (Alternate), ✓ 04-002-9082 (Alternate), ✓ 04-006-6528 (Alternate), ✓ 04-007-0049 (Alternate), ✓ 04-007-2808 (Alternate), ✓ 04-007-4388 (Alternate), ✓ 04-007-8659 (Primary), ✓ 04-008-0198 (Alternate), ✓ 04-008-0212 (Alternate), ✓ 04-008-0213 (Alternate), ✓ 04-008-0788 (Alternate), ✓ 04-012-8072 (Alternate), ✓ 04-016-9713 (Alternate)

**CAS Number - PR:** 13397-26-7 **Entry Date:** 09/01/2005 **Last Modification Date:** 09/01/2011
**Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Additional Reference | | Pilati, T., Demartin, F., Gramaccioli, C.M. Golden Book of Phase Transitions, Wroclaw 1, 1 (2002). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "Lattice-dynamical estimation of atomic displacement parameters in carbonates: Calcite and aragonite Ca C O3, dolomite Ca Mg (C O3)2, and magnesite Mg C O3". Pilati, T., Demartin, F., Gramaccioli, C.M. Acta Crystallogr., Sec. B: Struct. Sci. 54, 515 (1998). |

**01-071-3699** Jun 9, 2020 2:05 PM (fal-sharji2)

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca (C O3). ICSD Collection Code: 52151. Calculated Pattern Original Remarks: Zero-point contribution to Uik: Ca: .0028, .0028; C: .0028, .0032; O: .0031, .0048, .0056, .0024, -.00055, -.0011. Cell and positional parameters from 73446, calculated Uik. Stable up to 1260 K (2nd ref., Tomaszewski), above R3-m, m.p. 1520 K. Wyckoff Sequence: e b a(R3-CH). Unit Cell Data Source: Single Crystal.

**d-Spacings (77) - Ca ( C O3 ) - 01-071-3699 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.0480 | 3.855680 | 95 | 0 | 1 | 2 | | 80.9104 | 1.187140 | 5 | 3 | 1 | 2 | | 109.5033 | 0.943210 | 17 | 4 | 1 | 0 | |
| 29.3944 | **3.036060** | 999 | 1 | 0 | 4 | | 81.5038 | 1.179990 | 23 | 2 | 1 | 10 | | 110.4380 | 0.937835 | 9 | 2 | 2 | 12 | |
| 31.4327 | 2.843670 | 20 | 0 | 0 | 6 | | 82.0953 | 1.172980 | 3 | 0 | 1 | 14 | | 111.7493 | 0.930501 | 1 | 1 | 4 | 3 | |
| 35.9579 | 2.495500 | 143 | 1 | 1 | 0 | | 83.7388 | 1.154090 | 43 | 1 | 3 | 4 | | 113.9892 | 0.918510 | 3 | 3 | 2 | 7 | |
| 39.3975 | 2.285190 | 190 | 1 | 1 | 3 | | 84.7758 | 1.142600 | 20 | 2 | 2 | 6 | | 115.0813 | 0.912900 | 1 | 4 | 0 | 10 | |
| 43.1449 | 2.094990 | 152 | 2 | 0 | 2 | | 85.8495 | 1.131040 | 1 | 3 | 1 | 5 | | 117.8856 | 0.899174 | 7 | 2 | 3 | 8 | |
| 47.1008 | 1.927840 | 66 | 0 | 2 | 4 | | 86.4373 | 1.124850 | 5 | 1 | 2 | 11 | | 118.7250 | 0.895249 | 6 | 1 | 4 | 6 | |
| 47.4994 | **1.912590** | 195 | 0 | 1 | 8 | | 91.4592 | 1.075730 | 1 | 1 | 3 | 7 | | 119.2195 | 0.892975 | 8 | 2 | 1 | 16 | |
| 48.4938 | **1.875670** | 202 | 1 | 1 | 6 | | 91.8667 | 1.072020 | 1 | 0 | 4 | 2 | | 120.7489 | 0.886118 | 9 | 1 | 1 | 18 | |
| 56.5435 | 1.626250 | 34 | 2 | 1 | 1 | | 93.0395 | 1.061560 | 8 | 2 | 0 | 14 | | 127.1737 | 0.860062 | 2 | 5 | 0 | 2 | |
| 57.3794 | 1.604530 | 94 | 1 | 2 | 2 | | 94.6749 | 1.047490 | 26 | 4 | 0 | 4 | | 127.9124 | 0.857335 | 8 | 3 | 2 | 10 | |
| 58.0720 | 1.587030 | 10 | 1 | 0 | 10 | | 94.9680 | 1.045030 | 29 | 3 | 1 | 8 | | 128.5117 | 0.855161 | 2 | 1 | 2 | 17 | |
| 60.6489 | 1.525620 | 53 | 2 | 1 | 4 | | 96.1456 | 1.035330 | 14m | 1 | 0 | 16 | | 128.6587 | 0.854633 | 2 | 3 | 1 | 14 | |
| 60.9844 | 1.518030 | 24 | 2 | 0 | 8 | | 96.1456 | 1.035330 | m | 1 | 1 | 15 | | 130.7795 | 0.847242 | 7 | 0 | 5 | 4 | |
| 61.3625 | 1.509580 | 26 | 1 | 1 | 9 | | 97.6734 | 1.023170 | 2 | 2 | 1 | 13 | | 132.7947 | 0.840601 | 1 | 2 | 2 | 15 | |
| 63.0331 | 1.473530 | 21 | 1 | 2 | 5 | | 99.1280 | 1.012020 | 25 | 0 | 3 | 12 | | 133.9509 | 0.836954 | 7 | 0 | 1 | 20 | |
| 64.6372 | 1.440780 | 63 | 3 | 0 | 0 | | 102.1752 | 0.989941 | 3 | 3 | 2 | 1 | | 134.4319 | 0.835471 | 2 | 2 | 3 | 11 | |
| 65.6060 | 1.421830 | 34 | 0 | 0 | 12 | | 102.8929 | 0.984980 | 12 | 2 | 3 | 2 | | 135.6402 | 0.831833 | 4 | 3 | 3 | 0 | |
| 69.1674 | 1.357060 | 12 | 2 | 1 | 7 | | 103.4946 | 0.980889 | 3 | 1 | 3 | 10 | | 138.7335 | 0.823076 | 1 | 3 | 3 | 3 | |
| 70.2268 | 1.339160 | 20 | 0 | 2 | 10 | | 104.0977 | 0.976849 | 10 | 1 | 2 | 14 | | 141.4950 | 0.815910 | 1 | 2 | 4 | 1 | |
| 72.8728 | 1.296920 | 27 | 1 | 2 | 8 | | 105.7860 | 0.965856 | 9 | 3 | 2 | 4 | | 142.6350 | 0.813125 | 7 | 4 | 2 | 2 | |
| 73.6442 | 1.285230 | 6 | 3 | 0 | 6 | | 106.0906 | 0.963921 | 18 | 0 | 4 | 8 | | 144.6101 | 0.808533 | 1 | 0 | 4 | 14 | |
| 76.2436 | 1.247750 | 11 | 2 | 2 | 0 | | 107.3138 | 0.956296 | 5 | 0 | 2 | 16 | | 147.5330 | 0.802266 | 7 | 2 | 4 | 4 | |
| 77.1468 | 1.235380 | 20 | 1 | 1 | 12 | | 107.9828 | 0.952222 | 3 | 2 | 3 | 5 | | 148.0828 | 0.801156 | 6 | 5 | 0 | 8 | |
| 78.3985 | 1.218760 | 1 | 2 | 2 | 3 | | 108.5999 | 0.948524 | 1m | 0 | 0 | 18 | | 149.5093 | 0.798376 | 7 | 3 | 3 | 6 | |
| 80.2006 | 1.195850 | 1 | 1 | 3 | 1 | | 108.5999 | 0.948524 | m | 3 | 1 | 11 | | | | | | | | |

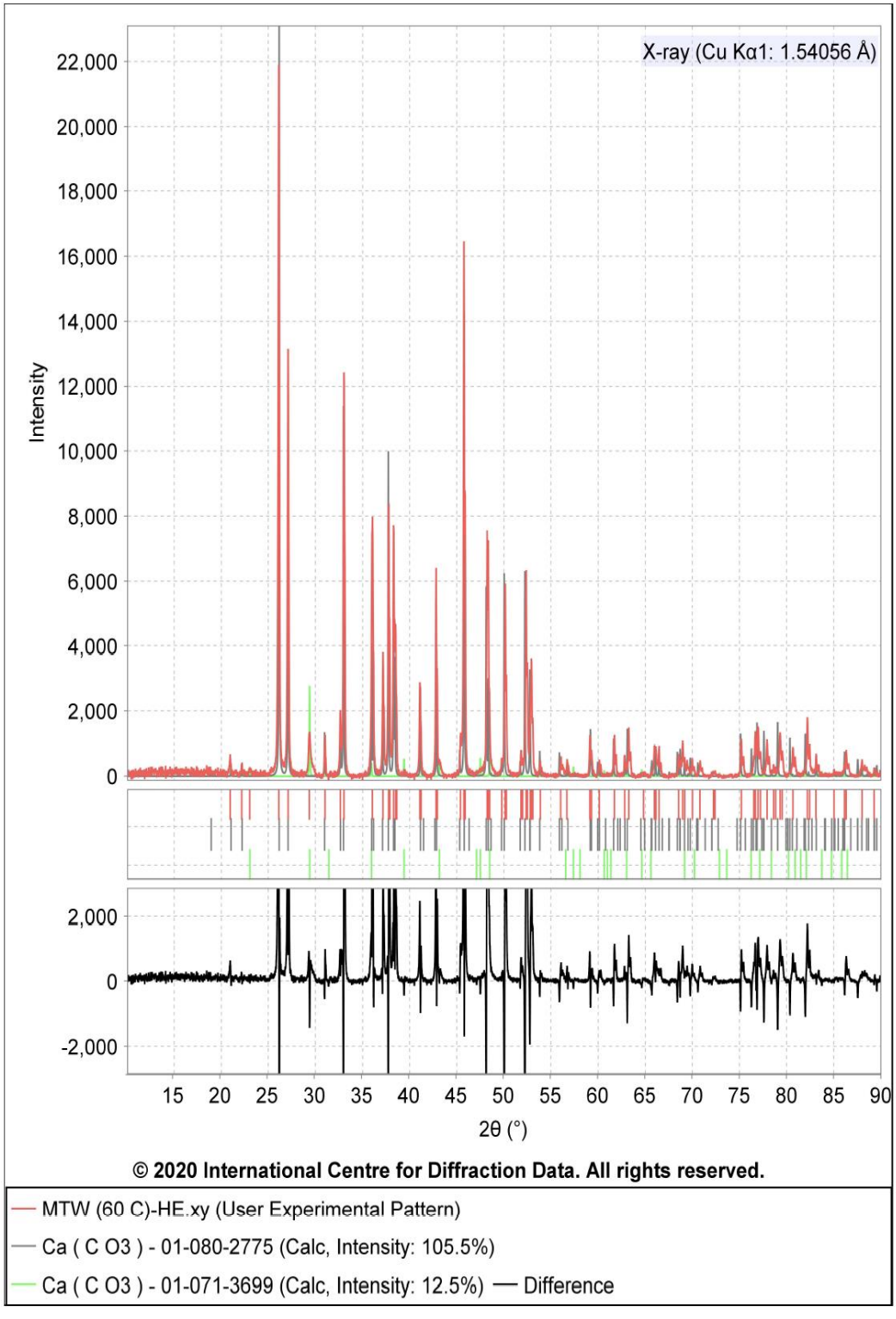


**Figure E.9 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 60 °C from accelerated scale simulation study**

# SIeve+ Report

## Experiment

**Search Line:** 1.976166 Å **D1 Range:** 1.970 Å - 1.982 Å
**Search Line:** 1.880833 Å **D1 Range:** 1.875 Å - 1.886 Å
**Search Line:** 2.372026 Å **D1 Range:** 2.363 Å - 2.381 Å
**Search Line:** 1.728285 Å **D1 Range:** 1.724 Å - 1.733 Å
**Search Line:** 1.741580 Å **D1 Range:** 1.737 Å - 1.746 Å
**Search Line:** 1.813554 Å **D1 Range:** 1.808 Å - 1.819 Å
**Search Line:** 2.489883 Å **D1 Range:** 2.480 Å - 2.500 Å
**Search Line:** 2.195541 Å **D1 Range:** 2.188 Å - 2.203 Å
**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (2)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 01-080-2775 | S | Calcium Carbonate | 1.055 | 89.416 | *1.14 | 96 |
| 2 | true | 01-071-3699 | S | Calcium Carbonate | 0.125 | 10.584 | 3.23 | 4 |

**01-080-2775** Jun 9, 2020 1:44 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Temperature (Non-ambient) **Chemical Formula:** Ca ( C O3 )
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Aragonite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 1.18 **I/Ic - ND:** 0.51

**SYS:** Orthorhombic **SPGR:** Pmcn (62)
**Author's Cell [ AuthCell a:** 4.9624(4) Å **AuthCell b:** 7.9989(6) Å **AuthCell c:** 5.7714(5) Å
**AuthCell Vol:** 229.09 Å³ **AuthCell Z:** 4.00 **AuthCell MolVol:** 57.27 ]
**Author's Cell Axial Ratio [ c/a:** 1.163 **a/b:** 0.620 **c/b:** 0.722 ]
**Density [ Dcalc:** 2.902 g/cm³ **Dstruc:** 2.9 g/cm³ ] **SS/FOM:** F(30) = 854.1(0.0011, 32)
**Temp:** 448.0 K (Author provided temperature) **R-factor:** 0.0338

**Space Group:** Pnam (62) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 5.771 Å **XtlCell b:** 7.999 Å **XtlCell c:** 4.962 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 229.09 Å³ **XtlCell Z:** 4.00 ]
**Crystal Data Axial Ratio [ c/a:** 0.860 **a/b:** 0.721 **c/b:** 0.620 ]
**Reduced Cell [ RedCell a:** 4.962 Å **RedCell b:** 5.771 Å **RedCell c:** 7.999 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 90.00° **RedCell Vol:** 229.09 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-008-5421** **ADP:** B
**Crystal (Symmetry Allowed):** Centrosymmetric

**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -x+1/2,-y+1/2,z+1/2 | 5 | x+1/2,-y,-z | 7 | -x,y+1/2,-z+1/2 |
| 2 | -x,-y,-z | 4 | x+1/2,y+1/2,-z+1/2 | 6 | -x+1/2,y,z | 8 | x,-y+1/2,z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Biso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 4c | m.. | 0.25 | 0.41508 | 0.24046 | 1.0 | 0.61095 | 9-a |
| C | 2 | 4c | m.. | 0.25 | 0.76211 | 0.08518 | 1.0 | 0.43867 | 3#a |
| O | 3 | 4c | m.. | 0.25 | 0.92224 | 0.09557 | 1.0 | 0.77616 | 1#a |
| O | 4 | 8d | 1 | 0.47347 | 0.68065 | 0.08726 | 1.0 | 0.70856 | 1#a |

**Anisotropic Displacement Parameters:**

| Atom | Num | Bani11 | Bani22 | Bani33 | Bani12 | Bani13 | Bani23 |
|---|---|---|---|---|---|---|---|
| Ca | 1 | 0.665479 | 0.670266 | 0.497141 | 0.0 | 0.0 | 0.0201231 |
| C | 2 | 0.442997 | 0.573788 | 0.299269 | 0.0 | 0.0 | 0.0073175 |
| O | 3 | 1.13407 | 0.540783 | 0.653666 | 0.0 | 0.0 | -0.05854 |
| O | 4 | 0.509938 | 0.926694 | 0.689106 | 0.180227 | -0.0136696 | 0.0841512 |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**Mineral Classification:** Aragonite (Group), carbonate (Subgroup) **Pearson Symbol:** oP20.00

**Cross-Ref PDF #'s:** 00-001-0628 (Deleted), 00-003-0405 (Deleted), 00-003-0425 (Deleted), 00-003-1067 (Deleted), 00-005-0453 (Alternate), 00-041-1475 (Primary), ✓ 00-061-0390 (Primary), 01-071-2392 (Alternate), 01-071-2396 (Alternate), 01-071-3700 (Alternate), 01-071-4891 (Alternate), 01-075-9982 (Alternate), 01-075-9983 (Alternate), 01-075-9984 (Alternate), 01-075-9985 (Alternate), 01-075-9986 (Alternate), 01-075-9987 (Alternate), 01-076-0606 (Alternate), 01-078-4337 (Alternate), 01-078-4338 (Alternate), 01-078-4339 (Alternate), 01-080-2768 (Alternate), 01-080-2769 (Alternate), 01-080-2770 (Alternate), 01-080-2771 (Alternate), 01-080-2772 (Alternate), 01-080-2773 (Alternate), 01-080-2774 (Alternate), 01-080-2789 (Alternate), 01-080-2790 (Alternate), ✓ 04-006-5441 (Alternate), ✓ 04-006-5444 (Alternate), ✓ 04-006-6531 (Alternate), ✓ 04-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate), ✓ 04-014-1837 (Alternate), ✓ 04-015-4109 (Alternate), ✓ 04-017-9180 (Alternate)

**Entry Date:** 09/01/2013

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "Temperature dependence of the structural parameters in the transformation of aragonite to calcite, as determined from in situ synchrotron powder x-ray-diffraction data". Antao, S.M., Hassan, I. Can. Mineral. 48, 1225 (2010). |

**01-080-2775** Jun 9, 2020 1:44 PM (fal-sharji2)

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca (C O3). ICSD Collection Code: 169897. Sample Source or Locality: Cuenca,Spain. Temperature of Data Collection: 448 K. Wyckoff Sequence: d c3 (PMCN). Unit Cell Data Source: Powder Diffraction.

**d-Spacings (199) - Ca ( C O3 ) - 01-080-2775 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 18.9456 | 4.680300 | 3 | 0 | 1 | 1 | | 78.4001 | 1.218740 | 7 | 2 | 5 | 2 | | 107.5222 | 0.955020 | m | 3 | 4 | 4 | |
| 21.0504 | 4.216830 | 15 | 1 | 1 | 0 | | 79.0549 | 1.210280 | 69m | 0 | 6 | 2 | | 108.3322 | 0.950121 | 1 | 5 | 2 | 1 | |
| 22.2087 | 3.999450 | 17 | 0 | 2 | 0 | | 79.0549 | 1.210280 | m | 2 | 4 | 3 | | 109.2380 | 0.944758 | 1m | 0 | 8 | 2 | |
| 26.1505 | **3.404840** | 999 | 1 | 1 | 1 | | 80.3567 | 1.193920 | 48 | 1 | 5 | 3 | | 109.2380 | 0.944758 | m | 1 | 0 | 6 | |
| 27.1032 | **3.287290** | 515 | 0 | 2 | 1 | | 80.6162 | 1.190730 | 3 | 2 | 2 | 4 | | 110.0530 | 0.940034 | 11m | 3 | 1 | 5 | |
| 30.9633 | 2.885700 | 55 | 0 | 0 | 2 | | 81.0953 | 1.184900 | 1 | 4 | 2 | 0 | | 110.0530 | 0.940034 | m | 3 | 7 | 0 | |
| 32.6482 | 2.740520 | 78 | 1 | 2 | 1 | | 81.9772 | 1.174370 | 53 | 2 | 6 | 0 | | 110.3172 | 0.938523 | 3m | 1 | 1 | 6 | |
| 32.9706 | 2.714460 | 486 | 0 | 1 | 2 | | 82.3428 | 1.170080 | 5 | 0 | 4 | 4 | | 110.3172 | 0.938523 | m | 5 | 0 | 2 | |
| 35.9716 | 2.494580 | 177 | 1 | 0 | 2 | | 82.7009 | 1.165920 | 1 | 3 | 4 | 2 | | 110.7513 | 0.936061 | 3 | 0 | 5 | 5 | |
| 36.1723 | 2.481200 | 166 | 2 | 0 | 0 | | 83.1561 | 1.160690 | 25 | 4 | 2 | 1 | | 110.8987 | 0.935231 | 1 | 0 | 2 | 6 | |
| 37.1124 | 2.420480 | 94 | 0 | 3 | 1 | | 84.0337 | 1.150790 | 1m | 2 | 6 | 1 | | 111.0742 | 0.934247 | 3 | 4 | 1 | 4 | |
| 37.7432 | 2.381460 | 412 | 1 | 1 | 2 | | 84.0337 | 1.150790 | m | 3 | 5 | 0 | | 111.4545 | 0.932129 | 8 | 5 | 1 | 2 | |
| 38.2893 | 2.348740 | 273 | 1 | 3 | 0 | | 84.7896 | 1.142450 | 1 | 0 | 1 | 5 | | 111.8164 | 0.930132 | 9 | 5 | 3 | 0 | |
| 38.4354 | 2.340150 | 168 | 0 | 2 | 2 | | 85.0386 | 1.139740 | 8m | 1 | 4 | 4 | | 112.2168 | 0.927943 | 9m | 1 | 8 | 2 | |
| 41.1426 | 2.192200 | 112 | 2 | 1 | 1 | | 85.0386 | 1.139740 | m | 4 | 0 | 2 | | 112.2168 | 0.927943 | m | 3 | 7 | 1 | |
| 41.4732 | 2.175490 | 6 | 1 | 3 | 1 | | 85.4828 | 1.134950 | 3 | 3 | 3 | 3 | | 112.3427 | 0.927259 | 12m | 2 | 4 | 5 | |
| 42.8566 | 2.108410 | 170 | 2 | 2 | 0 | | 86.1579 | 1.127780 | 31m | 3 | 5 | 1 | | 112.3427 | 0.927259 | m | 2 | 8 | 0 | |
| 45.3116 | 1.999720 | 34 | 0 | 4 | 0 | | 86.1579 | 1.127780 | m | 4 | 1 | 2 | | 112.8547 | 0.924500 | 4 | 4 | 4 | 3 | |
| 45.7786 | **1.980400** | 609 | 2 | 2 | 1 | | 86.8135 | 1.120940 | 1 | 0 | 7 | 1 | | 113.7347 | 0.919839 | 13 | 1 | 5 | 5 | |
| 46.3244 | 1.958330 | 4 | 0 | 3 | 2 | | 87.5577 | 1.113320 | 20m | 1 | 1 | 5 | | 114.0328 | 0.918283 | 1 | 5 | 3 | 1 | |
| 48.1157 | 1.889520 | 259 | 0 | 4 | 1 | | 87.5577 | 1.113320 | m | 1 | 7 | 0 | | 114.5427 | 0.915648 | 20m | 2 | 8 | 1 | |
| 48.3374 | 1.881370 | 131 | 2 | 0 | 2 | | 87.9842 | 1.109020 | 13 | 0 | 2 | 5 | | 114.5427 | 0.915648 | m | 4 | 2 | 4 | |
| 48.6376 | 1.870460 | 5 | 0 | 1 | 3 | | 88.4853 | 1.104030 | 2 | 4 | 3 | 1 | | 114.9232 | 0.913703 | 1m | 2 | 7 | 3 | |
| 49.7445 | 1.831400 | 21 | 2 | 1 | 2 | | 88.6849 | 1.102060 | 1 | 2 | 5 | 3 | | 114.9232 | 0.913703 | m | 5 | 2 | 2 | |
| 50.0299 | 1.821620 | 257 | 1 | 3 | 2 | | 89.2955 | 1.096100 | 10m | 0 | 6 | 3 | | 115.4961 | 0.910809 | 7 | 2 | 6 | 4 | |
| 51.7248 | 1.765840 | 18 | 1 | 4 | 1 | | 89.2955 | 1.096100 | m | 4 | 2 | 2 | | 116.0209 | 0.908194 | 9 | 4 | 6 | 0 | |
| 52.2198 | 1.750260 | 262 | 1 | 1 | 3 | | 89.5764 | 1.093390 | 13 | 1 | 7 | 1 | | 116.7083 | 0.904820 | 1 | 0 | 3 | 6 | |
| 52.7582 | 1.733660 | 141m | 0 | 2 | 3 | | 90.1687 | 1.087740 | 14m | 2 | 6 | 2 | | 117.8643 | 0.899275 | 5 | 3 | 5 | 4 | |
| 52.7582 | 1.733660 | m | 2 | 3 | 1 | | 90.1687 | 1.087740 | m | 3 | 0 | 4 | | 118.3779 | 0.896862 | 8m | 2 | 0 | 6 | |
| 53.8035 | 1.702420 | 30 | 2 | 2 | 2 | | 90.7457 | 1.082320 | 1 | 1 | 2 | 5 | | 118.3779 | 0.896862 | m | 4 | 6 | 1 | |
| 55.8925 | 1.643640 | 29 | 0 | 4 | 2 | | 91.2749 | 1.077420 | 5 | 3 | 1 | 4 | | 119.0117 | 0.893927 | 8 | 3 | 7 | 2 | |
| 56.1519 | 1.636660 | 1 | 1 | 2 | 3 | | 91.9297 | 1.071450 | 1 | 0 | 5 | 4 | | 119.8438 | 0.890144 | 13 | 1 | 3 | 6 | |
| 56.7868 | 1.619860 | 16 | 3 | 1 | 0 | | 92.2853 | 1.068250 | 8 | 3 | 5 | 2 | | 120.5055 | 0.887192 | 4m | 0 | 8 | 3 | |
| 59.1939 | 1.559600 | 60m | 0 | 3 | 3 | | 92.9406 | 1.062430 | 1m | 0 | 7 | 2 | | 120.5055 | 0.887192 | m | 4 | 3 | 4 | |
| 59.1939 | 1.559600 | m | 3 | 1 | 1 | | 92.9406 | 1.062430 | m | 3 | 4 | 3 | | 120.9397 | 0.885281 | 14 | 5 | 3 | 2 | |
| 59.3031 | 1.556990 | 22 | 2 | 4 | 0 | | 93.4123 | 1.058300 | 7m | 0 | 3 | 5 | | 121.4830 | 0.882920 | 4 | 2 | 8 | 2 | |
| 59.9532 | 1.541650 | 17 | 0 | 5 | 1 | | 93.4123 | 1.058300 | m | 2 | 4 | 4 | | 121.8023 | 0.881547 | 6 | 1 | 7 | 4 | |
| 60.1438 | 1.537220 | 8 | 2 | 3 | 2 | | 93.8852 | 1.054210 | 4 | 4 | 4 | 0 | | 122.4855 | 0.878647 | 2m | 0 | 9 | 1 | |
| 60.7815 | 1.522610 | 2 | 1 | 5 | 0 | | 94.6963 | 1.047310 | 5m | 1 | 5 | 4 | | 122.4855 | 0.878647 | m | 5 | 4 | 1 | |
| 61.6490 | 1.503250 | 45 | 2 | 4 | 1 | | 94.6963 | 1.047310 | m | 4 | 3 | 2 | | 122.9491 | 0.876708 | 12 | 5 | 1 | 3 | |
| 62.8392 | 1.477610 | 18 | 3 | 2 | 1 | | 95.7093 | 1.038890 | 12 | 1 | 7 | 2 | | 123.3306 | 0.875129 | 9m | 1 | 9 | 0 | |
| 63.0947 | 1.472240 | 61 | 1 | 5 | 1 | | 95.9342 | 1.037050 | 27m | 2 | 1 | 5 | | 123.3306 | 0.875129 | m | 2 | 2 | 6 | |
| 64.5333 | 1.442850 | 4 | 0 | 0 | 4 | | 95.9342 | 1.037050 | m | 4 | 4 | 1 | | 125.5349 | 0.866304 | 12m | 0 | 4 | 6 | |
| 64.9254 | 1.435080 | 1 | 3 | 0 | 2 | | 97.8841 | 1.021530 | 2m | 2 | 7 | 1 | | 125.5349 | 0.866304 | m | 4 | 6 | 2 | |
| 65.7049 | 1.419930 | 19m | 0 | 1 | 4 | | 97.8841 | 1.021530 | m | 3 | 6 | 1 | | 126.8364 | 0.861325 | 1 | 5 | 2 | 3 | |
| 65.7049 | 1.419930 | m | 2 | 2 | 3 | | 99.0670 | 1.012480 | 19 | 2 | 2 | 5 | | 127.3380 | 0.859451 | 1 | 1 | 6 | 5 | |
| 66.0930 | 1.412530 | 31 | 3 | 1 | 2 | | 99.5461 | 1.008890 | 17 | 4 | 2 | 3 | | 128.3957 | 0.855579 | 1 | 3 | 4 | 5 | |
| 66.4604 | 1.405610 | 28 | 3 | 3 | 0 | | 99.8251 | 1.006820 | 26 | 3 | 3 | 4 | | 129.6263 | 0.851209 | 4 | 4 | 4 | 4 | |
| 67.5551 | 1.385470 | 5m | 0 | 4 | 3 | | 100.4314 | 1.002370 | 3 | 2 | 6 | 3 | | 129.9563 | 0.850061 | 1m | 2 | 3 | 6 | |
| 67.5551 | 1.385470 | m | 1 | 0 | 4 | | 100.8007 | 0.999692 | 10m | 0 | 4 | 5 | | 129.9563 | 0.850061 | m | 5 | 4 | 2 | |
| 68.4081 | 1.370260 | 29 | 2 | 4 | 2 | | 100.8007 | 0.999692 | m | 0 | 8 | 0 | | 130.1498 | 0.849393 | 1 | 0 | 9 | 2 | |
| 68.6999 | 1.365150 | 33m | 1 | 1 | 4 | | 102.1380 | 0.990200 | 7 | 4 | 4 | 2 | | 131.0192 | 0.846433 | 1 | 3 | 8 | 1 | |
| 68.6999 | 1.365150 | m | 3 | 3 | 1 | | 102.5914 | 0.987053 | 14 | 3 | 5 | 3 | | 131.5382 | 0.844699 | 14 | 3 | 7 | 3 | |
| 69.1575 | 1.357230 | 16 | 0 | 2 | 4 | | 102.8627 | 0.985187 | 11m | 0 | 8 | 1 | | 131.9422 | 0.843366 | 1 | 5 | 5 | 0 | |
| 69.5363 | 1.350760 | 3 | 3 | 2 | 2 | | 102.8627 | 0.985187 | m | 5 | 1 | 0 | | 132.1871 | 0.842565 | 3m | 2 | 7 | 4 | |
| 69.7792 | 1.346650 | 22 | 1 | 5 | 2 | | 103.0872 | 0.983652 | 3 | 2 | 5 | 4 | | 132.1871 | 0.842565 | m | 3 | 6 | 4 | |
| 70.5904 | 1.333150 | 16 | 0 | 6 | 0 | | 103.7505 | 0.979167 | 11 | 0 | 6 | 4 | | 132.8600 | 0.840392 | 1 | 4 | 1 | 5 | |
| 71.3557 | 1.320720 | 1 | 2 | 3 | 3 | | 104.1254 | 0.976665 | 7m | 2 | 7 | 2 | | 133.8659 | 0.837218 | 14m | 1 | 9 | 2 | |
| 72.0641 | 1.309470 | 4m | 1 | 2 | 4 | | 104.1254 | 0.976665 | m | 3 | 6 | 2 | | 133.8659 | 0.837218 | m | 5 | 3 | 3 | |
| 72.0641 | 1.309470 | m | 2 | 5 | 1 | | 104.4964 | 0.974211 | 2 | 2 | 3 | 5 | | 134.4570 | 0.835394 | 9 | 2 | 8 | 3 | |
| 72.7407 | 1.298950 | 2 | 0 | 6 | 1 | | 105.0040 | 0.970891 | 12m | 4 | 3 | 3 | | 134.7494 | 0.834503 | 8 | 5 | 5 | 1 | |
| 75.1151 | 1.263670 | 54 | 3 | 3 | 2 | | 105.0040 | 0.970891 | m | 5 | 1 | 1 | | 135.7438 | 0.831527 | 1m | 3 | 0 | 6 | |
| 76.2768 | 1.247290 | 34 | 2 | 0 | 4 | | 105.6828 | 0.966515 | 2m | 1 | 8 | 1 | | 135.7438 | 0.831527 | m | 4 | 7 | 1 | |
| 76.7628 | 1.240600 | 45 | 4 | 0 | 0 | | 105.6828 | 0.966515 | m | 4 | 5 | 1 | | 137.3789 | 0.826814 | 15m | 4 | 2 | 5 | |
| 76.8720 | 1.239110 | 67 | 3 | 1 | 3 | | 106.1176 | 0.963750 | 18 | 1 | 7 | 3 | | 137.3789 | 0.826814 | m | 6 | 0 | 0 | |
| 77.5913 | 1.229410 | 55m | 0 | 5 | 3 | | 106.4112 | 0.961900 | 11 | 0 | 0 | 6 | | | | | | | | |
| 77.5913 | 1.229410 | m | 1 | 3 | 4 | | 107.5222 | 0.955020 | 1m | 0 | 1 | 6 | | | | | | | | |

**01-071-3699** Jun 9, 2020 1:44 PM (fal-sharji2)

**Status** Alternate **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca ( C O3 )
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**ANX:** ABX3 **Compound Name:** Calcium Carbonate **Mineral Name:** Calcite, syn

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Calculated **Intensity:** Calculated **I/Ic:** 3.23 **I/Ic - ND:** 0.9

**SYS:** Rhombohedral **SPGR:** R-3c (167)
**Author's Cell [ AuthCell a:** 4.991(2) Å **AuthCell c:** 17.062(2) Å **AuthCell Vol:** 368.07 Å³ **AuthCell Z:** 6.00
**AuthCell MolVol:** 61.34 ] **Author's Cell Axial Ratio [ c/a:** 3.419 ]
**Density [ Dcalc:** 2.709 g/cm³ **Dstruc:** 2.71 g/cm³ ] **SS/FOM:** F(30) = 999.9(0.0000, 30)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **R-factor:** 0.017

**Space Group:** R-3c (167) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 4.991 Å **XtlCell b:** 4.991 Å **XtlCell c:** 17.062 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 120.00° **XtlCell Vol:** 368.07 Å³ **XtlCell Z:** 6.00 ]
**Crystal Data Axial Ratio [ c/a:** 3.419 **a/b:** 1.000 **c/b:** 3.419 ]
**Reduced Cell [ RedCell a:** 4.991 Å **RedCell b:** 4.991 Å **RedCell c:** 6.376 Å **RedCell α:** 66.96°
**RedCell β:** 66.96° **RedCell γ:** 60.00° **RedCell Vol:** 122.69 Å³ ]

**Atomic parameters are cross-referenced from PDF entry 04-007-8659**
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -y,x-y,z | 5 | -x+y,-x,z | 7 | -y,-x,z+1/2 | 9 | x,x-y,z+1/2 | 11 | -x+y,y,z+1/2 |
| 2 | -x,-y,-z | 4 | y,-x+y,-z | 6 | x-y,x,-z | 8 | y,x,-z+1/2 | 10 | -x,-x+y,-z+1/2 | 12 | x-y,-y,-z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | IDP | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 6b | -3. | 0.0 | 0.0 | 0.0 | 1.0 | | 6-a |
| C | 2 | 6a | 32 | 0.0 | 0.0 | 0.25 | 1.0 | | 3#b |
| O | 3 | 18e | .2 | 0.2593 | 0.0 | 0.25 | 1.0 | | 1#a |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic), Pharmaceutical (Excipient), Pigment/Dye, Superconducting Material

**Mineral Classification:** Calcite (Supergroup), calcite (Group) **Pearson Symbol:** hR10.00

**Cross-Ref PDF #'s:** 00-001-0837 (Deleted), 00-002-0623 (Deleted), 00-002-0629 (Deleted), 00-003-0569 (Deleted), 00-003-0596 (Deleted), 00-003-0670 (Deleted), 00-004-0636 (Deleted), 00-004-0637 (Deleted), 00-005-0586 (Primary), 00-024-0027 (Deleted), 00-047-1743 (Primary), 01-072-1937 (Alternate), 01-072-4582 (Alternate), 01-075-6049 (Alternate), 01-078-3262 (Alternate), 01-078-4614 (Alternate), 01-078-4615 (Alternate), 01-080-2791 (Alternate), 01-080-2792 (Alternate), 01-080-2793 (Alternate), 01-080-2794 (Alternate), 01-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 01-080-2799 (Alternate), 01-080-2800 (Alternate), 01-080-2801 (Alternate), 01-080-2802 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2806 (Alternate), 01-080-2807 (Alternate), 01-080-2808 (Alternate), 01-080-2809 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-9775 (Alternate), 01-080-9776 (Alternate), 01-083-0577 (Alternate), 01-083-0578 (Alternate), 01-085-0849 (Alternate), 01-086-2334 (Alternate), 01-086-2339 (Alternate), 01-086-2340 (Alternate), 01-086-2341 (Alternate), 01-086-2342 (Alternate), 01-086-2343 (Alternate), ✓ 04-001-7249 (Alternate), ✓ 04-002-9082 (Alternate), ✓ 04-006-6528 (Alternate), ✓ 04-007-0049 (Alternate), ✓ 04-007-2808 (Alternate), ✓ 04-007-4388 (Alternate), ✓ 04-007-8659 (Primary), ✓ 04-008-0198 (Alternate), ✓ 04-008-0212 (Alternate), ✓ 04-008-0213 (Alternate), ✓ 04-008-0788 (Alternate), ✓ 04-012-8072 (Alternate), ✓ 04-016-9713 (Alternate)

**CAS Number - PR:** 13397-26-7 **Entry Date:** 09/01/2005 **Last Modification Date:** 09/01/2011
**Last Modifications:** Reflections

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Calculated from ICSD using POWD-12++. |
| Additional Reference | | Pilati, T., Demartin, F., Gramaccioli, C.M. Golden Book of Phase Transitions, Wroclaw 1, 1 (2002). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Structure | | "Lattice-dynamical estimation of atomic displacement parameters in carbonates: Calcite and aragonite Ca C O3, dolomite Ca Mg (C O3)2, and magnesite Mg C O3". Pilati, T., Demartin, F., Gramaccioli, C.M. Acta Crystallogr., Sec. B: Struct. Sci. 54, 515 (1998). |

**01-071-3699** Jun 9, 2020 1:44 PM (fal-sharji2)

**Database Comments:** ANX: ABX3. Analysis: C1 Ca1 O3. Formula from original source: Ca (C O3). ICSD Collection Code: 52151. Calculated Pattern Original Remarks: Zero-point contribution to Uik: Ca: .0028, .0028; C: .0028, .0032; O: .0031, .0048, .0056, .0024, -.00055, -.0011. Cell and positional parameters from 73446, calculated Uik. Stable up to 1260 K (2nd ref., Tomaszewski), above R3-m, m.p. 1520 K. Wyckoff Sequence: e b a(R3-CH). Unit Cell Data Source: Single Crystal.

**d-Spacings (77) - Ca ( C O3 ) - 01-071-3699 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 23.0480 | 3.855680 | 95 | 0 | 1 | 2 | | 80.9104 | 1.187140 | 5 | 3 | 1 | 2 | | 109.5033 | 0.943210 | 17 | 4 | 1 | 0 | |
| 29.3944 | **3.036060** | 999 | 1 | 0 | 4 | | 81.5038 | 1.179990 | 23 | 2 | 1 | 10 | | 110.4380 | 0.937835 | 9 | 2 | 2 | 12 | |
| 31.4327 | 2.843670 | 20 | 0 | 0 | 6 | | 82.0953 | 1.172980 | 3 | 0 | 1 | 14 | | 111.7493 | 0.930501 | 1 | 1 | 4 | 3 | |
| 35.9579 | 2.495500 | 143 | 1 | 1 | 0 | | 83.7388 | 1.154090 | 43 | 1 | 3 | 4 | | 113.9892 | 0.918510 | 3 | 3 | 2 | 7 | |
| 39.3975 | 2.285190 | 190 | 1 | 1 | 3 | | 84.7758 | 1.142600 | 20 | 2 | 2 | 6 | | 115.0813 | 0.912900 | 1 | 4 | 0 | 10 | |
| 43.1449 | 2.094990 | 152 | 2 | 0 | 2 | | 85.8495 | 1.131040 | 1 | 3 | 1 | 5 | | 117.8856 | 0.899174 | 7 | 2 | 3 | 8 | |
| 47.1008 | 1.927840 | 66 | 0 | 2 | 4 | | 86.4373 | 1.124850 | 5 | 1 | 2 | 11 | | 118.7250 | 0.895249 | 6 | 1 | 4 | 6 | |
| 47.4994 | **1.912590** | 195 | 0 | 1 | 8 | | 91.4592 | 1.075730 | 1 | 1 | 3 | 7 | | 119.2195 | 0.892975 | 8 | 2 | 1 | 16 | |
| 48.4938 | **1.875670** | 202 | 1 | 1 | 6 | | 91.8667 | 1.072020 | 1 | 0 | 4 | 2 | | 120.7489 | 0.886118 | 9 | 1 | 1 | 18 | |
| 56.5435 | 1.626250 | 34 | 2 | 1 | 1 | | 93.0395 | 1.061560 | 8 | 2 | 0 | 14 | | 127.1737 | 0.860062 | 2 | 5 | 0 | 2 | |
| 57.3794 | 1.604530 | 94 | 1 | 2 | 2 | | 94.6749 | 1.047490 | 26 | 4 | 0 | 4 | | 127.9124 | 0.857335 | 8 | 3 | 2 | 10 | |
| 58.0720 | 1.587030 | 10 | 1 | 0 | 10 | | 94.9680 | 1.045030 | 29 | 3 | 1 | 8 | | 128.5117 | 0.855161 | 2 | 1 | 2 | 17 | |
| 60.6489 | 1.525620 | 53 | 2 | 1 | 4 | | 96.1456 | 1.035330 | 14m | 1 | 0 | 16 | | 128.6587 | 0.854633 | 2 | 3 | 1 | 14 | |
| 60.9844 | 1.518030 | 24 | 2 | 0 | 8 | | 96.1456 | 1.035330 | m | 1 | 1 | 15 | | 130.7795 | 0.847242 | 7 | 0 | 5 | 4 | |
| 61.3625 | 1.509580 | 26 | 1 | 1 | 9 | | 97.6734 | 1.023170 | 2 | 2 | 1 | 13 | | 132.7947 | 0.840601 | 1 | 2 | 2 | 15 | |
| 63.0331 | 1.473530 | 21 | 1 | 2 | 5 | | 99.1280 | 1.012020 | 25 | 0 | 3 | 12 | | 133.9509 | 0.836954 | 7 | 0 | 1 | 20 | |
| 64.6372 | 1.440780 | 63 | 3 | 0 | 0 | | 102.1752 | 0.989941 | 3 | 3 | 2 | 1 | | 134.4319 | 0.835471 | 2 | 2 | 3 | 11 | |
| 65.6060 | 1.421830 | 34 | 0 | 0 | 12 | | 102.8929 | 0.984980 | 12 | 2 | 3 | 2 | | 135.6402 | 0.831833 | 4 | 3 | 3 | 0 | |
| 69.1674 | 1.357060 | 12 | 2 | 1 | 7 | | 103.4946 | 0.980889 | 3 | 1 | 3 | 10 | | 138.7335 | 0.823076 | 1 | 3 | 3 | 3 | |
| 70.2268 | 1.339160 | 20 | 0 | 2 | 10 | | 104.0977 | 0.976849 | 10 | 1 | 2 | 14 | | 141.4950 | 0.815910 | 1 | 2 | 4 | 1 | |
| 72.8728 | 1.296920 | 27 | 1 | 2 | 8 | | 105.7860 | 0.965856 | 9 | 3 | 2 | 4 | | 142.6350 | 0.813125 | 7 | 4 | 2 | 2 | |
| 73.6442 | 1.285230 | 6 | 3 | 0 | 6 | | 106.0906 | 0.963921 | 18 | 0 | 4 | 8 | | 144.6101 | 0.808533 | 1 | 0 | 4 | 14 | |
| 76.2436 | 1.247750 | 11 | 2 | 2 | 0 | | 107.3138 | 0.956296 | 5 | 0 | 2 | 16 | | 147.5330 | 0.802266 | 7 | 2 | 4 | 4 | |
| 77.1468 | 1.235380 | 20 | 1 | 1 | 12 | | 107.9828 | 0.952222 | 3 | 2 | 3 | 5 | | 148.0828 | 0.801156 | 6 | 5 | 0 | 8 | |
| 78.3985 | 1.218760 | 1 | 2 | 2 | 3 | | 108.5999 | 0.948524 | 1m | 0 | 0 | 18 | | 149.5093 | 0.798376 | 7 | 3 | 3 | 6 | |
| 80.2006 | 1.195850 | 1 | 1 | 3 | 1 | | 108.5999 | 0.948524 | m | 3 | 1 | 11 | | | | | | | | |

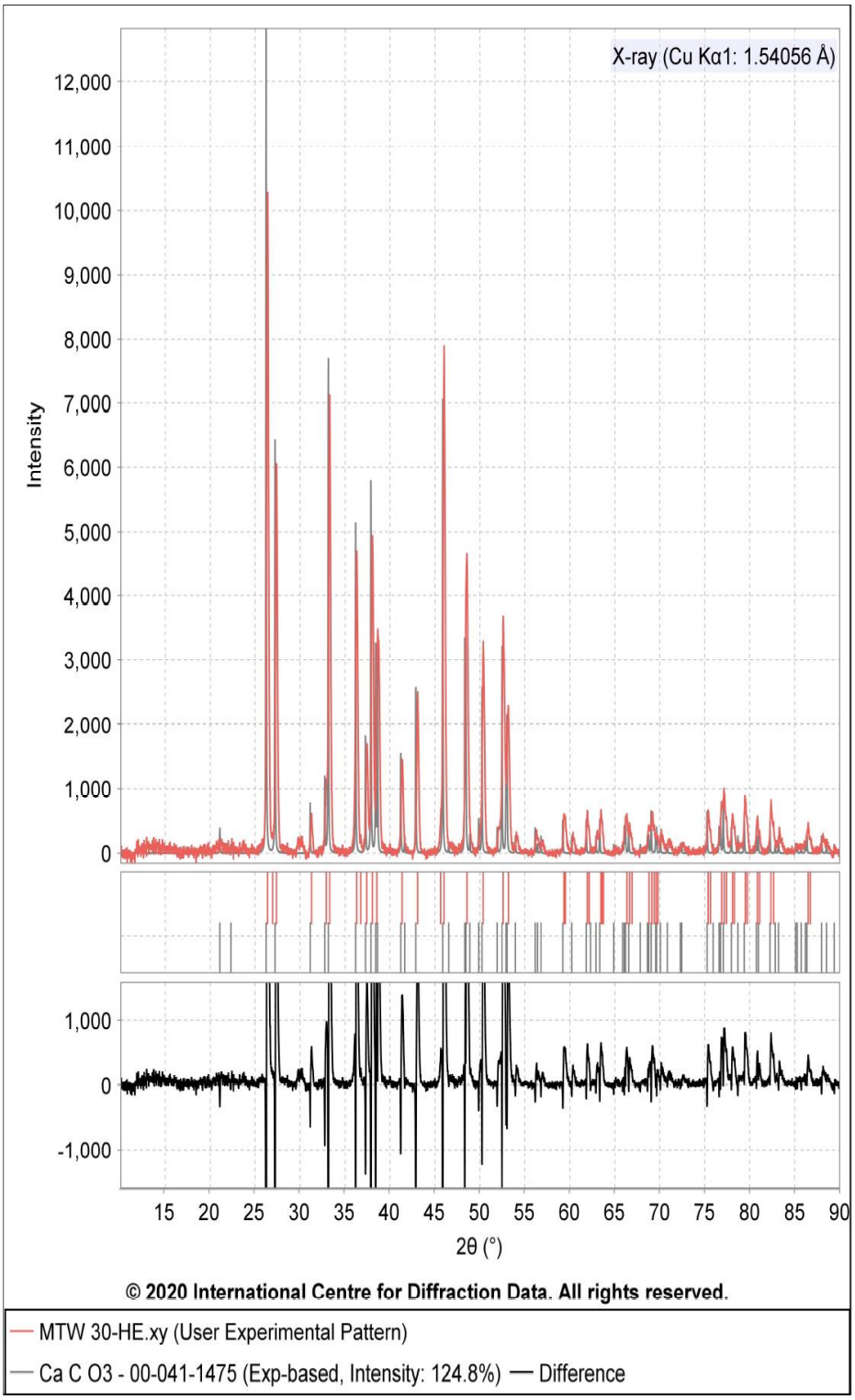


**Figure E.10 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 30 °C from accelerated scale simulation study**

# SIeve+ Report

## Experiment

**Search Line:** 3.376276 Å **D1 Range:** 3.357 Å - 3.395 Å
**Search Line:** 2.689511 Å **D1 Range:** 2.678 Å - 2.701 Å
**Search Line:** 3.255456 Å **D1 Range:** 3.238 Å - 3.273 Å
**Search Line:** 2.363400 Å **D1 Range:** 2.354 Å - 2.372 Å
**Search Line:** 2.098995 Å **D1 Range:** 2.092 Å - 2.106 Å
**Search Line:** 1.721028 Å **D1 Range:** 1.717 Å - 1.726 Å
**Search Line:** 1.872995 Å **D1 Range:** 1.868 Å - 1.878 Å
**Search Line:** 2.182236 Å **D1 Range:** 2.175 Å - 2.190 Å
**Rotation:** All 8 Rotations

## Preferences

**Radiation:** X-ray **Wavelength:** Cu Kα1 1.54056 Å **Search Method:** Hanawalt
**Search Window:** 0.15° **Match Window:** 0.15° **2nd Pass Filter:** Yes
**d-Spacings:** Weighted **Lowest Allowable GOM:** 2000

## Phases (1)

| # | Accepted | PDF # | QM | Compound Name | I Ratio | I % | I/Ic | Est Wt % |
|---|---|---|---|---|---|---|---|---|
| 1 | true | 00-041-1475 | S | Calcium Carbonate | 1.248 | 100 | *1.14 | 100 |

**00-041-1475** Jun 9, 2020 3:01 PM (fal-sharji2)

**Status** Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** Ca C O3
**Empirical Formula:** C Ca O3 **Weight %:** C12.00 Ca40.04 O47.95 **Atomic %:** C20.00 Ca20.00 O60.00
**Compound Name:** Calcium Carbonate **Mineral Name:** Aragonite

**Radiation:** CuKα1 **λ:** 1.5406 Å **d-Spacing:** Diff. **Intensity:** Diffractometer **I/Ic:** 1

**SYS:** Orthorhombic **SPGR:** Pmcn (62)
**Author's Cell [ AuthCell a:** 4.9623(3) Å **AuthCell b:** 7.968(1) Å **AuthCell c:** 5.7439(3) Å
**AuthCell Vol:** 227.11 Å³ **AuthCell Z:** 4.00 **AuthCell MolVol:** 56.78 ]
**Author's Cell Axial Ratio [ c/a:** 1.158 **a/b:** 0.623 **c/b:** 0.721 ]
**Density [ Dcalc:** 2.927 g/cm³ **Dmeas:** 2.95 g/cm³ ] **SS/FOM:** F(30) = 220.6(0.0040, 34)
**Temp:** 298.0 K (Ambient temperature assigned by ICDD editor) **Color:** Colorless

**Space Group:** Pnam (62) **Molecular Weight:** 100.09
**Crystal Data [ XtlCell a:** 5.744 Å **XtlCell b:** 7.968 Å **XtlCell c:** 4.962 Å **XtlCell α:** 90.00° **XtlCell β:** 90.00°
**XtlCell γ:** 90.00° **XtlCell Vol:** 227.11 Å³ **XtlCell Z:** 4.00 ]
**Crystal Data Axial Ratio [ c/a:** 0.864 **a/b:** 0.721 **c/b:** 0.623 ]
**Reduced Cell [ RedCell a:** 4.962 Å **RedCell b:** 5.744 Å **RedCell c:** 7.968 Å **RedCell α:** 90.00°
**RedCell β:** 90.00° **RedCell γ:** 90.00° **RedCell Vol:** 227.11 Å³ ]

**εα:** =1.5300 **πωβ:** =1.6810 **εγ:** =1.6854 **Sign:** =- **2V:** =18(calc.)°

**Atomic parameters are cross-referenced from PDF entry 04-012-0488** **ADP:** U
**Crystal (Symmetry Allowed):** Centrosymmetric
**SG Symmetry Operators:**

| Seq | Operator | Seq | Operator | Seq | Operator | Seq | Operator |
|---|---|---|---|---|---|---|---|
| 1 | x,y,z | 3 | -x+1/2,-y+1/2,z+1/2 | 5 | x+1/2,-y,-z | 7 | -x,y+1/2,-z+1/2 |
| 2 | -x,-y,-z | 4 | x+1/2,y+1/2,-z+1/2 | 6 | -x+1/2,y,z | 8 | x,-y+1/2,z+1/2 |

**Atomic Coordinates:**

| Atom | Num | Wyckoff | Symmetry | x | y | z | SOF | Uiso | AET |
|---|---|---|---|---|---|---|---|---|---|
| Ca | 1 | 4c | m.. | 0.25 | 0.41502 | 0.75985 | 1.0 | | |
| C | 2 | 4c | m.. | 0.25 | 0.76194 | -0.0824 | 1.0 | | |
| O | 3 | 4c | m.. | 0.25 | 0.92238 | -0.09453 | 1.0 | | |
| O | 4 | 8d | 1 | 0.47499 | 0.68012 | -0.08725 | 1.0 | | |

**Subfile(s):** Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Educational Pattern, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material (Superconductor Related Materials)

**Prototype Structure [Formula Order]:** Ca C O3 **Prototype Structure [Alpha Order]:** C Ca O3
**LPF Prototype Structure [Formula Order]:** Ca [ C O3 ],oP20,62
**LPF Prototype Structure [Alpha Order]:** C Ca O3,oP20,62
**Mineral Classification:** Aragonite (Group), carbonate (Subgroup) **Pearson Symbol:** oP20.00
**Cross-Ref PDF #'s:** 00-005-0453 (Alternate), 01-071-2392 (Alternate), 01-076-0606 (Alternate), ✓ 04-006-5441 (Alternate), ✓ 04-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate)
**CAS Number - PR:** 14791-73-2 **Entry Date:** 09/01/1991

**References:**

| Type | DOI | Reference |
|---|---|---|
| Primary Reference | | Keller, L., Rask, J., Buseck, P., Arizona State Univ., Tempe, AZ, USA. ICDD Grant-in-Aid (1989). |
| Crystal Structure | | Crystal Structure Source: LPF. |
| Optical Data | | Dana's System of Mineralogy, 7th Ed. II, 182 (1951). |
| Structure | | Jarosch, D., Heger, G. Tschermaks Mineral. Petrogr. Mitt. 35, 127 (1986). |

**Database Comments:** Additional Patterns: To replace 00-005-0453 and validated by calculated pattern 00-024-0025. See PDF 01-071-2392 and 01-076-0606. Analysis: Microprobe analyses (wt.%): major Ca, and trace Sr(<<1). Color: Colorless. General Comments: Antacid. Optical Data Specimen location: Optical data on specimen from Bilin, Bohemia, Czechoslovakia. Sample Source or Locality: Specimen from Sefrou, Morocco. Unit Cell Data Source: Powder Diffraction.

**d-Spacings (82) - Ca C O3 - 00-041-1475 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å**

| 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * | 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 21.0748 | 4.212000 | 3 | 1 | 1 | 0 | | 27.2153 | 3.274000 | 50 | 0 | 2 | 1 | | 33.1270 | **2.702000** | 60 | 0 | 1 | 2 | |
| 22.2959 | 3.984000 | 1 | 0 | 2 | 0 | | 31.1148 | 2.872000 | 6 | 0 | 0 | 2 | | 36.1753 | 2.481000 | 40 | 2 | 0 | 0 | |
| 26.2120 | **3.397000** | 100 | 1 | 1 | 1 | | 32.7406 | 2.733000 | 9 | 1 | 2 | 1 | | 37.2636 | 2.411000 | 14 | 0 | 3 | 1 | |

**00-041-1475** Jun 9, 2020 3:01 PM (fal-sharji2)

| 2θ (°) | d (Å) | I | h | k | l | * |
|---|---|---|---|---|---|---|
| 37.8829 | 2.373000 | 45 | 1 | 1 | 2 | |
| 38.4039 | 2.342000 | 25 | 1 | 3 | 0 | |
| 38.6095 | 2.330000 | 25 | 0 | 2 | 2 | |
| 41.1858 | 2.190000 | 12 | 2 | 1 | 1 | |
| 41.6231 | 2.168000 | 2 | 1 | 3 | 1 | |
| 42.8654 | 2.108000 | 20m | 1 | 2 | 2 | |
| 42.8654 | 2.108000 | m | 2 | 2 | 0 | |
| 45.8520 | **1.977400** | 55 | 2 | 2 | 1 | |
| 46.5339 | 1.950000 | 1 | 0 | 3 | 2 | |
| 48.3175 | 1.882100 | 25 | 0 | 4 | 1 | |
| 48.4435 | 1.877500 | 25 | 2 | 0 | 2 | |
| 48.8842 | 1.861600 | 2 | 0 | 1 | 3 | |
| 49.8579 | 1.827500 | 4 | 2 | 1 | 2 | |
| 50.2279 | 1.814900 | 20 | 1 | 3 | 2 | |
| 51.9156 | 1.759800 | 3 | 1 | 4 | 1 | |
| 52.4539 | 1.743000 | 25 | 1 | 1 | 3 | |
| 52.9114 | 1.729000 | 12 | 2 | 3 | 1 | |
| 53.0205 | 1.725700 | 16 | 0 | 2 | 3 | |
| 53.9411 | 1.698400 | 2 | 2 | 2 | 2 | |
| 56.1429 | 1.636900 | 3 | 0 | 4 | 2 | |
| 56.4018 | 1.630000 | 1 | 1 | 2 | 3 | |
| 56.7891 | 1.619800 | 2 | 3 | 1 | 0 | |
| 59.2273 | 1.558800 | 4 | 3 | 1 | 1 | |
| 60.2095 | 1.535700 | 2 | 0 | 5 | 1 | |
| 61.8292 | 1.499300 | 4 | 2 | 4 | 1 | |
| 62.2998 | 1.489100 | 1 | 2 | 1 | 3 | |
| 62.8965 | 1.476400 | 2 | 3 | 2 | 1 | |
| 63.3365 | 1.467200 | 4 | 1 | 5 | 1 | |
| 64.8787 | 1.436000 | 1 | 0 | 0 | 4 | |
| 65.8737 | 1.416700 | 1 | 2 | 2 | 3 | |
| 66.0576 | 1.413200 | 3 | 0 | 1 | 4 | |
| 66.1897 | 1.410700 | 4 | 3 | 1 | 2 | |
| 66.5465 | 1.404000 | 3 | 3 | 3 | 0 | |
| 67.8369 | 1.380400 | <1 | 0 | 4 | 3 | |
| 68.6339 | 1.366300 | 2 | 2 | 4 | 2 | |
| 68.7716 | 1.363900 | 2 | 3 | 3 | 1 | |
| 69.0430 | 1.359200 | 5 | 1 | 1 | 4 | |
| 69.5398 | 1.350700 | 2 | 0 | 2 | 4 | |
| 69.6578 | 1.348700 | 3 | 3 | 2 | 2 | |
| 70.0803 | 1.341600 | 2 | 1 | 5 | 2 | |
| 70.8439 | 1.329000 | 1m | 0 | 6 | 0 | |
| 70.8439 | 1.329000 | m | 1 | 4 | 3 | |
| 72.2986 | 1.305800 | 1 | 2 | 5 | 1 | |
| 72.4464 | 1.303500 | 1 | 1 | 2 | 4 | |
| 75.2667 | 1.261500 | 5 | 3 | 3 | 2 | |
| 75.9315 | 1.252100 | 1 | 1 | 6 | 1 | |
| 76.6095 | 1.242700 | 3m | 2 | 0 | 4 | |
| 76.6095 | 1.242700 | m | 3 | 4 | 1 | |
| 76.7628 | 1.240600 | 4 | 4 | 0 | 0 | |
| 77.0640 | 1.236500 | 6 | 3 | 1 | 3 | |
| 77.9611 | 1.224500 | 3m | 0 | 5 | 3 | |
| 77.9611 | 1.224500 | m | 1 | 3 | 4 | |
| 78.6958 | 1.214900 | 2 | 2 | 5 | 2 | |
| 79.3988 | 1.205900 | 4m | 0 | 6 | 2 | |
| 79.3988 | 1.205900 | m | 2 | 4 | 3 | |
| 80.7577 | 1.189000 | 3 | 1 | 5 | 3 | |
| 80.9714 | 1.186400 | 2 | 2 | 2 | 4 | |
| 82.2556 | 1.171100 | 3m | 1 | 6 | 2 | |
| 82.2556 | 1.171100 | m | 2 | 6 | 0 | |
| 82.8500 | 1.164200 | 1m | 0 | 4 | 4 | |
| 82.8500 | 1.164200 | m | 3 | 4 | 2 | |
| 83.2166 | 1.160000 | 2 | 4 | 2 | 1 | |
| 85.1161 | 1.138900 | 1 | 4 | 0 | 2 | |
| 85.2920 | 1.137000 | <1 | 0 | 1 | 5 | |
| 85.7309 | 1.132300 | 1 | 3 | 3 | 3 | |
| 86.1940 | 1.127400 | 1 | 4 | 1 | 2 | |
| 86.3656 | 1.125600 | 2m | 2 | 3 | 4 | |
| 86.3656 | 1.125600 | m | 3 | 5 | 1 | |
| 87.9962 | 1.108900 | 2m | 1 | 1 | 5 | |
| 87.9962 | 1.108900 | m | 1 | 7 | 0 | |
| 88.5389 | 1.103500 | 1m | 0 | 2 | 5 | |
| 88.5389 | 1.103500 | m | 4 | 3 | 1 | |
| 89.4092 | 1.095000 | <1 | 4 | 2 | 2 | |