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MAGNETIC WATER TREATMENT FOR SCALE PREVENTION ON WATER HEATER ELEMENTS

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By

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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.

Acknowledgement

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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This can't go on without stating that my friends and family who showcased genuine love, support, and were the ones who constantly pushed me to become the best version of myself and be able to face adversity in a logical manner rather than give up.

Forever indebted to my parents who paved the way for my education and taught me that one reaps the true benefits of learning in the long term. I can't find enough words that can truly reflect my sincere gratitude for my parents as they were the ones who enabled my journey to attain my master's degree. I dedicate this thesis to them.

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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.

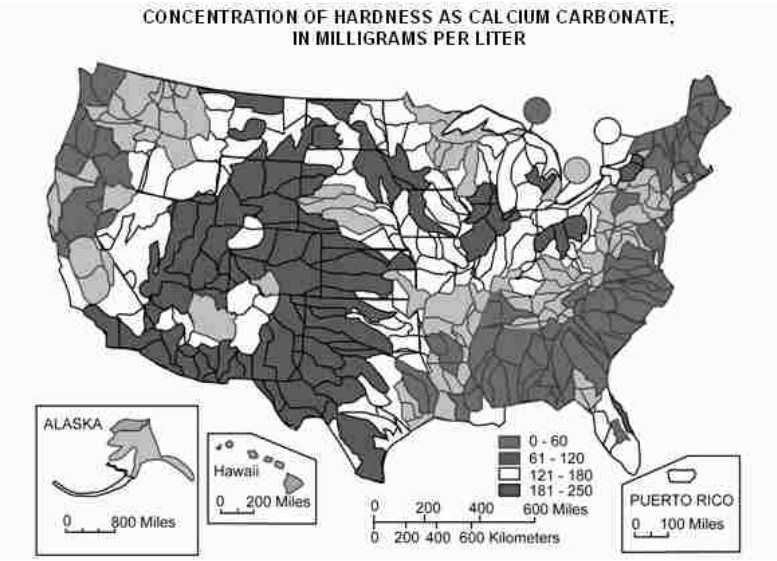

Figure 2.1 Mean hardness as calcium carbonate concentration levels. Source: USGS, (2019)

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.

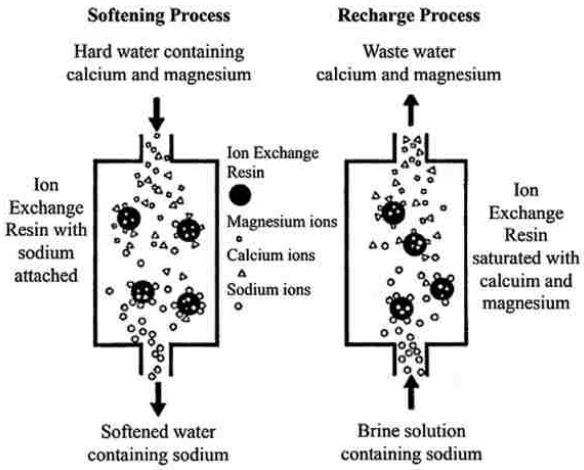

Figure 2.2 Water Softening and Regeneration Process.
Source: Skipton et al. (2008)

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.

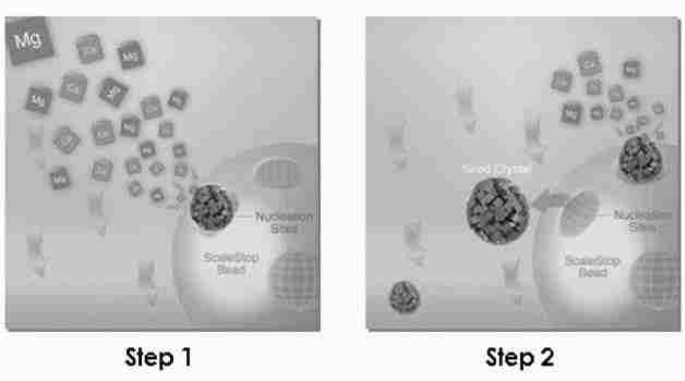

Figure 2.3 Template Assisted Crystallization (TAC) process. Source: Premier Water Technologies (2012)

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.

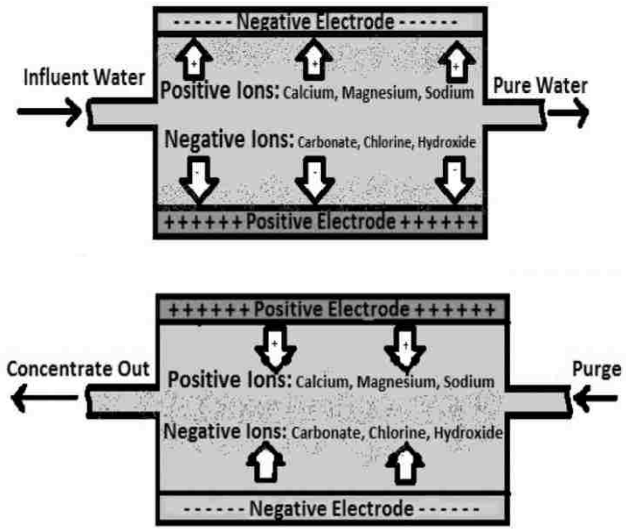

Figure 2.4 Capacitive Deionization (CDI) Process, Purification step (Top), Backwash Step (Bottom).
Source: Wiest et al. (2011)

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.

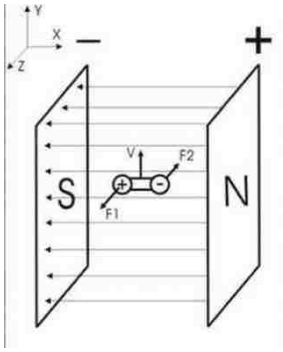

Figure 2.5 Physical Behavior. Source: Mosin and Ignatov, (2014)

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).

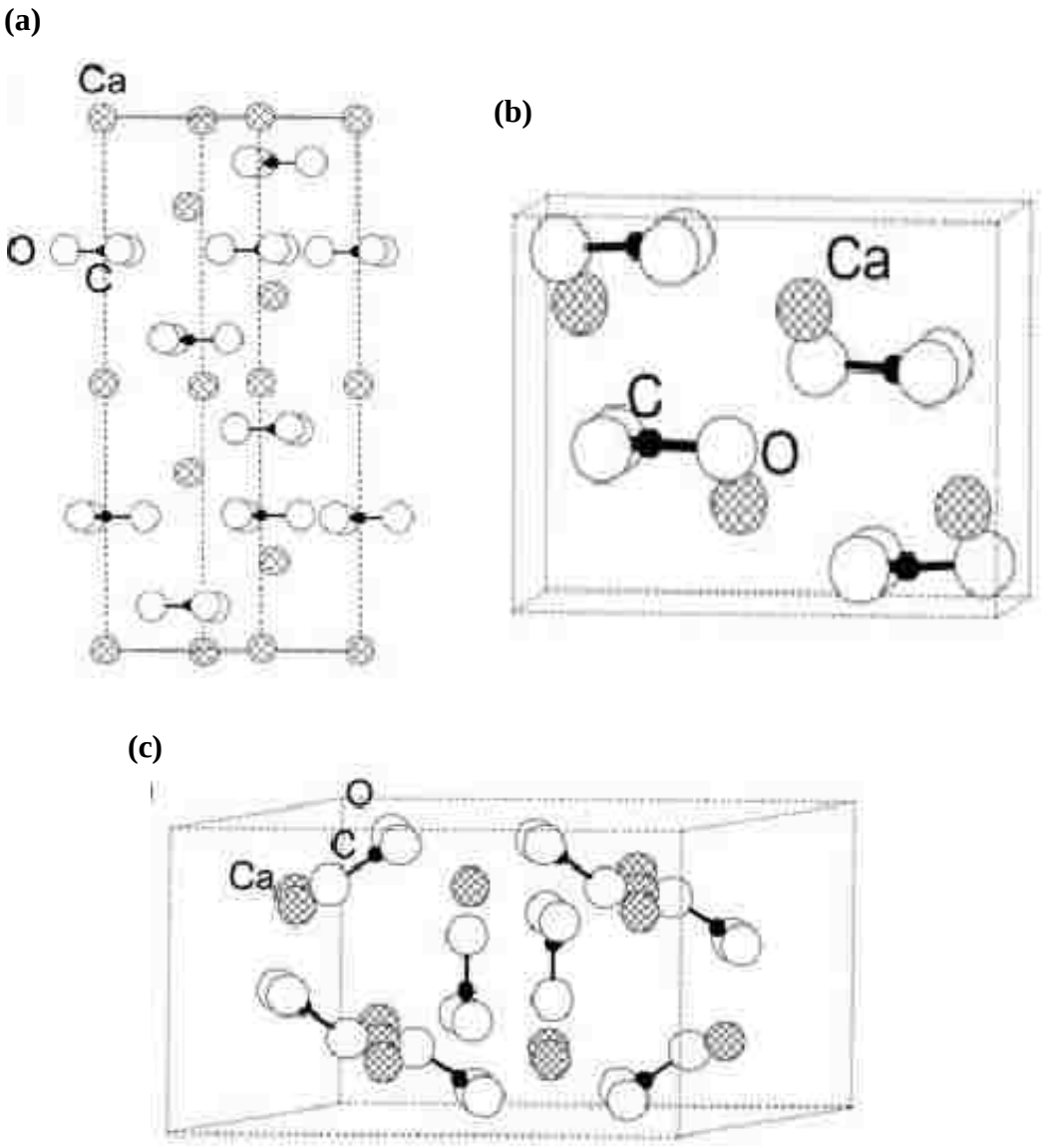

Figure 2.6 Schematic representation of crystallographic unit cells for (a) Calcite (b) Aragonite and (c) Vaterite. Source: Xu and Poduska, (2014)

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. 2θ is the angle between the incoming and outgoing beams direction. The lattice spacing, d, were calculated from the 2θ values using Braggs Law: $n\lambda = 2d \sin(\theta)$, where n is a positive integer (1, 2, 3, ...) λ 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 4th, 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 9th, 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.

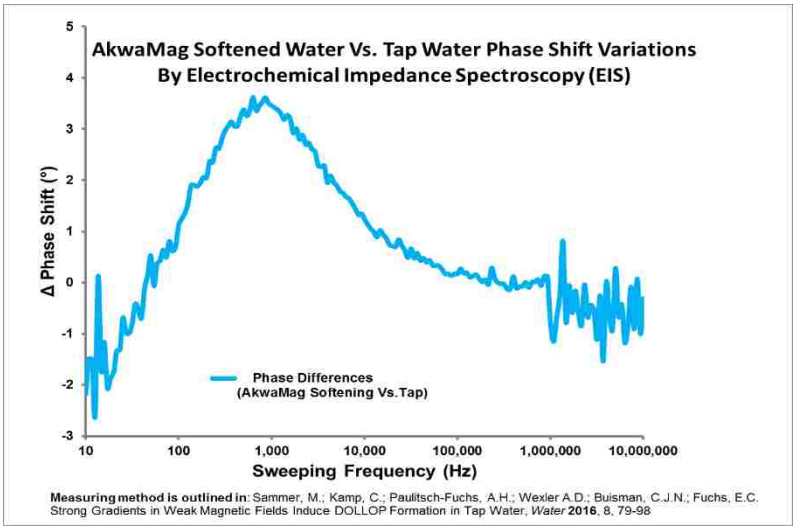

Figure 3.1 Impedance phase shift spectra of AkwaMag vs Tap water

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.

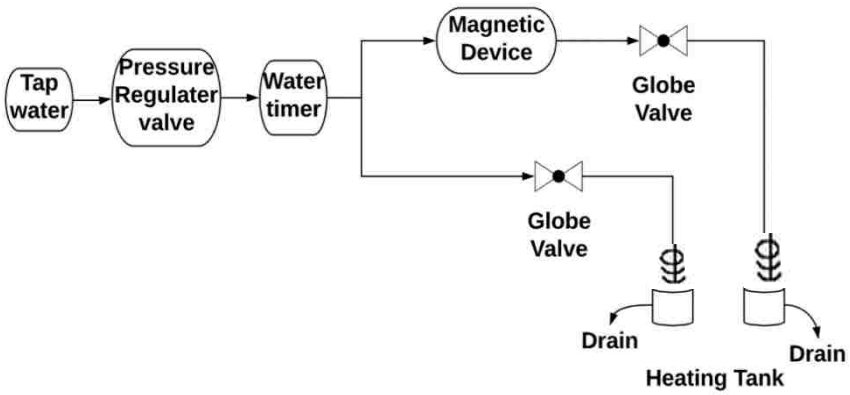

Figure 3.2 Heating System Apparatus Schematic

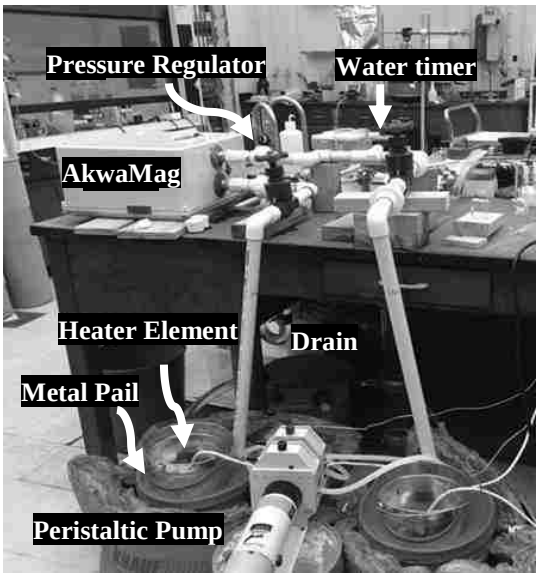

Figure 3.3 Experimental Set-Up for Water Heater Simulation test

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.

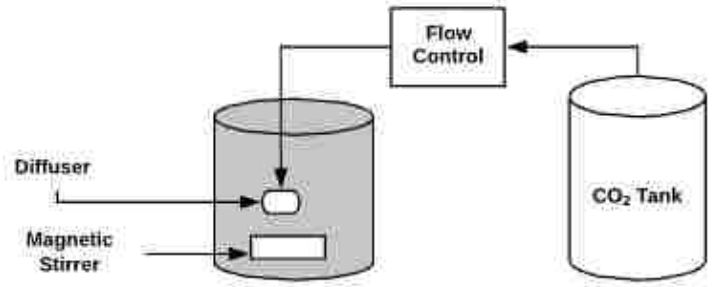

Figure 3.4 Feed preparation Set-Up

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.

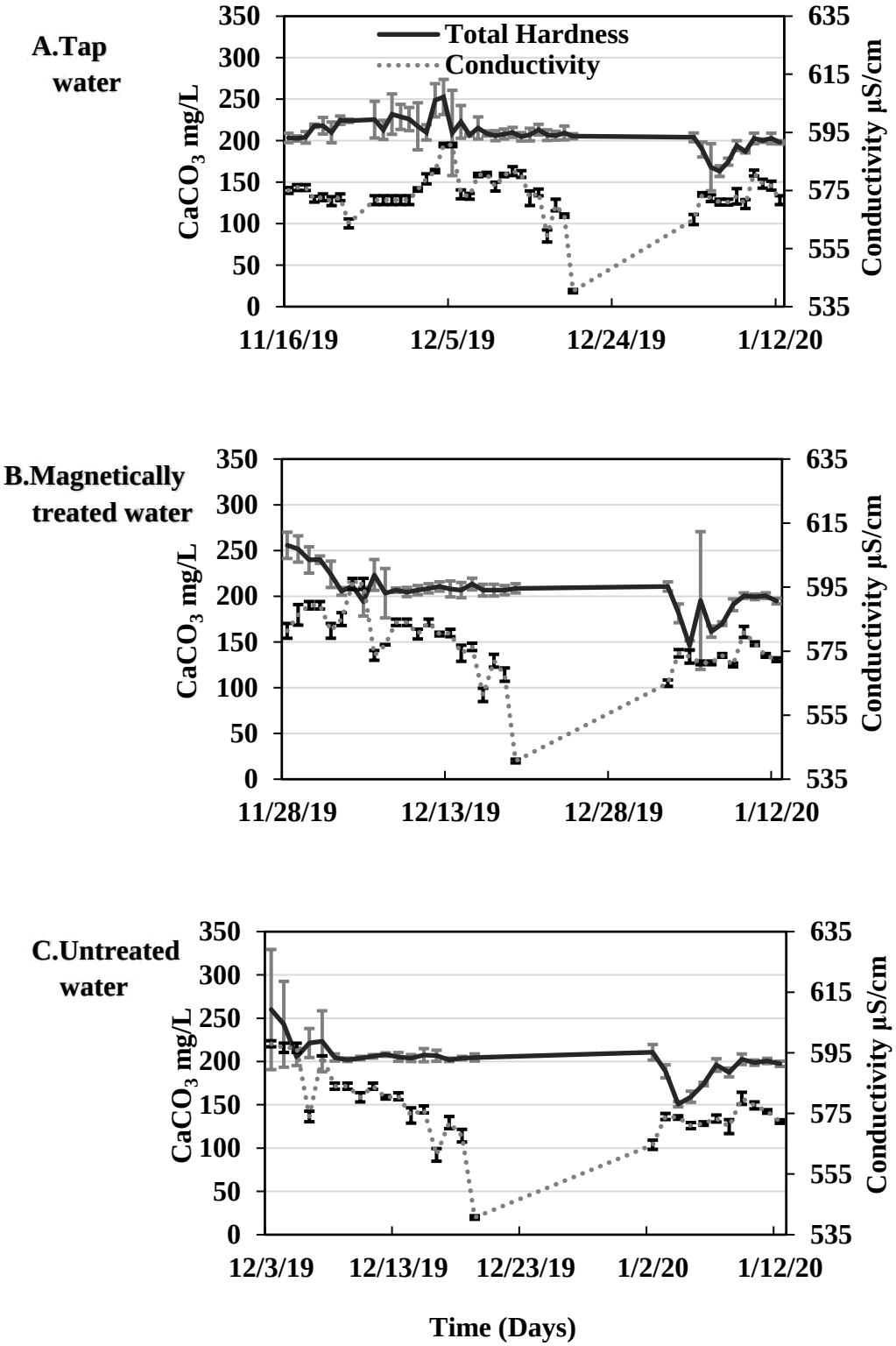

Figure 4.1 Influent water quality results from the experiment with a tank with 70.4 in^2 of exposed iron of (A) Tap water, (B) Magnetically treated water, (C) Untreated water

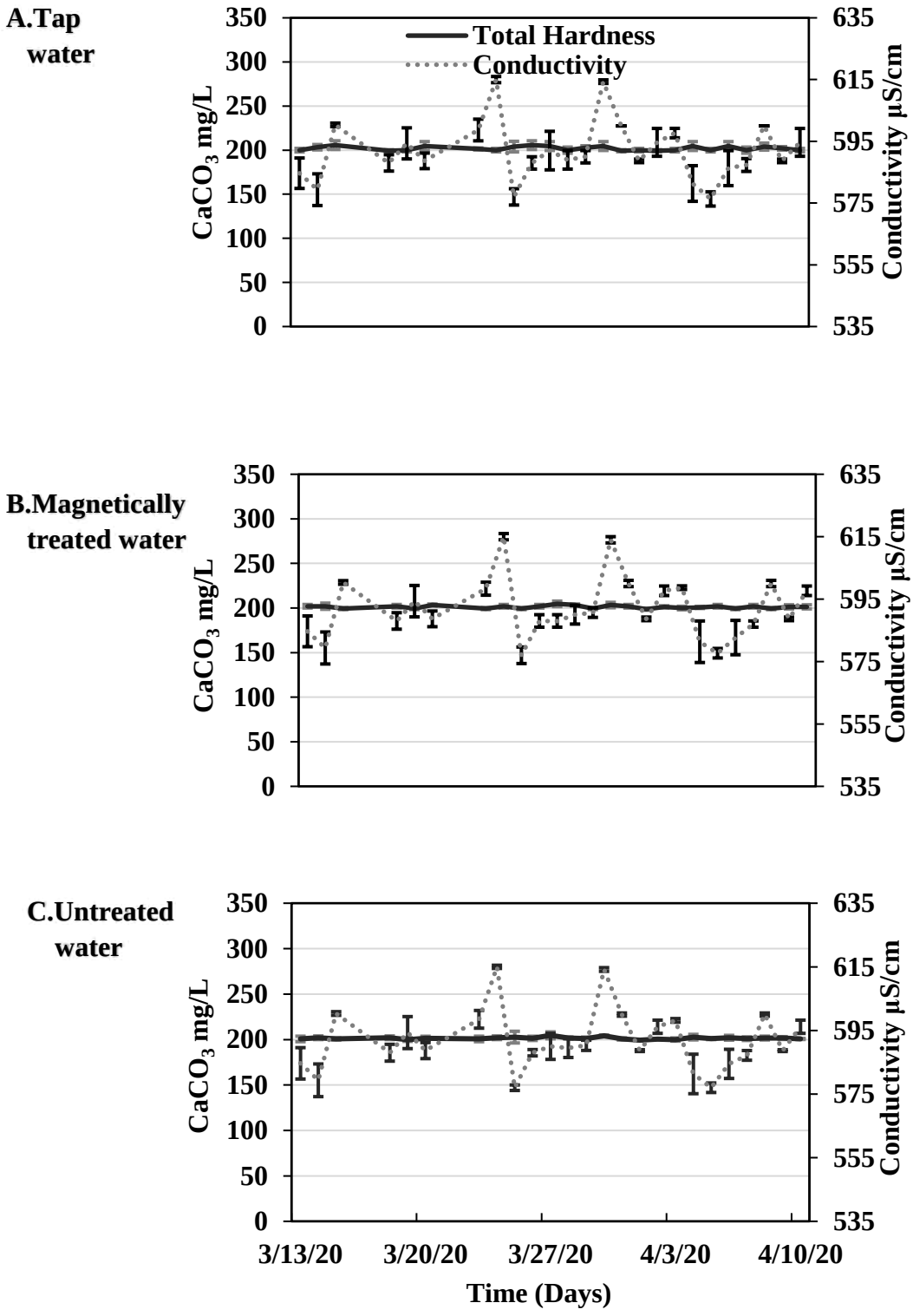

Figure 4.2 Influent water quality results from the experiment with a tank with little exposure of iron of (A) Tap water, (B) Magnetically treated water, (C) Untreated water

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

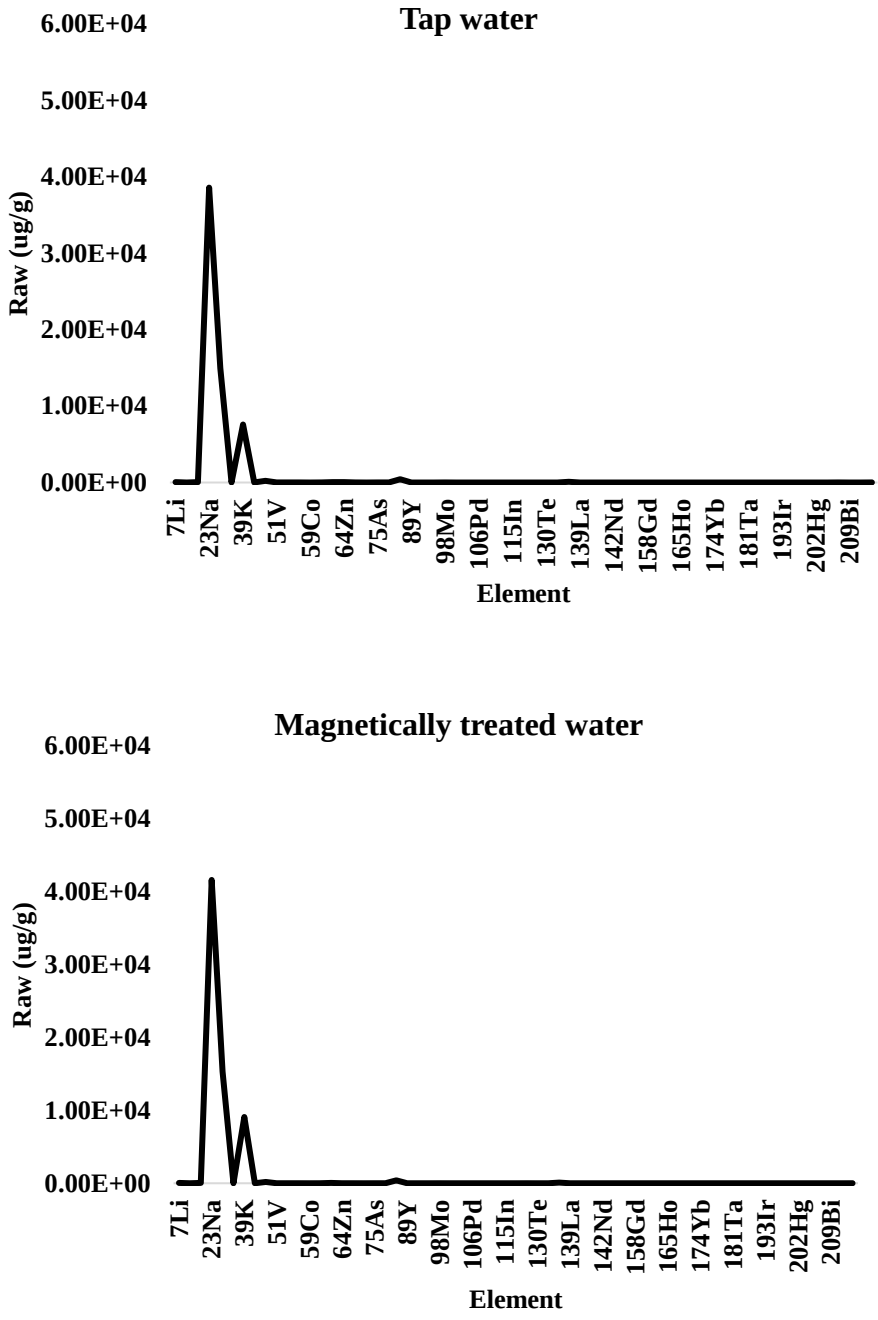

Figure 4.3. Semi-quantitative results for different elements

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.

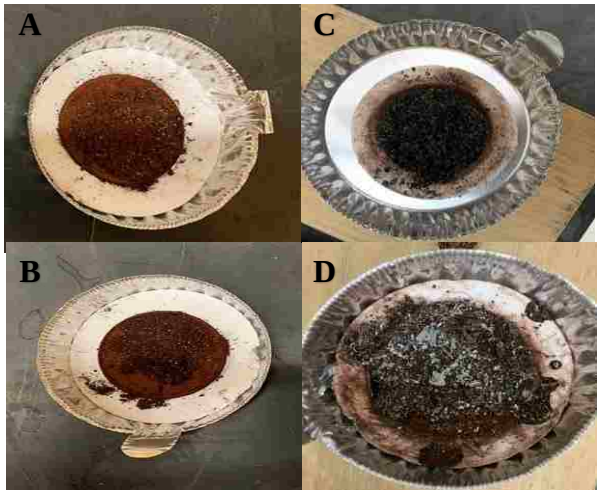

Figure 4.4 Solids formed from the experiment with a tank with 70.4 in^2 of exposed iron of (A) Untreated water tank (B) Magnetically treated water tank, and the experiment with a tank with little exposure of iron of (C) Untreated water tank (D) Magnetically treated water tank

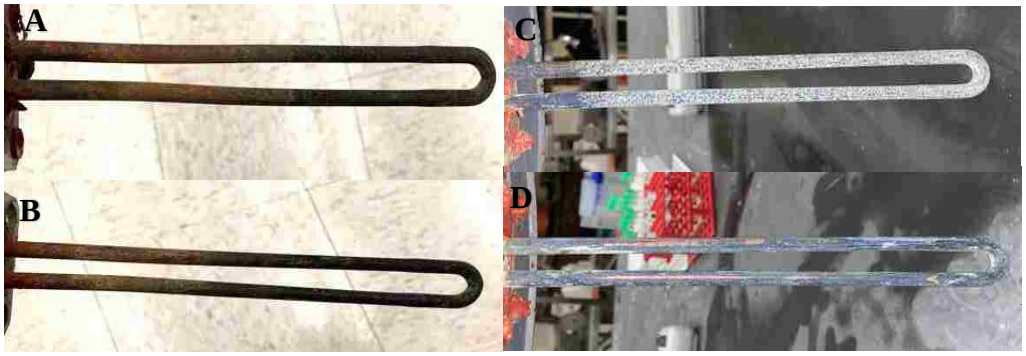

Figure 4.5 Scale formed on heater element from the experiment with a tank with 70.4 in^2 of exposed iron of (A) Untreated water (B) Magnetically treated water, and from the experiment with a tank with little exposure of iron of (C) Untreated water (D) Magnetically treated water

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.

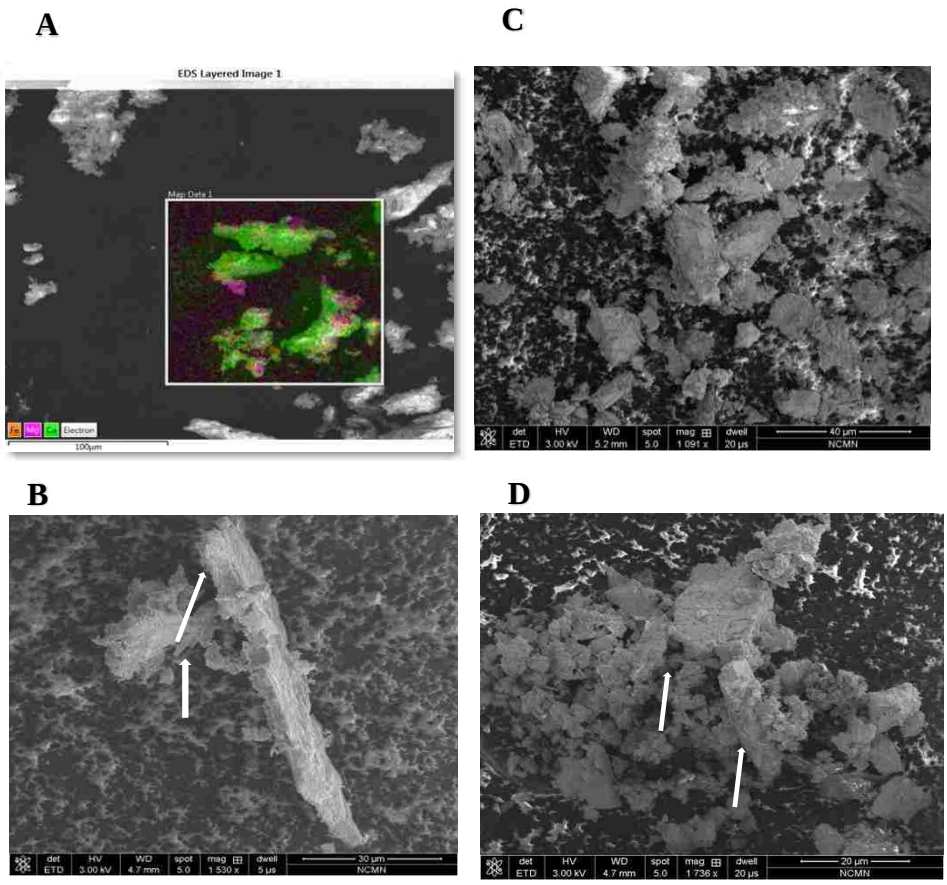

Figure 4.6 SEM Image of heating element from the experiment with a tank with 70.4 in^2 of exposed iron of (A) Untreated water (Electron Layer Image), (B) Magnetically treated water, and from the experiment with a tank with little exposure of iron of (C) Untreated water (D) Magnetically treated water

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.

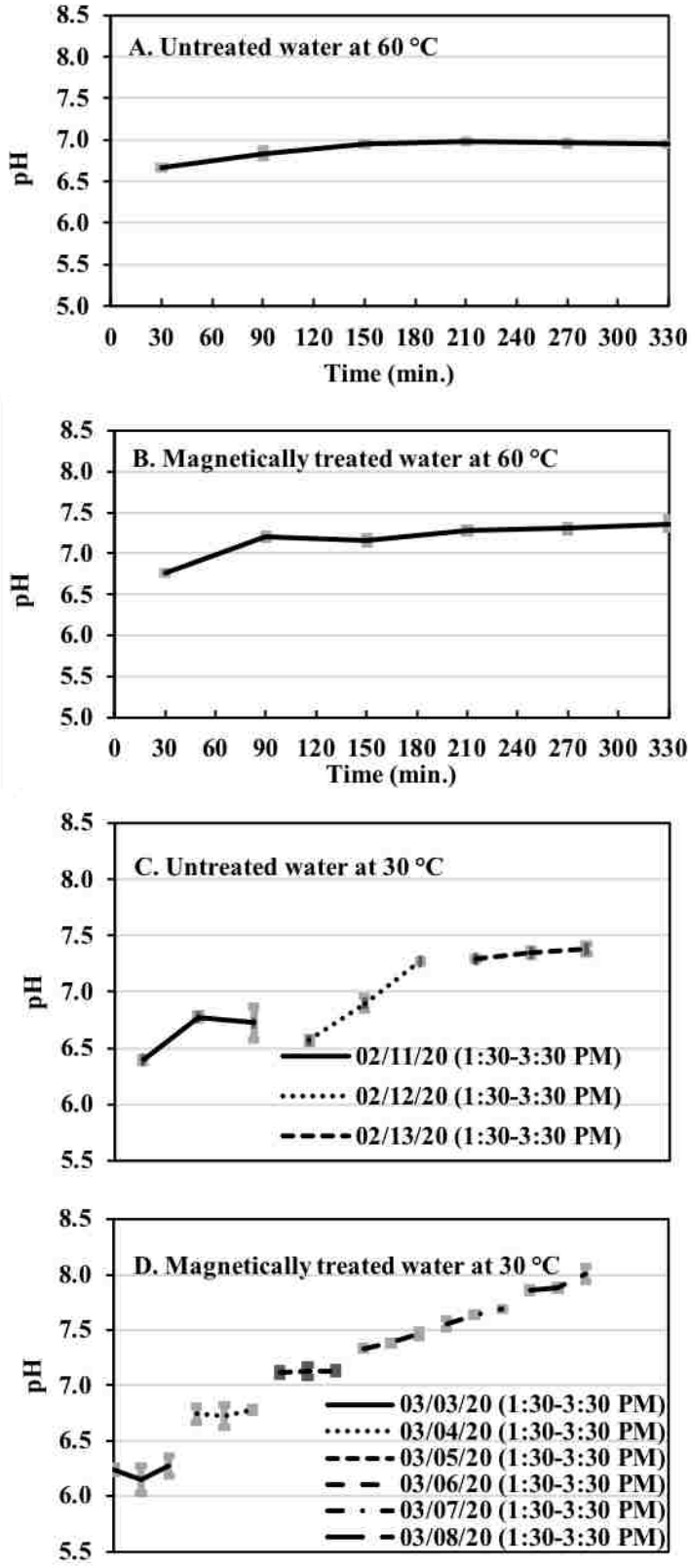

Figure 4.7 Effect of pH on (A) untreated water at 60 °C (B) magnetically treated water at 60 °C and (C) untreated water at 30 °C (D) magnetically treated water at 30 °C

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.

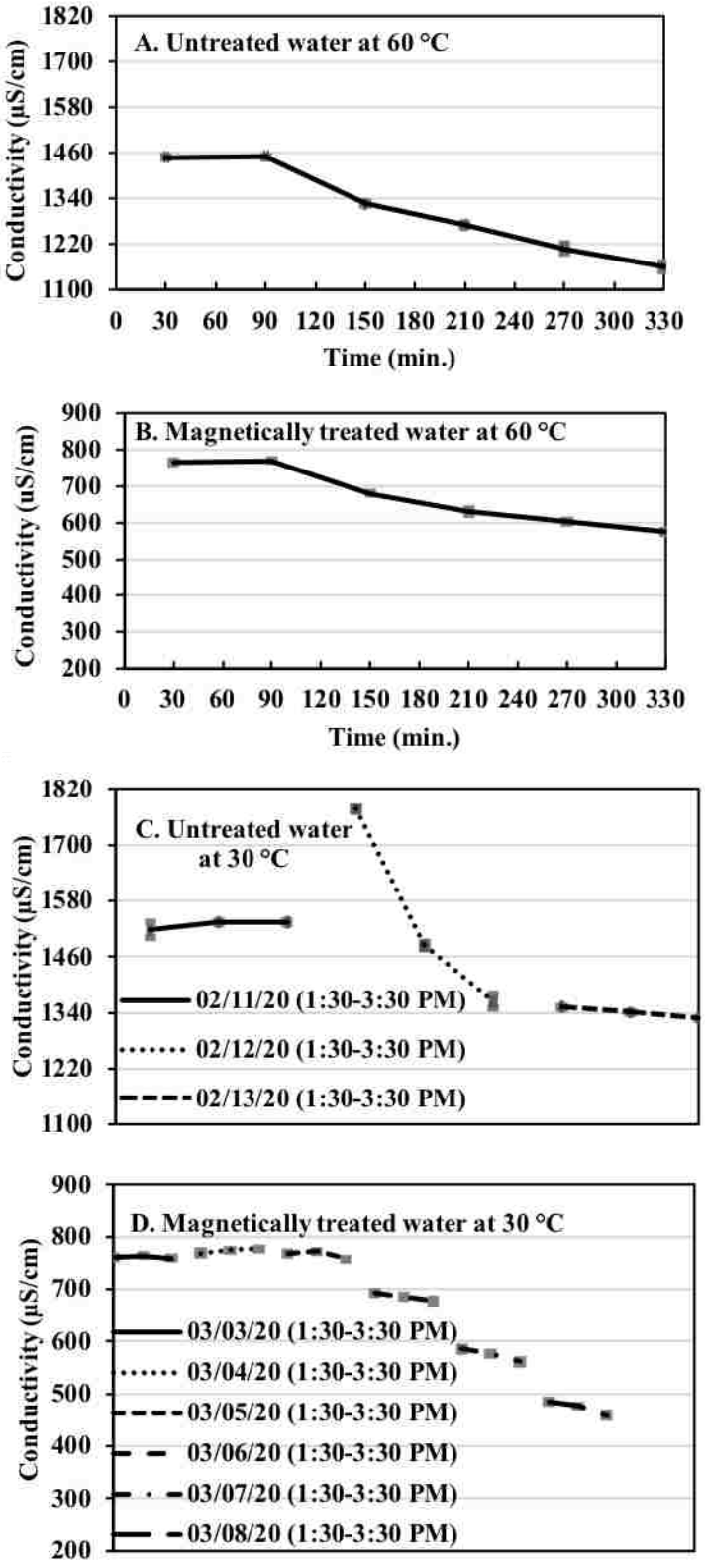

Figure 4.8 Effect of Conductivity on (A) untreated water at 60 °C (B) magnetically treated water at 60 °C and (C) untreated water at 30 °C (D) magnetically treated water at 30 °C

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.

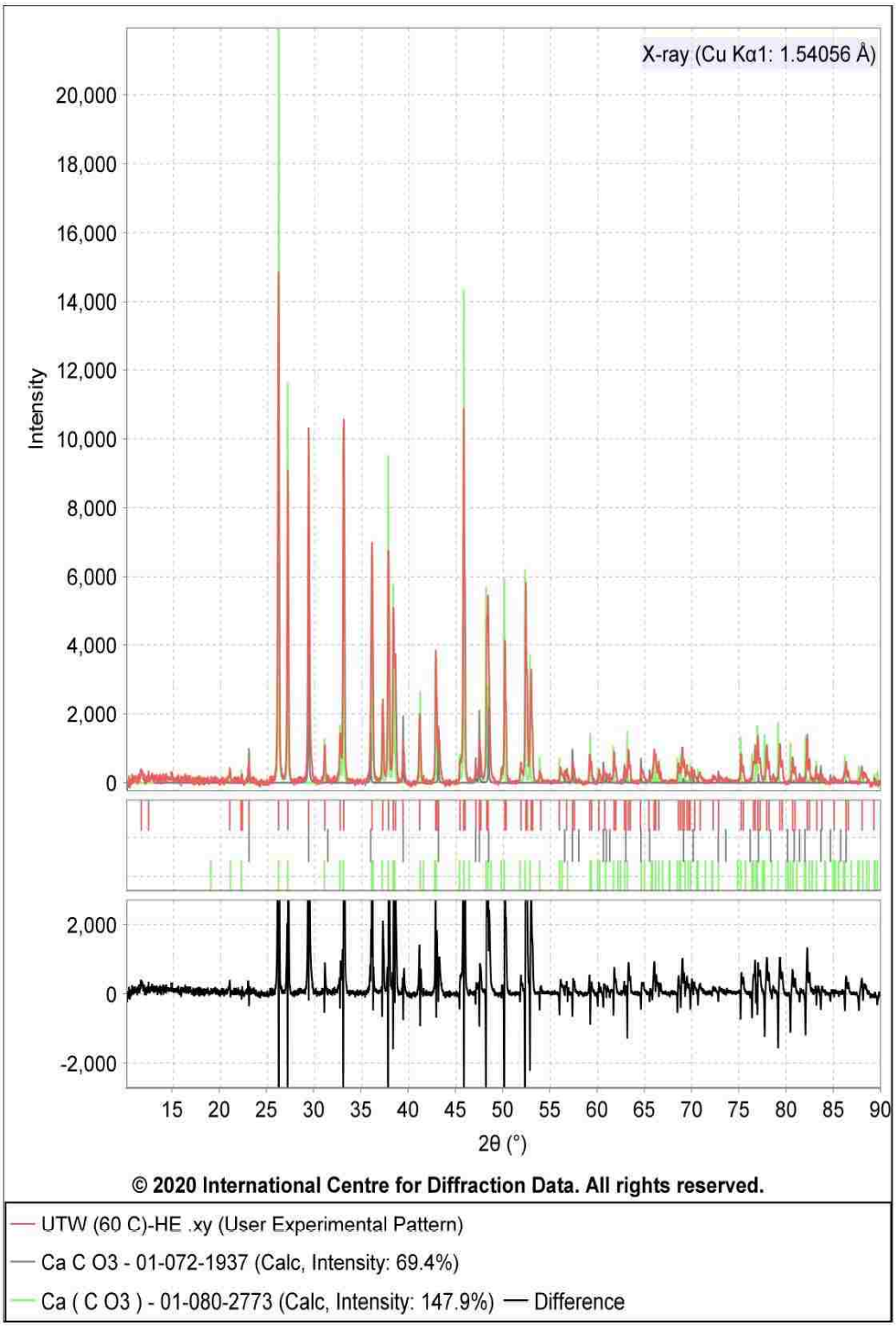

Figure 4.9 XRD patterns of substances precipitated from Untreated Water (UTW) heating element (HE) at 60 °C. Aragonite-PDF# 01-080-2773 **Calcite-**PDF# 01-072-1937

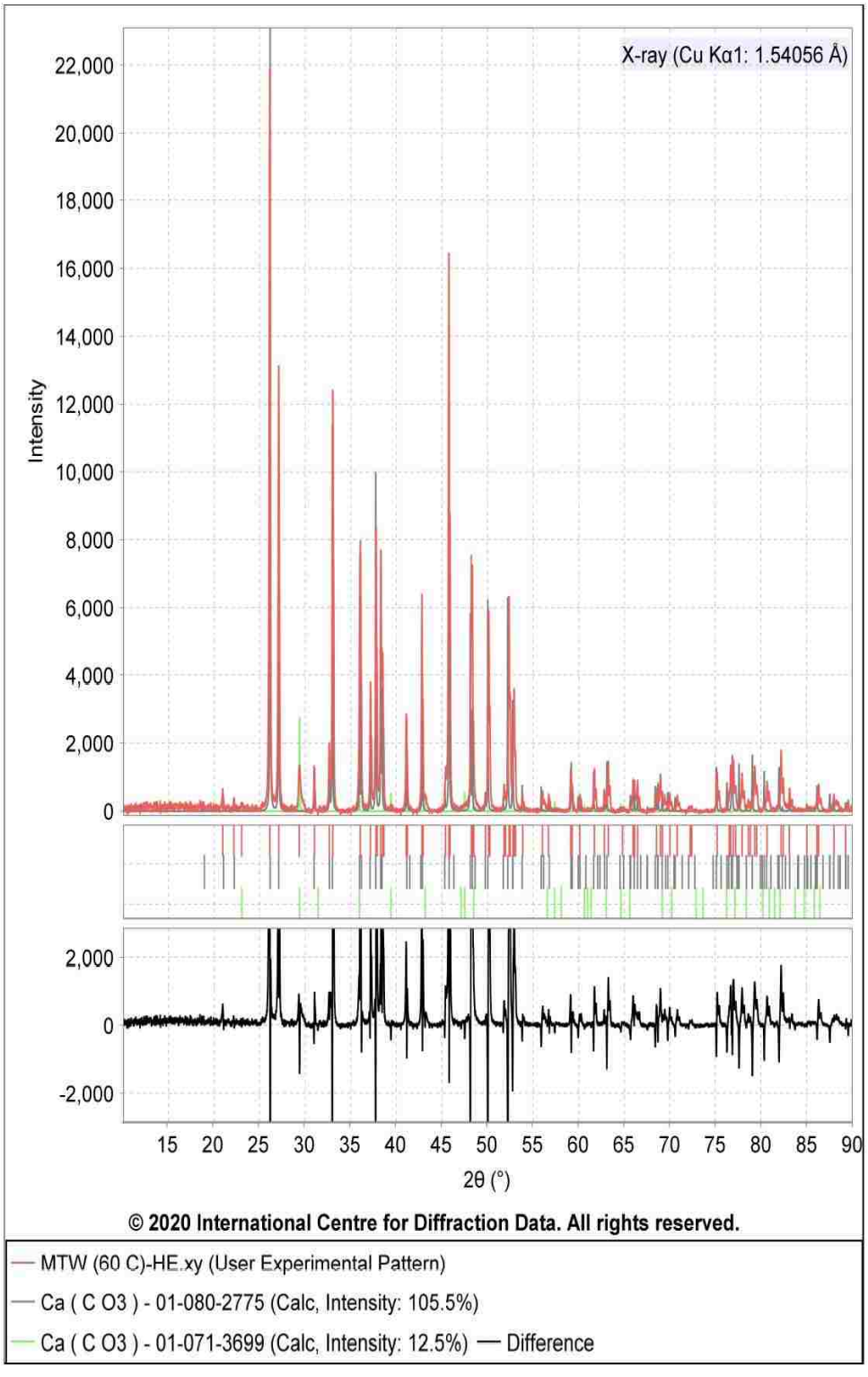

Figure 4.10 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element (HE) at 60 °C. Aragonite-PDF# 01-080-2775 **Calcite-** PDF# 01-071-3699

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.

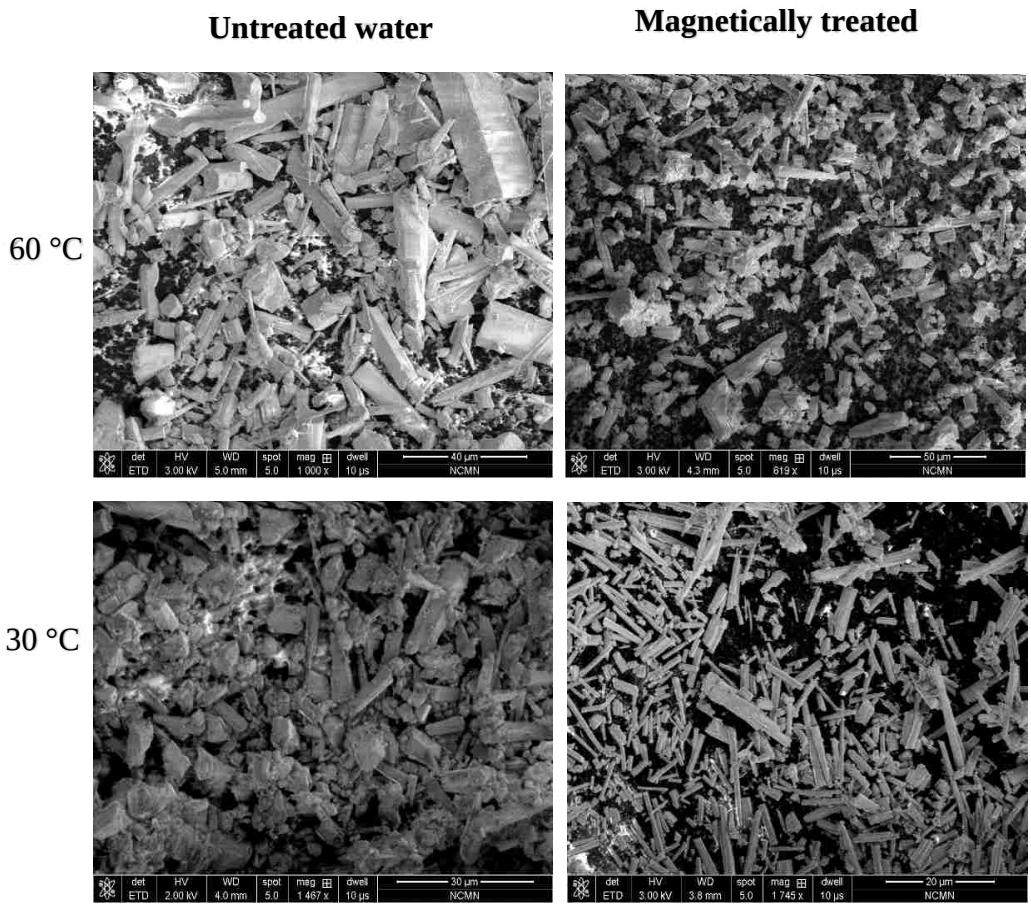

Figure 4.11 SEM Images of Calcite and Aragonite

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)

$$t = \frac{\overline{X_1} - \overline{X_2}}{S_{\overline{X_1} - \overline{X_2}}}$$

$$S_{\overline{X_1} - \overline{X_2}} = \sqrt{\frac{S_{X_1}^2}{n_1} + \frac{S_{X_2}^2}{n_2}}$$

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

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

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

$\overline{X_1}$ = 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)

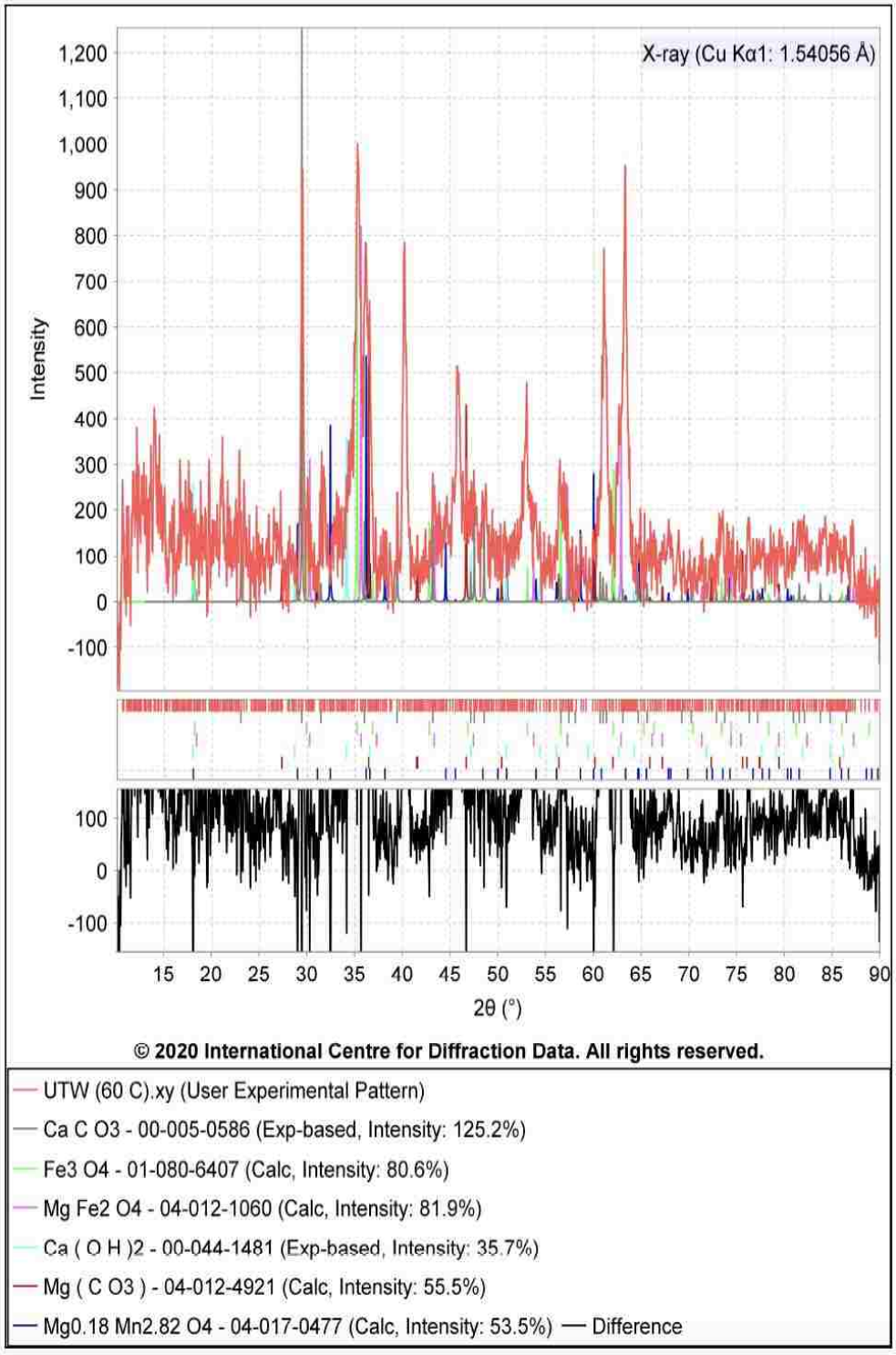

Figure E.1 XRD patterns of substances precipitated from Untreated Water (UTW) tank at 60 ˚C from experiment with a tank with 70.4 in^2 of exposed iron

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: CuKa1 **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 **mωβ:** =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 (Biooeramic), 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), 04-010-0489 (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 Ka1 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		84.6765	1.440000	6	3	0	0	
29.4049	3.035000	100	1	0	4		56.5630	1.626000	4	2	1	1		85.5972	1.422000	3	0	0	12	
31.4176	2.845000	3	0	0	6		57.4001	1.604000	8	1	2	2		89.2291	1.356000	1	2	1	7	
35.9654	2.495000	14	1	1	0		58.0732	1.587000	2	1	0	10		70.2364	1.339000	2	0	2	10	
39.4009	2.285000	18	1	1	3		60.8782	1.525000	5	2	1	4		72.6878	1.297000	3	1	2	8	
43.1447	2.095000	18	2	0	2		60.9857	1.518000	4	2	0	8		73.7284	1.284000	1	3	0	6	
47.1226	1.927000	5	0	2	4		61.3435	1.510000	3	1	1	9		76.2877	1.247000	1	2	2	0	
47.4686	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	*
80.9302	1.186800	<1	3	1	2	E
81.5449	1.179500	3	2	1	10	
82.1106	1.173000	<1	0	1	14	E
83.7648	1.153800	3	1	3	4	
84.7850	1.143500	1	2	2	8	
86.4804	1.124400	<1	1	2	11	
83.0891	1.061300	1	2	0	14	
84.6975	1.047300	3	4	0	4	
85.0075	1.044700	4	3	1	8	
86.1817	1.035200	2	1	0	16	
87.8440	1.023400	<1	2	1	13	
89.1573	1.014800	2	3	0	12	
102.2084	0.889500	<1	3	2	1	
102.9484	0.884800	1	2	3	2	
103.8850	0.878200	1	1	3	10	
104.1201	0.876700	3	1	2	14	
105.8419	0.865500	2	3	2	4	
106.1414	0.863600	4	0	4	8	
107.3295	0.856200	<1	0	2	18	
109.5566	0.842900	2	4	1	0	
110.4784	0.837600	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), 01-076-5428 (Alternate), 01-082-9851 (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), 04-002-3458 (Alternate), 04-002-3459 (Alternate), 04-002-3654 (Alternate), 04-002-3768 (Alternate), 04-002-3769 (Alternate), 04-002-5223 (Alternate), 04-002-5326 (Alternate), 04-002-5461 (Alternate), 04-002-5666 (Alternate), 04-002-5894 (Alternate), 04-002-5904 (Alternate), 04-002-5403 (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), 04-006-2451 (Alternate), 04-006-2459 (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 8 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 Ka1 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	4.823630	29	1	1	1		74.3982	1.274060	71	5	3	3		111.1053	0.934073	22	8	4	0	
30.2322	**2.953886**	375	2	2	0		76.4071	1.259500	16	6	2	2		114.2731	0.917037	1	8	1	1	
35.6110	**2.519010**	999	3	1	1		79.4003	1.206880	21	4	4	4		115.3482	0.911582	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	8	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	
47.3818	1.918680	1	3	3	1		90.1751	1.087680	89	7	3	1		129.2053	0.852888	89	8	4	4	
53.7028	1.706380	109	4	2	2		95.0530	1.044320	40	8	0	0		133.0887	0.839889	1	9	3	3	
57.2503	1.607840	229	5	1	1		97.9937	1.020980	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		144.9980	0.807870	55	9	5	1	
66.1109	1.412190	3	5	3	1		102.9486	0.984099	16	8	2	2		146.7319	0.803922	6	10	2	2	
67.1724	1.393430	1	4	4	2		105.9868	0.964706	55	7	5	1								
71.3395	1.320980	36	6	2	0		106.9828	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), 01-080-7583 (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), 04-002-3669 (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), 04-004-2836 (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), 04-007-8975 (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 Ka1 1.54056 Å

2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*
18.1890	4.878550	100	1	1	1		73.4200	1.288600	66	5	3	3		109.2431	0.944729	14	9	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	**2.547746**	999	3	1	1		76.3311	1.246640	17	4	4	4		113.3319	0.921960	1	9	4	2	
36.8160	2.439260	76	2	2	2		81.2348	1.183220	3	5	5	1		117.5610	0.900762	4	6	6	4	
42.7702	2.112470	202	4	0	0		86.0261	1.129170	23	6	4	2		120.8236	0.886799	28	9	3	1	
46.8263	1.938540	4	3	3	1		88.8867	1.100360	74	7	3	1		125.5480	0.862414	48	8	4	4	
53.0493	1.724820	82	4	2	2		93.6496	1.056240	27	8	0	0		130.1922	0.848247	1	9	3	3	
56.5482	1.626180	263	5	1	1		96.5183	1.032320	1	7	5	3		136.7568	0.828561	10	8	6	2	
62.0543	**1.493750**	231	4	4	0		97.4779	1.024700	1	8	4	4		141.1061	0.816883	29	9	5	1	
65.2723	1.426290	7	5	3	1		101.3395	0.995830	10	9	2	2		142.6488	0.813092	5	10	2	2	
66.3160	1.408320	1	4	4	2		104.2894	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 (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								

04-017-0477 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	
31.0838	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	6		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	1.179960	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		141.5684	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	

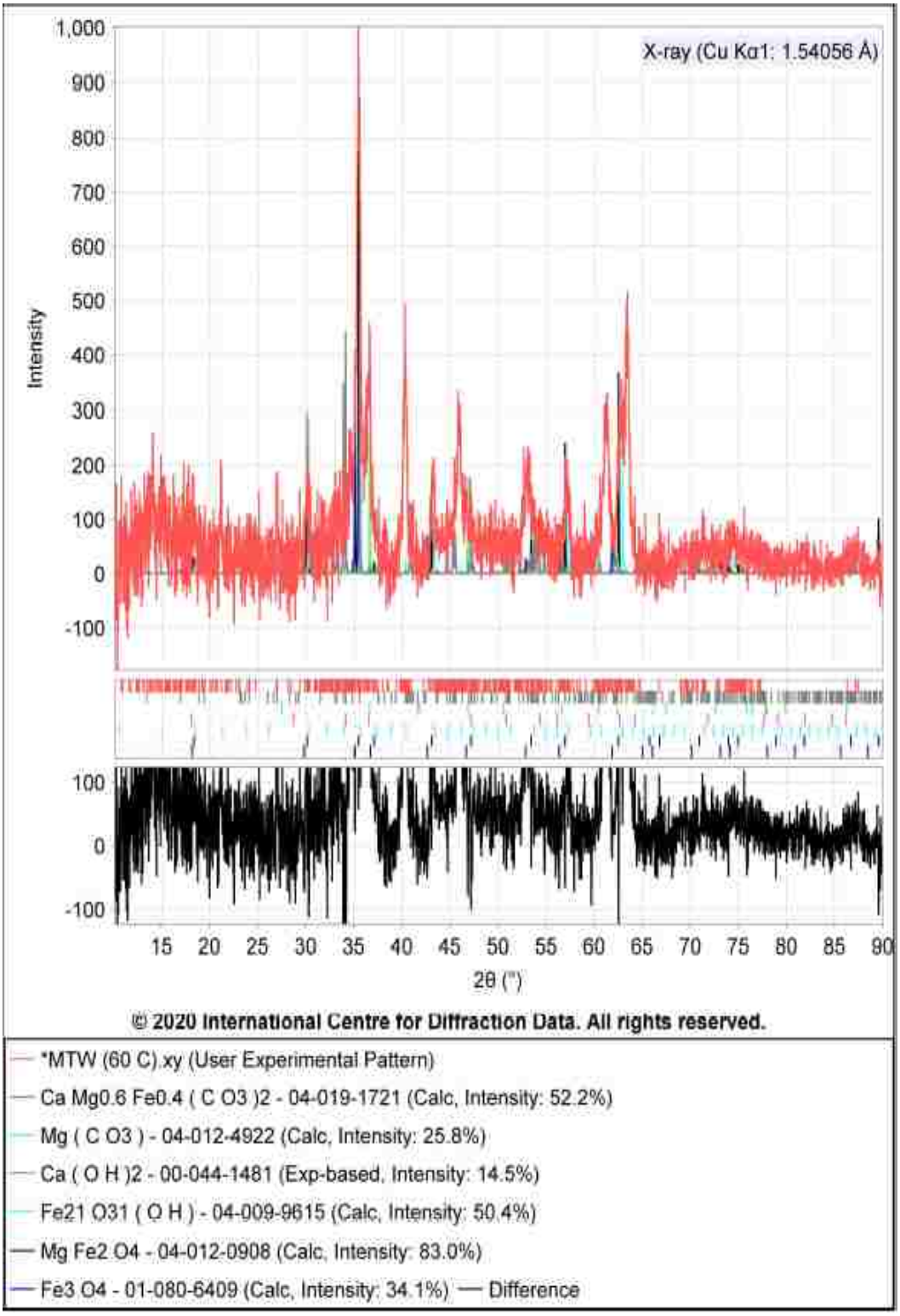

Figure E.2 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) tank at 60 °C from experiment with a tank with 70.4 in^2 of exposed iron

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	

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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	

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 (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								

04-009-9615 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								

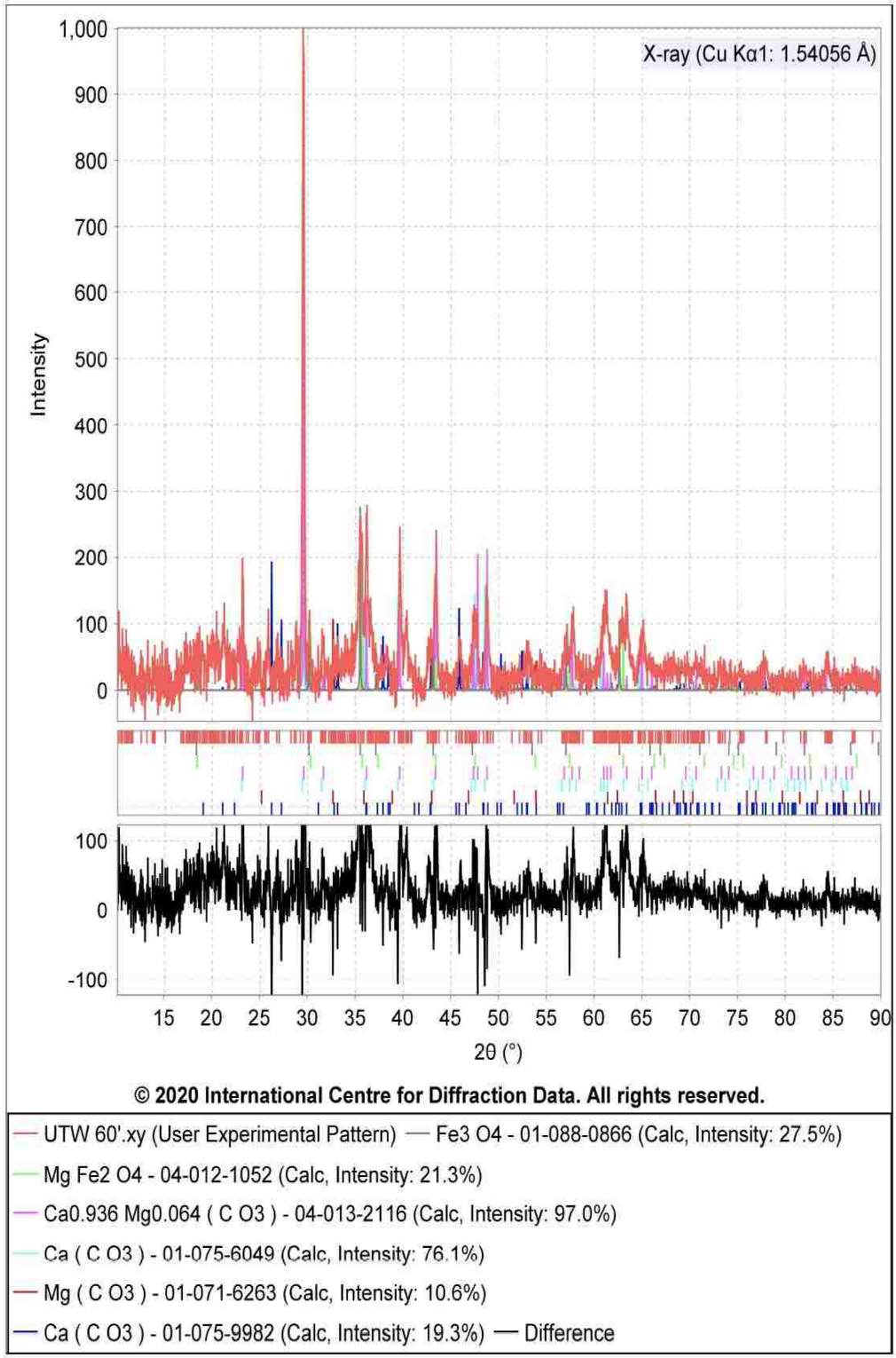

Figure E.3 XRD patterns of substances precipitated from Untreated Water (UTW) tank at 60 °C from experiment with a tank with little exposure of iron.

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	

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

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	1.006660	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	1.078200	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	
57.4138	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	
64.5811	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	
70.2464	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	0.808248	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								

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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).

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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	

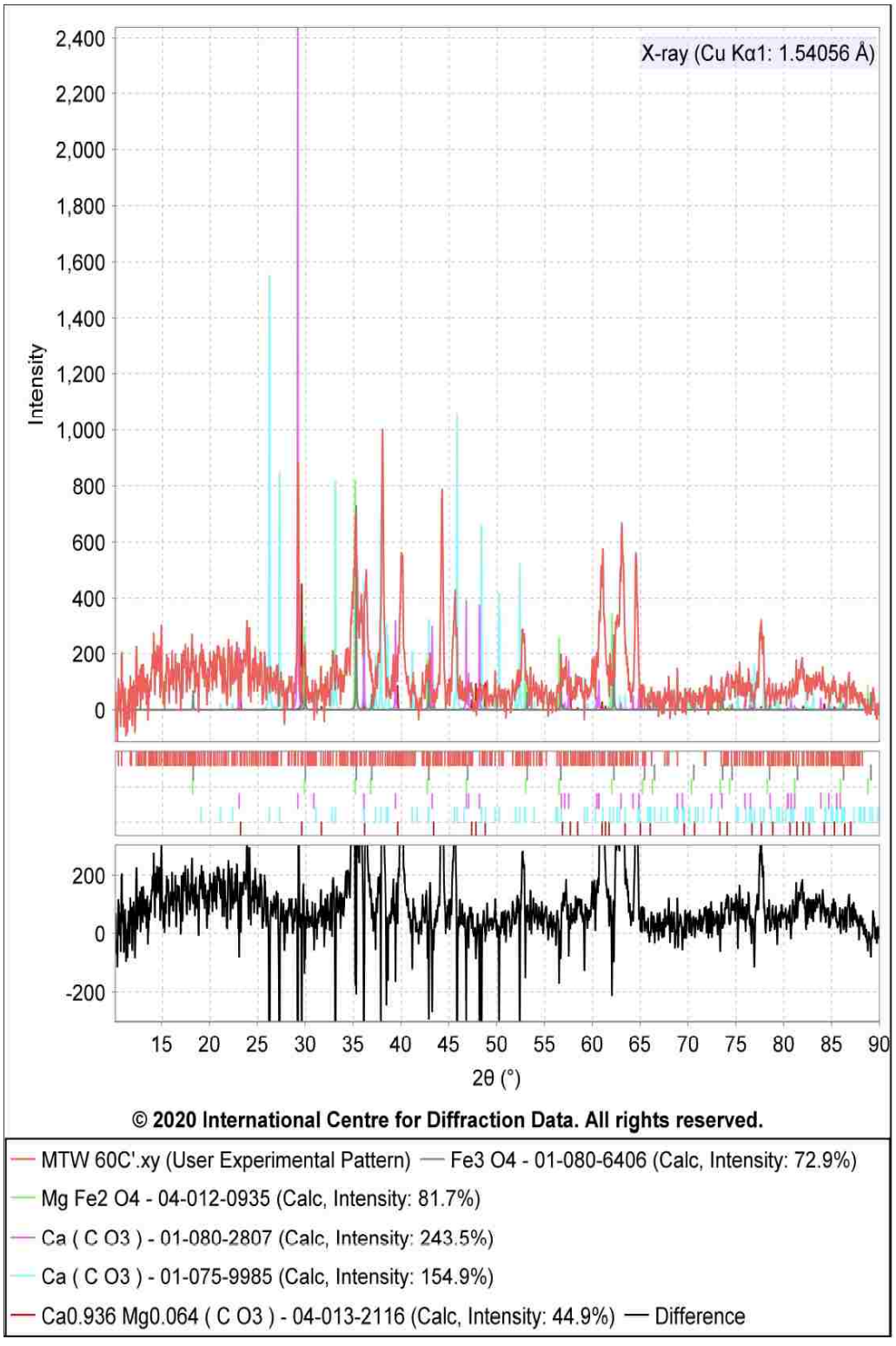

Figure E.4 XRD patterns of substances precipitated from Magnetically treated Water (MTW) tank at 60 °C from experiment with a tank with little exposure of iron.

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 (Biocerarnic), 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								

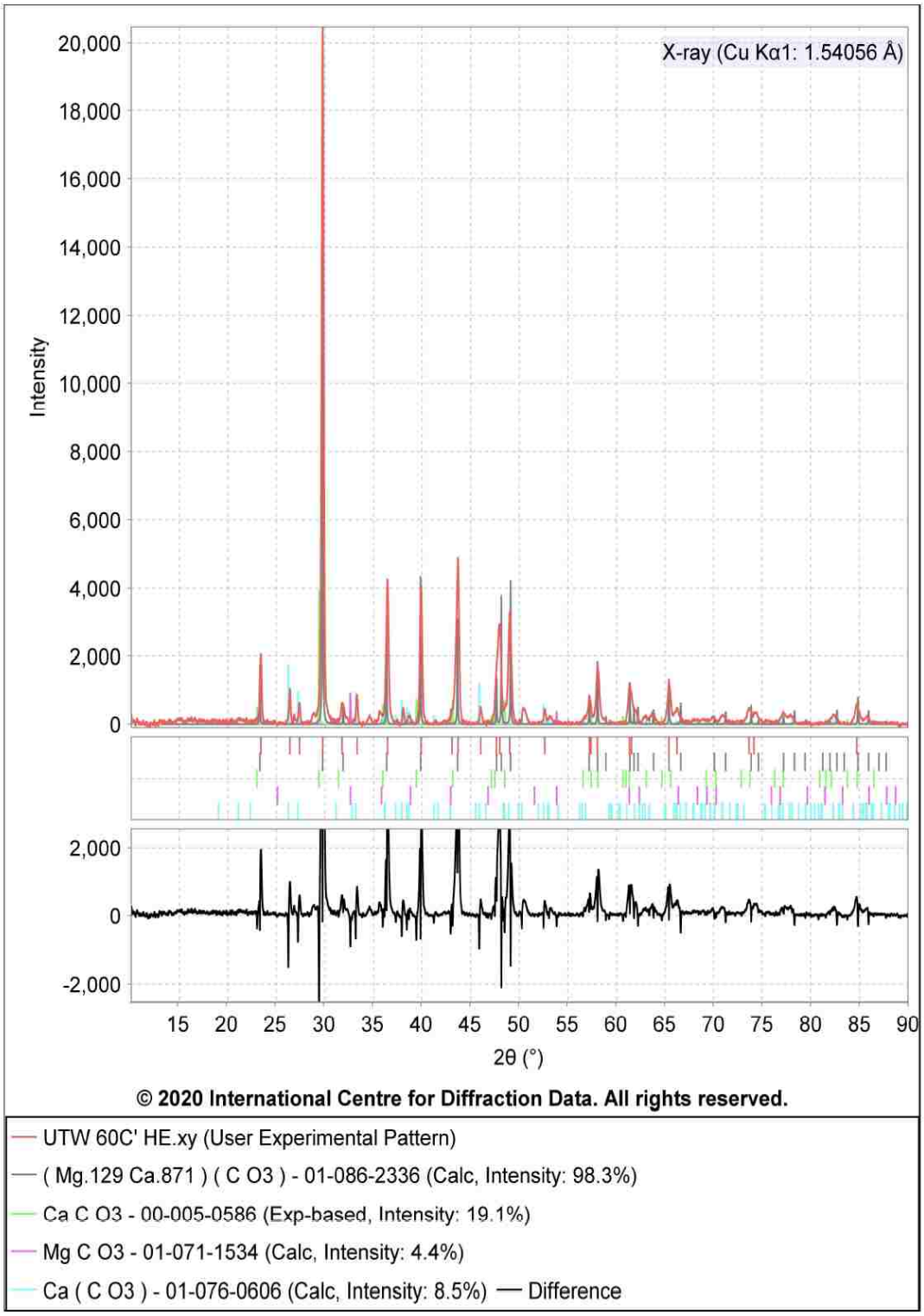

Figure E.5 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 60 °C from experiment with a tank with little exposure of iron.

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	

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	

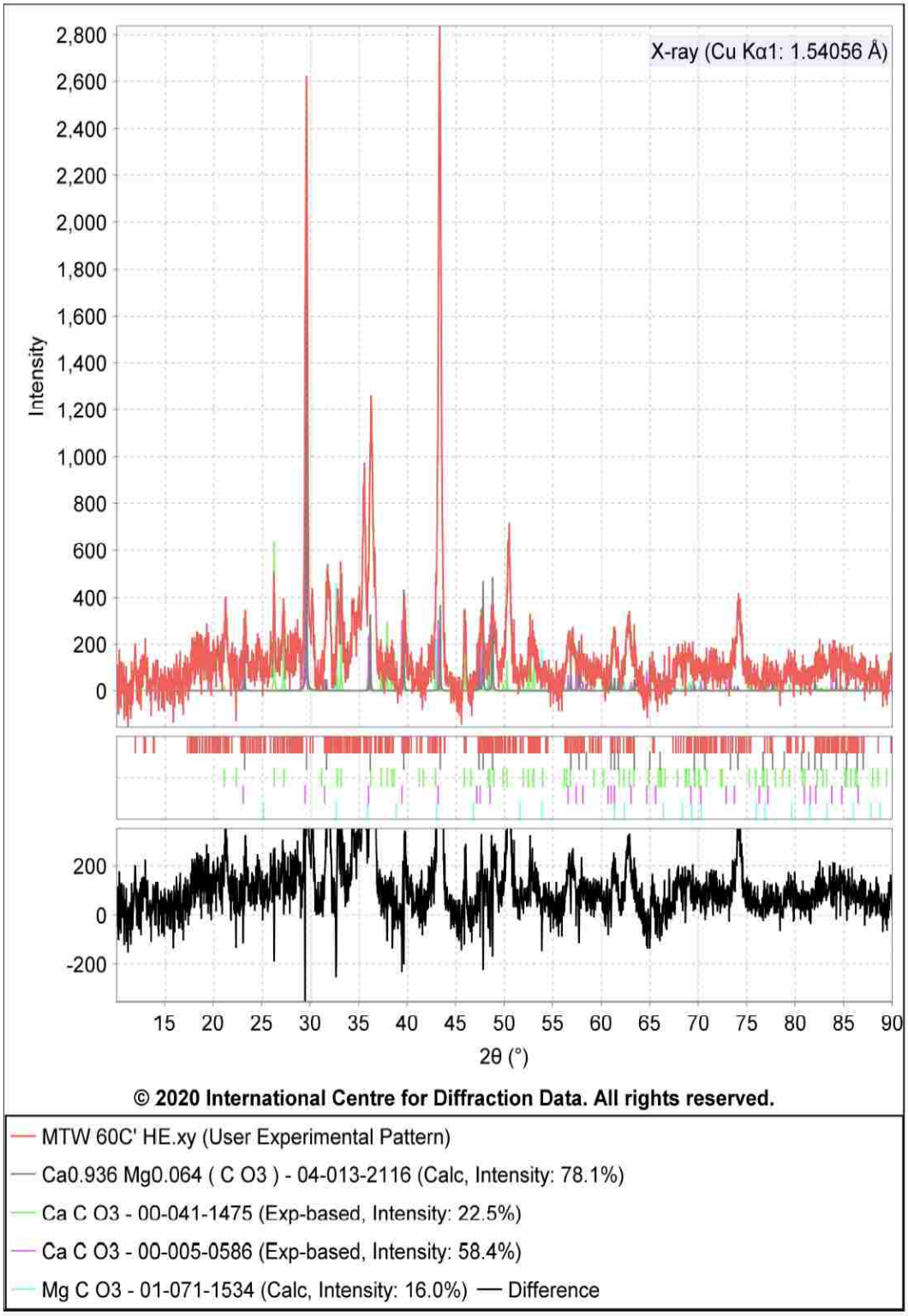

Figure E.6 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 60 °C from experiment with a tank with little exposure of iron.

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	0.00542	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	1.290250	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		112.5662	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	1.017650	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	

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		94.1457	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	
107.9999	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	

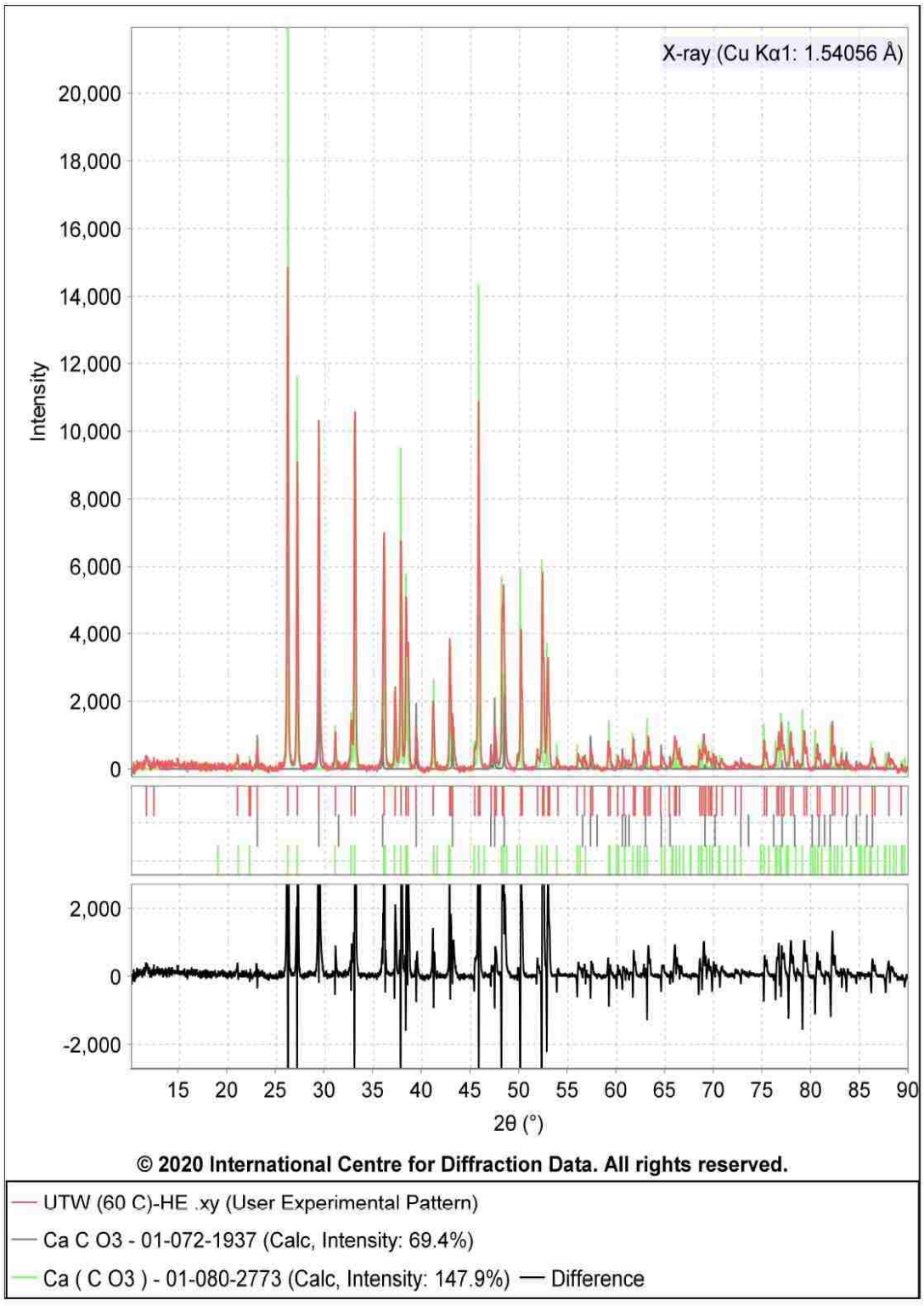

Figure E.7 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 60 °C from accelerated scale simulation study

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 (Biocceramic), 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.

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	3.856400	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		111.5455	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		99.0125	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	0.813518	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	

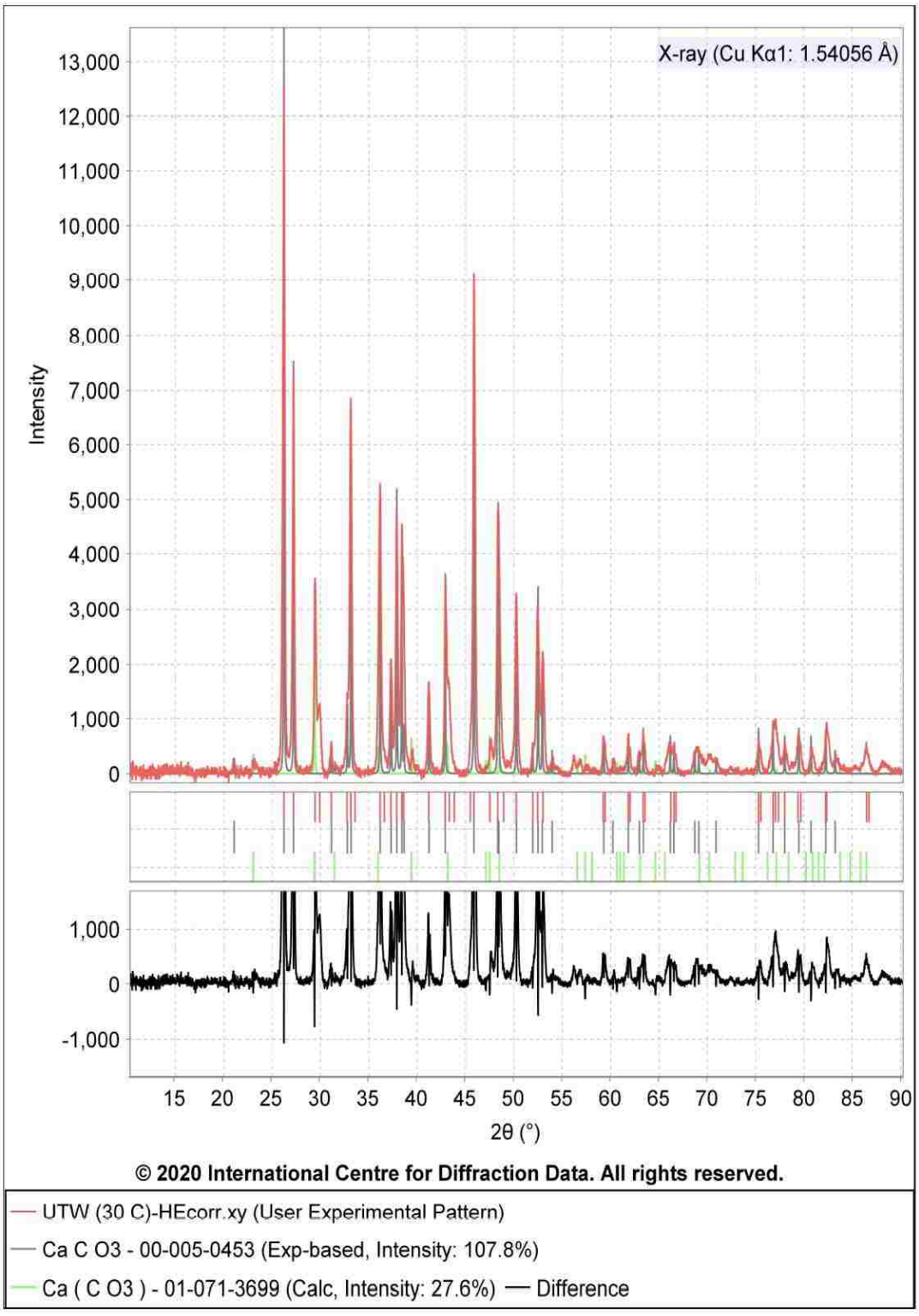

Figure E.8 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 30 °C from accelerated scale simulation study

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								

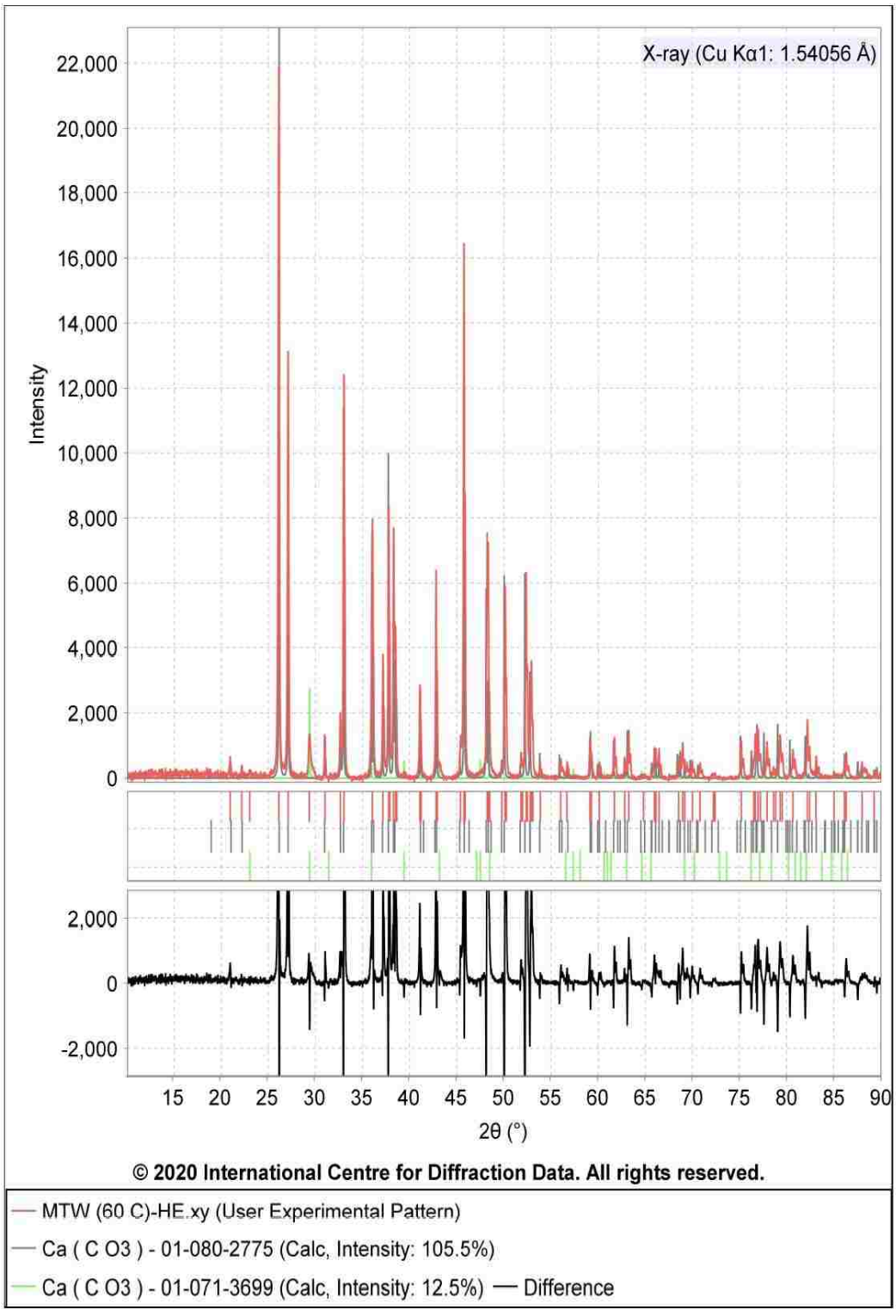

Figure E.9 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 60 °C from accelerated scale simulation study

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								

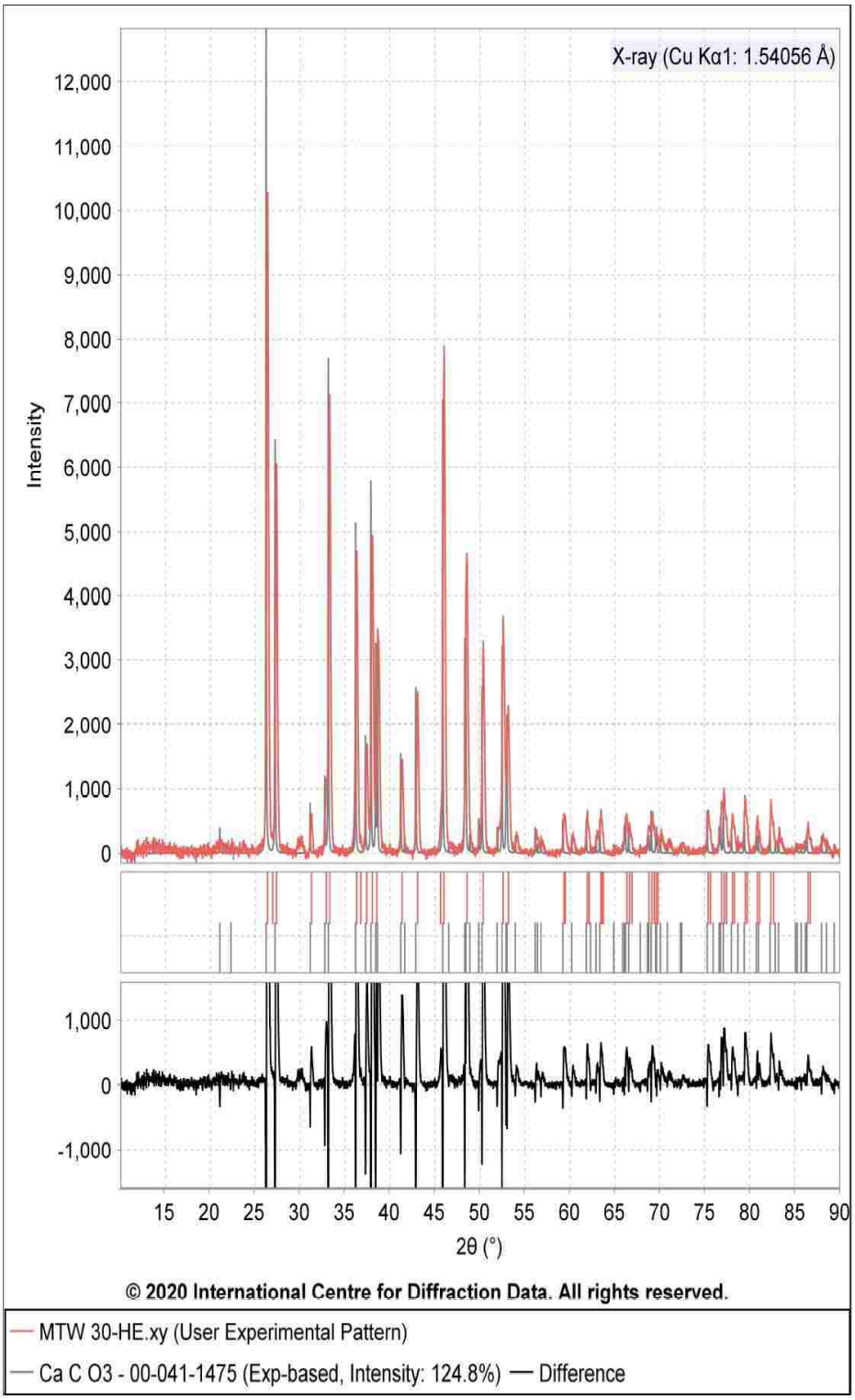

Figure E.10 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 30 °C from accelerated scale simulation study

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	

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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	