University of Nebraska - Lincoln DigitalCommons@University of Nebraska - Lincoln

Environmental Engineering Theses and Graduate Student Research

Environmental Engineering Program

Summer 7-30-2020

MAGNETIC WATER TREATMENT FOR SCALE PREVENTION ON WATER HEATER ELEMENTS

Fatma Al-Sharji University of Nebraska - Lincoln, fatmamnal@gmail.com

Follow this and additional works at: https://digitalcommons.unl.edu/envengdiss

Part of the Environmental Engineering Commons

Al-Sharji, Fatma, "MAGNETIC WATER TREATMENT FOR SCALE PREVENTION ON WATER HEATER ELEMENTS" (2020). *Environmental Engineering Theses and Graduate Student Research*. 20. https://digitalcommons.unl.edu/envengdiss/20

This Article is brought to you for free and open access by the Environmental Engineering Program at DigitalCommons@University of Nebraska - Lincoln. It has been accepted for inclusion in Environmental Engineering Theses and Graduate Student Research by an authorized administrator of DigitalCommons@University of Nebraska - Lincoln.

MAGNETIC WATER TREATMENT FOR SCALE PREVENTION ON WATER

HEATER ELEMENTS

By

Fatma Al-Sharji

A THESIS

Presented to the Faculty of

The Graduate College at the University of Nebraska

In Partial Fulfillment of Requirements

for the Degree of Master of Science

Major: Environmental Engineering

Under the Supervision of Professor Bruce I. Dvorak

Lincoln, Nebraska

July 2020

MAGNETIC WATER TREATMENT FOR SCALE PREVENTION ON WATER HEATER ELEMENTS Fatma Al-Sharji, M.S

University of Nebraska, 2020

Advisor: Bruce I. Dvorak

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 in² 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.

I would also like to acknowledge Don Chamberlain and Tuyen Vo for their effort in assisting me to carry out my research through the provision of the AkwaMag device as well as giving me research advice.

I would like to thank Dr. Yusong Li and Dr. Siamak Nejati for serving in my thesis committee and providing constructive feedback on my work.

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.

TABLE OF CONTENTS

Chapter 1 Introduction	1
1.1 Background	1
1.2 Goal and Specific Research Objectives	2
1.3 Organization of thesis	3
Chapter 2 Literature Review	4
2.1 Introduction	4
2.2 Softening methods	5
2.2.1 Ion Exchange	
2.2.2 Template assisted crystallization	
2.2.3 Capacitive deionization (CDI)	
2.2.4 Electrically induced precipitation	10
2.2.5 Magnetic Water Treatment	10
2.3 Scale Produced by Hard Water	12
2.3.1 Main Factors Affecting Scale Formation	
2.3.2 Properties of Calcium Carbonate Polymorphs	
Chapter 3 Methodology	17
3.1 Introduction	
3.2 Water Quality Testing	
3.2.1 Hardness	
3.2.2 Conductivity	
3.2.3 pH	
3.2.4 Iron, Manganese and other Different/Unknown Elements	
3.3 Scale Analysis	
3.3.1 X-ray Diffraction (XRD)	
3.3.2 Scanning Electron Microscopy (SEM)	
3.4 Magnetic Device	22
3.5 Water Heater Simulation	24
3.5.1 Experimental Apparatus	
3.5.2 Operational Schedule for Water Heater Simulation	
3.6 Accelerated Experimental Scale Simulation	29
3.6.1 Experimental Apparatus for Feed Preparation	30
3.6.2 Operational Schedule for Feed Preparation	
3.6.3 Apparatus for Accelerated Scale Formation	
3.6.4 Operational Schedule for Accelerated Scale Formation	31
Chapter 4 Results and Discussion	33
4.1 Introduction	33
4.2 Water Heater Simulation	33

4.2.1 Total Hardness and Conductivity of Influent Water	
 4.2.3 Analysis of precipitates with a tank with 70.4 in² of exposed iron and with a tank with little exposure of iron 4.2.4 Scanning Electron Microscope (SEM) Images 	
4.3 Accelerated Experimental Scale Simulation	
4.3.1 Effect of pH with respect to Time	
4.3.2 Effect of Induction Time	49
Simulation	51
Chapter 5: Conclusion and Recommendation	58
5.1 Introduction	58
5.2 Key Conclusions	59
5.3 Implications	60
5.4 Recommendation for future work	60
Reference	63
APPENDIX A: Statistical Analysis for Water Heater Simulation Influent Water	
Quality	71
APPENDIX B: Calculation for iron content in experiments with a tank with 70.4 in of exposed iron and with little exposure of iron in tank	
APPENDIX C: Calculation of Feed Preparation for Accelerated Experimental Sca Simulation	
APPENDIX D: Results of Feed Water for Accelerated Experimental Scale Simulation	78
APPENDIX D.1: Influent water quality analysis for untreated water	78
APPENDIX D.2: Influent water quality analysis for magnetically treated water '	78
APPENDIX E: X-Ray Diffraction (Results)	79

TABLE OF FIGURES

Figure 2.1 Mean hardness as calcium carbonate concentration levels. Source: USGS, (2019)
Figure 2.2 Water Softening and Regeneration Process. Source: Skipton et al. (2008) 7
Figure 2.3 Template Assisted Crystallization (TAC) process. Source: Premier Water Technologies (2012)
Figure 2.4 Capacitive Deionization (CDI) Process, Purification step (Top), Backwash Step (Bottom). Source: Wiest et al. (2011)
Figure 2.5 Physical Behavior. Source: Mosin and Ignatov, (2014)
Figure 2.6 Schematic representation of crystallographic unit cells for (a) Calcite (b) Aragonite and (c) Vaterite. Source: Xu and Poduska, (2014)
Figure 3.1 Impedance phase shift spectra of AkwaMag vs Tap water
Figure 3.2 Heating System Apparatus Schematic
Figure 3.3 Experimental Set-Up for Water Heater Simulation test
Figure 3.4 Feed preparation Set-Up
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 35
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 36
Figure 4.3. Semi-quantitative results for different elements
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
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
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
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

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 53
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
Figure 4.11 SEM Images of Calcite and Aragonite
Figure E.1 XRD patterns of substances precipitated from Untreated Water (UTW) tank at 60 $^{\circ}$ C from experiment with a tank with 70.4 in ² of exposed iron
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
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
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
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 120
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. 127
Figure E.7 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 60 °C from accelerated scale simulation study
Figure E.8 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 30 °C from accelerated scale simulation study
Figure E.9 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 60 °C from accelerated scale simulation study 144
Figure E.10 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 30 °C from accelerated scale simulation study

TABLE OF TABLES

Table 3.1 Product Specifications for the AkwaMag Device	22
Table 3.2 Experimental Set-up Equipment for Water Heater Simulation	27
Table 3.3 Sampling Location and Frequency for Water Heater Simulation experiment	28
Table 3.4 Operation Schedule for Accelerated Scale Formation	32
Table 4.1 ICP-MS Analysis	37
Table 4.2 Mass of solid and scale formed	41
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	
Table 4.4 Composition (Est Wt. %) of solid formed at 60 °C from the experiment with a tank with little exposure of iron.	
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.	
Table 4.6 Precipitates of scale formed composition at 60 and 30 $^{\circ}C$	55

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

1

(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 in² 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.

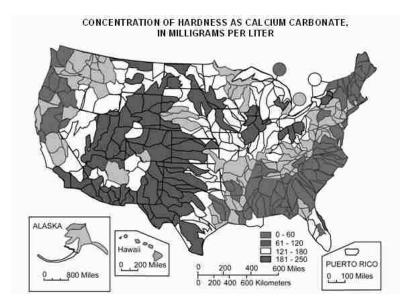


Figure 2.1 Mean hardness as calcium carbonate concentration levels. Source: USGS, (2019)

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.

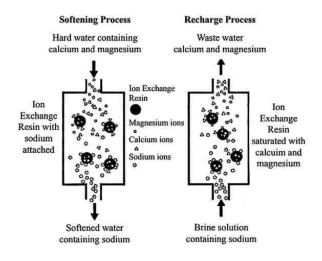


Figure 2.2 Water Softening and Regeneration Process. Source: Skipton et al. (2008)

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.

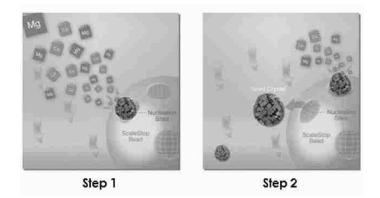


Figure 2.3 Template Assisted Crystallization (TAC) process. Source: Premier Water Technologies (2012)

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.

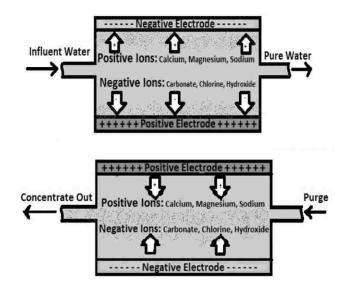


Figure 2.4 Capacitive Deionization (CDI) Process, Purification step (Top), Backwash Step (Bottom). Source: Wiest et al. (2011)

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 membranebased 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:

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

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 \rightarrow 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.

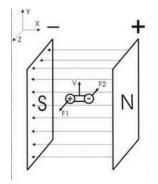


Figure 2.5 Physical Behavior. Source: Mosin and Ignatov, (2014)

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 (CaCO₃) as shown in the following equilibria reactions (Cho et al. 2005):

$$HCO_{3}^{-}(aq) \rightleftharpoons OH^{-}(aq) + CO_{2}(aq)$$
(2.2)

$$OH^{-}_{(aq)} + HCO_{3}^{-}_{(aq)} \rightleftharpoons CO_{3}^{2^{-}}_{(aq)} + H_{2}O$$

$$(2.3)$$

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

$$(2.4)$$

Overall reaction

$$Ca^{2+}_{(aq)} + 2HCO_3^{-}_{(aq)} \rightleftharpoons CaCO_{3(s)} + H_2O + CO_{2(aq)}$$
(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 (CaCO₃) 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).

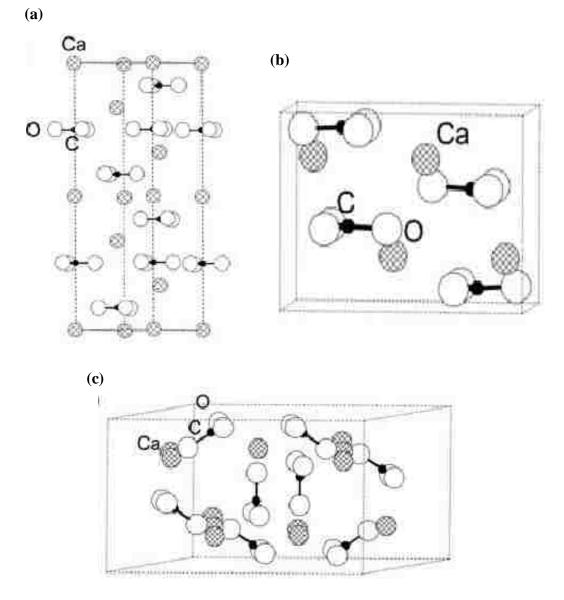


Figure 2.6 Schematic representation of crystallographic unit cells for (a) Calcite (b) Aragonite and (c) Vaterite. Source: Xu and Poduska, (2014)

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 in² 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 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 CaCO₃. 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 μ S/cm-1000 μ S/cm) using sodium chloride standard solution, 1000 \pm 10 μ S/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 μ g/L and 0.04 μ g/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.

20

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 k α radiation, $\lambda = 1.54056$ Å) were directed onto the sample and the scattered intensity is measured as a function of outgoing direction. 2 θ is the angle between the incoming and outgoing beams direction. The lattice spacing, d, were calculated from the 2 θ 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.

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 °F

 Table 3.1 Product Specifications for the AkwaMag Device

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.

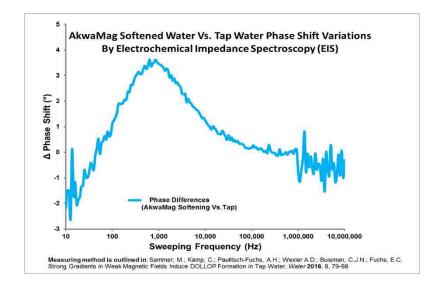


Figure 3.1 Impedance phase shift spectra of AkwaMag vs Tap water

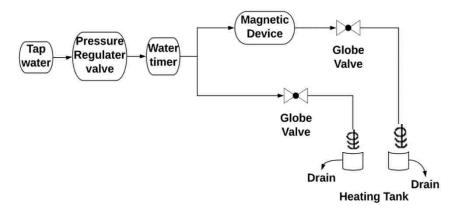
At frequency below 10⁶ Hz, ions in tap water move faster along with the field and eventually form layers at the electrodes causing electrode polarization. This causes the impedance phase to increase and eventually decrease at higher frequency unlike the AkwaMag softened water. Since the hydration shell 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 °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 °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.



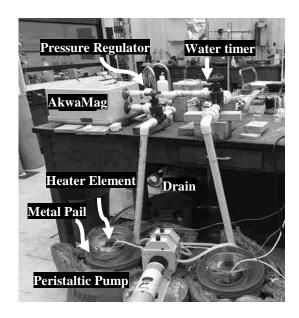


Figure 3.2 Heating System Apparatus Schematic

Figure 3.3 Experimental Set-Up for Water Heater Simulation test

A PVC pipe with ³/₄-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.

Equipment	Туре	Vendor/Model	Specifications
Pressure	Adjustable	Renator M11-	³ / ₄ inch Garden hose
Regulator Valve	Water Pressure	0660R	threads and NH
	Reducer with		threads
	Gauge		
Water Timer	Digital Watering	Homitt	³ / ₄ inch Hose thread
	Timer for		top and bottom
	Garden Lawn		connector
Globe Valve	Threaded PVC	Asahi/America	Pressure rating @
	Globe Valve	R	70°F: 150 psi, 1
			inch ID
Heater Element	Bolt On Style,	Grainger, 1500	L: 7-5/8 inches
	High-Watt	W, 120 V	
	Density		
Temperature	PID	Inkbird	With Heat Sink,
controller	Temperature		Solid State Relay
	Controller		and type K sensor
Metal Pail	leaktite	Home Depot	5-qt. Metal Pail
Water circulating	Rotary	Masterflex I/P	With controller
pump	Peristaltic		
Heater Tank	5 Gal. Bucket	Home Depot	20-qt
Drain Line	Clear PVC Vinyl	Everbilt	1-1/4 inches O.D. x
	Tubing		1 inches I.D. x 10 ft
Insulator	Fiberglass	Knauf	15 inches x 32ft.
	Insulation	Insulation Roll	

Table 3.2 Experimental Set-up Equipment for Water Heater Simulation

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	Sample tested in triplicate per day at	
faucet)	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	Sample tested in triplicate at the	
water bucket	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 in². 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:

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

This method is proved to yield better results in terms of accelerating scaling process as the dissolved CO₂ 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.

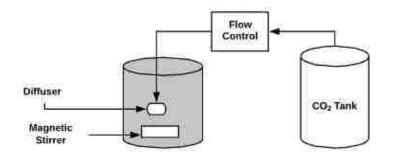


Figure 3.4 Feed preparation Set-Up

3.6.2 Operational Schedule for Feed Preparation

The desired total hardness of the feed was set to be approximately 400 mg/L as CaCO₃. 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.

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)

 Table 3.4 Operation Schedule for Accelerated Scale Formation

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 in² 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 in² 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 in² 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 in² 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 in² 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.

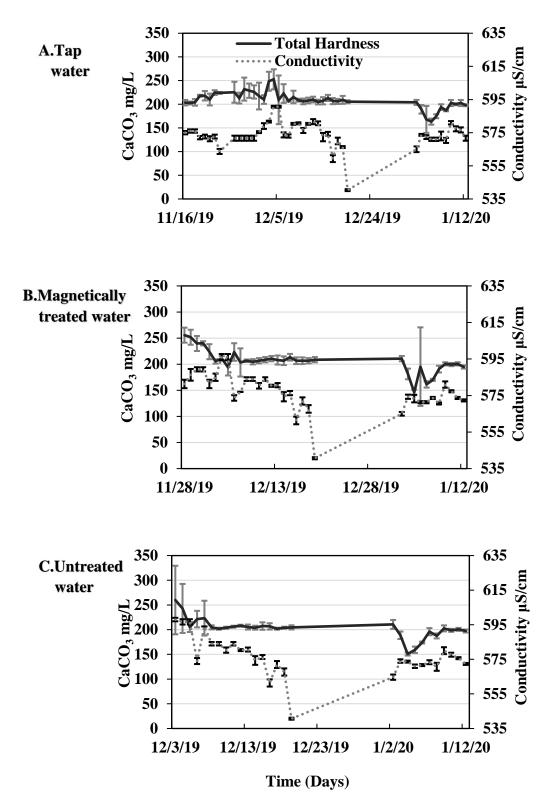


Figure 4.1 Influent water quality results from the experiment with a tank with 70.4 in² of exposed iron of (A) Tap water, (B) Magnetically treated water, (C) Untreated water

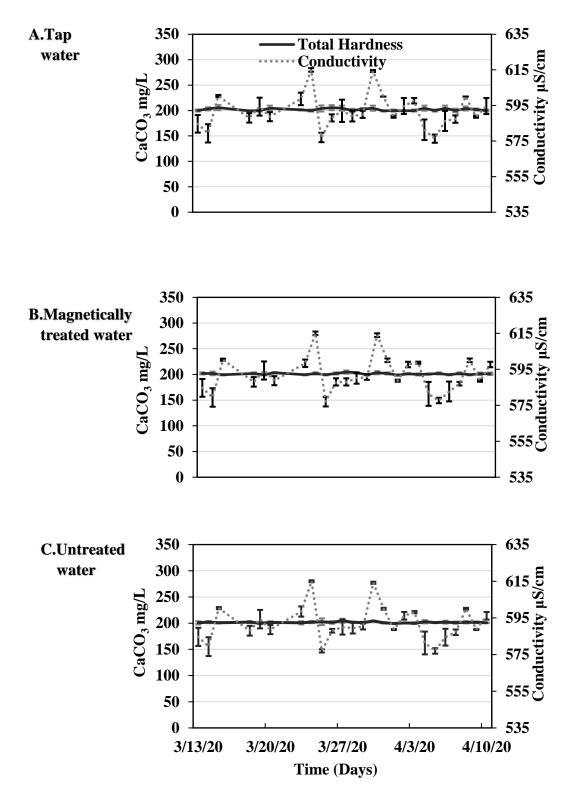


Figure 4.2 Influent water quality results from the experiment with a tank with little exposure of iron of (A) Tap water, (B) Magnetically treated water, (C) Untreated water

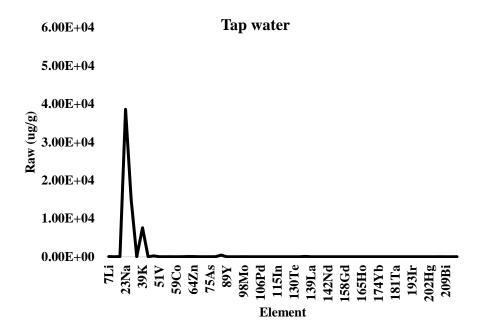
As shown in the previously provided figures, the influent total hardness and the conductivity of the solution did not change over the time. The statistical analysis using two-tail test (Dowdy et al. 2004) showed that the means of total hardness and conductivity are not statistically different between, 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.

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

Table 4.1 ICP-MS Analysis



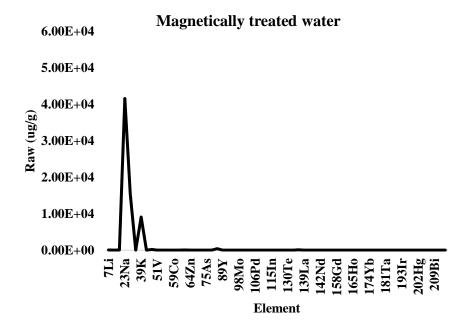


Figure 4.3. Semi-quantitative results for different elements

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 in² 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 in² 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

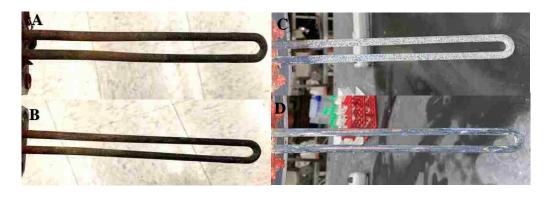


Figure 4.5 Scale formed on heater element from the experiment with a tank with 70.4 in² of exposed iron of (A) Untreated water (B) Magnetically treated water, and from the experiment with a tank with little exposure of iron of (C) Untreated water (D) Magnetically treated water

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 buildup.

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 in² 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.

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)	

Table 4.2 Mass of solid and scale formed

The scale formed were further analyzed using X-Ray Diffraction analysis. The Xray 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 in² 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 Fe³⁺ 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).

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 4.3 Composition (Est Wt. %) of solid formed at 60 °C from the experimentwith a tank with 70.4 in² of exposed iron

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.

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		

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

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 °Cfrom 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 CaCO₃ 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 CaCO₃. 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 in² 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.

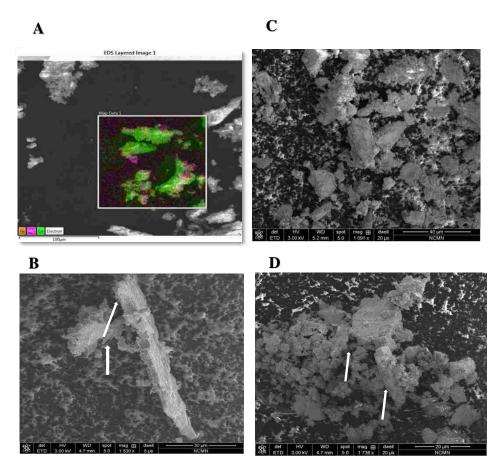


Figure 4.6 SEM Image of heating element from the experiment with a tank with 70.4 in² of exposed iron of (A) Untreated water (Electron Layer Image), (B) Magnetically treated water, and from the experiment with a tank with little exposure of iron of (C) Untreated water (D) Magnetically treated water

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.

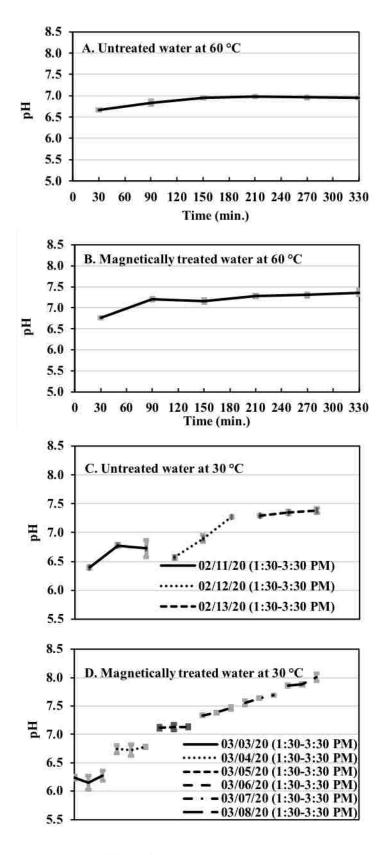


Figure 4.7 Effect of pH on (A) untreated water at 60 °C (B) magnetically treated water at 60 °C and (C) untreated water at 30 °C (D) magnetically treated water at 30 °C

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.

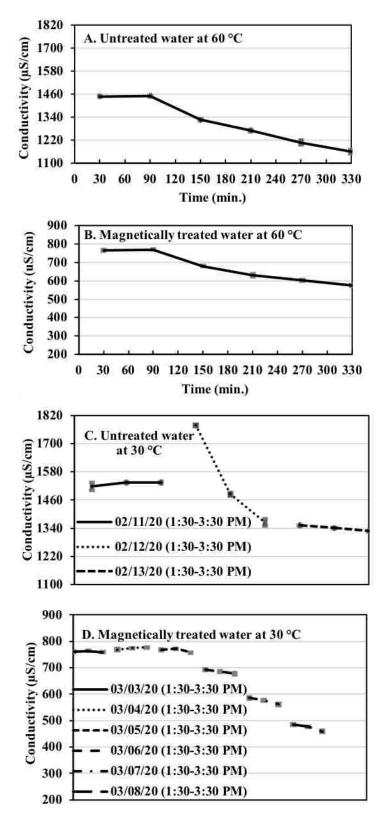


Figure 4.8 Effect of Conductivity on (A) untreated water at 60 °C (B) magnetically treated water at 60 °C and (C) untreated water at 30 °C (D) magnetically treated water at 30 °C

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 (2 θ) 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.

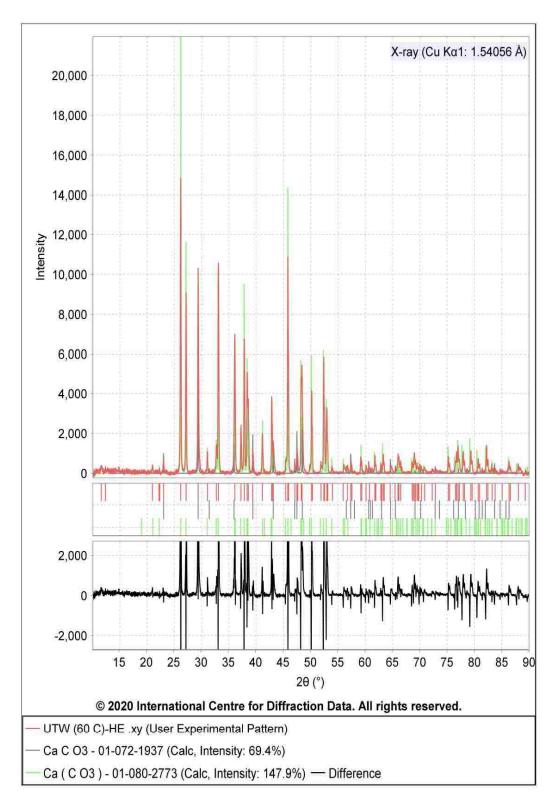


Figure 4.9 XRD patterns of substances precipitated from Untreated Water (UTW) heating element (HE) at 60 °C. Aragonite-PDF# 01-080-2773 Calcite-PDF# 01-072-1937

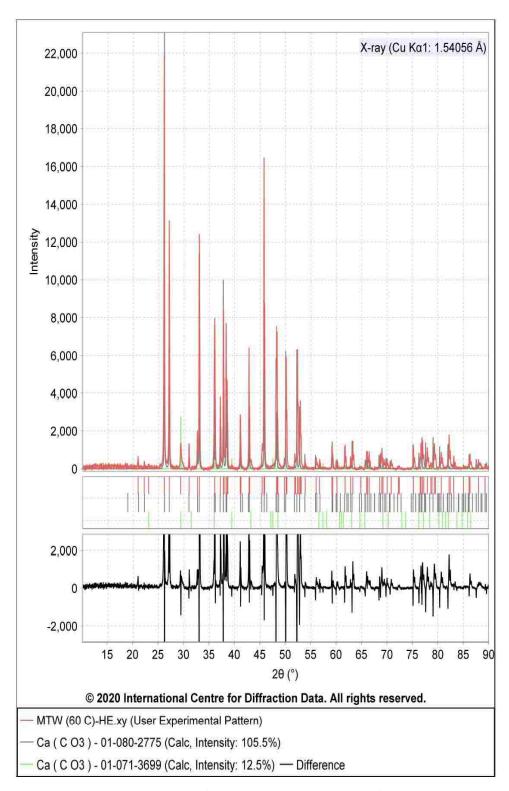


Figure 4.10 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element (HE) at 60 °C. **Aragonite-**PDF# 01-080-2775 **Calcite-** PDF# 01-071-3699

The figures above reveal that the crystals are aragonite and calcite. In Figure 4.9, aragonite formed at most intense peak of $26.17^{\circ} 2\theta$ (at d-value of 3.401 Å) while calcite formed at a most intense peak of $29.36^{\circ} 2\theta$ (at d-value of 3.038 Å). In Figure 4.10, aragonite formed at strongest peak of $26.19^{\circ} 2\theta$ (at d-value of 3.404 Å) while calcite formed at strongest peak of $29.39^{\circ} 2\theta$ (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.

	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	-

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

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 CaCO₃ polymorphs because they have different solubility products.

The supersaturation, Ω , depends on the (Ca²⁺) and (CO₃²⁻) ion activity according to the following equation:

$$\Omega = \frac{[Ca^{2+}][CO_3^{2-}]}{K_{so}}$$
(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 CO₂ from the solution to increase the concentration of CO₃²⁻. 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.

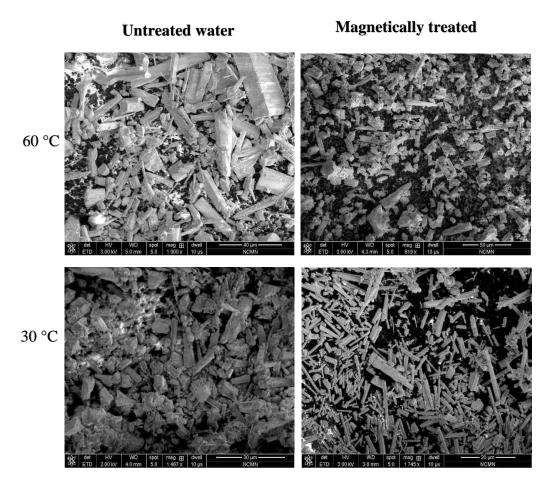


Figure 4.11 SEM Images of Calcite and Aragonite

The duration of the precipitation decreased as temperature was increased. The treated and untreated water samples gave rise to CaCO₃ 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 in² 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 $60 \degree C$ and $30 \degree C$. 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 CaCO₃ and CaSO₄ (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 CaCO₃ 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 °C and 80 °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.

Reference

- AkwaMag, Inc. (2014). "AkwaMag SpaceSaver PremiumTM, Owner's Manual." Palo Alto, CA, 94301.
- Alabi, A., Chiesa, M., Garlisi, C., and Palmisano, G. (2015). "Advances in anti-scale magnetic water treatment". *Environmental Science: Water Research & Technology*, 1(4), 408-425.
- American Public Health Association (APHA), American Water Works Association
 (AWWA), and Water Pollution Control Federation (WPCF) (2005), *Standard Methods for the Examination of Water and Wastewater 21st ed.*, American Public
 Health Association, New York.
- Amethyst Galleries, Inc (2019). "ARAGONITE (Calcium Carbonate)." Retrieved November 14,2019, from http://www.galleries.com/Aragonite .
- Andritsos, N., and Karabelas, A. J. (1999). "The Influence of Particulates on CaCO3 Scale Formation." *Journal of Heat Transfer*, 121(1), 225–227.
- Asano, T; Burton, F; Leverenz, H.; Tsuchihashi, R.; Tchobanoglous, G. (2006) Water Reuse: Issues, Technologies, and Applications; McGraw-Hill, New York.
- Behbahani, R. M., Müller-Steinhagen, H., and Jamialahmadi, M. (2008). "Investigation of Scale Formation in Heat Exchangers of Phosphoric Acid Evaporator Plants." *The Canadian Journal of Chemical Engineering*, 84(2), 189–197.
- Clifford, D. A. (1999). "Ion Exchange and Inorganic Adsorption. In: Water Quality and Treatment: A Handbook of Community Water Supplies", 5th ed.; Letterman, R.D., Ed.; McGraw-Hill: New York; pp 1–91.

- Cherkas, O., Beuvier, T., Zontone, F., Chushkin, Y., Demoulin, L., Rousseau, A., and Gibaud, A. (2018). "On the kinetics of phase transformations of dried porous vaterite particles immersed in deionized and tap water". *Advanced Powder Technology*, 29(11), 2872-2880.
- Chibowski, E., Hołysz, L., and Szcześ, A. (2003). "Adhesion of in situ precipitated calcium carbonate in the presence and absence of magnetic field in quiescent conditions on different solid surfaces." *Water Research*, 37(19), 4685-4692.
- Cho, Y. I., Lane, J., and Kim, W. (2005). "Pulsed-power treatment for physical water treatment." *International Communications in Heat and Mass Transfer*, 32(7), 861–871.
- Coetzee, P. P., Yacoby, M., Howell, S., (1996). "The role of zinc in magnetic and other physical water treatment methods for the prevention of scale." *Water SA* 22 319-326.
- Coetzee, P. P., Yacoby, M., Howell, S., & Mubenga, S. (1998). "Scale reduction and scale modification effects induced by Zn and other metal species in physical water treatment." *WATER SA-PRETORIA-*, *24*, 77-84.
- Dowdy, S. M., Wearden, S., and Chilko, D. M. (2004). *Statistics for Research*. Wiley-Interscience, Hoboken, NJ, 179-273
- Duffy E. A. (1977). "Investigation of magnetic water treatment devices". Thesis presented to the Clemson University in partial fulfillment of the requirement for the degree of Doctor of Philosophy in Materials Engineering.
- Dvorak, B. (2016). "Drinking Water Treatment: alt-Free Water "Softener" Options." G2275 Nebraska Extension.

Environmental Protection Agency (2020). "Drinking Water Treatability Database." Retrieved May 29, 2020, from https://iaspub.epa.gov/tdb/pages/treatment/treatmentOverview.do?treatmentProce

ssId=263654386.

- Esmaeilnezhad, E., Choi, H. J., Schaffie, M., Gholizadeh, M., and Ranjbar, M. (2017). "Characteristics and applications of magnetized water as a green technology." *Journal of Cleaner Production*, 161, 908–921.
- Fathi, A., Mohamed, T., Claude, G., Maurin, G., and Mohamed, B. A. (2006). "Effect of a magnetic water treatment on homogeneous and heterogeneous precipitation of calcium carbonate." *Water Research*, 40(10), 1941–1950.
- Flodman, H. R., and Dvorak, B. I. (2012). "Brine Reuse in Ion-Exchange Softening: Salt Discharge, Hardness Leakage, and Capacity Tradeoffs." *Water Environment Research*, 84(6), 535–543.
- Gabrielli, C., Maurin, G., Poindessous, G., and Rosset, R. (1999). "Nucleation and growth of calcium carbonate by an electrochemical scaling process". *Journal of Crystal Growth*, 200(1-2), 236-250.
- German Gas and Water Corporation. (1996). "Testing procedures to evaluate the effectiveness of water conditioning devices for the reduction of scaling."
 Technical Rules W512.
- Glater, J., York, J. L., and Campbell, K. S. (1980). "Scale Formation and Prevention." *Principles of Desalination*, 627–678. Academic Press, New York, 627-676.
- Hach Company.(1983). "Water Analysis Handbook Conductivity, Direct Measurement Method 8160." Retrieved February 10, 2020, from https://www.hach.com/wah.

- Hach Company. (1983). "Water Analysis Handbook Hardness, Calcium-Titration Method using EDTA Method 8204." Retrieved February 10, 2020, from https://www.hach.com/wah.
- Herzog, R., Shi, Q., Patil, J., and Katz, J. (1989). "Magnetic water treatment: the effect of iron on calcium carbonate nucleation and growth". *Langmuir*, 5(3), 861-867.
- Hoang, T. A., Ang, H. M., and Rohl, A. L. (2007). "Effects of temperature on the scaling of calcium sulphate in pipes." *Powder Technology*, 179(1-2), 31–37.
- Knez, S., and Pohar, C. (2005). "The magnetic field influence on the polymorph composition of CaCO3 precipitated from carbonized aqueous solutions." *Journal* of Colloid and Interface Science, 281(2), 377–388.
- Kozic, V., and Lipus, L. C. (2003). "Magnetic Water Treatment for a Less Tenacious Scale." *Journal of Chemical Information and Computer Sciences*, 43(6), 1815– 1819.
- Larson, T. E., and Buswell, A. M. (1942). "Calcium Carbonate Saturation Index and Alkalinity Interpretations." *Journal - American Water Works Association*, 34(11), 1667–1678.
- Lincoln Water System. (2019). "Annual Drinking Water Quality Report." Retrieved February 4, 2020, from https://www.lincoln.ne.gov/city/ltu/water/pdf/waterquality-report.pdf?2019.
- MacAdam, J., and Parsons, S. (2009). "The Effect of Metal Ions on Calcium Carbonate Precipitation and Scale Formation". Sustainability in Energy and Buildings, 137-146.

MathPortal. (2020). "Test calculator." Retrieved April 1, 2020, from

https://www.mathportal.org/calculators/statistics-calculator/t-test-calculator.php .

- Mosin, O., & Ignatov, I. (2014). "Basic Concepts of Magnetic Water Treatment." *European Journal of Molecular Biotechnology*, 4, 72–85.
- Muryanto, S. (2002). "*The role of impurities and additives in the crystallisation of gypsum*". Dissertation presented to the Curtin University in partial fulfillment of the requirement for the degree of Doctor of Philosophy in Chemical Engineering.
- Muryanto, S., Bayuseno, A., Sediono, W., Mangestiyono, W., and Sutrisno. (2012)."Development of a versatile laboratory project for scale formation and control." *Education for Chemical Engineers*, 7(3).
- Muryanto, S., Bayuseno, A., Ma'Mun, H., Usamah, M., and Jotho. (2014). "Calcium Carbonate Scale Formation in Pipes: Effect of Flow Rates, Temperature, and Malic Acid as Additives on the Mass and Morphology of the Scale." *Procedia Chemistry*, 9, 69–76.
- Naushad, M., and Al-Othman, Z. A. (2013). *A book on ion exchange, adsorption and solvent extraction*. Nova Science Publishers, Inc., Hauppauge, NY, pp. 15-44.
- Nebraska Center for Materials & Nanoscience. (2020). "Central Facilities." Retrieved from Jun 4, 2020, https://ncmn.unl.edu/central-facilities .
- Nebraska Water Center. (2020). "Facilities and Equipment." Retrieved Jun 1, 2020. from https://watercenter.unl.edu/facilities-and-equipment.
- Ni, M., and Ratner, B. D. (2008). "Differentiating calcium carbonate polymorphs by surface analysis techniques-an XPS and TOF-SIMS study." *Surface and Interface Analysis*, 40(10), 1356–1361.

- Ogino, T., Suzuki, T., and Sawada, K. (1987). "The formation and transformation mechanism of calcium carbonate in water." *Geochimica et Cosmochimica Acta*, 51(10), 2757–2767.
- Oren, Y. (2008). "Capacitive deionization (CDI) for desalination and water treatment past, present and future (a review)." *Desalination*, 228(1-3), 10–29.
- Parsiegla, K. I. (1998). "Effect of solution composition of calcite growth inhibition by copper (II) and zinc (II)." Dissertation presented to The Johns Hopkins University Baltimore in partial fulfillment of the requirement for the degree of Doctor of Philosophy.
- Pernot, B., Euvrard, M., and Simon, P. (1998). "Effects of iron and manganese on the scaling potentiality of water". *Journal of Water Supply: Research and Technology*—AQUA, 47(1), 21-29.
- Premier Water Technologies (2012). "Saltless Water Softeners: Fact Or Fiction?." Retrieved April 27, 2020, from https://www.premierwatermn.com/saltless-watersofteners-fact-fiction/.
- Provin, T and Pitt, J.L. (2017). "Managing Soil Salinity." E-60 Texas A&M AgriLife Extension.
- Rathilal, S. (2004). "The study of the mechanism of magnetic water treatment for the prevention of scale and corrosion." Thesis presented to the University of Durban-Westville in partial fulfillment of the requirements for the degree of Master of Science in Chemical Engineering.

- Sammer, M., Kamp, C., Paulitsch-Fuchs, A., Wexler, A., Buisman, C., and Fuchs, E. (2016). "Strong Gradients in Weak Magnetic Fields Induce DOLLOP Formation in Tap Water." *Water*, 8(3), 79.
- Sarkar, A., and Mahapatra, S. (2012). "Mechanism of unusual polymorph transformations in calcium carbonate: Dissolution-recrystallization vs additive-mediated nucleation." *Journal of Chemical Sciences*, 124(6), 1399–1404.
- Sangwal, K. (1996). "Effects of impurities on crystal growth processes". *Progress in Crystal Growth and Characterization of Materials*, 32(1-3), 3-43.
- Smith, C., Coetzee, P., and Meyer, J. (2004). "The effectiveness of a magnetic physical water treatment device on scaling in domestic hot-water storage tanks." *Water SA*, 29(3).
- Skipton, S; Dvorak, B.; and Niemeyer, S (2008). "Drinking Water Treatment: Water Softening (Ion Exchange)." G08-1491 Nebraska Extension.
- Stickford, G. J., and Johnson, O. (1984). "The effect of hard-water scale buildup on water heater life-cycle efficiency." *In ACEEE*, pp. E238-E25.
- Tang, Q., Meng, J., Liang, J., Nie, L., and Li, Y. (2010). "Effects of copper based alloys on the nucleation and growth of calcium carbonate scale". *Journal of Alloys and Compounds*, 491(1-2), 242-247.
- Tung, C.-H., Sheng, G. T. T., and Lu, C.-Y. (2003). "ULSI semiconductor technology atlas." John Wiley & Sons, Hoboken, NJ.
- USGS Geological Survey Office. (2019). "Hardness Of Water." Retrieved November 19, 2019 from https://www.usgs.gov/special-topic/water-science-

school/science/hardness-water?qt-science_center_objects=0#qtscience_center_objects .

- Water Quality Research Foundation. (2011). "Softened Water Benefits Study: Energy Savings • Detergent Savings." Retrieved May 22, 2020 from www.wqa.org/Portals/0/WQRF/ResearchStudy_BenefitsOfSoftenedWater_ExecS ummary.pdf.
- Wiest, M.; Fox, P.; Lee, W.; Thomure, T.(2011). "Evaluation of Alternatives to Domestic Ion Exchange Water Softeners." Proceedings of the 84th Annual Water environment Federation Technical Exposition and Conferences, Los Angeles, California, Oct 10-13; Water Environmental Federation: Alexandria, Virginia.
- Xu, B., and Poduska, K. M. (2014). "Linking crystal structure with temperature-sensitive vibrational modes in calcium carbonate minerals." *Phys. Chem. Chem. Phys.*, 16(33), 17634–17639.

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)

$$t = \frac{\overline{X_1} - \overline{X_2}}{S_{\overline{X}_1 - \overline{X}_2}}$$
$$S_{\overline{X}_1 - \overline{X}_2} = \sqrt{\frac{S_{\overline{X}_1}^2}{n_1} + \frac{S_{\overline{X}_2}^2}{n_2}}$$
$$d. o. f = \frac{\left(\frac{S_{\overline{X}_1}^2}{n_1} + \frac{S_{\overline{X}_2}^2}{n_2}\right)^2}{\frac{\left(\frac{S_{\overline{X}_1}^2}{n_1}\right)^2}{n_1 - 1} + \frac{\left(\frac{S_{\overline{X}_2}^2}{n_2}\right)^2}{n_2 - 1}}$$

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

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

$$\overline{X_1} = \text{Mean of data for group 1}$$

$$\overline{X_2} = \text{Mean of data for group 2}$$

$$S_{X_1} = \text{Standard deviation of data for group 2}$$

$$S_{X_2} = \text{Standard deviation of data for group 2}$$

$$d. o. f = \text{degrees of freedom}$$

$$n_1 = \text{Total number of values in first dataset}$$

n2 = Total number of values in second dataset

	Total Hardne	ss CaCO3 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	().6	-1.5		
d.o.f		59	59		
Critical value from T-table	2	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.			e means are not	

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).

Table A.2 Unpaired T- test to compare Tap Water and Untreated Water (From the experiment with a tank with 70.4 in² of exposed iron).

	Total Hardnes	s CaCO ₃ mg/L	Conduct	ivity 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		1.2	
d.o.f	50	50.0 43		43
Critical value from T-table	2.0		2	
Conclusion	t is smaller than cr (1.3<2.0), so the m significantly differ	eans are not	t is smaller than (0.3<2.0), so the significantly dif	e means are not

	Total Hardness CaCO ₃ mg/L Conductivity µS/cm			tivity 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	2.0	48		
Critical value from T-table	2.	00	2.00		
Conclusion	t is smaller than c (1.6<2.0), so the m significantly differ	eans are not	t is smaller than critical value (0.04<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).

 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 Hardnes	s CaCO ₃ mg/L	Conducti	ivity 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	3	6		48		
Critical value from T-table	2.	04		2		
Conclusion	(0.92<2.04), so t	n critical value he means are not y different.	(0.01<2.0), so t	an critical value the means are no tly different.		

Regression Slope analysis for influent water quality

	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.5 Regression Slope for influent water Total Hardness CaCO₃ mg/L (From the experiment with a tank with 70.4 in² of exposed iron)

Table A.6 Regression Slope for influent water Conductivity μ S/cm (From the experiment with a tank with 70.4 in² 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

	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.7 Regression Slope for influent water Total Hardness CaCO₃ mg/L

 (From the experiment with a tank with little exposure of iron)

Table A.8 Regression Slope for influent water	Conductivity µS/cm (From the experimen	t 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 in² of exposed iron and with little exposure of iron in tank

Assumptions	1. 1.							
					rmined by XRD is a	ccurate.		
That the form	ulas for each type of	f compond is co	rrect base	i on XRD	analysis			
PL-20090720091		11. 						
Experiment	with exposed iron i	<u>n tank</u>						
Untreated Ta	ip 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	
	Treated Tap wate							
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	MgF#2O4	200.00	16	0.16	(Fe/MgFe2O4)	0.28	0.05	
Calcium Magnesium Iron Carbonate	CaMg0.6Fe0.4(CO 3)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	
1		1				Sum	0.23	
Experiment v	without significant	exposed iron i	in tonk					
Untreated To								
MW Iron	Contraction of the second	Mass of	5.650			-		
(g/mol)	55.84	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 wate	ar .						
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	Fe304	231.55	5	0.05	(Fe/Fe2O4)	0.24	0.01	
Magnesium Iron Oxide	MgFe2O4	199.99	Ť	0.07	(Fe/MgFe2O4)	0.28	0,01	
() () () () () () () () () ()						Sum	0.82	

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

(A) Untreated water influent (400 ppm as Ca²⁺):

Number of moles of $CaCO_3 = mass / molar mass$

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

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

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

 $0.04 \text{ moles} \times 40 \text{ g/mol.} = 1.6 \text{ g}$

Calcium conc. (mg/L as Ca²⁺) = 1600 mg/4L = **400 ppm as Ca²⁺** Total Hardness (mg/L as CaCO₃) = 2.5 $\frac{\left(\frac{\text{mg as CaCO3}}{\text{mmol.}}\right)}{\left(\frac{\text{mg Ca2+}}{\text{mmol.}}\right)} \times \text{Calcium conc. (mg/L as Ca²⁺)} + 4.12 \frac{\left(\frac{\text{mg as CaCO3}}{\text{mmol.}}\right)}{\left(\frac{\text{mg Mg2+}}{\text{mmol.}}\right)} \times \text{Magnesium conc. (mg /L as Mg²⁺)}$ Total Hardness (mg/L as CaCO₃) = 2.50 $\frac{\left(\frac{\text{mg CaCO3}}{\text{mmol.}}\right)}{\left(\frac{\text{mg Ca2+}}{\text{mmol.}}\right)} \times 400$ ppm as Ca²⁺ = **1,000 ppm as CaCO3**

(B) Magnetically treated water influent (400 ppm as CaCO₃):

Mass of $CaCO_3$ powder required = 1.6 g

Volume of high purity water required = 4 L

Total Hardness concentration (mg/L as CaCO₃) = 1600 mg \div 4 L = 400 ppm as CaCO₃

Molecular weight of CaCO₃: $\frac{100 \text{ mg}}{\text{mmol.}}$, Ca²⁺: $\frac{40 \text{ mg}}{\text{mmol.}}$, Mg²⁺: $\frac{24.3 \text{ mg}}{\text{mmol.}}$

Calcium conc. (mg/L as Ca²⁺) = 400 ppm as CaCO₃ / 2.50 = 160 mg/L as Ca²⁺

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

	Number of Replicate =3				
		T ₁		T ₂	
Parameter	Unit	Average	SD	Average	SD
Total Hardness	CaCO ₃ mg/L	~1000	0	~1000	0
рН	-	6.14	0.03	6.13	0.05
Conductivity	μS/cm	1439	1.5	1509	1.5

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

SD: Standard Deviation

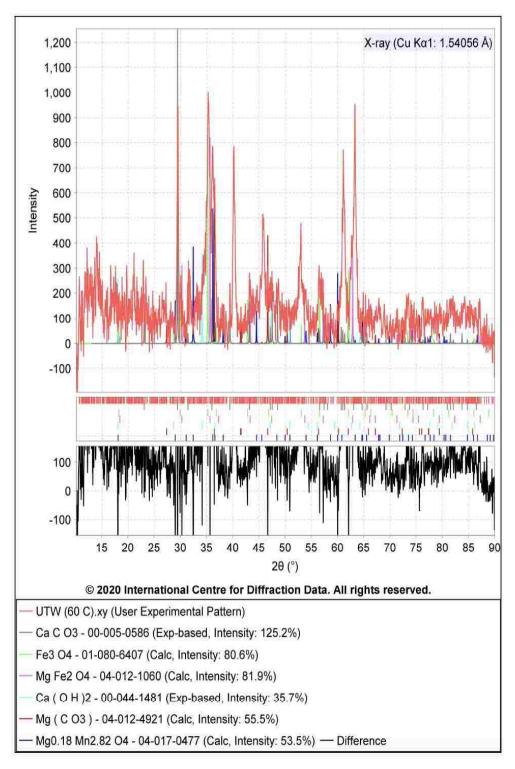
APPENDIX D.2: Influent water quality analysis for magnetically treated water

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.

		Nun	ber of l	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

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

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 in² of exposed iron

SIeve+ Report

Experiment

Search Line:	1.467772 Å	D1 Range:	1.465 <mark>Å</mark> - 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 <mark>Å</mark> - 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 <mark>Å</mark> - 1.516 Å
Search Line:	2.458280 Å	D1 Range:	2.449 <mark>Å</mark> - 2.468 Å
Search Line:	2.509879 Å	D1 Range:	2.500 Å - 2.520 Å
Rotation: All	8 Rotations		

Preferences

Radiation: X-rayWavelength: Cu Ka1 1.54056 ÅSearch Method: HanawaltSearch Window: 0.15°Match Window: 0.15°2nd Pass Filter: Yesd-Spacings: WeightedLowest Allowable GOM: 2000

Phases (6)

<u>#</u>	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	1	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

Jun 9, 2020 2:37 PM (fal-sharii2) Status Primary QM: Star Pressure/Temperature: Ambient Chemical Formula: Ca C 03 Empirical Formula: C Ca C3 Weight %; C12:00 Ca40.04 O47.95 Atomic %; C20:00 Ca20.00 O60.00 Compound Name: Caldum Carbonate Mineral Name: Caldie, syn Radiation: CuKo1 A: 1,5405 Å Filter: Ni Beta Intensity: Diffractometer Mic. 2 SYS: Rhombohedral SPGR: R-3c (167) Author's Cell [AuthCell s: 4.389 Å AuthCell s: 17.052 Å AuthCell Vol: 367.78 Å* AuthCell Z: 6.00 AuthCell MolVol: 61:30] Author's Cell Axial Ratio [c/a: 3.420] Density [Deale: 2.711 g/cm* Drivers: 2.71 g/cm*] SS/FOM: F \$5/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 Spate Group: Net (107) Weitzellar Veigini 103.05 Crystal Data [XilCell a: 4.589 Å XilCell b: 4.989 Å XilCell c: 17,052 Å XilCell a: 90.00° XilCell β: 90.00° XilCell γ: 120.00° XilCell Voi: 367.76 Å' XilCell Z: 6.90] Crystal Data Actal Ratio [c/a: 3.420 wb: 1.000 c/b: 3.420] Reduced Cell [RedCell a: 4.989 Å RedCell b: 4.589 Å RedCell c: 6.375 Å RedCell α: 66.97° RedCell β: 66.97° RedCell γ: 60.00° RedCell Voi: 122.59 Å'] εα: =1.487 muß; =1.659 Sign: =-Atomic parameters are cross-referenced from PDF entry 04-012-8072 ADP. U

Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators:

00-005-0586

2	Ay Z	or	y y x y	z.	5	-11	Y, A.Z		g.g.t+12		XJAY 2+1/2	500	-a+y.y.z+1/2
Z	A/¥.5	and the second second	E (3)/85	(2)	4	89	N/4	1	¥.4. #*1/2	10	-x, org. 2+1/2	12	X9,9,3*12
Atom	ic Coort	finatest											
Atom	Nam	Wyckoff	Semmet	NX.	¥.	:	SOF	Uise	AET				
Ca:	1	SE.	-3	0.0	0.0	0.0	1.0	0,01525					
C	20	fla	32	0.0	0.0	0.25	1.0	0,02084					
a :	3	1.84	2	0.04	0,0	0.25	1.0	10,02408-4					

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

Minoral 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), 04-007-4388 (Alternate), 04-007-8559 (Primar 04-007-858) (Alternate), 04-007-8559 (Primar 04-008-0788 (Alternate), 04-012-0489 (Primary), 04-012-8072 (Alternate) 04-007-8659 (Primary), -CAS Number - PR: 13397-26-7 Entry Date: 09/01/1955

References Type DOI Seferance Primary Haference Crystal Structure Swanson, Fuyat, Natl. Bar, Stand. (U. S.), Con. 539 8, 51 (1953). Crystal Structure Source: CPF. Dana's System of Mineralogy, 7th Ed. 8, 142 Optical Clebs

Additional Patterns: See PDF 01-072-1214 . 01-072-1937, 01-081-2027, 01-083-6577 and 01-083-0578. Analysis: Spectroscopic analysis: <0.1% Sr. <0.01% Ba; <0.001% Al, B, Cs, Cu, K, Mg, Na; SL Sr. <0.0001% Ag, Cr, Fe, Li, Mn. Color, Colorless. General Comments: Additional weak reflections indicated by brackets) were observed. Other form: arogonate. Pattern reviewed by Parks. J. McCarthy, G. North Dakotas State Univ., Fargo, North Dakota, USA. (CDD Grant-n-Aid (1992). Agrees well with experimental and calculated patterns. Antaold. Sample Source or Locality: Sample from Mallinckrodt Chemical Works, Temperature of Data Collection. Pattern taken at 299 K. Unit Cell Data Source: Powder Diffraction.

28 (*)	(A) b	1	h.		1		29.0%	# (Å)	1	. 11	1	1		28.(*)	d (Å)	1	. 8		1	
23.0218	3,000000	12	0	-31	2		48.6122	1.875000	57	18		8.		64.6765	1.440000	6	3	.0	0	
29.4048	2.035000	100	1.8	1	- 4		56.6630	1.825000	4	-2-	-32	111		48.5972	1.422900	12	- a	12	:12	
11.4176	2.845000	- 3	- 61	0	- 1 5		57,4001	1.804600		14	21	2		69.2291	1.256000	2 #	2	÷.	2	
5.0054	2,495000	14	1		4		58,0720	1.587000	2	14	÷.	10		70.2364	1.220000	2		-2	10	
D 4005	2.285000	18	- 11	. 9	3		00.0702	1.525000	5	2	10	4		72.0070	1.297000	2	- t:	2	11	
3.1447	2.095000	12	- 21	0	-2		00.08:07	1.510000	4	12	0	1		73,7294	1,254000	1	2	10	1	
0,1226	1.927000	-5	- 10 -	2	- 4		61.3435	1.510000	2	11	10	. 9		76.2877	1.247000	- H	2.	2	û.	
7.40EH	1.01000	17	10	1	18		63.0654	1.473000	2.1	11	20	5		77.1740	1,235000	-2	11	1	12	
5 2020	Internatio	Inna	Ce	nte	a fo	r Dil	fraction	Data All	right	in in	16.0	inie	d.	- 100 Prod 110	CONTRACTOR OF METHOD				Pa	ae 1

00-005-0586 20(*) 0(A) 00 9302 1,8690 81,5440 1,7785 62,1106 1,7290 63,7648 1,5300 64,7650 1,4298 65,4804 1,22440 83,0981 1,06130 Jun 9, 2020 2:37 PM (fal-sharji2) 28 (*) d(A) 1 h k (* 103,8650 0.978200 1 1 3 10 104,1201 0.978700 3 1 2 14 105,8416 0.965500 2 3 2 4 106,1414 0.965500 4 0 4 8 107,3095 0.95560 0.94200 2 4 1 0 110,4784 0.837000 2 2 2 12 20 (*) 54,6975 56,0075 56,1817 57,5440 50,1570 102,2984 102,9484 4 (Å) 1 047300 1 044700 1 035200 1 023400 1 011800 0 889500 0 984800 • E ٠ 1 1 1 ħ. k 1 186900 1 178500 1 178500 1 172900 1 153000 1 142500 1 124400 1 001300 30010100 2 E 10 E 4 E 11 43101023 2020121 40,000 040202-

© 2020 International Centre for Diffraction Data, All rights reserved.

04-012-1060

Jun 9, 2020 2:38 PM (fal-sharji2)

Aton	us Alternate mical Formula: nic %: Fe28.57 eral Name: Mag	Mg14.29 O5	Empirical 7.14 ANX:	Formula: F	e2 Mg (04	Temperature (No Weight %: Fe ame: Magnesiu	55.85 N	/lg12.15 O32.00
Radi	iation: CuKα1	λ: 1.5406	Å d-Spac	ing: Calcul	ated	Inten	sity: Calculated	l/lo	:: 4.07 I/Ic - ND : 1.5
Auth Dens	: Cubic SPC nor's Cell [Autl sity [Dcalc: 4. p: 920.0 K (Au	556 g/cm ³	460(9)Å Dstruc: 4.56		SS/FO	M: F	AuthCell Z: (30) = 999.9(0.0 blor: Brown		AuthCell MolVol: 72.89]
Crys Redu Redu ADP	ell γ: 90.00° stal Data Axial I uced Cell [Red Cell β: 60.00° : U Origin: ymmetry Operat	Cell a: 5.908 RedCell γ: O2 Cryst	.000 c/b: 3 Å RedCo	XtlCell Z: 1.000] ell b: 5.908 edCell Vol: y Allowed):	Å R e 145.79	ų]		RedC	ell α: 60.00°
Seg	Operator	Seq Opera	ator S	eg Operato	r				
	x,y,z					Seq	Operator	Seq	Operator
1 2 3 4 5 6 7 8 9 10	x,y,z x,-y,-Z x,-y+1/4,-z+1/4 -x,y+3/4,2+3/4 -x+1/4,y,-z+1/4 x+3/4,-y,2+3/4 -x+1/4,-y+1/4,z x+3/4,y+3/4,-z z,x,y -z,-x,-y	12 -z,x+3, 13 -z+1/4 14 z+3/4, 15 -z+1/4 16 z+3/4,; 17 y,z,x 18 -y,-z,-) 19 y,-z+1,	/4,-y+1/4 2 /4,-y+3/4 22 /x,-y+1/4 22 /x,-y+3/4 24 /x,-x+1/4, y 25 /x+3/4,-y 26 /x+3/4,-y 26 /4,-x+1/4 22 /4,x+3/4 30	y+1/4,z, y+3/4,z, y+3/4,z, y+3/4,z+ x,z,y x,z,y x,z+1/4, y-x,z+1/4, y-x+1/4,z, y-x+1/4,z,	x+1/4 +1/4,x 3/4,-x y+1/4 y+1/4 y+1/4	Seq 31 32 33 34 35 36 37 38 39 40	Operator -x+1/4,-z+1/4,y x+3/4,z+3/4,-y y,-x,-z y,-x+1/4,-z+1/4 -y,x+3/4,-z+3/4 -y+1/4,x,-z+1/4 y+3/4,x,-z+3/4 -y+1/4,-x+1/4,z	Seq 41 42 43 44 45 46 47 48	$\begin{array}{l} \hline \textbf{Operator} \\ z.y.x \\ -z.y-x \\ z.y+1/4, x+1/4 \\ -z.y+3/4, x+3/4 \\ -z+1/4, y.x+1/4 \\ z+3/4, -y, x+3/4 \\ -z+1/4, y+1/4, x \\ z+3/4, y+3/4, -x \end{array}$
2 3 4 5 6 7 8 9 10	-x, y, -z x, -y+1/4, -z+1/4 -x, y+3/4, 2+3/4 -x+1/4, y, -z+1/4 x+3/4, -y, 2+3/4 -x+1/4, y+1/4, z x+3/4, y+3/4, -z z, x, y	12 -z,x+3, 13 -z+1/4 14 z+3/4, 15 -z+1/4 16 z+3/4,; 17 y,z,x 18 -y,-z,-) 19 y,-z+1,	/4,y+3/4 22 ,x,-y+1/4 23 -x,y+3/4 24 ,-x+1/4,y 25 x+3/4,-y 26 x+3/4,-y 27 x+26 (4,-x+1/4 25)	y+1/4,z, y+3/4,z, y+3/4,z, y+3/4,z+ x,z,y x,z,y x,z+1/4, y-x,z+1/4, y-x+1/4,z, y-x+1/4,z,	x+1/4 +1/4,x 3/4,-x y+1/4 y+1/4 y+1/4	31 32 33 34 35 36 37 38 39	-x+1/4,-z+1/4,y x+3/4,z+3/4,-y y,x,z -y,-x,-z y,-x+1/4,-z+1/4 -y,x+3/4,z+3/4 -y+1/4,x,-z+1/4 y+3/4,-x,z+3/4	41 42 43 44 45 46 47	Z.y.x -Zy.x Zy+1/4.x+1/4 -z+1/4.y.x+3/4 -z+1/4.y.x+1/4 z+3/4.y.x+3/4 -z+1/4.yix+1/4
2 3 4 5 6 7 8 9 10 Atom	-x,-y,-z x,-y+1/4,-z+1/4 -x,y+3/4,z+3/4 -x+1/4,y,-z+1/4 x+3/4,-y,z+3/4 -x+1/4,-y+1/4,z x+3/4,y+3/4,-z z,x,y -z,-x,-y	12 -z,x+3, 13 -z+1/4 14 z+3/4, 15 -z+1/4 16 z+3/4,, 17 y,z,x 18 -y,-z,-1 19 y,-z+1, 20 -y,z+3,	/4,y+3/4 2; ,x,-y+1/4 2; -x,y+3/4 2; -x,y+3/4 22 x+3/4,-y 22 x+3/4,-y 22 (4,-x+1/4 25 (4,-x+1/4 25 (4,x+3/4 30)	y+1/4,z, y+3/4,z, y+1/4,z- y+3/4,z- x,z,y,	x+1/4 (+3/4 +1/4,x 8/4,-x y+1/4 y+3/4 y+1/4 (+3/4 SOF	31 32 33 34 35 36 37 38 39	-x+1/4,-z+1/4,y x+3/4,z+3/4,-y y,x,z y,-x-1/4,-z+1/4 y,x+3/4,-z+1/4 y+3/4,-x,z+3/4 -y+1/4,x,-z+1/4 y+3/4,x+3/4,-z y+3/4,x+3/4,-z	41 42 43 44 45 46 47	Z.y.x -Zy.x Zy+1/4.x+1/4 -z+1/4.y.x+3/4 -z+1/4.y.x+1/4 z+3/4.y.x+3/4 -z+1/4.yix+1/4

 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
 Pearson Symbol:
 cF56.00

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1/2

04-012-1060						Jun 9, 2	020 2:38 FM	itai-snarii
20002-000	00-017-0464 (F 01-075-9708 (/ 01-098-1935 (/	Primary), 00- Alternate), 01 Alternate), 01	036-0398 (Pri -078-5428 (Al JOR9-1037 (Al	nary), 01-0 ternatel, 01 ternatel, 01	73-1960 (Alte -082-9881 (A JAR-1034 (A	mate), 01-073 itemate), 01-0	-2410 (Alternate 188-1935 (Altern 188-1939 (Altern	ate).
	01-088-1940 (Alternate), 01	-088-1941 (A	ternate), 01	-088-1942 A	ternate) 01-0	88-1943 (Altern	ate),
	01-089-3084 (A	Alternate), 01 Alternate),	-089-4924 (A) 04-001-7921 ((atemate), U1 Atemate),	-089-018/ (A	Bernate), 01-0 38 (Alternate),	188-1943 (Altern 189-6188 (Altern) 04-002-0587	(Alternate).
	04-002-0619 (A	Alternate),	04-002-2458	Alternate :	04-002-249	59 (Alternate) 13 (Alternate)	04-002-3054	(Alternate).
			04-002-5555	Alternate).	04-002-589	A (Atemate), A (Atemate),	04-002-5904	(Alternate), (Alternate)
	04-002-5403 (/	Alternate), -	04-002-8191	Alternate .	04-002-820	4 (Alternate).	04-005-7127	(Alternate).
	04-006-0427 {/	Alternate).	04-005-1839	Alternate), Alternate),	/ 04-005-248	Alternate	/ 04-005-2469	(Alternate), (Alternate)
	04-006-4005 (#	Albernate .	04-006-6673	Alternate?	04-006-66	6 Alternate). 9 Alternate)	04-006-6677	Alternate)
	04-007-5530 //	Alternate)	04-008-2382	Alternate), Alternate)	04-010-612	(Pnmary)	04-011-9002 (Alternate
	04-011-9003 (#	Alternate), Alternate),	04-012-0906 04-012-0912	Alternate).	04-012-090	9 Alternate 3 Alternate	04-012-0910	(Alternate).
	04-012-0915 (#	Alternate	04-012-0916 (Atemate).	04-012-091	Alternate).	04.017-0918	Alternate
	04-012-0919 (/ 04-012-0923 (/	Alternate), -	04-012-0920 04-012-0924	Alternate . Alternate .	04-012-09	21 (Alternate). 25 (Alternate).	04-012-0922 04-012-0926	(Alternate) (Alternate)
	04-012-0927	liternate).	04-012-0928	Alternate).	04-012-093	9 (Alternate).	04-012-0930	(Alternate)
Cross-Ref PDF #'s:	04-012-0931 (/ 04-012-0935 (/	Alternate), Alternate),	04-012-0932 04-012-0935	Alternate . Alternate .	04-012-09	33 (Alternate). 37 (Alternate).	04-012-0934	(Alternate), (Alternate),
atosa-not PDP # 5.	04-012-0939 (A	Alternate).	04-012-0940	Alternate).	04-012-094	[] (Alternate).	04-012-0942	(Alternate).
	04-012-0943 (/	Alternate)	04-012-0944 04-012-0946	Alternate .	04-012-09	45 (Alternate), 19 (Alternate),	04-012-0946	Alternate).
	04-012-0951 //	Alternate)	04-012-1050	Afternate)	04-012-105	51 (Alternate).	04-012-1052	(Alternate),
	04-012-1053 // 04-012-1057 //	Alternate), Alternate),	04-012-1054 04-012-1058	Alternate),	04012-10	6 (Alternate) 9 (Alternate)	04-012-1056	(Alternate), (Alternate),
	04-012-1062 (A	Alternate),	04-912-1053	Ademate)	04012-10	4 (Alternate), 8 (Alternate),	04-012-1065 04-012-1069	(Alternate)
		Alternate), Alternate), -	04-012-1067 (04-012-1071 (Alternate . Alternate .	04-012-108	58 (Alternate), 72 (Alternate),	04-012-1069	(Alternate)
	04-012-1074 (A	litemate),	04-012-1075	Alternate)	84812-10	6 (Atemate).	04-012-1077	(Aitemate)
		Alternate), -	04-012-1079	Alternate),	04-012-108	30 (Alternate), 34 (Alternate).	04-012-1081 04-014-3695	(Alternate)
	04-014-3696 (7	Alternate),	04-014-3697	Alternate).	8181139	Alternate)	/ 04-014-3699	(Alternate),
		Alternate), Alternate),	04-014-3701 04-014-3705	Alternate),	04-014-370)2 (Alternate), X6 (Alternate),	04-014-3703	(Alternate), (Alternate),
		MINESS 1021 ET 1.	04-014-01001		01 01 07	(Alternate)	01.014.2711	(Alternate)
	04-014-3704 (A 04-014-3708 (A	Alternate),	04-014-3709	Alternate),	/ 04-014-3/1	of choten inspect	ALALASI 11	
	04-014-3708 // 04-014-3712 // 04-014-3716 //		04-014-3213	Atternate)	04-014-37		04-014-3711 04-014-3715 04-014-3719	(Alternate).
	04-014-3708 // 04-014-3712 // 04-014-3716 //	Alternate	04-014-37171	Alternate), Alternate), Alternate),	04-014-37	8 (Alternate).	04-014-3719	(Alternate) (Alternate) (Alternate)
	04-014-3708 04-014-3712 04-014-3716 04-014-3716 04-014-3720 04-014-3724	Alternate), Alternate), Alternate)	04-014-3717 04-014-3721 04-014-3725	Alternate), Alternate), Alternate),	04-014-37	18 (Alternate), 22 (Alternate), 26 (Alternate),	04-014-3719 04-014-3723 04-014-3727	(Alternate) (Alternate) (Alternate) (Alternate)
	04-014-3708 // 04-014-3712 // 04-014-3716 //	Alternate), Alternate), Alternate)	04-014-37171	Alternate), Alternate), Alternate),	04-014-37	8 (Alternate).	04-014-3719 04-014-3723 04-014-3727 04-014-3731	(Alternate) (Alternate) (Alternate) (Alternate)
Entry Date: 09/01/2	04-014-3708 / 04-014-3712 / 04-014-3716 / 04-014-3720 / 04-014-3724 / 04-014-3728 / 04-014-3728 /	Alternate), Alternate), Alternate), Alternate), Alternate),	04-014-3717 04-014-3721 04-014-3725	Atemate), Atemate), Atemate), Atemate), Atemate),	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37	18 (Alternate), 22 (Alternate), 26 (Alternate), 30 (Alternate),	04-014-3719 04-014-3723 04-014-3727 04-014-3731 04-015-7027	(Alternate) (Alternate) (Alternate) (Alternate)
laferences:	04-014-3708 / 04-014-3712 / 04-014-3716 / 04-014-3720 / 04-014-3724 / 04-014-3728 / 04-014-3728 /	Alternate), Alternate), Alternate), Alternate), Alternate),	04-014-3717 04-014-3721 04-014-3725 04-014-3729 04-014-3733	Atemate), Atemate), Atemate), Atemate), Atemate),	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37	(8 (Alternate), 22 (Alternate), 36 (Alternate), 30 (Alternate), 34 (Alternate),	04-014-3719 04-014-3723 04-014-3727 04-014-3731 04-015-7027	(Alternate) (Alternate) (Alternate) (Alternate)
Entry Date: 29101/2 References Proc. 29 Partury References	04-014-3708 () 04-014-3712 () 04-014-3715 () 04-014-3724 () 04-014-3724 () 04-014-3728 () 04-014-3732 () 04-014-3732 () 2009 Last Mc	Alternate), Alternate), Alternate), Alternate), Alternate),	04-014-3717 04-014-3721 04-014-3725 04-014-3729 04-014-3733 04-014-3733 Inte: 09/01/20	Atemate), Atemate), Atemate), Atemate), Atemate),	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37	(8 (Alternate), 22 (Alternate), 36 (Alternate), 30 (Alternate), 34 (Alternate),	04-014-3719 04-014-3723 04-014-3727 04-014-3731 04-015-7027	(Alternate) (Alternate) (Alternate) (Alternate)
Referencesi Date Di Himary Reference	04-014-3708 () 04-014-3712 () 04-014-3716 () 04-014-3720 () 04-014-3722 () 04-014-3732 () 04-014-3732 () 2009 Last Me 21 Beference Calculated fro	Alternate), Alternate), Alternate), Alternate), Alternate), odification () odification () odification ()	04-014-3717 04-014-3725 04-014-3725 04-014-3725 04-014-3725 04-014-3723 late: 09/01/20	Atternate), Atternate, Atternate, Atternate, Atternate, Atternate, Dt1 Las	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 1 Modificanto	18 (Alternate), 22 (Alternate), 6 (Alternate), 10 (Alternate), 14 (Alternate), 14 (Alternate), 15 (Alternate), 16 (Alternate), 16 (Alternate), 16 (Alternate), 16 (Alternate), 16 (Alternate), 17 (Alternate), 18 (Alternate), 19 (Alternate), 10 (Alternate),	04-014-3713 04-014-3723 04-014-3727 04-014-3727 04-015-7027 ns	(Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate)
Referencesi Date Di Himary Reference	04-014-3708 () 04-014-3712 () 04-014-3716 () 04-014-3720 () 04-014-3722 () 04-014-3732 () 04-014-3732 () 2009 Last Me 21 Beference Calculated fro	Alternate), Alternate), Alternate), Alternate), Alternate), odification () odification () odification () odification ()	04-014-3717 04-014-3725 04-014-3725 04-014-3725 04-014-3725 04-014-3723 late: 09/01/20	Atternate), Atternate, Atternate, Atternate, Atternate, Atternate, Dt1 Las	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 1 Modificanto	18 (Alternate), 22 (Alternate), 6 (Alternate), 10 (Alternate), 14 (Alternate), 14 (Alternate), 15 (Alternate), 16 (Alternate), 16 (Alternate), 16 (Alternate), 16 (Alternate), 16 (Alternate), 17 (Alternate), 18 (Alternate), 19 (Alternate), 10 (Alternate),	04-014-3719 04-014-3723 04-014-3727 04-014-3727 04-014-3727 04-015-7027	(Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate)
leferencest Dros Ri	04-014-3708 () 04-014-3712 () 04-014-3715 () 04-014-3720 () 04-014-3724 () 04-014-3732 () 04-014-3732 () 009 Last Mo 209 Last Mo 2009 Last Mo 2000 L	Alternate), Alternate), Alternate), Alternate), addition D am LPF using T affection up 005) Color, brown	04-014-3717 04-014-3725 04-014-3725 04-014-3725 04-014-3723 04-014-3733 (late: 09/01/21 POWD-12+4. 6 high temports m1420 X and II 11, in Situ Conc	Atternate), Abernate), Atternate,	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 1 Modification cridering in mag E.M., Hossen 1 d capsule (cr	(8) (Alternate), 22 (Alternate), 23 (Alternate), 30 (Altern	04-014-3719 04-014-3723 04-014-3727 04-014-3727 04-015-7027 ns	(Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) Code:
laferencesi (vola Di himary Refamoce Structure	04-014-3708 () 04-014-3715 () 04-014-3715 () 04-014-3720 () 04-014-3728 () 04-014-3728 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 04-014-3728 () 04-014	Alternate), Alternate), Alternate), Alternate), Alternate), odification D ant LPF using T ph pressure an diffactor up loss) Color, brows ample Prepa	04-014-3717 04-014-3725 04-014-3725 04-014-3729 04-014-3733 leate: 09/01/20 *5WD:12++ 6 high temporation to 12-04 c high temporation temporati	Attemate), Alternate), Alternate), Alternate), Alternate), Alternate), Alternate), Alternate), Alternate, Alternate, Matemate, Matemate, Matemate, Alterna	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 1 Modification cedaring in may E.M. Hossan 1 d capsule (cr abort solid-st	18 (Alternate), 21 (Alternate), 26 (Alternate), 30 (Alternate), 44 (Aternate), 44 (Aternate), 45 (Alternate), 44 (Aternate), 45 (Alternate), 46 (Alternate), 46 (Alternate), 46 (Alternate), 46 (Alternate), 46 (Alternate), 47 (Alternate), 48 (Alternate), 48 (Alternate), 49 (Alternate), 49 (Alternate), 40 (Alternate), 4	04-014-3719 04-014-3723 04-014-3727 04-015-7027 ns of=204, coing in a Partse J.B. Am. V	(Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Code: 223 K for 1
leferences Cros P Innuty Reference Etsetum Database Common	04-014-3708 () 04-014-3712 () 04-014-3715 () 04-014-3720 () 04-014-3728 () 04-014-3732 () 04-014-3732 () 009 Last Mo 209 Last Mo 209 Last Mo 201 Reference Calculated fro 2 Flocts of hig 2 may powder 1000, 1984 () 000, 1984 () Diffraction, Diffraction,	Alternate), Alternate), Alternate), Alternate), atternate), odification D atternate), odification D atternate atternate obj Color: brow ample Prepa Datacollectio	04-014-3717 04-014-3725 04-014-3725 04-014-3725 04-014-3723 04-014-3733 (leate: 09/01/25 POWD-12+4 6 high temperate st12:00 x and if h, in Situ Contration: Composition: Composition: Composition: Composition: Composition: SigPa, Ter	Atternate), Abernate), Aternate), Aternate), Aternate, Aternate, Aternate, Aternate, Aternate, Aternate, aternate, the second the se	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 Modification in Modification in Modification	(8) (Alternate), 2) (Alternate), 20 (Alternate), 30 (Alternate), 30 (Alternate), 30 (Alternate), 30 (Alternate), 30 (Alternate), 30 (Alternate), 30 (Alternate), 30 (Alternate), 30 (Alternate), 31 (Alternate), 32 (Alternate), 32 (Alternate), 33 (Alternate), 34 (Alternate), 35 (Alternate), 36 (Alternate), 36 (Alternate), 36 (Alternate), 36 (Alternate), 36 (Alternate), 36 (Alternate), 36 (Alternate), 36 (Alternate), 37 (Alternate), 36 (Alternate), 37 (Altern	04-014-3719 04-014-3723 04-014-3727 04-014-3727 04-015-7027 ns pf=204, using in a Partise J.B. Am. M	(Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Code: 223 K for 1
laferences: (vic. P Immary References Platabase Comment I-Specings (34) - Mg	04-014-3708 () 04-014-3712 () 04-014-3715 () 04-014-3720 () 04-014-3728 () 04-014-3732 () 04-014-3732 () 009 Last Mo 209 Last Mo 209 Last Mo 201 Reference Calculated fro 2 Flocts of hig 2 may powder 1000, 1984 () 000, 1984 () Diffraction, Diffraction,	Alternate), Alternate), Alternate), Alternate), atternate), odification D atternate), odification D atternate), atternate	04-014-3717 04-014-3725 04-014-3725 04-014-3725 04-014-3723 04-014-3733 (leate: 09/01/25 POWD-12+4 6 high temperate st12:00 x and if h, in Situ Contration: Composition: Composition: Composition: Composition: Composition: SigPa, Ter	Atternate), Abernate), Aternate), Aternate), Aternate, Aternate, Aternate, Aternate, Aternate, Aternate, aternate, the second the se	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 Modification in Modification in Modification	18 (Alternate), 27 (Alternate), 26 (Alternate), 30 (Alternate), 44 (Aternate), 44 (Aternate), 50 (Alternate), 50 (Alternate),	04-014-3719 04-014-3723 04-014-3727 04-014-3727 04-015-7027 ns pf=204, using in a Partise J.B. Am. M	(Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Code: 223 K for 1
References: Discussion	04-014-3708 () 04-014-3712 () 04-014-3715 () 04-014-3724 () 04-014-3724 () 04-014-3732 () 2009 Last Mo 20 Reference Catculated fro % frag powder 1000 1681 (2) ANX: A3X4 to: T601271, S Pressure of Diffraction. Fe2 04 - 94-011 1 h k 1 29 1 1	Alternate), Alternate), Alternate), Alternate), Alternate), additication D an LPF using 7 presents an diffection up 005) Color: brows ample Prepa Distacollectio 2-1960 (Stici 2-29 (*), 74, 1982	04-014-3717 04-014-3725 04-014-3725 04-014-3725 04-014-3733 late: 09/01/25 *0WD-12++ 6 high temporation tel/12-00 K and II 1. If Situ Conc region: Composi- in: 5 GPa. Ter 1. If And Skit Im d (Å) 1. If Alogo	Aftemate), Abernate), Aftemate), Aftemate), Attemate), Attemate, A	04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 1 Modificano sodaring in ma E.M. Hassan 1 d capsule (cr ation: solid-st f Cata Collect a Ka1 1,54054 1 20 1 20 1 11 1 20 1 11 1 111	18 (Alternate), 27 (Alternate), 20 (Alternate), 30 (Al	04-014-3719 04-014-3723 04-014-3727 04-014-3727 04-015-7027 ns f=204, ming in a Parter J.B. Am. W LEPF Collection sample dried at 4 nt Cell Data Sou	(Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Alternate) (Code: 223 K for 1
Ileferencesi Pros D Primary Refumece Database Comment Database Comment Despecings (34) - My 29 (*) d (Å) 15 3761 4.823600 00.2222 2.953868	04-014-3708 () 04-014-3712 () 04-014-3715 () 04-014-3726 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 2009 Last Mo 20 Reference Calculated fro 2 Sector of lig 2 ANX: A3X4, 1000 11021 (2) ANX: A3X4, 1000 11021 (2) Calculated fro 2 Sector of lig 2 Pressure of Diffraction. 1 h k 1 29 1 1 1	Ahemate), Alternate), Alternate), Alternate), Alternate), additication D am LPF using 1 pressues un diffaction up 005) Color: brows ample Prepa Diatabolischic 2-1060 (Stick M. 407) Te 4000	04-014-3717 04-014-3725 04-014-3725 04-014-3723 04-014-3733 late: 09/01/25 *0WD-12++ 4 high temporation to Situ Conto *0WD-12++ 4 high temporation to Situ Conto *0WD-12++ *0WD-1	Attemate), Abemate), Attemate), A	o4-014-37 04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 1 Modificano stdning is me E.M. Hessen 1 d capsule (cr stdn: solid-st f Data Collect 1 1 54054 1 2 9 1 11 2 111 2 1	18 (Alternate), 27 (Alternate), 26 (Alternate), 30 (Alternate)	D4-014-3719 04-014-3723 04-014-3727 04-014-3727 04-015-7027 ns of=204, using in a Parties J.B. Am. W LEPF Collection fample dried at 4 nt Cell Data Soc t h k T3 22 t 4 17 t 1 t 4	(Alternate) (Alter
Inferences: Principal Intrany References Printrany References	04-014-3708 () 04-014-3712 () 04-014-3715 () 04-014-3720 () 04-014-3728 () 04-014-3732 () 04-014-372 () 04-	Alternate), Alternate), Alternate), Alternate), Alternate), odification D an LPF using 1 ph processes an diffication D ph processes an diffication D ph processes an diffication D ph processes an diffication D ph processes an diffication D diffication D and D at according to the diffication D at according to the	04-014-3717 04-014-3725 04-014-3729 04-014-3729 04-014-3729 04-014-3729 atas: 09/01/20 PCWD-12+4 6 high temports to 12.00 K and 0 to 12.00 K and 0 12.00 K and 0 12.00 K and 1 12.00 K and 1 10.00 K a	Attemate), Abemate), Attemate), Attemate), Attemate, Att	od-014-37 04-014-37 04-014-37 04-014-37 04-014-37 04-014-37 i Modification Modification d capsule (or stion: solid-st f Data Collect a Kal 1.54054 1 * 29 3 * 111 1 * 115	18 (Alternate), 27 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 27 (Alternate), 26 (Alternate), 27 (Alternate), 26 (Alternate), 27 (Alternate), 26 (Alternate), 27 (Alternate)	D4-014-3713 04-014-3723 04-014-3723 04-014-3727 04-015-7027 ns pf=204, caing in a Partise J.B. Am. M LEPF Collection sample dired at 4 nit Cell Data Soc <u>I h k</u> 12 2 1 4 4 13 2 4 4 14 5 1 4 4 15 5 6 16 5 7 17 5 7 18 5 19 5 7 19 5 7 1	(Alternate) (Alter
Inferences: Participation Intrusy References Participation Intrusy References Intrusy References Intrusy References In	04-014-3708 () 04-014-3712 () 04-014-3715 () 04-014-3726 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 04-014-3732 () 090 Last Mo 20 Reference Calculated for 255cm of hig X-ray powder 1000 1905 () Reference Calculated for 255cm of hig X-ray powder 1000 1905 () Reference Calculated for 255cm of hig X-ray powder 1000 1905 () 1001271 Si Pressure of Diffraction. () Fe2 04 - 94-01 1 h k 1 29 1 1 1 375 2 0 1 1	Ahemate), Alternate), Alternate), Ahemate), Ahemate), Aternate), additication D odification D odific	04-014-37171 04-014-37251 04-014-37251 04-014-37259 04-014-37231 late: 09/01/20 *0WD-12++ d high temporati- tel/30 K and if h, in Situ Contri ration: Compo nr. 5 GPa, Ter d (Å) 12/4060 12/05880 11/65800 11/65800 11/65800	Attemate), Abemate), Attemate), Attemate), Attemate, Att	odo14.37 04-014.37 04-014.37 04-014.37 04-014.37 04-014.37 04-014.37 1 Modification solid-state f Data Collect 1 State Collect 2 Kin1 1.54054 1 2 111 2 1111 2 111 2 111 2 111	(Alternate), 20 (Alternate), 20 (Alternate), 20 (Alternate), 20 (Alternate), 20 (Alternate), 20 (Alternate), 30 (Alternate), 44 (Aternate), 44 (Aternate), 44 (Aternate), 44 (Aternate), 50 (C)	O4-014-3719 O4-014-3723 O4-014-3723 O4-014-3727 O4-014-3727 O4-015-7027 ns Farlos J.B. Am. M LPF Collection Sample dried at A nt Cell Data Sou I h k T1 22 1 4 T1 1 4 T1 2 1 4 O	(Alternate) (Alter
Inferences DX Voice DX Viscury Refumeces DX Principy Refumeces </td <td>04-014-3708 04-014-3712 04-014-3715 04-014-3720 04-014-3724 04-014-3724 04-014-3732 04-014-3732 04-014-3732 04-014-3732 0209 Last Mo 2009 Last Mo 2009 2009 Last Mo 2009 Last Mo 2000 Last Mo 2009</td> <td>Ahemate), Alternate), Alternate), Alternate), Alternate), adification D odification D</td> <td>04-014-3717 04-014-3725 04-014-3725 04-014-3725 04-014-3723 1ate: 09/01/25 *0WD-12+4 6 high temporation to Stitu Control to Statu Control to S</td> <td>Attemate), Abemate), Abemate), Atemate), Atemate</td> <td>ordaning is may ordaning is may ordaning is may is Modification display to the streng is may is modification display to the display to the di</td> <td>(Alternate), 27 (Alternate), 27 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 30 (</td> <td></td> <td>(Alternate) (Alter</td>	04-014-3708 04-014-3712 04-014-3715 04-014-3720 04-014-3724 04-014-3724 04-014-3732 04-014-3732 04-014-3732 04-014-3732 0209 Last Mo 2009 Last Mo 2009 2009 Last Mo 2009 Last Mo 2000 Last Mo 2009	Ahemate), Alternate), Alternate), Alternate), Alternate), adification D odification D	04-014-3717 04-014-3725 04-014-3725 04-014-3725 04-014-3723 1ate: 09/01/25 *0WD-12+4 6 high temporation to Stitu Control to Statu Control to S	Attemate), Abemate), Abemate), Atemate), Atemate	ordaning is may ordaning is may ordaning is may is Modification display to the streng is may is modification display to the display to the di	(Alternate), 27 (Alternate), 27 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 30 ((Alternate) (Alter
Inferences: Differences: (vice Differences: **many Refurences: Differences: Database Comment Differences: -Specings (34) - Mg Differences: 0.01202 2.958865 Differences: 0.01203 2.411710 Differences: 0.31702 1.701360 Differences:	04-014-3708 () 04-014-3712 () 04-014-3715 () 04-014-3728 () 04-014-3728 () 04-014-3732 () 04-014-3732 () 009 Last Me 20 Reference Calculated % 209 Effection 20 Reference Calculated % 20 Reference Calculated % 20 Reference Calculated % 20 Reference Calculated % 20 Reference 1000 1908 () 21 Reference 1000 1908 () 22 Reference 1000 1908 () 23 Reference 1000 1908 () 24 Reference 1000 1908 () 24 Reference 1000 1908 () 25 Reference 1000 1908 () 27 Reference 1000 1908 () 28 Reference 1000 1908 () 29 Reference 1000 1908 () 20 Reference 1000 1908 () 20 Reference 20	Ahemate), Alternate), Alternate, Alternate	04-014-3717 04-014-3725 04-014-3725 04-014-3725 04-014-3723 1ate: 09/01/25 *0WD-12++ 4 high temporation (A fined Skit Int 12/0580 12/05800 11/058	Attemate), Abemate), Attemate), Attemate), Attemate), Attemate), Attemate), Attemate), Attemate), Attemate), Attemate, Attemate), Attemate, Attema	ordening in may ordening in may in Modification in Modificatio	18 (Alternate), 27 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 26 (Alternate), 27 (Alternate)		(Alternate) (Alter

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 2/2

01-080-6407 Jun 9, 2020 2:38 PM (fal-sharji2) Status Alternate QM: Star Pressure/Temperature: Temperature (Non-ambient) Chemical Formula: Fe3 t34 Empirical Formula: Fe3 04 Weight %: Fe72.36 027.64 Atomic %: Fe42.86 057.14 ANX: A3X4 Compound Name: Iron Oxide Mineral Name: Magnetite Common Name: Iron(II) diiron(III) tetraoxide d-Specing: Calculated Rediation: CuKo1 A: 1.5406 L Intensity: Calculated Ma: 472 10c - ND: 125 SYS: Cubic SPGR: Fd-3m (227) Author's Cell | AuthCell a: 8.4499(5) Å AuthCell Vol: 603.33 Å* AuthCell Z: 8.00 Density | Deale: 5.098 gicm* Distruc: 5.1 gicm*] \$\$/FOM: F(30) = 999.9(0.0000, 30) AuthCell MolVal: 75:421 Temp: 773.0 K (Author provided temperature) R-factor: 0.0264 Space Group: Fd-3m (227) Molecular Weight: 231.54 Crystal Data (XilCell a: 5.450 Å XtiCell b: 5.450 Å XIICall c: 5.450 Å XIICall o: 90.00" XIICall B: 90.00" XtiCell y: 90.00° XtiCell Vol: 603.33 Å* XtiCell 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 c: 60.00* RedColl y: 60.00" RedCell B: 50.00* RedCell Vol: 150.63 4*] Crystal (Symmetry Allowed): Centrosymmetric Subfile(s): Common Phase, Forensic, Inorganic, Metais & Alloys, Mineral Related (Mineral , Natural) Prototype Structure [Formula Order]: Mg Al2 04 Prototype Structure [Alpha Order]: Al2 Mg 04 Pearson Symbol: cF56.00 D0-001-1111 (Deleted), 00-002-1035 (Deleted), 00-003-0862 (Deleted), 00-007-0322 (Deleted), 00-011-0614
 Deleted), 00-019-0529 (Firmary), 00-055-0731 (Primary), 01-071-4918 (Alternate), 01-072-2303 (Alternate), 01-075-1909 (Alternate), 01-075-1910 (Alternate), 01-075-1910 (Alternate), 01-075-1910 (Alternate), 01-075-1910 (Alternate), 01-075-1910 (Alternate), 01-075-1910 (Alternate), 01-076-1949 (Alternate), 01-075-5948 (Alternate), 01-075-6086 (Alternate), 01-080-6402 (Alternate), 01-080-6403 (Alternate), 01-080-6403 (Alternate), 01-080-6405 (Alternate), 01-080-6405 (Alternate), 01-080-6403 (Alternate), 01-080-6405 (Alternate), 01-080-6405 (Alternate), 01-080-7833 (Alternate), 01-080-7833 (Alternate), 01-080-7834 (Alternate), 01-080-9086 (Alternate), 01-080-3854 (Alternate), 04-002-3658 (Alternate), 04-002-2054 (Alternate), 04-002-2054 (Alternate), 04-002-2056 (Alternate), 04-002-2568 (Alternate), 04-002-256
 Ort-002-0076 (Alternate)
 Ort-002-0060 (Alternate)
 Ort-002-2481 (Alternate)

 04-002-5709 (Alternate)
 04-002-5831 (Alternate)
 04-002-5632 (Alternate)

 04-002-5903 (Alternate)
 04-002-5863 (Alternate)
 04-002-5632 (Alternate)

 04-002-5903 (Alternate)
 04-002-5863 (Alternate)
 04-002-5633 (Alternate)

 04-002-4828 (Alternate)
 04-002-5633 (Alternate)
 04-002-5635 (Alternate)

 04-004-2838 (Alternate)
 04-005-4307 (Alternate)
 04-005-6268 (Alternate)

 04-005-4751 (Alternate)
 04-005-9733 (Alternate)
 04-005-6256 (Alternate)

 04-005-252 (Alternate)
 04-005-9733 (Alternate)
 04-005-6268 (Alternate)

 04-005-252 (Alternate)
 04-005-6268 (Alternate)
 04-005-6268 (Alternate)

 04-005-252 (Alternate)
 04-005-6268 (Alternate)
 04-005-6268 (Alternate)

 04-005-6059 (Alternate)
 04-005-6268 (Alternate)
 04-005-6497 (Alternate)

 04-005-6050 (Alternate)
 04-005-875 (Alternate)
 04-005-6497 (Alternate)

 04-005-6115 (Alternate)
 04-007-6507 (Alternate)
 04-008-6497 (Alternate)

 04-005-6115 (Alternate)
 04-008-8145 (Alternate)
 04-008-8145 (Alternate)

 04-008-8148 (Alternate)
 04-002-5683 (Alternate) 04-002-8141 (Alternate) 04-003-1446 (Alternate) 04-003-1446 (Alternate) 04-005-4704 (Alternate) 04-005-9786 (Alternate) 04-005-9786 (Alternate) 04-005-9786 (Alternate) 04-005-558 (Alternate) 04-005-558 (Alternate) 04-007-9083 (Alternate) 04-008-4511 (Alternate) 04-008-8147 (Alternate) 04-009-8418 (Atemate) 04-009-8418 (Atemate) 04-009-8422 (Atemate) 04-009-8420 (Atemate) 04-009-8430 (Atemate) 04-009-8434 (Alternate), 04-009-8438 (Alternate), 04-009-6439 (Alternate), 04-009-6436 (Alternate), 04-009-8443 (Alternate), 04-009-8440 (Alternate), 04-009-8443 (Alternate), 04-013-9807 (Alternate), 04-013-9806 (Alternate), 04-013-9807 (Alternate), 04-015-8203 (Alternate), 04-015-8301 (Alternate), 04-015-8203 (Alternate), 04-015-8304 (Alternate), 04-015-8203 (Alternate), 04-015-8304 (Alternate), 04-009-0431 Attentate 04-013-7099 Attentate 04-013-9608 Attentate 04-013-9608 Attentate 04-014-1396 Attentate 04-015-8207 Attentate 04-009-0436 Alternate 04-013-842 (Ahternate 04-013-9609 Ahternate) 04-014-9564 (Ahternate) 04-015-8200 (Ahternate) 04-015-8209 (Atternate) 04-015-8211 (Alternate), 04-015-8213 (Alternate), 04-015-8214 (Alternate), 04-017-1024 (Alternate)

Entry Date: 09/01/2013

References: Type	100	Reference
Primary Reference		Calcutded from ICSD using POWD-12++
Structure		"Structure of magnetite (Fe3 O4) scove the Curte temperature: a calico ordering study" Levy, Q., Giustello, R., Hoser, A. Phys. Chem. Molec. 39, 169 (2012).

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1/2

01-080-6407 Jun 9, 2020 2:38 PM (fal-sharji2) ANX: A3X4. Analysis: Fe3 04. Formula from original source: Fe3 04. ICSD Collection Code: 183974. Sample Source of Locality: Brosso mining area. Tirrea, Italy. Structures: Magnetic structure also determined. Temperature of Data Collection: 773 K. Wyckoff Sequence: e d a (FD3-MZ). Unit Cell Data Source: Provder Diffraction.

29(*)	# (A)	1	h.			28 (*)	d (A)	1	1.	. 8	1.	29.00	d (Å)	1	h	k	1	11
2.1890	4.878650	100	1	- ±		72.4200	1288608	6.6		<u>a</u>	3	109:2431	0.644728	34	- 2	4	0	
\$ 8832	2.987490	294	2	- 21	0	34,4112	1273870	23	1	2	20	112 2008	0.927487	÷.	. 0	- 1	1	
5.1062	2.547740	999	3	- 11	3	78.2311	1218540	뀨	-4	-4	4	113,3319	1:921060	1		4	12	
6.0100	2 439280	74	2	-2	2	01.2340	1.180220	3	- 5	- 5	1.	117.6610	10990762	4	. 6	6	14	
2 7702	2112470	202	4	10	0	00.0201	1.129170	22	181	4	21	120 2236	d 8867990	28		1	ίŧ.	
0.8253	1.1138640	4	31	- 20	1	88.8867	1.100080	24	12	-3	1	125.5400	0.862414	40	1.8	4	-4	
1.0463	1.734830	12	4	-20	2	82.6438	1.056240	21	18	0	b.:	136 1922	0.849247	1		3	1	
0.5462	1.626180	263	- W.	- 30	(#)(90.0185	1,0101000	ार २	.7	12	2	136.7568	0.020501	:10	. 8	.6	-2	
2.0143	1.493750	331	-4	- 40	10	07.4779	1.034700	1.1	18	-4	4	141,1001	0.0166603	25	2 Q L	5	64	
5.2723	1.428290	17	6	- 36	182	101,3395	0.9966830	10	(港)	-2	21	142.6488	0.813082	8.	12	2	7	
6.3168	1.400320	31	4	- 4	2	104,2594	0.875710	36	7	18	1.	010000000000						
0.4144	1.33868-0	24	4	2	0	106.2541	0.969270	7	- 6	.6	22							

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 2/2

04-012-4921 Jun 9, 2020 2:39 PM (fal-sharji2) Status Alternate QM: Indexed Pressure/Temperature: Pressure (Non-ambient) Chemical Formula: Mg (CO3) Empirical Formula: C Mg 03 Weight %: C14.25 Mg28.83 056.93 Atomic %: C20.00 Mg20.00 060.00 ANX: ABX3 Compound Name: Magnesium Carbonate Mineral Name: Magnesite Radiation: CuKa1 A: 1.5406 Å d-Spacing: Calculated Intensity: Calculated Vic: 1.24 Vic - ND: 1.15 SYS: Rhombohedral SPGR: R-3c (167) Author's Cell [AuthCell a: 4.3530(4) Å
 Author's Cell [AuthCell a: 4.3530(4) Å
 AuthCell c: 13.0325(29) Å
 AuthCell Vol: 213.86 ų
 AuthCell Z: 6.00

 AuthOr's Cell [AuthCell a: 4.3530(4) Å
 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 Space Group: R-32 (107) Molecular weight: 04.31 Crystal Data [XtCell is: 4.353 Å XtCell is: 4.353 Å XtCell i: 13.033 Å XtICell α: 90.00° Xt XtICell γ: 120.00° XtICell Vol: 213.86 Å³ XtICell Z: 6.00] Crystal Data Axial Ratio [*ci*: 2.994 a/b: 1.000 *cib*: 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] XtiCell c: 13,033 Å XtiCell α: 90.00° XtiCell β: 90.00° Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: Seg Operator Seg Operator Seg Operator Seg Operator Seq Operator Seq Operator x,y,z -x,-y,-z 3 -y,x-y,z y,-x+y,-z 5 -x+y,-x,z 6 x-y,x,-z 7 -y,-x,z+1/2 8 y,x,-z+1/2 9 10 x,x-y,z+1/2 -x,-x+y,-z+1/2 11 -x+y,y,z+1/2 12 x-y,-y,-z+1/2 Atomic Coordinates: Atom Num Wyckoff Symmetry x
 x
 y
 z
 501

 0.3066
 0.0
 0.25
 1.0

 0.0
 0.0
 0.0
 1.0

 0.0
 0.0
 0.25
 1.0
 SOF IDP AET 18e 6b 6a O Mg 123 232
 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]:
 Ca O3,hR30,167
 Cross-Ref PDF #'s: 04-012-4921 (Alternate), < 04-012-4918 (Alternate), < 04-012-4919 (Alternate), < 04-012-4920 (Alternate), 04-012-4917 (Alternate), < 04-012-4918 (Alternate), < 04-012-4919 (Alternate), < 04-012-4920 (Alternate), Cross-Ref PDF #'s: 04-012-4922 (Alternate), < 04-012-4923 (Alternate), < 04-012-4923 (Alternate), 04-012-4921 (Alternate), < 04-013-2018 (Alternate), < 04-014-4830 (Primary), < 04-014-4846 (Alternate), < 04-013-2018 (Alternate), < 04-014-4830 (Primary), < 04-014-4846 (Alternate), < 04-013-2018 (Alternate), < 04-014-4830 (Primary), < 04-014-4846 (Alternate), < 04-013-2018 (Alternate), < 04-014-4830 (Primary), < 04-014-4846 (Alternate), < 04-013-2018 (Alternate), < 04-014-4830 (Primary), < 04-014-4846 (Alternate), < 04-013-2018 (Alternate), < 04-014-4830 (Primary), < 04-014-4846 (Alternate), < 04-013-2018 (Primary), < 04-014-4846 (Primary Entry Date: 09/01/2009 Last Modification Date: 09/01/2011 Last Modifications: Reflections References: DOI Reference Type Primary Reference Calculated from LPF using POWD-12++. "Structural refinements of magnesite at very high pressure". Figuet G., Guyot F., Kunz M., Matas J., Andrault D., Hanfland M. Am. Mineral. 87, 1261,1265 (2002). Structure ANX: ABX3. In Situ Condition: Powdered samples were placed in diamond anvil without pressure ANA, ADAS: In Silu Conductor, Powdered stamples were placed in diamond artivit windout 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 Kn1 1.54056 Å 28 (°) d (Å) * <u>28 (°)</u> d (Å) 28 (°) h k l I hkl d (Å)
 d(A)
 I
 h
 k

 1.416410
 14
 2
 1

 1.305470
 93
 2
 1

 1.305470
 93
 2
 1

 1.256600
 187
 3
 0

 1.256200
 187
 3
 0

 1.232530
 31m
 1
 0

 1.232530
 31m
 1
 1

 1.232530
 65
 1
 1

 1.31510
 4
 2
 1
 I h 15m 0 m 2 34 0 42m 0 m 1 27 2 1 1 3 3 49 1 3.263090 2.465050 2.176500 2.176500 1.945930 1.810670 1.631550 1.537450 1.495410 65,8889 67,1976 72,3197 75,6117 76,0646 77,3583 77,3583 79,4216 85,8052 90.1149 90.1149 90.3488 91.8137 93.7204 95.3068 96.5146 101.3787 27 3080 36,4176 41,4530 41,5413 46,6369 50,3534 56,3434 60,1339 62,0078 1.088250 1.088250 1.086040 1.072500 1.072500 1.072500 111 124051897 0 101010211 240002400 320222313 601210831 999 81 133 760 119 97 284 133 012010 042210 0.995551 Page 1/2 © 2020 International Centre for Diffraction Data. All rights reserved.

04-012														Jun	9,2020	2:39	P	М (fal-sharji2)
28 (°)	d (Å)	I	h	k		•	28 (°)	d (Å)	I	h	k			28 (°)	d (Å)	1	h	k	+
104,6862	0.972965	29	2	2	6		116.9294	0.903747	2	0	1	14	1.1	139.2518	0.821685	73	0	3	12
104.8676	0.971779	9	- 5	1	12		122,1849	0.879917	33	3	1	8		139,9297	0.819898	3	2	1	13
105,0803	0.970395	2	3	- 31	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	Ū	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-sharii2)
 Status Primary
 QM: Star
 Pressure/Temperature:
 Ambient
 Chemical Formula:
 Ca (0 H)2

 Empirical Formula:
 Ca H2 02
 Weight %:
 Ca54.09 H2.72 043.19
 Atomic %:
 Ca20.00 H40.00 040.00
 Compound Name: Calcium Hydroxide Mineral Name: Portlandite.svn Radiation: CuKo1 A: 1.5406 Å Filter: Graph Mono d-Spacing: Diff. Cutoff: 15.00 Intensity: Diffractometer VIc: 2.9 SYS: Hexagonal SPGR: P-3m1 (164) Author's Cell [AuthCell a: 3.5899(4) Å
 Sigg(4) Å
 AuthCell c:
 4.916(3) Å
 AuthCell Vol:
 54.87 Å*
 AuthCell

 Author's Cell Axial Ratio [c/a:
 1.369]
 Density [Dcalc:
 2.242 g/cm³]
 AuthCell Z: 1.00 AuthCell MolVol: 54.87] 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 Space Group: P-3m1 (164) Molecular Weight: 74.09 Crystal Data [XtiCell a: 3,590 Å XtiCell b: 3,590 Å XtiCell c: 4,916 Å XtiC XtiCell y: 120.00° XtiCell Vol: 54.87 Å XtiCell 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 XtiCell c: 4.916 Å XtiCell α: 90.00* XtiCell β: 90.00* RedCell a: 90.00" RedCell β: 90.00° RedCell γ: 120.00° RedCell Vol: 54.87 Å*] Atomic parameters are cross-referenced from PDF entry 04-006-9147 ADP: U Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: Seg Operator Seq Operator Seq Operator Seq Operator Seg Operator Seg Operator x,x-y,z -x,-x+y,-z x,y,z -x,-y,-z -y,x-y,z y,-x+y,-z -x+y,-x,z x-y,x,-z -y,-x,z y,x,-z 5 8 9 10 11 -x+y,y,z 12 x-y,-y,-z Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Uiso AEL 0.0 0.0 0.33333 0.66666 0.33333 0.66666 0.0 1.0 0.234 1.0 0.4256 1.0 0.01194 0.01203 0.04203 Ca O H 123 1a 2d 2d -3m 3m 3m Anisotropic Displacement Parameters: Atom Num Uani11 Uani22 Uani33 Uani12 Uani13 Uani23 0.0083 0.0106 0.0528 0.0083 0.0106 0.0528 0.0193 0.0149 0.0205 0.0042 0.0053 0.0264 0.0 Ca 0.0 123 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 ✓ 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 DOI Reference Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA. ICDD Grant-in-Aid (1992). Crystal Structure Source: LPF. Winchell, A., Winchell, H. Microscopic Character of Artificial Inorg. Solid Sub. 69 (1964). Type Primary Reference Crystal Structure Optical Data 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 Ko1 1.54056 Å 28 (°) d (Å) hkl * 28 (°) d (Å) I hkl 28 (°) d (Å) I 56.0907 59.4244 62.6319 64.2314 64.2314 71.8086 77.6520 18.0073 28.6709 34.1013 36.5257 47.1200 4.922000 3.111000 2.627000 2.458000 1.927100 1.638300 1.554100 1.482000 1.448900 1.448900 79.0924 81.9069 84.7484 84.7484 86.1940 93.2060 96.0263 72 27 100 1 30 31 14 1397m 61 1.209800 1.175200 1.142900 1.142900 1.142900 1.127400 1101010 01 0000011 225 ENSO 0221120 0000100 0010004 1012201 1212222 10111 1,795400 1.313500 1.060100 50.8120 54.3565 © 2020 International Centre for Diffraction Data. All rights reserved. Page 1/2

Jun 9, 2020 2:38 PM (fal-sharji2) <u>20 (*) d(A) T h k 1 *</u> 118.2628 0.897400 1 2 2 0 00-044-1481 28 (°) d (Å) 28 (°) 28 (°) d (A) h k . h k 1.013900 1.013900 0.983300 106.0623 0.964100 107.5746 0.954700 110.5164 0.937390 2 0 2 1 1 0 2m m <1 1 1 4 3 0 1 0 0 5 1 2 <1 98.8790 435

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: CuKa1 A: 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 is: 57.550(3)Å AuthCell c: 9.4365(8)Å AuthCell Vol: 312.54Å* AuthCell Z: 4.00 AuthCell MolVol: 78.14] Author's Cell Axial Ratio [c/a: 1.640] Density [Dealc: 47.46 g/cm² Distruc: 4.75 g/cm²] SS/FOM: F(30) = 703.9(0.0013, 33) Temp: 296.0 K (Author provided temperature) R-factor: 0.0268
 Space Group:
 141/amd (141)
 Molecular Weight:
 223.30

 Crystal Data [XtlCell a:
 5,755 Å
 XtlCell b:
 5,755 Å
 XtlCell c:
 9,436 Å
 XtlCell a:
 90.00°
 XtlCell β:
 90.00°
 RedCell β:
 117.50°

 RedCell β:
 117.50°
 RedCell γ:
 90.00°
 RedCell VI:
 156.27 Å*
 1
 ADP: U Origin: O2 Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators:
 Seq
 Operator

 5
 -y+1/4,x+3/4,z+1/4

 6
 y+3/4,x+1/4,z+3/4

 7
 y+1/4,x+1/4,z+3/4

 8
 -y+3/4,x+3/4,z+1/4

 Seq
 Operator

 9
 -x+1/2,y-z+1/2

 10
 x+1/2,y-z+1/2

 11
 x-y-z

 12
 -x,y.z

 Seq
 Operator

 13
 y+1/4,x+3/4,-z+1/4

 14
 -y+3/4,-x+1/4,2+3/4

 15
 -y+1/4,-x+1/4,-z+3/4

 16
 y+3/4,-x+3/4,2+1/4
 Seq Operator x,y,z -x,-y,-z -x+1/2,-y,z+1/2 x+1/2,y,z+1/2 Atomic Coordinates:
 SDF
 Uise

 0.83
 0.00581

 0.17
 0.00581

 1.0
 0.00392

 1.0
 0.00528
 Atom Num Wyckoff AET Symmetr 0 0 0 25 0 875 0 0 0 25 0 875 0 0 0 25 0 875 0 0 0 5 0 5 0 0 0 47265 0 25827 4a 4a 8d 15h -4m2 -4m2 .2/m Mn Mg Mn 1 2034 n m ropic Displac int Para Atom Num Uani11 Uani22 Uani33 Uani12 Uani13 Uani23 Mn Mg Mn Q
 0.00572
 0.00572
 0.006
 0.0

 0.00572
 0.00572
 0.006
 0.0

 0.00572
 0.00572
 0.006
 0.0

 0.00337
 0.00247
 0.00593
 0.0

 0.00425
 0.00411
 0.00749
 0.0
 0.0 0.0 0.0 -6.5E-4 2.8E-4 1234 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 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++. *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). Structure 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 Database Comments: rt, flux dissolved in HCI solution. CRUCIBLE: platinum crucible ATMOSPHERE: air SOLVENT: Na2B407 Thux. 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 Mo2.82 O4 - 04-017-0477 (Stick, Fixed Slit Intensity) - Cu Ko1 1.54056 Å d-Spacings (87) - mgv.se 26 (*) d (Å) I 18 0392 4 913360 335 28 9506 3.061580 334 31 0538 2.877500 140 32 4099 2.760130 765 36 1449 2.483020 999 36 5460 2.465680 155 35 6149 2.14
 btck, incertsity:
 intensity:
 Cu Kal 1.54056 A <u>26 (°)</u> 60.8106 63.3461 64.7396 65.5256 67.8559 67.8559 67.8559 67.8559 <u>h k 1 * 20(°) d(Å)</u> d (A) 6 112031240 45.4992 1.991910 7 2 1 3 46.3782 1.879680 1 3 0 1 49.9493 1.824370 54 2 0 4 50.8748 1.793330 223 1 0 5 53.9662 1.687950 83 3 1 2 56.1097 1.537790 78 3 0 3 58.6079 1.537790 78 3 0 3 58.6079 1.537390 78 3 2 1 59.9001 1.540790 525 2 2 4 1.521950 12 1.467000 21 1.438750 193 1.42380 15 1.380060 34m 1.380060 m 1.345360 46 1.312540 1 2-4324 560361 38.1144 2.359120 214 2.034700 248 69.8559 71.8693 305

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1/2

04-017 28 (*)	-0477 d (Å)	I	h	*	a.	28 (°)	d.(Å)	I	ĥ	k	6	•	Jun 9	, 2020 2	:39 Pl	М (fal	sharji2)
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	- 21	2	03	98.4260	1.017350	42m	- 5	÷	0		119,1089	0.893481	1	6	4	2
74.2783	1.275820	88	- 5	а.	3	98.4260	1.017350	m	Þ	-21	5		120.2033	0.888534	2	6	0	£
76.6963	1.241510	43	- 12	2	×.	99.1480	1.011870	23 S	- 20	2	3		123.0381	0.876338	33	12	2	9
77.6715	1 228340	49	4	2	÷.	101.3222	0.995953	21	4	2	5		124,7125	0.869538	0	-2	2	8
78.4008	1.218730	13	3	-	5	102.1908	0.989832	1.		- 31	8		126.0811	0.864194	32	. 8.	- 11	4
80.3356	1.194180	47	2		1	103 2314	0.982671	50	- #3	3	2		128,7291	0.854381	31	6	3	3
80.6791	1.189960	21	3	.2	6	104.9850	0.971014	32	- 2	-21	9		130.2696	0.848981	108m	1	0	22
81,5398	1.179560	38		0	8	105_7534	0.966064	5	2	3	2		130.2696	0.848981	ED:	6	2	4
84.7822	1.142530	6	D	0	- E	105.8489	0.959167	3	0	0	0		131.2111	0.845789	2	0	1	2
85.9750	1.129710	17	4	2	÷5.	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	- 16 m	3	0	1	111.0849	0.934187	16	- 51	- 5	4		134.2615	0.835994	ō	5	3	8
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	Ð	8	113,8468	0.919258	-4	- 1	- 11	10		140.3172	0.818893	9m	6	0	6
90.8973	1.080910	58	- 4	3	3	114.2865	0.916967	6	5	1	6		140,3172	0.818893	111	- 7	0	1
93.0019	1.051890	26m	4	Q	-6	115.2229	0.912184	59	- 40	0	8		141,5684	0.815480	1	5	- 10	8
93.0019	1.061890	TTS .	5	2	1	115.6687	0.909945	17m	5	3	4		142.3364	0.813845	1	2	1	11
95.6180	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	з	2	7	116.4627	0.906019	1	б	1	3		147.6466	0.802035	9	7	1	2
97.1618	1.027190	7	з	3	6	118,4202	0.896665	8	2	٥.	10		149.6682	0.798075	-4	6	4	0

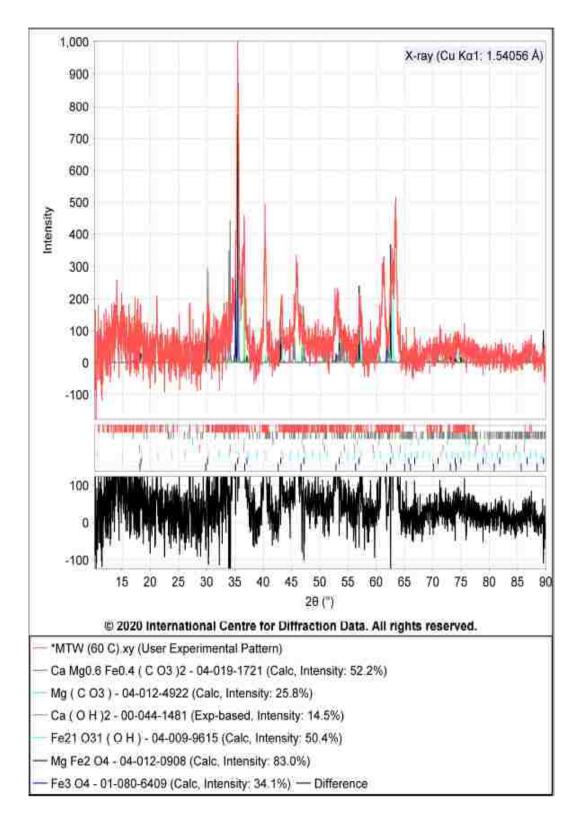


Figure E.2 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) tank at 60 °C from experiment with a tank with 70.4 in² of exposed iron

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-rayWavelength: Cu Ko1 1.54056 ÅSearch Method: HanawaltSearch Window: 0.15°Match Window: 0.15°2nd Pass Filter: Yesd-Spacings: WeightedLowest Allowable GOM: 2000

Phases (6)

#	Accepted	PDF #	QM	Compound Name	I Ratio	I %	I/Ic	Est Wt %
1	true	04-019-1721	4	Calcium Magnesium Iron Carbonate	0.522	20.088	0.8	53
2	true	04-012-4922	1	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	T	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

Status Primary QM: Indexed Pressure/Temperature: Pressure (Non-ambient)
 Chemical Formula:
 Ca Mg0.6 Fe0.4 (CO3)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
 Compound Name: Calcium Magnesium Iron Carbonate Mineral Name: Dolomite ANX: ABC2X6 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) AuthCell c: 6.743(1) Å Author's Cell [AuthCell a: 4.7407(10) Å AuthCell b: 5.3885(10) 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 y: 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 a: 78.58° RedCell 6: 89.27° RedCell y: 84.28° RedCell Vol: 168.00 Å3] ADP: U Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: Seq Operator Seq Operator X,V,Z 2 -x,-y,-z Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Uiso AET -0.2 -0.2 -0.2418 0.3 0.7473 0.7473 0.7926 0.73 0.74 0.586 0.1226 0.742 0.863 0.5819 0.791 -0.2016 -0.2016 0.3039 0.0167 0.0167 0.0167 0.013 0.6 0.4 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 Mg Fe C C C C O O O O O O O O O 2 234 -0.486 0.3 0.262 0.143 -0.129 0.546 0.493 0.349 0.041 -0.486 -0.014 -0.147 -0.123 0.026 -0.372 -0.638 -0.447 0.013 0.018 0.0143 0.0206 0.0201 0.0139 567 89 10 11 0.019 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: DOI Reference Type Calculated from LPF using POWD-12++. Primary Reference "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). Structure 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, Database Comments: Vizille, Vaulnavys, 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 Ku1 1.54056 Å 20 (°) d (Å) h k | * 20 (°) d (Å) h k ï. * 20 (°) d (Å) I 6.609330 5.255810 4.716970 4.578260 3.852540 3.826500 3.766820 3.697390 26 (°) 25.9738 26.5916 26.9579 28.2235 28.9077 29.1829 31.4605 32.9551 3.427610 3.349360 3.304670 3.159300 3.086060 3.057580 2.841220 2.715700 2.697460 2.645640 2.627910 2.577370 2.523610 2.399000 2.394980 13.3854 16.8550 18.7970 19.3719 23.0670 33.1844 33.8537 34.0891 34.0891 34.7786 28 123 54 0 207 720 879m 00101101 0-12-21-12-2 2201 101110 15 001 021211 10-1 0011 000-1-1 0-10-1-1-1 3 5 19 21 216 m 48 999 44 40 1 55 12201 30 2 28 35.5439 37.4570 37.5222 23.2261 23.5994 110 24 0401 © 2020 International Centre for Diffraction Data. All rights reserved. Page 1/2

(°)	d (Å)	I	h	k	1 *	20 (°)	d (Å)	I	h	k	1 *	20 (°)	23, 2020 d (Å)	I	h	k	<u> </u>
8.1249 8.8667	2.358490 2.315170	153 82	2	0	0	60.3652 60.5100	1.532110 1.528790	10 40	-3	0	1	75.3284 75.5940	1.260620 1.256850	m 8m	-2 0	-2	4
9.3269	2.289130	78m	0	2	1	60.5809	1.527170	42m	0	-3	3	75.5940	1.256850	m	-1	4	1
9.3269	2.289130	m	õ	-2	2	60,5809	1.527170	m	3	0	ĭ	76.3049	1.246900	1	3	-2	3
0.2985	2.236150	14	-2	1	0	61.2528	1.512020	1	-2	1	3	76.6036	1.242780	23m	0	-4	3
0.4835	2.226360	2	-2	0	1	61.9719	1.496190	51	-1	2	3	76.6036	1.242780	m	2	1	4
0.7602	2.211880	53	1	1	2	62.0719		95m	0	1	4	76.9734	1.237730	7m	-1	3	3 3
0.8997 0.8997	2.204660	63m m	0	0 2	3 0	62.0719 62.1949	1.494020	m 69	2 -3	-3 1	1	76.9734 77.0862	1.237730 1.236200	m 3	-3 -2	1	3
1.1419	2.192240	13	ó	-1	3	62.2859	1.491300	58m	-3	-2	4	77,2097	1.234530	3m	1	4	0
1.5879	2.169750	43	2	-1	1	62,2859	1.489400	m	1	-3	3	77.2097	1.234530	m	-1	-4	ž
2.2539	2.137080	75	-1	2	1	62.8084	1.478260	5	-2	3	0	77.3635	1.232460	4	-3	3	0
2.4306	2.128590	98	1	-2	2	63.3476	1.466970	14	3	1	0	77.6108	1.229150	8m	1	-4	3
3.6888	2.070160	12	-2	1	1	64.1155	1.451240	9m	2	1,	3	77.6108	1.229150	m	-1	-2	5
4.5886 4.9599	2.030450 2.014540	82 6	-2 1	-1	1 3	64.1155 64.4392	1.451240 1.444730	m 32	-3 -1	-1	1	77.8213 77.8213	1.226350 1.226350	14m	0	12	5 4
5.2659	2.0014540	105	4	0	3	64.7113	1.439310	32 16m	2	-2	2	78,4031	1.218700	m 7	2	4	1
5.4825	1.992600	164m	1	ŏ	3	64.7113	1,439310	m	-1	1	ã.	79,1707	1.208800	3	3	-3	2
5.4825	1.992600	m	1	2	1	64.9341	1.434910	12	0	3	2	79.6259	1.203030	2	2	-3	4
6.2195	1.962530	2	-1	-1	3	65.1283	1.431100	15	3	-1	2	79.9073	1.199500	9	-2	4	0
5.9243	1.934680	38	2	1	1	65.3721	1.426350	2	-2	-2	3	80.0685	1.197490	16	2	-4	2
7.1416	1.926270	245	-2	0	2	65.5049	1.423780	1	-3	0	2	80.2555	1.195170	4	-1	1	5
7.2454	1.922280	241 27	22	-1 0	2	65.9167 66.2146	1.415880 1.410230	34 20m	3 1	0 1	2 4	80.5688 80.8718	1.191310 1.187610	4 5	1	3	3 3
8.2818	1.883410	76m	õ	2	2	66.2146	1.410230	m	3	-2	1	81.3027	1.182400	16m	2	3	2
8.2818	1.883410	m	0	-2	3	66.4294	1.406190	10	-1	3	2	81.3027	1.182400	m	-3	3	ĩ
9.3415	1.845410	99	2	-2	1	67.0225	1.395180	3	-2	3	1	81.5667	1.179240	11m	2	-1	5
9.8139	1.829010	9	-2	-1	2	67.8079	1.380920	17	2	-1	4	81.5667	1.179240	m	4	0	0
0.7872	1.796220	57	-1	2	2	68.0930	1.375830	38	-3	1	2	81.8562	1.175800	6m	-1	-4	3
1.0098	1.788900	74m m	1-2	-2 1	32	68.2714 69.0494	1.372670 1.359090	22 9	-3	-1-3	2 1	81.8562 81.9738	1.175800 1.174410	m 5	1	1	0
2.1660	1.751940	44	0	3	õ	69,1214	1.357850	10	-2	õ	4	82,1327	1.172540	1	ó	-3	5
2.5860	1.738930	13	1	1	3	69,6838	1.348260	9m	2	0	4	82.3737	1,169720	5	-3	-2	3
3.0354	1.725250	46	1	-3	1	69.6838	1.348260	m	3	-2	2	82.8040	1.164730	20m	3	2	2
3.1520	1.721740	47	-2	2	1	69.9333	1.344060	10	2	3	0	82.8040	1.164730	m	4	-1	1
3.4174	1.713810	67	2	-2	2	70.0719	1.341740	47m	0	-3	4	83.0110	1.162350	5	-4	0	1
3.6961 3.9490	1.705570	118 118	1	23	0	70.0719	1.341740 1.331630	m 32m	2	-4	3	83.2034 83.2034	1.160150	11m m	3	0	4
1.0650	1.694800	129m	0	-3	2	70,6831	1.331630	m	-2	-3 2	3	83.4286	1.157590	5	-2	2	4
1.0650	1.694800	m	2	1	2	71,1186	1.324540	7	ĩ	-4	ĭ	83,5117	1.156650	6	-2 -2	0	5
1.7998	1.673800	166m	0	-1	4	71.2252	1.322820	6m	0	0	5	83.7255	1.154240	1	1	-3	5
1.7998	1.673800	m	2	2	0	71.2252	1.322820	m	2	-2	4	84.0714	1.150370	2m	2	0	5
5.9573	1.641890	80 4	12	-3	23	71.4768	1.318780 1.313950	7 19m	-2 0	-3 4	2 0	84.0714 84.5959	1.150370	m	2 0	-2	5 4
6.2582 6.9286	1.633820 1.616160	4 19m	õ	-1 3	1	71.7802 71.7802	1.313950	m	ŏ	4	2	84.5959	1.144570	52m m	-2	3	3
5.9286	1.616160	m	-1	-3	1	71,9637	1.311050	18	3	1	2	84,7264	1.143140	22m	3	-3	3
7.3907	1.604240	3	2	0	3	72,6090	1.300980	2	1	-1	5	84,7264	1.143140	m	-3	0	4
7.8879	1.591640	57m	1	3	0	72.8057	1.297950	4m	1	-4	2	85.3171	1.136730	3	-1	4	2
7.8879	1.591640	m	1	-1	4	72.8057	1.297950	m	3	-1	3	85.4800	1.134980	7	3	0	4
B.3695	1.579650	89m	-2	-1	3	73.0684	1.293930	14m	3	2 -2	0	85.6062	1.133630	5	1	43	4
8.3695 8.6681	1.579650 1.572320	m 29	-2	-2 0	2	73.0684 73.4140	1.293930	m 8m	-3 0	2	1	85.7262 85.7262	1.132350	7m m	-2	-5	4
8.9492	1.565490	37	-1	-1	4	73,4140	1.288690	m	-1	-1	5	85.8721	1.130800	6	3	-2	4
9.0553	1.562930	44	-1	0	4	73.8370	1.282350	11	-2	1	4	86.2302	1.127020	21	4	1	ō
9.3467	1.555950	40	1	0	4	74.0782	1.278770	3	2	3	1	86.5514	1.123660	5	Ó	-1	6
9.6644	1.548420	157m	-1	-3	2	74.3689	1.274490	10m	-1	0	5	86.8881	1.120170	4m	4	-1	2
9.6644	1.548420	m	-3	1	0	74.3689	1.274490	m	-2	3	2	86.8881	1.120170	m	-4	-1	1
9.8941 9.8941	1.543030 1.543030	56m m	0	2	3 4	74.8567 75.3284	1.267390	1 25m	-1	-32	4						

Status Alternate Empirical Formu ANX: ABX3 (Weight %:	C14.25 Mg28.8	the state of the second s	on-ambient) tomic %: C20 e: Magnesite	0.00 Mg20.00	ormula: Mg (CO3) O60.00
Radiation: CuKe	r 1 A: 1.5406	5Â d-Spac	ing: Calculate	d Intensity:	Calculated	I/Ic: 1.36	I/Ic - ND: 1.1
SYS: Rhombohe Author's Cell [A AuthCell MolVol Density [Dcalc: Femp: 293.0 K (uthCell a: 4.3 35.22] A 3.975 g/cm³	Author's Cell A Dstruc: 3.97	uthCell c: 12. Ixial Ratio [c/ 'g/cm³] S		AuthCell Vol: = 309.2(0.003		AuthCell Z: 6.00
Space Group: R Crystal Data [Xt KtlCell y: 120.00 Crystal Data Axi Reduced Cell [R RedCell ß: 64.2:	ICell a: 4.340 * XtlCell Vo al Ratio [c/a: tedCell a: 4.34	l: 211.31 ų 2.985 a/b: 0 Å RedCo	: 4.340 Å Z XtlCell Z: (2.985] RedCell c:	nandat i soor one ne	ll a: 90.00° edCell a: 64	XtiCeil β: 90.00°
Crystal (Symmel G Symmetry Ope		Centrosymmetr	ic				
eg Operator	<u>Sea Opera</u>	tor Sea	Operator	Seg Operat	or Sea	Operator	Seg Operator
x,y,z -x,-y,-z	3 -y,x-y, 4 yx+y	z 5 -z 6	-x+y,-x,z x-y,x,-z	7 -y,-x,z+ 8 y,x,-z+1	1/2 9 /2 10	x,x-y,z+1/2 -x,-x+y,-z+1/2	11 -x+y,y,z+1/2 12 x-y,-y,-z+1/2
tomic Coordinat	11C- 110		1999 -	319-11			
tom Num Wy				DP AET			
1 18e	2	0.2967 0.0	0.25 1.0				
1a 2 6b	-3.	0.0 0.0	0.0 1.0				
: 3 6a Subfile(s): Inorg .PF Prototype S	32 anic, Mineral Re tructure [Form tructure [Alpha	0.0 0.0 elated (Mineral ula Order]: C a Order]: C C	0.0 1.0 0.25 1.0 , Natural) F a (C O3),hR3 a O3,hR30,167	Pearson S	ymbol: hR10	.00	12-4916 (Alternate), √
2 3 6a Subfile(s): Inorg .PF Prototype S .PF Prototype S Cross-Ref PDF #	32 anic, Mineral R tructure (Form 01-080-010 04-012-491 's: 04-012-492 04-012-492 04-013-202	0.0 0.0 elated (Mineral ula Order]: C C a Order]: C C 11 (Alternate), 7 (Alternate), 6 (Alternate), 80 (Alternate),	0.0 1.0 0.25 1.0 , Natural) I a (C O3),hR3 a O3,hR30,167 01-063-1761 (A 04-012-4918 04-012-4923 04-013-2017	0,167 Pearson S Nternate), 01-08 (Alternate), - 0 (Alternate), - 0 (Alternate), - 0 (Alternate), - 0	ymbol: hR10 6-0175 (Alterr)4-012-4919 (/)4-012-4924 (/)4-013-2018 (/	.00 hate), √ 04-01 Viternate), √ 0 Viternate), √ 0 Primary), √ 04	12-4916 (Alternate), / 14-012-4920 (Alternate), 14-012-4925 (Alternate), 14-013-2019 (Alternate), 1-014-4846 (Alternate)
C 3 6a Subfile(s): Inorg LPF Prototype S LPF Prototype S Cross-Ref PDF # Entry Date: 09/(References:	32 anic, Mineral R/ tructure [Form tructure [Alpha 01-080-010 04-012-492 04-012-492 04-012-492 04-013-202 11/2009 Last	6.0 0.0 elated (Mineral ula Order]: C a Order]: C C 11 (Alternate), (7 (Alternate), 6 (Alternate), 90 (Alternate), 10 (Alternate), 10 (Alternate), 10 (Alternate), 10 (Alternate),	0.0 1.0 0.25 1.0 , Natural) F a (C O3),hR3 a O3,hR30,167 01-083-1761 (A 04-012-4918 04-012-4928 04-013-2017 / 04-013-2021	0,167 Pearson S Nternate), 01-08 (Alternate), - 0 (Alternate), - 0 (Alternate), - 0 (Alternate), - 0	ymbol: hR10 16-0175 (Alterr 14-012-4919 (/ 14-012-4924 (/ 14-013-2018 (/ 14-014-4830 (F	.00 hate), √ 04-01 Viternate), √ 0 Viternate), √ 0 Primary), √ 04	04-012-4925 (Alternate), 04-013-2019 (Alternate),
C 3 6a Subfile(s): Inorg LPF Prototype S Cross-Ref PDF # Entry Date: 09/C References: Type	32 anic, Mineral R/ tructure [Form tructure [Alpha 01-080-010 04-012-492 04-012-492 04-012-492 04-013-202 11/2009 Las	6.0 0.0 elated (Mineral ula Order]: C a Order]: C C 11 (Alternate), C 7 (Alternate), C 14 (Alternate), 16 (Alternate), 10 (Alt	0.0 1.0 0.25 1.0 Natural) I a (C O3),hR3 03,hR30,167 01-083-1761 (A 04-012-4918 04-012-4918 04-012-4918 04-013-2017 04-013-2021 Date: 09/01/2	0,167 Pearson S Nternate), 01-08 (Alternate), - 0 (Alternate), - 0 (Alternate), - 0 (Alternate), - 0	ymbol: hR10 16-0175 (Alterr 14-012-4919 (/ 14-012-4924 (/ 14-013-2018 (/ 14-014-4830 (F	.00 hate), √ 04-01 Viternate), √ 0 Viternate), √ 0 Primary), √ 04	04-012-4925 (Alternate), 04-013-2019 (Alternate),
C 3 6a Subfile(s): Inorg LPF Prototype S LPF Prototype S	32 anic, Mineral R tructure (Form tructure (Alpha 01-880-010 04-012-490 04-00	6.0 0.0 elated (Mineral ula Order]: C a Order]: C C 11 (Alternate), C 11 (Alternate), 11 (Alternate), 12 (Alternate), 10 (Alte	0.0 1.0 0.25 1.0 Natural) II a (C O3),hR3 a O3,hR30,167 01-083-1761 (A 04-012-4918 04-012-4918 04-013-2017 04-013-2021 Date: 09/01/2 POWD-12++ magnesite at ver	0,167 7 Pearson S (Alternate), 01-08 (Alternate), / 0 (Alternate), / 0 (Alternate), / 0 (Alternate), / 0 (Alternate), / 0	ymbol: hR10 6-0175 (Alterr 44-012-4919 (/ 44-012-4924 (/ 44-013-2018 (/ 44-013-2018 (/ 04-014-4830 (F odifications:	.00 hate), √ 04-01 Vternate), √ 0 Vternate), √ 0 Primary), √ 04 Reflections	04-012-4925 (Alternate), 04-013-2019 (Alternate),
C 3 6a Subfile(s): Inorg LPF Prototype S Cross-Ref PDF # Entry Date: 09/C References: Type Frimary Reference	32 anic, Mineral R tructure [Aph. 01-080-01 04-012-491 04-012-492 04-012-492 04-012-492 04-012-492 04-013-202 1//2009 Las DOI Referense Calculate "Structure M.Am. M ANX: AE transmiti anneale ents: Code: 11 focused Datacoli	0.0 0	0.0 1.0 0.25 1.0 . Natural) f a (C O3),hR3 a O3,hR30,167 11-083-1761 (4 04-013-2017 04-013-2017 04-013-2021 Date: 09/01/2 bate: 01/2 bate: 09/01/2 bate: 09/01/2 ba	0,167 Pearson S Utemate), 01-06 (Alternate), (Alternate), (Alternate), (Alternate), (Alternate), (Alternate), (Old Last M y high pressure* red samples we um was used a cowed to cool be acompound Pre pressure step. Compound Pre pre pressure step. Compound Pre p	ymbol: hR10 6-0175 (Altern 14-012-4919 (/ 14-012-4919 (/ 14-013-2018 (/ 14-013-2018 (/ 14-014-4830 (F odifications: Fiquet G., Guyol replaced in di s pressure cal efore diffraction effert diffraction: anne RUCIBLE: di Remarks: LP	.00 hate), < 04-01 kiternate), < 0 kiternate), < 0 Primary), < 04 Reflections F, Kunz M, M ibrant. At each in data was co n data was co n data was co n data was co F Editor Comr	94-012-4925 (Alternate), 14-013-2019 (Alternate), 1-014-4846 (Alternate)
2 3 6a Subfile(s): Inorg .PF Prototype S .PF Prototype S Cross-Ref PDF # Entry Date: 09/C References: Evice	32 anic, Mineral R tructure (App. 01-080-01 04-012-491 04-012-492 04-013-202 04-013-202 04-014 04-01	0.0 0	0.0 1.0 0.25 1.0 . Natural) F a (C O3),hR3 a O3,hR30,167 10.083.1761 (4 04-012-4918 04-012-4918 04-013-2017 04-013-2021 Date: 09/01/2 tes (2002). notice: Powde owdered platin th laser and all e Preparation: Powde evaluated erature: Temps int Cell Data SC ick, Fixed Sitt I	0,167 Pearson S Vitemate), 01-06 (Alternate), (Alternate), (Othernate), (Othernate),	ymbol: hR10 6-0175 (Altern 4-012-4919 (/ 4-012-4919 (/ 4-013-2018 (/ 4-013-2018 (/ 4-014-4830 (F odifications: Figuet G., Guyol rep placed in di s pressure cal fore diffraction garation: anne RUCIBLE: di Collection: 293 Diffraction.	.00 hate), < 04-01 klternate), < 0 klternate), < 0 Primary), < 04 Reflections F, Kunz M., M ismond anvil k brant. At each n data was co aled by local amond anvil p F Editor Coll K. Minor Wa	J4-012-4925 (Alternate), J4-013-2019 (Alternate), I-014-4846 (Alternate) I-014-4846 (Altern
2 3 6a Subfile(s): Inorg PF Prototype S PF Prototype S Cross-Ref PDF # Entry Date: 09/C References: Inve: Database Comm I-Spacings (48) - 18 (c) d (Å)	32 anic, Mineral R tructure (Form tructure (Alphi 01-080-010 04-012-491 94-012-492 04-012-492 04-012-492 04-013-202 11/2009 Lasi Calculate *Structure M. Am. X ANX: AE transmit anneale ents: Code: 11 focused Datacoli coordina reported	6.0 0.0 elated (Mineral ula Order]: C a Order]: C C if (Alternate), C if (Alter	0.0 1.0 0.25 1.0 . Natural) I a (C 03),hR3 a (C 03),hR3 (04-012-4918 (04-013-2017 Date: 09/01/2 Date: 09/01/2 pate: 09/01/2 pat	0,167 Pearson S Vitemate), 01-06 (Alternate), (Alternate), (Alternate),	ymbol: hR10 16-0175 (Alterr 16-0175 (Alterr 16-0175 (Alterr 14-012-4919 (/ 14-012-4924 (/ 14-013-2018 (/ 14-013-4919 (/	.00 nate), < 04-01 Viternate), < 0 Viternate), < 0 Primary), < 04 Reflections F., Kunz M., M isonant. At each n data was co isolad by local amond anvil p F Editor Comr K. Minor Wa d (Å)	Al-012-4925 (Alternate), 4-013-2019 (Alternate), 1-014-4846 (Alternate) I-014-4846 (Alternate) I-0
2 3 6a Subfile(s): Inorg PF Prototype S PF Prototype S Cross-Ref PDF # Entry Date: 09/(Type Primary Reference Vive Database Comm 1-Spacings (48) - 28 (*) 4 (Å) 77.4125 3 25088	32 anic, Mineral R tructure (Form tructure (Alphon 01-080-01 04-012-491 04-012-492 04-01	0.0 0	0.0 1.0 0.25 1.0 . Natural) I a (C 03),hR3 a (C 03),hR3 (04-012-4918 (04-013-2017 Date: 09/01/2 Date: 09/01/2 Date: 09/01/2 bate: 09/01/2 Date: 09/01/2 Dat	0,167 Pearson S Utemate), 01.067 (Alternate), (Alternate), (Alternate), (Alternate), (Alternate), (Alternate), (Alternate), (Old Last M y high pressure* red samples we um was used a cowed to cool be compound Pre pressure step. (Computer Signature of Data abuve compound Pre pressure step.) Compound Pre pressure step. (Computer Signature of Data abuve computer Pointern Original arature of Data intensity) - Cu K 1 h k 1 1 h k 1 	ymbol: hR10 16-0175 (Alterr 16-0175 (Alterr 16-0172 (Alterr 14-012-4919 (/ 14-012-4919 (/ 14-012-4919 (/ 14-012-4919 (/ 14-013-4919 (/ 14-013-4919 (/ 14-013-4919 (/ 14-013-4919 (/ 16-013-4919 (/	.00 nate), < 04-01 Viternate), < 0 Viternate), < 0 Viternate), < 0 Primary), < 04 Reflections F, Kunz M, M iamond anvil p F Editor Comm K. Minor Wa d (Å) 2 1.065020 5 1.085020	Al-012-24925 (Alternate), 4-013-2019 (Alternate), 1-014-4846 (Alternate) I-014-4846 (Alternate) I-
2 3 6a Subfile(s): Inorg Subfile(s): Inorg PF Prototype S S Cross-Ref PDF # Entry Date: Entry Date: 09/C Primary References: YPE Vac Sinucture Database Comm 1-Spacings (48) - 616 (*) d (A) 7.4125 3 25088 615666 2.45340 1.5819 2.17005	32 anic, Mineral R tructure (Form tructure (Alpm tr	0.0 0.0 elated (Mineral ula Order]: C 0 a Order]: C 0 a Order]: C 0 a Order]: C 0 a Order]: C 0 (Alternate), . 1 (Alternate), . 1 (Alternate), . 0 (at form LPF using the line . 0 (at form Caser ection, 60.2 GT, Samp days the line . 0 (at startard) . 0 67.43 (at startard) . 1 67.43 (b) 7.587 75.87 75.87	0.0 1.0 0.25 1.0 . Natural) I a (C 03),hR3 a (C 03),hR3 (04-012-49/18 (04-013-2017 Date: 09/01/2 Date: 09/01/2 Date: 09/01/2 bare: 09/01/2 Date: 09/01/2 Da	0,167 Pearson S Vitemate), 01-06 (Alternate), (Alternate), (Alternate),	ymbol: hR10 16-0175 (Alterr 16-0175 (A	.00 nate), < 04-01 Viternate), < 0 Viternate), < 0 Viternate), < 0 Primary), < 04 Reflections : F., Kunz M., M isamond anvil p brant. At each n data was co n data so n data	Al-012-24925 (Alternate), 44-013-2019 (Alternate), 4-013-2019 (Alternate), 4-013-2019 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4926 (Alternate), 4-014-4846 (Altern
2 3 6a Subfile(s): Inorg Subfile(s): Inorg PF Prototype S S Cross-Ref PDF # Entry Date: Entry Date: 09/C Prototype S S Cross-Ref PDF # S Entry Date: 09/C Primary References: Yme Database Comm S Database Comm S ISS96 2.4540 115819 2.17005 6.8146 1.9386 0.5263 1.80488	32 anic, Mineral R tructure (Form tructure (Alpm tr	0.0 0.0 elated (Mineral ula Order]: C 0 a Order]: C 0 a Order]: C 0 a Order]: C 0 a Order]: C 0 (Alternate), . 7 (Alternate), . 1 (Alternate), . 0 (Alternate), . 0 <td< td=""><td>0.0 1.0 0.25 1.0 . Natural) I a (C 03),hR3 a (C 03),hR3 (04-012.4921 (04-013.2021 Date: 09/01/2 Date: 09/01/2 Date: 09/01/2 powdered platin th laser and all e Preparation. Powdered platin th laser and all e Preparation. Powdered platin th laser and all e Preparation. Eacludated (A () 25 14/2160 3 1387640 3 1387660 3 1387660 3 1387660 3 1387660 3 138760 3 1387660 3</td><td>0,167 Pearson S Vitemate), 01-06 (Alternate), (Alternate), (Alternate),</td><td>ymbol: hR10 16-0175 (Alterr 16-0175 (A</td><td>.00 nate), < 04-01 Viternate), < 0 Viternate), < 0 Viternate), < 0 Primary), < 04 Reflections F., Kunz M., M iamond anvil p F.Editor Comm K. Minor Wa d (Å) 2 1.085020 5 1.075890 5 1.065520 5 1.075890 5 1.075890 5 1.075890 5 1.065520 5 1.075890 5 1.075800 5 1.07</td><td>Al-012-24925 (Alternate), 44-013-2019 (Alternate), 4-013-2019 (Alternate), 4-013-2019 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4926 (Alternate), 4-014-4846 (Altern</td></td<>	0.0 1.0 0.25 1.0 . Natural) I a (C 03),hR3 a (C 03),hR3 (04-012.4921 (04-013.2021 Date: 09/01/2 Date: 09/01/2 Date: 09/01/2 powdered platin th laser and all e Preparation. Powdered platin th laser and all e Preparation. Powdered platin th laser and all e Preparation. Eacludated (A () 25 14/2160 3 1387640 3 1387660 3 1387660 3 1387660 3 1387660 3 138760 3 1387660 3	0,167 Pearson S Vitemate), 01-06 (Alternate), (Alternate), (Alternate),	ymbol: hR10 16-0175 (Alterr 16-0175 (A	.00 nate), < 04-01 Viternate), < 0 Viternate), < 0 Viternate), < 0 Primary), < 04 Reflections F., Kunz M., M iamond anvil p F.Editor Comm K. Minor Wa d (Å) 2 1.085020 5 1.075890 5 1.065520 5 1.075890 5 1.075890 5 1.075890 5 1.065520 5 1.075890 5 1.075800 5 1.07	Al-012-24925 (Alternate), 44-013-2019 (Alternate), 4-013-2019 (Alternate), 4-013-2019 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4846 (Alternate), 4-014-4926 (Alternate), 4-014-4846 (Altern
3 6a Bubfile(s): Inorg Bubfile(s): Inorg PF Prototype S S Cross-Ref PDF # Entry Date: Entry Date: 09// teferences: ypc trimary Reference Structure Database Comm	32 anic, Mineral R tructure (Form tructure (Alph- 01-080-01 04-012-491 04-012-492 04-012-492 04-013-202 04-013-202 11/2009 Las DOI Referense Calculate "Structure "Structure "Structure "Man. M ANX: AE transmiti anneale cordina cordina cordina Calculate "Structure "Mag(C O3) - 04 1 h k 0 999 1 0 1 H k 1 0 150 67 1 1 0 151 2 0 0 76 0 2	0.0 0.0 elated (Mineral ula Order]: C 0 a Order]: C 0 a Order]: C 1 a Order]: C 0 a Order]: C 0 a Order]: C 0 (Alternate), 11 (Alternate), 12 (Alternate), 00 (Alter	0.0 1.0 0.25 1.0 . Natural) F a (C O3),hR3 a (C O3),hR3 (O4-013-2017 (O4-013-2017 (O4-013-2017 (O4-013-2021 Date: 09/01/2 Date: 1.256 Comparison: 1.25680 Comparison: 1.25680 Compariso	0,167 Pearson S Uternate), 01-06 (Alternate), / (Alternate), / (Alternate), / (Alternate), / (Alternate), / (Old Last M y high pressure* red samples we um was used a lowed to cool be compound Pre pressure step. (Compound Pre pressure step.) Computer Original rature of Data uurce: Powder E I h k I I h k I 1 60 1 2 2 1 1 50 3 0 0 1 3 1 2 5	ymbol: hR10 16-0175 (Alterr 16-0175 (A	00 hate), < 04-01 Viternate), < 0 Viternate), < 0 Primary), < 04 Reflections F., Kunz M., M iamond anvil 1 birant. At eacl amond anvil 2 ibrant. At eacl to 6 1.08630 5 1.078480 5 1.06580 1.06580 1.06580 1.06580 1.06580 1.06580 1.06580 1.052310 1.055	J4-012-24925 (Alternate), J4-013-2019 (Alternate), I-014-4846 (Alternate), I-014-4846 (Alternate), I-014-4846 (Alternate), Iatas J., Andrault D., Hanflau without pressure h pressure samples were llected. LPF Collection K ressure cell. Pressure collectorion k rement: editor took fixed rming: No R factors 1 h 1 0 3 0 30 0 30 0 31 2 32 1 34 0 14 0

 Status
 Primary
 QM: Star
 Pressure/Temperature:
 Ambient
 Chemical Formula:
 Ca (OH)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 Ceil [AuthCell a: 3.5899(4) Å AuthCell c: 4.916(3) Å AuthCell Vol: 54.87 Å³ AuthCell MolVol: 54.87] Author's Cell Axial Ratio [c/a: 1.369] Density [Dcalc: 2.242 g/ SS/FOM: F(25) = 51.7(0.0167, 29) Temp: 298.0 K (Ambient temperature assigned by ICDD editor) AuthCell Z: 1.00 Density [Dcalc: 2.242 g/cm³] Color: White Space Group: P-3m1 (164) Molecular Weight: 74.09
 Space Glob, 1 = 0.001, 1001, 1001, 1001, 14:05
 Vergetal Data [XtiCell a: 3.590 Å
 XtiCell b: 3.590 Å
 XtiCell c: 4.916 Å
 XtiCell a: 90.00°
 XtiCell y: 120.00°
 XtiCell Vei; 54.87 ų
 XtiCell 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 a: 90.00°

 RedCell β: 90.00°
 RedCell y: 120.00°
 RedCell Vol: 54.87 ų]
 RedCell y: 120.00°
 RedCell Vol: 54.87 ų]
 XtiCell c: 4.916 Å XtiCell α: 90.00° XtiCell β: 90.00° Atomic parameters are cross-referenced from PDF entry 04-006-9147 ADP: U Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: <u>Seg Operator Seg Operator Seg Operator Seg Operator Seg Operator</u> Seg Operator 12 X,Y,Z -X,-Y,-Z 34 -y,x-y,z y,-x+y,-z 5 -X+y,-X,Z X-y,X,-Z 78 -y,-x,z y,x,-z 9 x,x-y,z 10 -x,-x+y,-z 11 -x+y,y,z 12 x-y,-y,-z Atomic Coordinates: Atom Num Wyckoff Symmetry x SOF Uiso AET -3m. 3m. 3m. Ca O H 0.0 0.0 0.0 1.0 0.33333 0.66666 0.234 1.0 0.33333 0.66666 0.4256 1.0 0.01194 0.01203 0.04203 1a 2d 2d 22 Anisotropic Displacement Parameters: Uani11 Uani22 Uani33 Uani12 Uani13 Uani23 Atom Num 0.0083 0.0106 0.0528 0.0193 0.0149 0.0205 0.0042 0.0053 0.0264 Ca O H 0.0083 0.0 0.0 0.0 0.0 0.0528 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 ✓ 04-006-9147 (Alternate), ✓ 04-006-9148 (Alternate), ✓ 04-006-9149 (Alternate), ✓ 04-006-9150 (Alternate),
 Cross-Ref PDF #s: ✓ 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: DOI Reference Type Primary Reference Crystal Structure Optical Data Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA. ICDD Grant-In-Aid (1992). Crystal Structure Source: LPF. 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: Downter Difference
 Powder Diffraction. d-Spacings (28) - Ca (O H)2 - 00-044-1481 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å 28 (°) d (Â) <u>h k l *</u> 28 (°) d (Å) I hkl 28 (°) d (Å) 72 27 100 4.922000 3.111000 2.627000 2.458000 1.927100 1.795400 1.686400 0 1 0 0 0 1 0 2 0 2 1 0 1 1 56.0907 59.4244 62.6319 64.2314 64.2314 71.8086 77.6520 1.638300 1.554100 1.482000 1.448900 1.448900 1.313500 1.228600 1.209800 1.175200 1.142900 1.142900 1.142900 1.127400 1.060100 18.0073 0000100 79.0924 2 2 5m 2 3 2 0110111 0221120 3013224 1212223 1101010 3041 28.6709 34.1013 36.5257 47.1200 50.8120 3 9 7m 81.9069 84.7484 84.7484 1 30 31 14 m 6 1 86.1940 93.2060 320 54.3565 96.0263 1.036300 © 2020 International Centre for Diffraction Data. All rights reserved. Page 1/2

Status Primary QM: Indexed Pressure/Temperature: Ambient Chemical Formula: Fe21 031 (0H) Weight %: Fe69.57 H0.06 O30.37 Empirical Formula: Fe21 H O32 Atomic %: Fe38.89 H1.85 O59.26 ANX: A21X32 Compound Name: Iron Oxide Hydroxide Mineral Name: Maghemite, syn d-Spacing: Calculated Radiation: CuKa1 A: 1,5406 Å 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 ų
 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° XtiCell y: 90.00° XtiCell 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 a: 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 Seg Operator Seg Operator Seg Operator X,Y,Z Z,X,Y Y,Z,X X,Z,Y 9 10 11 12 y,-z,-x x,-z,-y y,-x,-z z,-y,-x 13 14 15 16 -X,Y,-Z -Z,X,-Y -Y,Z,-X -X,Z,-Y -y,x,-z -z,y,-x -x,-y,z -z,-x,y 21 22 23 24 -y,-Z,X -x,-Z,y -y,-X,Z -Z,-y,X y,x,z z,y,x 17 18 19 20 5 6 X,-Y,-Z Z,-X,-Y Я 7 ă 8 **Atomic Coordinates:** Atom Num Wyckoff Symmetry x SOF IDP AET 0.125 0.125 0.375 1.0 1.0 1.0 1.0 0 4-a m .m -42.m 6-a 4-a 2 12 0.125 0.125 0.625 Fe Fe H O Fe Fe O 3c 4e 4e 12i 3 0.0 0.5 0.5 .3m .3m 0.25 0.25 0.25 4-a 0.625 0.375 -0.125 0.25 0.625 0.625 3#a .m .3m -0.125 1.0 1.0 6 7 0.375 -0.125 4-a 4e 1b 89 -43m -43m 0.5 0.5 0.5 1.0 4-a 0.0 1a 4-a 0.375 10 4e .3m 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 032,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:

Туре	DOI	Reference
Primary Reference Structure		Calculated from LPF using POWD-12++. "Ein Fehistellenuberstruktur-Modell fur y-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.

20 (°)	d (Å)	I	h	k	1 *	20 (°)	d (Å)	I	h	k	1	*	20 (º)	d (Å)	I	h	k	1	*
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	23	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	
© 2020	Internatio	onal	Cer	ntre	for	Diffraction	Data, All	riaht	s re	ese	rve	d.				- 25		P	age 1

04-009		10	121	141	041-040	147212121	100000	20		1411	1021-2355			12:		M	(fal-sharji2
20 (°)	d (Å)	I	h	k	1 *	20 (°)	d (Å)	I	h	ĸ	*	20 (°)	d (Å)	I	h	k	*
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	8 6	25	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		4	1	137.3935	0.826773	1	7	7	2
92.1894	1.069110	1	6	5	0	113.3049	0.922103	1	8	4	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	<u>.</u>	9	5	0
96.1013	1.035690	7	6		2	116.5310	0.905685	1	8		0	145.1968	0.807225	36	9	5	1
97.0835	1.027810	5	7	5 4	1	117.6262	0.900404	3	7	26	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

5 32e .3m

Jun 23, 2020 12:43 PM (fal-sharji2)

z,y,x

z, y, x -z, -y, -x z, -y+1/4, -x+1/4 -z, y+3/4, x+3/4 -z+1/4, y, -x+1/4 z+3/4, -y, x+3/4 -z+1/4, -y+1/4, x z+3/4, y+3/4, -x

QM: Star Pressure/Temperature: Temperature (Non-ambient) Chemical Formula: Mg Fe2 04 Status Alternate 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: Ed-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 a:
 90.00°
 XtlCell β:
 90.00°
 XtiCell y: 90.00° XtiCell Vol: 592.08 Å3 XtiCell 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 a: 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 Seg Operator Seg Operator Seq Operator Operator -y+1/4,z,x+1/4 y+3/4,-z,x+3/4 -y+1/4,-z+1/4,x y+3/4,z+3/4,-x x,z,y x,-z+1/4,-y+1/4 -x,z+3/4,y+3/4 -x+1/4,z,y+3/4 x+3/4,-z,y+3/4 z,-x+1/4,-y+1/4 -z,x+3/4,y+3/4 -z+1/4,x,-y+1/4 z+3/4,-x,y+3/4 -z+1/4,-x+1/4,y z+3/4,x+3/4,-y -x+1/4,-z+1/4,y x+3/4,z+3/4,-y 41 42 43 44 45 46 47 48 11 12 13 14 15 16 17 18 19 20 31 32 33 34 35 36 37 38 39 40 x,y,z 21 22 23 24 25 26 27 28 29 30 x,y,z -x,-y,-Z x,-y+1/4,-z+1/4 -x+1/4,y,-z+1/4 -x+1/4,y,-z+3/4 -x+1/4,y-z+3/4 -x+1/4,-y+1/4,z x+3/4,y+3/4,-z z,x,y -z,-x,-y x+3/4,z+3/4,-y y,xz -y,-x,-z y,-x+1/4,-z+1/4 -y+1/4,z+1/4 -y+1/4,x,-z+1/4 y+3/4,-x,2+3/4 -y+1/4,-x+1/4,z y+3/4,x+3/4,-z 3 6 y,z,x -y,-z,-x y,-z+1/4,-x+1/4 -y,z+3/4,x+3/4 8 9 10 Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Uiso AET 8a 8a 16d 16d 0.125 0.125 0.5 0.5 0.125 0.125 0.5 0.5 0.125 0.125 0.5 0.5 0.841 0.159 0.579 0.0011 0.0011 0.0022 0.0022 -43m -43m .-3m .-3m Fe Mg Fe Mg O 12 34 0.421

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

0.0052

LPF Prototype Structure [Alpha Order]: Al2 Mg 04,cF56,227 Pearson Symbol: cF56.00

0.2548 0.2548 0.2548 1.0

04-012-0908	Jun 23, 2020 12:43 PM (fal-sharji	
	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 (Alternat	
	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), 01-089-6189 (Alternate), 001-7928 (Alternate), <001-7928 (Alternate), <001-928 (Altern	
	01-089-6188 (Alternate), 01-089-6189 (Alternate), 7 04-001-7921 (Alternate), 7 04-001-9288 (Alternate)	
	04-002-0587 (Alternate), < 04-002-0619 (Alternate), < 04-002-2458 (Alternate), < 04-002-2459 (Alternate),	
	U4-002-3054 (Alternate), ✓ 04-002-3768 (Alternate), ✓ 04-002-3769 (Alternate), ✓ 04-002-5223 (Alternate),	
	04-002-5328 (Alternate), V 04-002-5461 (Alternate), V 04-002-5666 (Alternate), V 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), V 04-006-4005 (Alternate), V 04-006-6673 (Alternate), V 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).	
	04-011-9002 (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), < 04-012-0910 (Alternate), < 04-012-0912 (Alternate), < 04-012-0919 (Alternate), < 04-012-0910 (Alternate),	
	04-012-0910 (Alternate), < 04-012-0910 (Alternate), < 04-012-0917 (Alternate), < 04-012-0910 (Alternat	
	04-012-0912 (Alternate), √ 04-012-0920 (Alternate), √ 04-012-0925 (Alternate), √ 04-012-0926 (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),	
Cross-Ref PDF #'s	. 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 (Alternat	
	04-012-0947 (Alternate), < 04-012-0948 (Alternate), < 04-012-0949 (Alternate), < 04-012-0950 (Alternate), 04-012-0951 (Alternate), < 04-012-0950 (Alternate), < 04-012-1051 (Alternate), < 04-012-1052 (Alternate	
	04-012-0951 (Alternate), < 04-012-1050 (Alternate), < 04-012-1051 (Alternate), < 04-012-1052 (Alternate), 04-012-1053 (Alternate), < 04-012-1056 (Alternate), < 04-012-1055 (Alternate), < 04-012-1056 (Alternate), 04-012-1057 (Alternate), < 04-012-1058 (Alternate), < 04-012-1059 (Alternate), < 04-012-1050 (Alternate)	
	04-012-1057 (Alternate), v 04-012-1058 (Alternate), v 04-012-1059 (Alternate), v 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 (Alternat	
	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)	
	04-012-1081 (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),	
	04-014-3/07 (Alternate), / 04-014-3/08 (Alternate), / 04-014-3/09 (Alternate), / 04-014-3/10 (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), < 04-014-3710 (Alternate), < 04-014-3717 (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)	
	04-014-3/27 (Alternate) / 04-014-3/28 (Alternate) / 04-014-3/29 (Alternate) / 04-014-3/30 (Alternate)	
	04-014-3731 (Alternate), v 04-014-3732 (Alternate), v 04-014-3733 (Alternate), v 04-014-3734 (Alternate), 04-015-7027 (Alternate)	
Entry Date: 09/01/		
andy bate. 03/01/		
lype D	ODI Reference	
lype D	Calculated from LPF using POWD-12++.	
Ype D Primary Reference	Calculated from LPF using POWD-12++.	
References: Type D Primary Reference Structure	Calculated from LPF using POWD-12++. "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).	
ype D rimary Reference Structure	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 160110 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173	
ype D rimary Reference Structure	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 160110 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 for 10 d, quenched in air. CRUCIBLE: sealed evacuated silica tube lined with silver foil. Temperature of	
ype D rimary Reference itructure	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 160110 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173	
ype D rimary Reference tructure Database Commer	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 160110 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 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.	
ype <u>D</u> trimary Reference itructure Database Commer -Spacings (34) - M	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 1601101 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 for 10 d, quenched in air. CRUCIBLE: sealed evacuated silica tube lined with silver foil. Temperature of	
rype <u>D</u> Primary Reference Sitructure Database Commer I-Spacings (34) - M. 88 (°) d (Å)	Calculated from LPF using POWD-12++. "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). 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 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. g Fe2 04 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å I h k 1 h k * 20 (°) d (Å) I h k *	
type D Primary Reference Structure Database Commer	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 1601100 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 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. g Fe2 04 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å I h k i 34 1 1 73.9587 1280540 79 5 3 346 2 0 74.9599 12805900 19 5 1 1 9 1	
Type D Primary Reference Structure Database Commer	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 1601100 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 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. g Fe2 04 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å I h k i 34 1 1 73.9587 1280540 79 5 3 346 2 0 74.9599 12805900 19 5 1 1 9 1	
Type D Primary Reference Structure Database Commer	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 1601100 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 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. g Fe2 04 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å I h k l * 20 (°) d(Å) I h k l * 34 1 1 1 7 39587 1.280540 79 5 3 3 110.2654 0.938818 25 8 4 0 3 1 1 7 2 2 2 21 2 12010 23 4 4 4 111.8525 1.17820 2	
Type D Primary Reference Structure Structure Structure Database Commer A Ref (*) d (Å) R8 (*) d (Å) R0 (*) d (Å) R0 (*) d (Å) R0 (*) 2.968800 10 0759 2.968800 10 759 2.968800 10 752 2.968100 17.0562 2.424020 13.0527 2.099260 13.0527 2.19926410	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 1601100 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 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. g Fe2 04 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å 1 h <th colspan<="" td=""></th>	
Type D Primary Reference Structure Structure	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 1601100 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 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. g Fe2 04 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å 1 h <th colspan<="" td=""></th>	
Type D Primary Reference Structure Structure Structure Database Commer Ref (*) 4:Spacings (34) - M M 8:264 4 484030 0.0759 2.968800 10:759 2.968800 2.531800 17:0562 2.424020 13.0527 2.098260 13:0527 2.098260 13.26410 13:4097 1.714040 16.60210	Calculated from LPF using POWD-12++. "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). 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 i 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. g Fe2 04 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å 1 h h h h h h h k h k h k h k h k h k <th< td=""></th<>	
Type D Primary Reference Structure Structure Structure Database Commer Structure I-Spacings (34) - M. (Å) 8.2844 4.848030 0.0759 2.968800 15.4251 2.531800 13.0577 2.099260 13.0527 2.099260 13.34097 1.714040 26.3434 1.616010 2.5192 1.844400	Calculated from LPF using POWD-12++. "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). 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 i 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. gFe2 04 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Â 1 h k l * 20 (°) d (Â) I h k l * 24 (°) d (Â) I h k l * 20 (°) d (Â) I h k l * 34 1 1 1 7.35687 1.280540 79 5 3 3 110.2654 0.398818 25 8 4 0 34 1 1 1 7.39587 1.280540 79 5 3 3 110.2654 0.398818 25 8 4 0 34 1 1 1 7.39587 1.280540 79 5 3 3 110.2654 0.398818 25 8 4 0 99 3 1 7.89587 1.280540 79 5 3 3 110.2654 0.398818 25 8 4 0 1 91 7.89587 1.280540 79 5 3 3 110.2654	
Type D Primary Reference Structure Structure Structure Database Commer (A) - M. (B) (2) (2) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3	Calculated from LPF using POWD-12++. "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). ANX: A3X4. Color: brown. In Situ Condition: In quartz capillary open to air. LPF Collection Code: 160/1106 Sample Preparation: Compound Preparation: mixed, ground under ethanol for 2 h, dried, heated at 1173 i 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. g Fe2 04 - 04-012-0908 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å 1 h h h h h h h k h k h k h k h k h k k k k k k k Colspan="2">k k k k k k k k k k k k k <th col<="" td=""></th>	

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 2/2

Status Alternate	QM: Star Pressure/Temperature: Temperature (Non-ambient) Chemical Formula: Fe3 04
Empirical Formula	
Compound Name:	
Radiation: CuKa1	A: 1.5406 Å d-Spacing: Calculated Intensity: Calculated I/Ic: 4.61 I/Ic - ND: 1.16
Author's Cell [Aut Density [Dcalc: 5	SR: Fd-3m (227) Cell a: 8,4814(5)Å AuthCell Vol: 610.10Å ² AuthCell Z: 8.00 AuthCell MolVol: 76.26] 041 g/cm ² Datrue: 5.04 g/cm ²] SS/FOM: F(30) = 999.9(0.0001, 30) thor provided temperature) R-factor: 0.0219
Space Group: Fd- Crystal Data [XtlC KtlCell γ: 90.00° Crystal Data Axial Reduced Cell [Rec RedCell β: 60.00°	ell a: 8.481 Å XtiCell b: 8.481 Å XtiCell c: 8.481 Å XtiCell α: 90.00° XtiCell β: 90.00° XtiCell Vol: 610.10 Å? XtiCell Z: 8.00] Ratio [a/b: 1.000 c/b: 1.000]
Crystal (Symmetry	Allowed): Centrosymmetric
Pearson Symbol: Cross-Ref PDF #'s	00-001-1111 (Dolsted), 00-002-0125 (Deleted), 00-003-0862 (Doleted), 00-007-0322 (Deleted), 00-011-0652 (Deleted), 01-0752 (Deleted

Entry Date: 09/01/2013

	1.00			
Re	fei	ren	ce	s:

Туре	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).

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1/2

and the second second second													e: Fe3 O4.							
Databas	e Commer	nts:	Sam Nvc	koff	So	aue	or Locality nce: e d a (-D3-MZ), I	Unit (area Cell [i, ivi Data	Sou	taly.	Powder D	iffraction.	a Co	lecti	on:	97.	3 K.
			2			2	5	10												
d-Spacin	gs (34) - Fe	3 04	- 01	L-08	0-6	409	(Stick, Fixe	d Slit Inter	usity)	- Ci	ı Ka	1 1.5	405	6 Å						
28 (°)	d (Å)	I	h	k			20 (°)	d (Å)	I	h	k	1.1		20 (°)	d (Å)	I	h	k	L	
18.1010	4.896740	104	1	1	1	- 15	73,1032	1,293400	54	5	3	3	-	108.6461	0.948249	12	8	4	0	-
29,7697	2,998630	300	2	ż	0		74.0884	1.278620	22	564567	2	2		111.6669	0.930955	1		1	1	
35.0612	2.557240	999	3	1	1		77.9854	1.224180	16	4	4	4		112.6876	0.925397	1	986989	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		3	1		125.7088	0.865629	41	8	46040	4	
52.8370	1.731260	80	4	- 2	2		93.1980	1.060170	24	8	8	0		129 2832	0.852413	1	9	3	3	
56.3171	1.632250	257	5	- 52	1		96.0423	1.036170	1	1	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 70.1145	1.413570	1	4	- 2	2		103.7236	0.979348	32		074549004756	3								
	1.341030	23	0	- : Z :	- U		104 6987	0.972883	0	6	- 6	4								

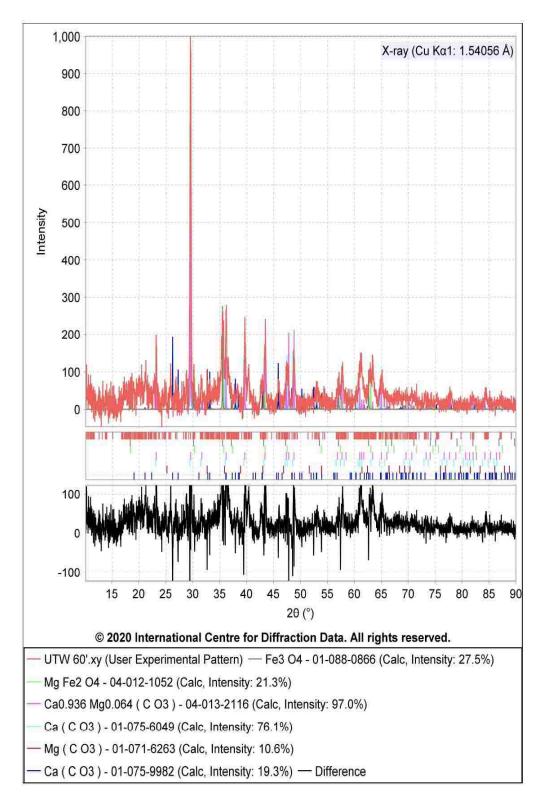


Figure E.3 XRD patterns of substances precipitated from Untreated Water (UTW) tank at 60 °C from experiment with a tank with little exposure of iron.

SIeve+ Report

Experiment

Search Line: 2	.080316 Å	D1 Range:	2.073 Å - 2.087 Å
Search Line: 1	5 14557 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	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 <mark>Å</mark> - 1.471 Å
Rotation: All 8	Rotations		

Preferences

Radiation: X-ray Wa	velength: Cu Kal 1.54056 Å	Search Method: Hanawalt
Search Window: 0.15°	Match Window: 0.15°	2nd Pass Filter: Yes
d-Spacings: Weighted	Lowest Allowable GOM: 2	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

Status Alternate Empirical Formula: Compound Name: 1	Fe3 O4 Weight	%: Fe72	perature: Aml 2.36 O27.64 Magnetite	Atom	Chemical Form ic %: Fe42.86 O non Name: iron	57.14	ANX: AB2X4
Radiation: CuKa1	λ: 1.5406 Å d	-Spacing	: Calculated	Inte	nsity: Calculated	1/10	c: 4.93 I/Ic - ND: 1.5
SYS: Cubic SPG Author's Cell [Author Density [Dcalc: 5.2 Temp: 298.0 K (Amt	18 g/cm ³ Dstruc	: 5.22 g/	cm ³] SS/I	FOM:	AuthCell Z: F(30) = 999.9(0.0 actor: 0.033		AuthCell MolVol: 73.68] 0)
Crystal Data [XtlCel XtlCell γ: 90.00° Crystal Data Axial R Reduced Cell [RedC RedCell β: 60.00° Atomic parameters a Crystal (Symmetry A	XtlCell Vol: 589.47 atio [a/b: 1.000 Cell a: 5.929 Å RedCell γ: 60.00 are cross-reference	7Å3 X c/b: 1.1 RedCell ° Red ed from I	tlCell Z: 8.00 000] 5: 5.929 Å Cell Vol: 147.] RedC 37 Å ³]	ell c: 5.929 Å	RedC	90.00° XtlCell β: 90.00° ell α: 60.00° gin: O2
SG Symmetry Operato							
Seq Operator 1 x,y,z 2 -x,-y,-z 3 x,-y+1/4,-z+1/4 4 -x,y+3/4,z+3/4 5 -x+1/4,y,-z+1/4 6 x+3/4,-y,-z+3/4 7 -x+1/4,-y+1/4, z+1/4 8 x+3/4,-y+3/4,-z 9 z,x,y 10 -z,-x,-y Atomic Coordinates:	$\begin{array}{c c} \underline{Seq} & \underline{Operator} \\ 11 & z_{-}x+1/4, -y+1/4 \\ 12 & -z_{-}x+3/4, y+3/4 \\ 13 & -z+1/4, x_{-}y+3/4 \\ 14 & z+3/4, -x, y+3/4 \\ 15 & -z+1/4, -x+1/4, \\ 16 & z+3/4, x+3/4, -y \\ 17 & y_{-}z_{-}x \\ 18 & -y_{-}z_{-}x \\ 19 & y_{-}z-1/4, -x+1/4 \\ 20 & -y_{-}z+3/4, x+3/4 \end{array}$	4 21 22 4 23 24 7 25 26 27 28 4 29	Operator -y+1/4,z,x+1/4 y+3/4,-z,x+3/4 -y+1/4,-z,+1/4,x y+3/4,z+3/4,-x x,z,y x,-z+1/4,-y+1/4 -x,z+3/4,y+3/4 -x+1/4,z,y+3/4	Sec 31 32 33 34 35 36 37 38 39 40	$\begin{array}{c} \textbf{Operator} \\ -x+1/4,-z+1/4,y \\ x+3/4,z+3/4,-y \\ y,x+2/4,z+3/4,-y \\ y,-x+1/4,-z+1/4 \\ -y,-x+3/4,-z+3/4 \\ -y+1/4,-x,z+1/4 \\ y+3/4,-x,z+3/4 \\ -y+1/4,-x+1/4,z \\ y+3/4,x+3/4,-z \end{array}$	Seq 41 42 43 44 45 46 47 48	$\begin{array}{c} \hline \textbf{Operator} \\ z.y.x \\ zy-X \\ z.y+3/4, x+3/4 \\ -z.y+3/4, x+3/4 \\ -z+1/4, yx+1/4 \\ z+3/4, -y.x+3/4 \\ -z+1/4, -y+1/4, x \\ z+3/4, y+3/4, -x \end{array}$
Atom Num Wyckof	f Symmetry x	V	z SOF	Biso	AET		
Fe 1 16d Fe 2 8a O 3 32e	3m 0.5 -43m 0.125 .3m 0.254		0.5 1.0 0.125 1.0	0.47 0.37 0.64	6-a 4-a 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-sharii2
01-000-0000	
	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), <
0	04-006-0425 (Alternate), < 04-006-1668 (Alternate), < 04-006-2406 (Alternate), < 04-006-2467 (Alternate), <
Cross-Ref PDF #'s:	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 (Alternat
	04-015-8211 (Alternate), < 04-015-8213 (Alternate), < 04-015-8214 (Alternate), < 04-017-1024 (Alternate)
	vervio-ozi i (niteinate), « vervio-ozi i (niteinate), « 04-010-0z14 (niteinate), « 04-017-10z4 (niteinate)

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

Rei	erences:

Туре	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: Database Comments: ANX: AB2X4. Analysis: Fe3 04. Formula from original source: Fe3 04. 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.

20 (°)	d (Å)	I	h	k		*	20 (°)	d (Å)	1	h	ĸ		*	20 (°)	d (Å)	I	h	k	1	3
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	5	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	
7.2115	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	
2.6216	1.482220	368	4	4	0		98,4992	1.016790	1	6	4	4		143,7141	0.810580	50	9	5	1	
55.8438	1.417270	8	5	3	1		102.4334	0.988146	14	8	2	2		145.3818	0.806818	7	10	2	2	
36.8993	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								

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 2/2

	us Alternate	QM: S	tar Pressure	e/Tem	perature: F	Pressure &	Temperature (N	Ion-am	bient)
	mical Formula:								Mg12.15 O32.00
	mic %: Fe28.57						ame: Magnesiu		
Min	eral Name: Mag	gnesiofe	errite, Syn				1900-1900 - 19 7 9		
		-							
Rad	iation: CuKa1	λ: 1.	.5406 Å d-S	pacing	: Calculate	d Inten	sity: Calculated	d M	c: 4.06 I/Ic - ND: 1.5
SYS	: Cubic SPG	R: Fd-	-3m (227)						
Aut	hor's Cell [Auth	Cell a:	8.33588(8) Å	Aut	hCell Vol:	579.23 Å ³	AuthCell Z:	8.00	AuthCell MolVol: 72.40]
	sity [Dcalc: 4.						(30) = 999.9(0.0)	0001, 3	0)
Ten	np: 885.0 K (Aut	hor prov	vided temperatu	ıre)	R-factor: (0.082 C	olor: Brown		
	a ava								
	ce Group: Fd-3						orrestore 0 - 22/24		
	stal Data [XtlCe				3.336 Å 🛛 🕽		8.336 Å Xtl	Cell a:	90.00° XtiCell β: 90.00°
	ell γ: 90.00°		l Vol: 579.23 Å		tlCell Z: 8.	.00]			
Cry	stal Data Axial F	Ratio [a	a/b: 1.000 c	/b: 1.0	000]				
Red	uced Cell [Red	Cell a:	5 804 Å Re	dCell	h: 5 804 Å	RedCe	I c: 5 894 Å	RedC	ell a: 60.00°
	uced Cell [Red				b: 5.894 Å		ll c: 5.894 Å	RedC	cell α: 60.00°
	luced Cell [Red Cell β: 60.00°						ll c: 5.894 Å	RedC	:ell α: 60.00°
Red	Cell β: 60.00°	RedC	Cell γ: 60.00°	Red	Cell Vol: 14	44.81 ų]		RedC	:ell α: 60.00°
Red ADF		RedC		Red	Cell Vol: 14	44.81 ų]		RedC	:ell α: 60.00°
Red ADF SG S	Cell β: 60.00° P: U Origin:	RedC O2 ors:	Cell γ: 60.00°	Red	Cell Vol: 14	44.81 Å ³] entrosymn			ell α: 60.00°
Red ADF SG S Seq 1	Cell β: 60.00° P: U Origin: Symmetry Operato Operator x,y,z	O2 ors: <u>Seq</u> 11	Crystal (Symm Operator z,-x+1/4,-y+1/4	Red netry A <u>Seq</u> 21	Cell Vol: 14 Mowed): C Operator -y+1/4,z,-x+1	44.81 Å ³] :entrosymn 	netric <u>Operator</u> -x+1/4,-z+1/4,y	<u>Seq</u> 41	
Red ADF SG S Seq 1	Cell β: 60.00° P: U Origin: Symmetry Operat Operator x,y,z -x-y,-z	02 02 ors: <u>Seq</u> 11 12	Crystal (Symm <u>Operator</u> z,-x+1/4,-y+1/4 -z,x+3/4,y+3/4	Red netry A Seg 21 22	Cell Vol: 14 Illowed): C Operator -y+1/4,z,-x+3 y+3/4,-z,x+3	44.81 Å ³] centrosymn <u>5eq</u> 1/4 31 /4 32	Operator -x+1/4,-z+1/4,y x+3/4,z+3/4,-y	<u>Seq</u> 41 42	Operator Z.y.x -ZYX
ADF SG S Seq 1	Cell β: 60.00° Construction 000000000000000000000000000000000000	RedC 02 tors: <u>Seq</u> 11 12 13	Crystal (Symm <u>Operator</u> z,-x+1/4,-y+1/4 -z,x+3/4,y+3/4 -z+1/4,x,-y+1/4	Red netry A Seq 21 22 23	Cell Vol: 14 Jlowed): C Operator -y+1/4,z,x+3 -y+1/4,-z,+1/4	44.81 Å ³] centrosymn <u>Seq</u> 1/4 31 /4 32 4,x 33	Operator -x+1/4,-z+1/4,y x+3/4,z+3/4,-y y,x,z	<u>Seq</u> 41 42 43	Operator Z.y.x -Zy-X Z.y+1/4 -X+1/4
ADF SG S Seq 1 2 3 4	Cell β: 60.00° P: U Origin: Symmetry Operator X,y.z X,y.z xyZ xyZ XyZ xy.4/4,z+1/4,z+3/4 X-4/4,z+3/4 X-4/4	RedC 02 cors: <u>Seq</u> 11 12 13 14	Crystal (Symm Crystal (Symm <u>Operator</u> Z,-x+1/4,-y+1/4 -z,+3/4,y+3/4 -z+1/4,x,-y+1/4 z+3/4,-xy+3/4	Red netry A 21 22 23 24	Cell Vol: 14 Jlowed): C Operator -y+1/4,z,-x+3 y+3/4,-z,+3/4, y+3/4,z+3/4,	44.81 Å ³] centrosymn //4 31 /4 32 4,x 33 -x 34	Operator -x+1/4,-z+1/4,y x+3/4,z+3/4,-y y,X,z -y,-X,-z	<u>Seq</u> 41 42 43 44	Operator z,y,x -z,-y-X z,-y+1/4 -z,y+3/4 x+3/4
ADF SG S Seq 1 2 3 4	Cell β: 60.00° Construction 000000000000000000000000000000000000	RedC O2 cors: <u>Seq</u> 11 12 13 14 15	Crystal (Symm <u>Operator</u> z,-x+1/4,-y+1/4 -z,x+3/4,y+3/4 -z+1/4,x,-y+1/4	Red netry A Seq 21 22 23	Cell Vol: 14 Jlowed): C Operator -y+1/4,z,x+3 -y+1/4,-z,+1/4	44.81 Å ³] centrosymn 1/4 31 1/4 32 4,x 33 -x 34 35 36	Operator -x+1/4,-z+1/4,y x+3/4,z+3/4,-y y,x,z	<u>Seq</u> 41 42 43	Operator Z, y, x -Z, -y+1/4 -Z, y+1/4 -Z, y+3/4, x+3/4 -2, +2/4 -2, +2
ADF SG 5 Seq 1 2 3 4 5 6 7	Cell β: 60.00° C: Origin: Symmetry Operator Xy,Z -x-y-Z x-y+1/4, z+1/4 -x,y+3/4, z+3/4 z+1/4, y,z+1/4 -x+1/4, y,z+1/4 x+3/4, -y,z+3/4 -x+1/4, y-1+1/4, z x+1/4, y-1+1/4, z	RedC 02 ors: <u>Seq</u> 11 12 13 14 15 16 17	Crystal (Symr Crystal (Symr 2x+1/4y+1/4 -z+1/4y+1/4 -z+1/4y+1/4 -z+1/4y+1/4 -z+1/4y+1/4 -z+1/4y+1/4.y z+3/4.x+3/4y y.z.x	Red netry A 21 22 23 24 25 26 27	Cell Vol: 14 sllowed): C Operator -y+1/4,z,x+3 -y+1/4,z+1/4 +3/4,-z,x+3 -y+1/4,z+1/4 x,z,y -x,-z,-y x,-z,-y x,-z,-y	44.81 Å ³] eentrosymm //4 31 /4 32 4,x 33 -x 34 36 1/4 37	Operator -x+1/4,-z+1/4,y x+3/4,-z+3/4,-y y,-x+1/4,-z+1/4 -y,-x+3/4,-z+3/4 -y+1/4,-z+1/4	Seq 41 42 43 44 45 46 47	Operator Z, y, x -Z, -y-1X -Z, y+1/4, -x+1/4 -Z, y+3/4, x+3/4 -z+1/4, -y, x+1/4 -z+3/4, -y, x+3/4 -z+1/4, -y+1/4, x
ADF SG S Seq 1 2 3 4 5 6 7 8	Cell β: 60.00° Cymmetry Operator Coperator x,y,z -x,-y+1/4,-z+1/4 -x+1/4,-y-1/4 -x+1/4,-y-1/4,-y-1/4 -x+1/4,-y-1/4 -x+1/4,-y-1/4,-y-1/4 -x+1/4,-y-1/4,-y-1/4 -x+1/4,-y-1/4 -x+1/4	RedC 02 ors: <u>Seq</u> 11 12 13 14 15 16 17 18	Crystal (Symr Crystal (Symr 2, x+1/4, -y+1/4 - z, x+3/4, y+3/4 - z+1/4 x, y+1/4 z+3/4, -x, y+3/4 - z+1/4, -x, y+3/4 - z+1/4, -x, y+3/4 - z+3/4, -x, y+3/4 - y, z, -x	Red netry A 21 22 23 24 25 26 27 28	Cell Vol: 14 Jlowed): C Operator y+1/4,2,x+1 y+3/4,2,x+3 y+3/4,2,x+3 y+3/4,2,x+3/4 x,2,y x,-2,-y x,-2,-y x,-2,+1/4,y+1 x,2,4/y+3 x,3/y+3	44.81 Å ³] centrosymn 1/4 31 1/4 32 4,x 33 -x 34 36 36 1/4 37 1/4 38	Operator -x+1/4,-z+1/4,-y +3/4,z+3/4,-y -yx,-z -yx+1/4,-z+1/4 -y+1/4,z+3/4,- +3/4,-x+3/4	Seq 41 42 43 44 45 46	Operator Z.y.x -ZYX Zy+14,-x+1/4 -z+14,-x+1/4 -z+14,-yx+1/4 z+3(4,-y,+x+3)4
ADF SG 5 Seq 1 2 3 4 5 6 7 8 9	Cell β: 60.00° Cymmetry Operato Operator x,yz	RedC 02 ors: <u>Seq</u> 11 12 13 14 15 16 17 18 19	Crystal (Symm Crystal (Symm 2, ** 1/4, -y+1/4 -2, ** 3/4, -y+1/4 2*3/4, -x, y*1/4 2*3/4, -x, y*1/4 2*3/4, -x, y*3/4 -y-2; -x, -y, -y, -z, -x y, -z+1/4, -x+1/4	Red netry A 21 22 23 24 25 26 27 28 29	Cell Vol: 14 Jlowed): C Operator -y+1/4,z,x+i y+3/4,z+1/4 y+3/4,z+1/4 y+3/4,z+3/4, x,z,y x,-z+1/4,y+i -x,z+3/4,y+3 -x+1/4,z,y+i	44.81 Å ³] centrosymn //4 31 /4 32 /x 33 -x 34 36 //4 37 //4 38 //4 39	Operator -x+1/4,z+1/4,y x+3/4,z+3/4,zy y,x,z -y,-x+1/4,-z+1/4 -y+1/4,-z+1/4 +y+1/4,-z+1/4 +y+1/4,-z+1/4 +y+1/4,-z+1/4	Seq 41 42 43 44 45 46 47	Operator Z, y, x -Z, -y-1X -Z, y+1/4, -x+1/4 -Z, y+3/4, x+3/4 -z+1/4, -y, x+1/4 -z+3/4, -y, x+3/4 -z+1/4, -y+1/4, x
Red ADF SG S Seq 1 2 3 4 5 5 6 7 7 8 9 10	Cell β: 60.00° Cymmetry Operator Coperator x,y,z -x,-y+1/4,-z+1/4 -x+1/4,-y-1/4 -x+1/4,-y-1/4,-y-1/4 -x+1/4,-y-1/4 -x+1/4,-y-1/4,-y-1/4 -x+1/4,-y-1/4,-y-1/4 -x+1/4,-y-1/4 -x+1/4	RedC O2 ors: <u>Seq</u> 11 12 13 14 15 16 17 18 19	Crystal (Symr Crystal (Symr 2, x+1/4, -y+1/4 - z, x+3/4, y+3/4 - z+1/4 x, y+1/4 z+3/4, -x, y+3/4 - z+1/4, -x, y+3/4 - z+1/4, -x, y+3/4 - z+3/4, -x, y+3/4 - y, z, -x	Red netry A 21 22 23 24 25 26 27 28	Cell Vol: 14 Jlowed): C Operator y+1/4,2,x+1 y+3/4,2,x+3 y+3/4,2,x+3 y+3/4,2,x+3/4 x,2,y x,2,y x,-2,-y x,-2,-y x,-2,+1/4,y+1 x,2,4/y+3 x,4/y+3	44.81 Å ³] centrosymn //4 31 /4 32 /x 33 -x 34 36 //4 37 //4 38 //4 39	Operator -x+1/4,-z+1/4,-y +3/4,z+3/4,-y -yx,-z -yx+1/4,-z+1/4 -y+1/4,z+3/4,- +3/4,-x+3/4	Seq 41 42 43 44 45 46 47	Operator Z, y, x -Z, -y-1X -Z, y+1/4, -x+1/4 -Z, y+3/4, x+3/4 -z+1/4, -y, x+1/4 -z+3/4, -y, x+3/4 -z+1/4, -y+1/4, x
Red ADF SG S Seq 2 3 3 4 5 5 6 6 7 8 9 10 Ator	Cell β: 60.00° Cymmetry Operator Coperator xy,z -x,-y,-z -x,-y+1/4,-z+1/4 -x+1/4,-y+1/4,-z +x+1/4,-y-2+3/4 -x+1/4,-y+1/4,z -x+3/4,-y-2+3/4 -x+1/4,-y+1/4,z -x+3/4,-y-2+3/4 -x+1/4,-y+1/4,z -x+3/4,-y-2-3/4 -x+1/4,-y+1/4,z -x-3/2 -x-3/2 -x-3/2 mic Coordinates:	RedC 02 02 11 12 13 14 15 16 17 18 19 20	Crystal (Symm Crystal (Symm 2, ** 1/4, -y+1/4 -2, ** 3/4, -y+1/4 2*3/4, -x, y*1/4 2*3/4, -x, y*1/4 2*3/4, -x, y*3/4 -y-2; -x, -y, -y, -z, -x y, -z+1/4, -x+1/4	Red netry A 21 22 23 24 25 26 27 28 29	Cell Vol: 14 Jlowed): C Operator -y+1/4,z,x+3 y+3/4,z,x+3 y+3/4,z,x+3 y+3/4,z,x+3 y+3/4,z+3/4 x,z,y -x,z+1/4,-y+1 x,z+3/4,y+3 -x+1/4,z,y+3 x+3/4,-z,y+3	44.81 Å ³] centrosymn //4 31 /4 32 /x 33 -x 34 36 //4 37 //4 38 //4 39	Operator -x+1/4,-z+1/4,-y y:X,z y:X,z y:X+1/4,-z+1/4 y+1/4,-z+1/4 y+1/4,-z+2/3/4 y+1/4,-z+2/3/4 y+1/4,-z+1/4 y+1/4,-z+1/4 y+1/4,-z+1/4 y+1/4,-z+1/4 y+1/4,-z+1/4 y+3/4,-z-1/4	Seq 41 42 43 44 45 46 47	Operator Z, y, x -Z, -y-1X -Z, y+1/4, -x+1/4 -Z, y+3/4, x+3/4 -z+1/4, -y, x+1/4 -z+3/4, -y, x+3/4 -z+1/4, -y+1/4, x
Red ADF SG S Seq 1 2 3 4 5 6 7 8 9 10 Ator Fe	Cell β: 60.00° C: Origin: Symmetry Operator Xy,z x,y,z, x,y+1/4, z+1/4 x,y+1/4, z+2/4 x+1/4, y,z+3/4, z+2/4 x+1/4, y,z+1/4 x+1/4, y,z+3/4, z+2/4 x+1/4, z,z+1/4 x+1/4, y,z+1/4 x+3/4, y-2,z+3/4 x+1/4, y,z+1/4, z x+3/4, y-3/4, z x-y-ir z,x-y Dic Coordinates: Num Wyckoo 1 8a	RedC 02 ors: <u>Seq</u> 11 12 13 14 15 16 17 18 19 20 <i>ff</i> Sym -43n	Crystal (Symm Operator z,-x114,-y+114 -zx+34/y+3/4 -z+1/4,x-y+13/4 -z+1/4,x-y+13/4 -z+1/4,x-y+13/4 -z+1/4,x+3/4,-y y,z,x y,z,x y,z,x+1/4,x+3/4,-y y,z,x+1/4,x+3/4,-y meetry x n 0.125	Red netry A 21 22 23 24 25 26 27 28 29 30 v 0.125	Cell Vol: 14 Jlowed): C Operator -y+1/4,2,x+1 y+3/4,2,x+1 y+3/4,2,x+1 y+3/4,2,x+1 x,2,y -x,2+1/4,2,+1 x,2,y -x,2+1/4,2,y+3 x+3/4,2,y+3 x+3/4,2,y+3 2 0.125 0	44.81 Å ³] ientrosymn ient	Operator -x+1/4, z+1/4, y x+3/4, z+3/4, -y y,x,z y,x,z,z y-x+1/4, z+1/4 y+1/4, x,z+2/4 y+1/4, x,z+3/4, -z y+1/4, x+3/4, -z AET 9	Seq 41 42 43 44 45 46 47	Operator Z, y, x -Z, -y-1X -Z, y+1/4, -x+1/4 -Z, y+3/4, x+3/4 -z+1/4, -y, x+1/4 -z+3/4, -y, x+3/4 -z+1/4, -y+1/4, x
ADF SG S Seq 1 2 3 4 5 6 7 8 9 10 Ator Fe Ma	Cell β: 60.00° Cymmetry Operator Coperator x,y,z -x,-y,-z -x,-y+1/4,-z+1/4 -x+1/4,-y-2+1/4 -x+1/4,-y-2+1/4 -x+1/4,-y-2+1/4 -x+1/4,-y-2+1/4 -x+1/4,-y-2+3/4 -x+1/4,-y-1/4,-z -x+3/4,-y-2+3/4 -x+1/4,-y-1/4,-z -x+3/4,-y-2+3/4 -x+1/4,-y-1/4,-z -x+3/4,-y-2+3/4 -x+1/4,-y-1/4,-z -x+3/4,-y-2 -x-3/4,-z -	RedC 02 ors: 5eq 11 12 13 14 15 16 17 18 19 20 ff Sym -43n -43n	Operator Z,x+114,-y+114 -z,x+114,-y+114 -z,x+134,y+334 -z+114,z,y+114 -z+114,z,y+114 -z+114,z,y+134,-y -z+114,z,y+134,-y -z+34,x+344,-y y,zz,-x y,zz,+114,-x+114,-y,z+34,x+344 unetry x n 0.125	Red netry A <u>Seq</u> 21 22 23 24 25 26 27 28 29 30 v 0.125 0.125	Cell Vol: 14 Jlowed): C Operator -y+1/4,2,x+1 y+3/4,2,x+3 -y+1/4,2,x+1 y+3/4,2,x+3 -y+1/4,2,x+1 x-2,-y -y,-2,-y x,-2,-y -y,-2,-4 x-2,-y -y,-2,-4 x-2,-y -y,-2,-4 x-2,-y -y,-3/4,y+3 x+1/4,2,-y+1 -y+1/4,2,-y+3 z S 0.125 0 0.125 0 0 125 0	44.81 Å ³] tentrosymm tentrosymm t/4 31 t/4 32 4.x 33 -x 34 36 1/4 37 t/4 38 t/4 39 t/4 30 OF Uiso 095 0.009 092 0.009	Operator -x+1/4, z+1/4, y x+3/4, z+3/4, -y y, z, z -y, x+3/4, z+3/4, -y+3/4, x, z+1/4 y+3/4, x, z+1/4, -z+3/4, -y+3/4, x, z+3/4, -y+3/4, x, z+3/4, -y+3/4, x, z+3/4, -z AET 9	Seq 41 42 43 44 45 46 47	Operator Z, y, x -Z, -y-1X -Z, y+1/4, -x+1/4 -Z, y+3/4, x+3/4 -z+1/4, -y, x+1/4 -z+3/4, -y, x+3/4 -z+1/4, -y+1/4, x
ADF SG S Seq 123345567789100 Atom Fe Fe Fe	Cell β: 60.00° Cymmetry Operato xy,z x,y/Z x/Y/Z X/Z	RedC 02 cors: <u>Seq</u> 11 12 13 14 15 16 17 18 19 20 <i>ff</i> Sym -43n -3m	Crystal (Symm Operator z,-x114,-y+114 -z,x314,-y+34 -z'+1/4, y+34 z*314,xy+34,-y y,zx y,zx y,zx y,z+1/4,x+3/4,-y mnetty n 0.125 n 0.25	Red netry A <u>Seq</u> 21 22 23 24 25 26 27 28 29 30 v 0.125 0.5	Zell Vol: 14 Jlowed): C Operator	44.81 Å ³] eentrosymm isentr	Operator -x+1/4, z+1/4, y x+3/4, z+3/4, -y y,x,z y,x,z,z y-x+1/4, z+2/4, -y y+1/4, x,z+3/4, -z y+1/4, x,z+3/4, -z AET 9 9 4	Seq 41 42 43 44 45 46 47	Operator Z, y, x -Z, -y-1X -Z, y+1/4, -x+1/4 -Z, y+3/4, x+3/4 -z+1/4, -y, x+1/4 -z+3/4, -y, x+3/4 -z+1/4, -y+1/4, x
ADF SG S Seq 1 2 3 3 4 5 5 6 7 8 9 10 Ator Fe Ma	Cell β: 60.00° Cymmetry Operator Coperator x,y,z -x,-y,-z -x,-y+1/4,-z+1/4 -x+1/4,-y-2+1/4 -x+1/4,-y-2+1/4 -x+1/4,-y-2+1/4 -x+1/4,-y-2+1/4 -x+1/4,-y-2+3/4 -x+1/4,-y-1/4,-z -x+3/4,-y-2+3/4 -x+1/4,-y-1/4,-z -x+3/4,-y-2+3/4 -x+1/4,-y-1/4,-z -x+3/4,-y-2+3/4 -x+1/4,-y-1/4,-z -x+3/4,-y-2 -x-3/4,-z -	RedC 02 ors: 5eq 11 12 13 14 15 16 17 18 19 20 ff Sym -43n -43n	Crystal (Symm Operator z,**1/4,-y+1/4 -z,**3/4,+'3/4 -z+1/4, x,y+1/4 z*3/4, x,y+1/4 z*3/4, x,y+1/4 z*3/4, x,y+3/4 y,z,x y,-z+1/4, x,+1/4 y,-z+1/4, x,+1/4 y,-z+3/4, x+3/4, x+3/4 metry x n 0,125 n 0,125 0,5 0,5	Red netry A <u>Seq</u> 21 22 23 24 25 26 27 28 29 30 v 0.125 0.125	Cell Vol: 14 Jlowed): C Operator -y+1/4,2,x+1 y+3/4,2,x+3 y+3/4,2,x+1 y+3/4,2,x+1 y+3/4,2,x+1 y+3/4,2,x+1 x+2,y+1 x-2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+3/4,2,y+1 x+1/4,2,y+1 x+1/4,2,y+1 y+3/4,2,y+1 y+	44.81 Å ³] tentrosymm tentrosymm t/4 31 t/4 32 4.x 33 -x 34 36 1/4 37 t/4 38 t/4 39 t/4 30 OF Uiso 095 0.009 092 0.009	Operator -x+1/4, z+1/4, y x+3/4, z+3/4, -y y.x.z y.x+1/4, z+1/4 -y+1/4, z+2/3/4 -y+1/4, z+2	Seq 41 42 43 44 45 46 47	Operator Z, y, x -Z, -y +1/4, -x + 1/4 -Z, y + 3/4, -x + 3/4 -z + 1/4, -y, -x + 1/4 -z + 3/4, -y, -x + 3/4 -z + 1/4, -y + 1/4, -x

04-012-1052

 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: 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Jun 9, 2020 11:58 AM (fal-sharji2) 0-017-0464 (Primary), 00-036-0398 (Primary), 01-073-1960 (Alternate), 01-073-2410 (Alternate), 1-075-9708 (Alternate), 01-078-5428 (Alternate), 01-088-1938 (Alternate), 01-088-1938 (Alternate), 1-088-1936 (Alternate), 01-088-1937 (Alternate), 01-088-1938 (Alternate), 01-088-1939 (Alternate), 1-088-3084 (Alternate), 01-088-1937 (Alternate), 01-088-1943 (Alternate), 01-088-1943 (Alternate), 1-089-3084 (Alternate), 01-089-4924 (Alternate), 01-089-6187 (Alternate), 04-002-0587 (Alternate), 4-002-3768 (Alternate), 04-002-3769 (Alternate), 04-002-5223 (Alternate), 04-002-5364 (Alternate), 4 4-002-3768 (Alternate), 04-002-2458 (Alternate), 04-002-5223 (Alternate), 04-002-5094 (Alternate), 4 4-002-6403 (Alternate), 04-002-8191 (Alternate), 04-002-5084 (Alternate), 04-002-5094 (Alternate), 4 4-002-6403 (Alternate), 04-002-8191 (Alternate), 04-002-5084 (Alternate), 04-002-6403 (Alternate), 04-005-6434 (Alternate), 40-005-6436 (Alternate), 40-005-6436 (Alternate), 40-005-6436 (Alternate), 40-005-6436 (Alternate), 40-005-6436 (Alternate), 40-005-6437 (Alternate), 04-005-6439 (Alternate), 40-005-6436 (Alternate), 40-005-6436 (Alternate), 40-005-6529 (Alternate), 40-005-6529 (Alternate), 40-005-6529 (Alternate), 40-007-4269 (Alternate), 40-005-6529 (Alternate), 40-005-6530 (Alternate), 04-012-0912 (Alternate), 40-010-6157 (Primary), 40-4012-0910 (Alternate), 40-012-0911 (Alternate), 40-012-0913 (Alternate), 40-012-0910 (Alternate), 40-012-0910 (Alternate), 40-012-0911 (Alternate), 40-012-0922 (Alternate), 40-012-0913 (Alternate), 40-012-0910 (Alternate), 40-012-0910 (Alternate), 40-012-0921 (Alternate), 40-012-0921 (Alternate), 40-012-0928 (Alternate), 40-012-0938 (Altern
Entry Date: 09/01/200	09 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) - Mn Fe	e2 04 - 04-012-1052 (Stick, Fixed Slit Intensity) - Cu Ka1 1.54056 Å
<u>20 (°) d (Å) I</u>	<u>hkl* 20(°) d(Å) Ihkl* 20(°) d(Å) Ihkl*</u>
18.4197 4.812720 31 30.3018 2.947180 38	3 2 2 0 75,6060 1,256680 17 6 2 2 114,6725 0,914982 2 9 1 1
35.6938 2.513360 99 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 19 47.5049 1.912380 1	4 4 0 0 87.4976 1.113930 35 6 4 2 123.6454 0.873838 44 9 3 1 3 3 1 90.4338 1.085240 100 7 3 1 129.7501 0.850777 92 8 4 4
53.8332 1.701550 10 57.3907 1.604240 30	9 4 2 2 95.3333 1.041990 41 8 0 0 1.33.6832 0.837788 1 9 3 3 5 5 1 1 98.2905 1.018390 1 7 3 3 140.9014 0.817400 19 8 6 2
63.0302 1.473590 40 66.2788 1.409020 4	9 4 4 0 99.2811 1.010870 1 6 4 4 145.8216 0.805860 58 9 5 1 5 3 1 103.2723 0.982393 16 8 2 2 147.6047 0.802120 9 10 2 2
67.3434 1.389310 1 71.5243 1.318020 34	4 4 2 106.3086 0.962545 57 7 5 1

04-013-2116 Jun 9, 2020 12:03 PM (fal-sharji2)
 Status
 Primary
 QM:
 Star
 Pressure/Temperature:
 Ambient
 Chemical Formula:
 Ca0.936 Mg0.064 (CO3)

 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: CuKo1 A: 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]
 AuthCell Z: 6.00
 AuthCell Z: 6.00

 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 Space Group: K-50 (107) Molecular Weight: 99.06 Crystal Data (XtiCell a: 4.967 Å XtiCell b: 4.967 Å XtiCell c: 16.963 Å XtiCell a: 90.00° XtiCell β: 90.00° XtiCell γ: 120.00° XtiCell Vol: 362.47 Å³ XtiCell Z: 6.00] Crystal Data Axial Ratio [c/a: 3.415 a) (1.000 c/b: 3.415] Reduced Cell [RedCell a: 4.967 Å RedCell b: 4.967 Å RedCell c: 6.340 Å RedCell a: 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
 Se Seg Operator 9 x,x-y,z+1/2 11 -x+y,y,z+1/2 10 -x,x+y,-z+1/2 12 x-y,-y,-z+1/2 x,y,z -x -y -z -y,x-y,z y,-x+y,-z 5 -x+y,-x,z 6 x-y,x,-z nic Coordinates: Atom Num Wyckoff Symmetry x SOF Uiso AET
 Y
 Z
 501
 0130

 0.0
 0.0
 0.0
 0.936
 0.01473

 0.0
 0.0
 0.004
 0.01473

 0.0
 0.0
 0.255
 1.0
 0.01426

 0.2575
 0.0
 0.25
 1.0
 0.02852
 6b 6b 6a 18e 3.3.22 Ca Mg C O -NWA Anisotropic Displacement Parameters: Atom Num Uani11 Uani22 Uani33 Uani12 Uani13 Uani23 0.00755 0.00755 0.00642 0.00849 0.0151 0.0151 0.0128 0.0161 0.0151 0.0151 0.0128 0.0336 0.014 0.014 0.0172 0.0306 0.0 0.0 0.0 -0.018 0.0 0.0 0.0 -0.0089 Ca Mg õ 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
 Pearson Symbol: hR10.00 References: DOI Reference Type Calculated from LPF using POWD-12++. Primary Reference "Single-crystal X-ray structure refinements of two biogenic magnesian calcite crystals". Paquette J., Reeder R.J. Am. Mineral. 75, 1151, 1158 (1990). Structure ANX: ABX3. LPF Collection Code: 1213141. Calculated Pattern Original Remarks; same sample studied in Database Comments: 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 Ku1 1.54056 Å <u>I h k l *</u> <u>28 (°)</u> 28 (°) hkl d (Å) d (Å) I hkl * 28 (°) d (Å)
 d (A)
 1

 1,865910
 193

 1.618510
 29

 1.596850
 85

 1.578050
 11

 1.518170
 53

 1.51010
 22

 1.501410
 22

 1.466240
 17
 d (A) 1.433940 1.413590 1.350180 1.331940 1.290260 1.278850 1.241820 1.228540 23.1645 29.5539 31.6208 36.1354 39.6004 43.3640 47.3501 47.7829
 0 (A)
 1
 0
 A

 3.836550
 89
 0
 1
 2

 3.836550
 89
 1
 0
 4

 2.827180
 20
 0
 0
 6

 2.483650
 14.3
 1
 1
 0

 2.483650
 14.3
 1
 1
 3

 2.0804910
 148
 2
 0
 2

 1.918270
 67
 0
 2
 4

 1.901900
 188
 0
 1
 8
 48.7639 56.8384 57.6812 58.4344 60.9781 61.3431 61.7328 63.3828 1 1 6 1 2 1 2 1 2 10 2 1 2 1 1 8 9 5 64.9834 66.0371 69.5704 70.6641 73.3101 74.0728 76.6736 77.6565 300122021 30201321 0 12 56 30 9 18 27 6 11 19 7 10 8 6 0 12 Page 1/2

© 2020 International Centre for Diffraction Data. All rights reserved.

Jun 9, 2020 12:03 PM (fal-sharji2) 04-013-2116 28 (°) d (Å) ٠ 28 (°) d (Å) h k l Ι h k l 78.8492 80.6619 81.3802 82.0256 82.279 85.2939 86.3723 87.0123 92.4362 93.7158 95.2986 96.8846 96.8846 98.3856 99.8440 102.8556 103.5836 104.2421 104.9024 106.65202 106.8537 108.1942 108.7518 109.6438 110.2807 111.3060 112.5652 114.8627 116.0013 118.8360 119.6750 120.3057 121 9071 121 9071 129 1066 129 9353 129 9353 139 9353 139 9353 139 9353 134 2180 135 5383 135 8378 135 8378 137 0012 140 2177 143 0935 144 2906 146 5426 149 4824 0.881099 1 212920 0.985236 0.980289 293884421 18 13 231113212340010113 321130023042434212 233224231012120341 7 EN 6 2 E5 11 121014 8 16 5 11 8 0 12 3 7 10 8 6 16 13022151213334244 1.190170 1.181470 1.173800 1.168270 1.148520 1.136980 1.125530 1.118890 1.076400 1.055670 1.042450 1.039800 1.029390 1.029390 1.029390 1.017660 0.975891 0.971552 0.961217 0.959137 0.950949 0.947622 0.943648 0.942394 0.938731 0.932954 0.926056 0.914011 0.908291 0.894736 0.880096 0.880096 0.855969 0.853037 0.853037 0.850134 0.843184 0.840279 0.836128 0.832135 0.831250 0.827883 0.819150 0.812033 0.819150 0.812033 0.809256 0.809256 0.804320 0.798427 0201201 210 14 465 117 2 14 48 165 13 12 5 20 3 36 16 531304202332402 2101714 49152011031 1 4 1 7 20 24 12m 2 21 613-10-6 14 8 1 2 1 6 6 7 02431120 14

Status Alternate	QM: Star	Prosente	Tomo	erature:	Ambient	Chamical	Formu	la: Ca (C O3	1	
Empirical Formula:		Weight %	: C12	00 Ca40.0	4 047 9		%: C2	0.00 Ca20.00		
Radiation: CuKo1	A: 1.5406	Å d-Sp	pacing:	Calculate	ed In	tensity: Calc	ulated	l/ic: 3.2	l/lc - N	D: 0.89
SYS: Rhombohedri Author's Cell [Aut AuthCell MolVol: (Density [Dcalc: 2 Temp: 297.0 K (Au	hCella: 4.98 51.27] A 713 g/cm ³	uthor's Ce Dstruc:	AuthCe all Axial 271 g/c		/a: 3.41 SS/FOM			5.2000 V	AuthCell	Z : 6.00
Space Group: R-3 Crystal Data [XtlC KtlCell γ: 120.00° Crystal Data Axial Reduced Cell [Red RedCell β: 66.97°	ell a: 4.988 / XtlCell Vo Ratio [c/a:	l: 367.61/ 3.420 av 8 Å Re-	lib: 4. Å' X /b: 1.00 dCelib:	988 Å tlCell Z:	6.00] 3.420 Red	Cell c: 6.375		əll a: 90.00° RedCəll a: 61		xII β: 90.00°
Atomic parameters Crystal (Symmetry IG Symmetry Opera	Allowed): (tors:	Centrosymn	netric	55.0507.5% * Vi						
Seg Operator	Seq Opera			erator		Operator		Operator		Operator
1 x.y.z 2 -x,-y,-z Atomic Coordinates:	3 -y.x-y. 4 yx+y.	2	-X* XY	yxz x,-z	8	-y,-x,z+1/2 y,x,-z+1/2	9 10	x,x-y,z+1/2 -x,-x+y,-z+1/2	11 12	-x+y,y,z+1/2 x-y,-y,-z+1/2
	off Symmetr		y z	SOF						
Ca 1 6b C 2 6a	-3 32	0.0	0.0 0.0							
0 3 18e	.2 t and Hydratic	0.0 0.2593	0.0 0.2 0.0 0.2 Cerami	5 1.0 5 1.0 c (Biocera	6-= 3# 1#	a ommon Phase	, Foren	sic, Inorganic	, Mineral	Related (Mineral
O 3 18 Subfile(a): Cemen Natural Prototype Structur Mineral Classificati Cross-Rof PDF #s:	2 t and Hydratic I, Pharmaceu Generation (Control Control Control Calcite 00-001-083 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0280-207 01-0280-207 01-0280-2080-208 01-0280-2080	0.0 0.2593 in Product, tical (Exclp Inder): Ca Supergrou 7 (Deleted) 2 (Alternati 9 (Alternati 7 (Alternati 9 (Alternati 2 (Alternati 9 (Alternati 2 (Alternati 3 (Alternati 3 (Alternati 3 (Alternati 3 (Alternati	0.0 0.2 Cerrami itent), St (C O3 (p), Cald (C 03 (Celet (C 03 (Celet (C 03 (Celet (C 03 (Celet (C 03 (Celet (C), 01-0 (Celet (C), 01-0 (C), 01-0 (C), 01-0 (Celet (C), 01-0 (C),	5 1.0 c (Biocera percondu Prototy te (Group 2-0623 (D ed) 00-00 7-1743 (P 78-3262 (J 80-2796 (J 80-2796 (J 80-2804 (J 80-2804 (J 80-2804 (J 80-2804 (J 80-2804 (J 86-2341 (J 86-	3# amic), C. acting M. acting M. actinge	b a cture [Alpha arson Symbo 00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-000-000 (00-000-000-000 (00-000-000-000 (00-000-000-000) (00-000-000-000-000-000-000-0000 (00-000-000-000-000-000-000-000-000-000	Order]: hR10 Deleter 004-06 Alterna 4 (Alter 3 (Alter 3 (Alter 5 (Alter 5 (Alter 5 (Alter 5 (Alter 5 (Alter 6 (Alter 2 (Alter 5 (Alter) 6 (Alter 5 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (C Ca O3 1.00 1.00 1.00-003-056 77 (Deleted), 1.01-072-11 nate), 01-072-11 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 Alternate), - Primary), - 0 Alternate), -	59 (Delet 00-005-0 337 (Afte 4615 (A 2798 (A -2798 (A -2802 (A -2802 (A -2802 (A -2802 (A -2393 (A -2343 (A 0577 (A -2343 (A 04-007-1)	ed) 00-003-0596 588 (Primary), mate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate)
O 3 198 Subfile(a): Cemen Natural Prototype Structur Mineral Classificati Cross-Rof PDF #s: Cross-Rof PDF #s:	2 t and Hydratic I, Pharmaceu Generation (Control Control Control Calcite 00-001-083 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0280-207 01-0280-207 01-0280-2080-208 01-0280-2080	0.0 0.2593 an Product, tical (Excipation) fical (Excipation) fical (Excipation) fical (Excipation) fical (Excipation) fical (Supergroup) for (Deleted) 2 (Alternation) 6 (Alternation) 9 (Alte	0.0 0.2 Cerrami itent), St (C O3 (p), Cald (C 03 (Celet (C 03 (Celet (C 03 (Celet (C 03 (Celet (C 03 (Celet (C), 01-0 (Celet (C), 01-0 (C), 01-0 (C), 01-0 (Celet (C), 01-0 (C),	5 1.0 c (Biocera percondu Prototy te (Group 2-0623 (D ed) 00-00 7-1743 (P 78-3262 (J 80-2796 (J 80-2796 (J 80-2804 (J 80-2804 (J 80-2804 (J 80-2804 (J 80-2804 (J 86-2341 (J 86-	3# amic), C. acting M. acting M. actinge	b a a cture [Alpha arson Symbo 00-002-0629] (Deleted), 00- 01-071-3699 0, 01-078-461 2, 01-080-279 3, 01-080-279 3, 01-080-280 3, 01-080-280 3, 01-080-280 3, 01-080-280 3, 01-086-233 3, 01-086-233 3, 01-086-233 4, 01-086-233 3, 01-086-233 4, 01-086-233 3, 01-086-233 4, 01-086-233 3, 01-086-234 3, 01-086-236 3,	Order]: hR10 Deleter 004-06 Alterna 4 (Alter 3 (Alter 3 (Alter 5 (Alter 5 (Alter 5 (Alter 5 (Alter 5 (Alter 6 (Alter 2 (Alter 5 (Alter) 6 (Alter 5 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (C Ca O3 1.00 1.00 1.00-003-056 77 (Deleted), 1.01-072-11 nate), 01-072-11 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 Alternate), - Primary), - 0 Alternate), -	59 (Delet 00-005-0 337 (Afte 4615 (A 2798 (A -2798 (A -2802 (A -2802 (A -2802 (A -2802 (A -2393 (A -2343 (A 0577 (A -2343 (A 04-007-1)	ed), 00-003-0596 596 (Primary), mate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), (094 (Alternate),
3 3 18e Subfile(a): Cemen Natural Prototype Structur Minoral Classificati Cross-Ref PDF #s: Entry Date: 09/01/7 References:	2 t and Hydratic I, Pharmaceu Generation (Control Control Control Calcite 00-001-083 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0274-002 01-0280-207 01-0280-207 01-0280-2080-208 01-0280-2080	0.0 0.2593 in Product, tical (Excip Inder): Ca Supergrou 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 9 (Alternati 0 (Alternati 8 (Alternati 8 (Alternati 8 (Alternati 8 (Alternati 3 (Alternati 3 (Alternati 3 (Alternati 3 (Alternati	0.0 0.2 Cerrami itent), St (C O3 (p), Cald (C 03 (Celet (C 03 (Celet (C 03 (Celet (C 03 (Celet (C 03 (Celet (C), 01-0 (Celet (C), 01-0 (C), 01-0 (C), 01-0 (Celet (C), 01-0 (C),	5 1.0 c (Biocera percondu Prototy te (Group 2-0623 (D ed) 00-00 7-1743 (P 78-3262 (J 80-2796 (J 80-2796 (J 80-2804 (J 80-2804 (J 80-2804 (J 80-2804 (J 80-2804 (J 86-2341 (J 86-	3# amic), C. acting M. acting M. actinge	b a cture [Alpha arson Symbo 00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-000-000 (00-000-000-000 (00-000-000-000 (00-000-000-000) (00-000-000-000-000-000-000-0000 (00-000-000-000-000-000-000-000-000-000	Order]: hR10 Deleter 004-06 Alterna 4 (Alter 3 (Alter 3 (Alter 5 (Alter 5 (Alter 5 (Alter 5 (Alter 5 (Alter 6 (Alter 2 (Alter 5 (Alter) 6 (Alter 5 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (C Ca O3 1.00 1.00 1.00-003-056 77 (Deleted), 1.01-072-11 nate), 01-072-11 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 Alternate), - Primary), - 0 Alternate), -	59 (Delet 00-005-0 337 (Afte 4615 (A 2798 (A -2798 (A -2802 (A -2802 (A -2802 (A -2802 (A -2393 (A -2343 (A 0577 (A -2343 (A 04-007-1)	ed), 00-003-0596 596 (Primary), mate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), (094 (Alternate),
3 3 18 Subfile(s): Cement Natural Prototype Structur Mineral Classificati Cross-Rof PDF #s: Entry Date: 09/01// References: Type	2 and Hydraidi, Pharmaceu e [Formula C 00-001-082 (Deletend), C 00-024-002 01-072-458 01-080-279 01-080-279 01-080-279 01-080-279 01-080-279 01-080-280 01-080 01-080-280	0.0 0.2593 in Product, tical (Excip Inder): Ca Supergrou 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 7 (Deleteid 0-003-067) 9 (Alternati 0 (Alternati 8 (Alternati 8 (Alternati 8 (Alternati 8 (Alternati 3 (Alternati 3 (Alternati 3 (Alternati 3 (Alternati	0.0 0.2 0.0 0.2 Cerami isent), St. C C O3 (p), calci 0.00-00 0 (Deilet 0, 01-0 e), 0	5 1.0 5 1.0 c (Biocerr apercondu Protoly ts (Group 2-0623 (D -00- 00-207 7-1743 (P - 80-2792 (J 80-2792 (J 80-2796 (J 80-2796 (J 80-2796 (J 80-2796 (J 80-2796 (J 80-2808 (J 80-2808 (J 80-2808 (J 90-2808	3# i# amic), Ci zcting M. pe Stru) Pec eleted), M-lo636 rimary), Atlernate At	b a cture [Alpha arson Symbo 00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-000-000 (00-000-000-000 (00-000-000-000 (00-000-000-000) (00-000-000-000-000-000-000-0000 (00-000-000-000-000-000-000-000-000-000	Order]: hR10 Deleter 004-06 Alterna 4 (Alter 3 (Alter 3 (Alter 5 (Alter 5 (Alter 5 (Alter 5 (Alter 5 (Alter 6 (Alter 2 (Alter 5 (Alter) 6 (Alter 5 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (Alter) 7 (Alter) 6 (Alter) 7 (C Ca O3 1.00 1.00 1.00-003-056 77 (Deleted), 1.01-072-11 nate), 01-072-11 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 nate), 01-080 Alternate), - Primary), - 0 Alternate), -	59 (Delet 00-005-0 337 (Afte 4615 (A 2798 (A -2798 (A -2802 (A -2802 (A -2802 (A -2802 (A -2393 (A -2343 (A 0577 (A -2343 (A 04-007-1)	ed), 00-003-0596 596 (Primary), mate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), (094 (Alternate),
0 3 18e	2 and Hydraidi, Pharmaceu e (Formula G 00-001-082 (Deliteda), 10 00-001-082 (Deliteda), 10 00-077-084 01-080-278 01-080-278 01-080-278 01-080-278 01-080-278 01-080-278 01-080-280 01-080-282 01-080-28 0 00-08	0.0 0.2593 in Product, tical (Excip Prder): Ca Supergrou 7 (Deleted) 0.003-067 7 (Deleted) 2 (Alternati 9 (Al	0.0 0.2 (2) Ceramini isent), SU CO3 (C CO3 (C CO3 (C CO3) (C C	5 1.0 5 1.0 c (Biocerr apercondu Protoly ts (Group 2-0623 (D -00- 00-207 17173 (P - 80-2796 (J 80-2796 (J 80-2796 (J 80-2796 (J 80-2796 (J 80-2804 (J 80-2805 (3# 1# amic), Ci acting M. pe Stru Pecesson of the structure of the structure	b a cture [Alpha arson Symbo 00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-002-0629 (00-000-000 (00-000-000-000 (00-000-000-000 (00-000-000-000) (00-000-000-000-000-000-000-0000 (00-000-000-000-000-000-000-000-000-000	Order): 1: hR10 Deletec 004-06: Alterna 4 (Alterna 3 (Alterna 4 (Alterna 5 (Alterna 9 (Alterna 9 (Alterna 9 (Alterna 4 (Alterna 9 (Alterna 1 (Alterna 9 (Alterna 9 (Alterna 9 (Alterna 1 (Alterna 9 (Alterna 1 (Alterna 9 (Alterna 1 (Alterna 1 (Alterna 9 (Alterna 1 (Altern	C Ca O3 .00 1, 00-003-063 7) (Deleted), 19 (Del	59 (Delet 00-005-0 337 (Afte 4615 (A 2798 (A -2798 (A -2802 (A -2802 (A -2802 (A -2802 (A -2393 (A -2343 (A 0577 (A -2343 (A 04-007-1)	ed), 00-003-0596 596 (Primary), mate), iternate), iternate), iternate), iternate), iternate), iternate), iternate), iternate), iternate), (0-94 (Alternate),
O 3 18 Subfile(a): Cement Natural Prototype Structur Mineral Classificati Cross-Rof PDF #s: Entry Date: 09/01// References: Type Primary Reference	2 and Hydraidi, Pharmaceu e (Formula G 00-001-082 (Deleted), (00-024-002 00-024-002 00-024-002 00-024-002 00-024-002 00-024-002 00-080-280 01-080 01-080-280 01-080-	0.0 0.2593 in Product, tical (Excip Prder): Ca Supergrou 7 (Deleted) 0.003-067 7 (Deleted) 2 (Alternati 9 (Al	0.0 0.2 Ceramini isent), S. S. Co C. Caramini isent), S. Co C. Co Co C. Co Co Co Co Co Co Co Co Co Co Co Co Co C	5 1.0 5 1.0 c (Biocerc upercondu Prototy is (Group 2.0623 (D ed) 00-00 7.1743 (P 78.3282 80-2796 (80-2806 (80-2806 (80-2806 (80-2806 (90-2806 (3# 1# amic), Ci acting M. pe Stru Pecesson of the structure of the structure	b ammon Phase alenai arson Symbo 00-002-052 (Cleated), 00- 01-071-3599), 01-082-279), 01-080-279), 01-080-279), 01-080-279), 01-080-279), 01-080-279), 01-080-289), 01-080-289), 01-080-281), 01-081-281), 01-081-281)	Order): 1: hR10 Deletec 004-06: Alterna 4 (Alterna 3 (Alterna 4 (Alterna 5 (Alterna 9 (Alterna 9 (Alterna 9 (Alterna 4 (Alterna 9 (Alterna 1 (Alterna 9 (Alterna 9 (Alterna 9 (Alterna 1 (Alterna 9 (Alterna 1 (Alterna 9 (Alterna 1 (Alterna 1 (Alterna 9 (Alterna 1 (Altern	C Ca O3 .00 1, 00-003-063 7) (Deleted), 19 (Del	59 (Delet 00-005-0 337 (Afte 4615 (A 2798 (A -2798 (A -2802 (A -2802 (A -2802 (A -2802 (A -2393 (A -2343 (A 0577 (A -2343 (A 04-007-1)	ed), 00-003-0596 596 (Primary), mate), iternate), iternate), iternate), iternate), iternate), iternate), iternate), iternate), iternate), (0-94 (Alternate),

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1 / 2

		a (C (1.27			5-60-	49 (Stick, F		tensit		Cu	Kal	1.54		100222		(31)		120	
2 0 (=)	d (A)	I	<u>h</u>	k		-	28 (*)	d (Å)	1	h	k	1		28 (*)	d (Å)	1	h	k	1	4
23.0594	3.8537.90	96	0	1	2		80.9689	1.186430	5	32	1	2		109.6009	0.942643	17	4	1	۵	
29.4642	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	0123	1	14		111.8486	0.929955	1	4	1	3	
35.9803 39.4185	2 494000 2 284020	146	1		03		83.7967 84.8299	1.153440	41	1	324	5		114.0818	0.918028	¥	3	20	10	
43,1706		157	1		2		85,9079		18	- 6	÷.	6				1	- 2	3	8	
43.1700	2.093800 1.926900	67	20	2	-		85.9079	1.130420	1	1	-	31		117.9818	0.898720	4	2	3	6	
47 5076	1.912280	194	ŏ	1	2		91.5171	1.124500	-	3	23	7		119 2626	0.892778	6	2	1	16	
48 5128	1.874980	201	1	2	6		91,9375	1.071380	1.0		1	2		120 7744	0.886006	8	1.5		18	
55.5803	1.625280	33	2		4		93.0622	1.061360	B	ž	400	14		127.3113	0.859550	2		ò	2	
57.4158	1.603600	93	1	+	ż.		94,7450	1 046900	24	4	ŏ	4		128.0214	0.856937	7	53	2	10	
58.0805	1.586820	11	1	20	10		95.0279	1.044530	28	0040	3	8		128 5609	0.854984		14	5	17	
60.5846	1.524810	53 23	2	1	4		96.1567	1.035240	13m	ž	0	16		128,7386	0.854347	22	3	2	14	
61.0066	1.517530	23	NN	0	8		96 1567	1.035240	m	4	÷.	15		130.9248	0.846751	6	304	5	4	
61 3800	1.509190	24	1	0	8		97,7080	1.022900	2	2032	1			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	14	2	2	15	
64.6811	1,439910	60	3	00	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	11	2	3	11	
69 2017	1.356470	11	Z	1	7		103.5560	0.980475	3	1	323332A24	10		135.8096	0.831333	4	023324	3	0	
70 2484	1.338800	19	G	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	б	100	NNONT	6		105.1654	0.963448	17	0	4	8		142.8378	0.812640	7		2	2	
76.2977	1.247000	12	2	2	0		107.3394	0.956139	5	D	23	16		144.7406	0.808240	1	0	4	. 14	
77.1638	1.235150	20		1	12		108.0712	0.951689	2	NODNO	3	5		147.7630	0.801799	1	025	4	4	
78.4523	1.218060	1	2	2	3		108.6635	0.948146	1m	0	0	\$8		148.2937	0.800736	5	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)

        Weight %:
        C14.25 Mg28.83 O56.93
        Atomic %:
        C20.00 Mg20.00 O60.00

Empirical Formula: C Mg O3
                                  Compound Name: Magnesium Carbonate
                                                                                                                                         Mineral Name: Magnesite
ANX: ABX3
                                                                                                                                                                                                           I/Ic: 1.83
Radiation: CuKa1 A: 1,5406 Å
                                                                                     d-Spacing: Calculated Intensity: Calculated
                                                                                                                                                                                                                                         V/Ic - ND: 1.08
SYS: Rhombohedral SPGR: R-3c (167)

        SYS:
        Khombonedral
        SPGR: K-3C (167)

        Author's Cell [ AuthCell a: 4,6339(4) Å
        AuthCell c: 15.0177(9) Å
        AuthCell Vol: 279.2'

        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
        0.035

                                                                                                 AuthCell c: 15.0177(9) Å AuthCell Vol: 279.27 Å<sup>3</sup> AuthCell Z: 6.00
Space Group: R-3c (167) Molecular Weight: 84.31

        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°
        XtlXtlCell a: 12.018 Å
        XtlCell α: 90.00°
        XtlCell 
                                                                                                                                      XtiCell c: 15.018 Å XtiCell α: 90.00° XtiCell β: 90.00°
Atomic parameters are cross-referenced from PDF entry 04-009-2317
                                                                                                                                                                             ADP: B
Crystal (Symmetry Allowed): Centrosymmetric
SG Symmetry Operators:
                                                                                                                                             Seg Operator
Seg Operator
                                               Seg Operator Seg Operator
                                                                                                                                                                                             Seg Operator
                                                                                                                                                                                                                                             Seq Operator
                                    -
12
          x,y,z
-x,-y,-z
                                               3
                                                           -y,x-y,z
y,-x+y,-z
                                                                                               5 -x+y,-x,z
6 x-y,x,-z
                                                                                                                                             7 -y,-x,z+1/2
8 y,x,-z+1/2
                                                                                                                                                                                               9 x,x-y,z+1/2
10 -x,-x+y,-z+1/2
                                                                                                                                                                                                                                             11 -x+y,y,z+1/2
12 x-y,-y,-z+1/2
Atomic Coordinates:
Atom
              Num Wyckoff
                                                   Symmetry
                                                                                                                                                           AET
                                                                                                                         SOF
                                                                                                                                      Biso
                                                                                                                                     0.36879 1#a
0.34715 3#b
0.35475 6-a
                                                                              0.2775
0.0
0.0
                                                                                                0.0 0.25
0.0 0.25
0.0 0.0
                              18e
6a
6b
                                                                                                                       1.0
1.0
1.0
0
               123
                                                     232
C
Mg
Anisotropic Displacement Parameters:
                                                   Bani22
                                                                         Bani33
                                                                                                      Bani12
                                                                                                                            Bani13
Atom Num Bani11
                                                                                                                                                      Bani23
                                                    0.646158
0.506867
0.51525
                                                                           0.0496549 0.323079 -0.0386154
0.0277294 0.253433 0.0
0.034178 0.257947 0.0
                              0.469464
0.506867
0.51525
                                                                                                                                                      -0.0772308
0.0
0.0
O
C
Mg
                2
Subfile(s): Cement and Hydration Product, Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural)
Pearson Symbol: hR10.00
                                               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), 

        (Alternate), 
        04-009-2317 (Primary), 
        04-010-3138 (Alternate), 
        04-012-1188 (Alternate), 
        04-012-1189 (Alternate), 

Cross-Ref PDF #'s:
Entry Date: 09/01/2005 Last Modification Date: 09/01/2011 Last Modifications: Reflections
References:
                                        DOI Reference
Type
Primary Reference
Crystal Structure
Structure
                                                     Calculated from ICSD using POWD-12++.
Crystal Structure Source: LPF,
"The equation of state and high pressure behavior of magnesite". Ross, N.L., Reeder, R.J. Am. Mineral. 82, 682 (1997).
ANX: ABX3. Analysis: C1 Mg1 O3. Formula from original source: Mg (C O3). ICSD Collection Code: 77481.
Database Comments: 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<mark>-</mark>071-6263 (Stick, Fixed <mark>S</mark>lit Intensity) - Cu Ku1 1.54056 Å
                                                                                   •
28 (°) d (Å)
                                                                                                20 (°)
                                                                                                                    d (Å)
                                                                                                                                             I
                                                                                                                                                                                                 28 (0)
                                                                                                                                                                                                                        d (Å)
                                                            hkl
                                                                                                                                                             hkl
                                                                                                                                                                                                                                                               h
                                                                                                                                                                                                                                                                     k
                                                                                                                                                                                                20 (°)

81.5198

81.5198

83.3502

86.0753

87.8866

88.7806

88.7806

92.4117

94.2217
25,1404
32,6343
35,8472
38,8356
42,9799
46,8258
51,6050
53,8763
53,8763
61,3832
                                                                                                20 (°)
62,4084
66,4204
68,3757
69,3443
69,3443
70,3153
75,9765
76,9153
79,6823
                                                                                                                      1,486770
1,406360
1,406360
1,370830
1,354030
1,354030
1,354030
1,251470
1,238520
1,202320
                                                                                                                                                                                                                       d (A)

1.179800

1.179800

1.158480

1.128650

1.10980

1.101120

1.01120

1.067120

1.067120

1.051330
                                                                                                                                                                                                                                                                    2 8
0 2 3
2 3 1
1 12
3 1 12
3 1 10
2 3
1 10
2 6
                      3 539310
                                                                                                                                              71
60m
                                                                                                                                                                                                                                               20m
                                                             0
                                                                                                                                                                   2010120012
                                                                                                                                                                           2104895012710
                                                                   1001102111
                                                                          2460324861
                                                                                                                                                            112211
                                                                                                                                                                                                                                                              1322113122
                      3.539310
2.741660
2.502950
2.316950
2.102650
1.938520
1.769660
1.700290
                                            999
131
62
501
130
51
400m
                                                                                                                                                                                                                                               m
                                                            1
                                                                                                                                             m
19
88m
                                                                                                                                                                                                                                                9
                                                            120012
                                                                                                                                                                                                                                              1
10m
72m
m
22
                                                                                                                                             m
119
43
17
17
                                                                                                                                                              13020
                       1.700290
                                             m
46
© 2020 International Centre for Diffraction Data. All rights reserved.
                                                                                                                                                                                                                                                                     Page 1/2
```

01-071- 28 (°)	6263 d (Å)	I	h	k	ĵ.	20 (°)	d (Å)	1	h	k	Ĩ	ø	Jun 9, 28 (°)	2020 12 d (Å)	:05 P I	M (fal	-sharji2
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	Ő	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	- M	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	Ő	14	126,4923	0.862625	4	1	4	3		149,6285	0.798150	m	5	Ó	2
113.8860	0.919048	24m	1	1	15	129,9324	0.850144	10m	0	2	16			SUMPORTS/		- 27	- 2	

5 759555 YE DECEMPTING 7 1

01-075-9982

Jun 9, 2020 12:05 PM (fal-sharji2)

Chemical Formula: Ca (CO3) Status Alternate QM: Star Pressure/Temperature: Ambient 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: CuKa1 d-Spacing: Calculated Intensity: Calculated I/Ic - ND: 0.58 λ: 1.5406 Å I/Ic: 1.14 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 ų
 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 β: 90.00° XtlCell y: 90.00° XtiCell 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 RedC RedCell c: 7.964 Å RedCell a: 90,00° RedCell 6: 90.00° RedCell y: 90.00° RedCell Vol: 227.30 Å3] ADP: B Atomic parameters are cross-referenced from PDF entry 04-008-5421 Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: Seg Operator Seg Operator Seg Operator Seq Operator -x+1/2,-y+1/2,z+1/2 x+1/2,y+1/2,-z+1/2 -x,y+1/2,-z+1/2 x,-y+1/2,z+1/2 x,y,z -x,-y,-z 3 4 56 x+1/2,-y,-z -x+1/2,y,z 8 2 Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Biso AET 0.25 0.25 0.25 0.47347 0.41508 0.76211 0.92224 0.68065 0.24046 0.08518 0.09557 0.08726 1.0 1.0 1.0 1.0 0.61095 0.43867 0.77616 0.70856 4c 4c 4c 8d 9-a 3#a 1#a 1#a Ca C m. m. ŏ 34 m. 1 Anisotropic Displacement Parameters: Atom Num Bani11 Bani22 Bani33 Bani12 Bani13 Bani23 0.670266 0.573788 0.540783 0.926694 0.665479 0.442997 0.497141 0.299269 0.0 0.0 0.0201231 0.0073175 Ca 12 0.653666 0.689106 õ 3 13407 0.0 0.180227 0.0 0.0841512 0.509938 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

 on:
 Aragonite (Group), carbonate (Subgroup)
 Pearson Symbol: oP22.00

 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), 01-075-9986
 (Alternate), 01-075-9986 (Alternate), 01-075-9987 (Alternate), 01-076-0606

 (Alternate), 01-074-337 (Alternate), 01-078-4338 (Alternate), 01-078-4339 (Alternate), 01-080-2768
 (Alternate), 01-080-2769 (Alternate), 01-080-2777 (Alternate), 01-080-2775 (Alternate), 01-080-2778

 (Alternate), 01-080-2773 (Alternate), 01-080-2774 (Alternate), 01-080-2775 (Alternate), 01-080-2778
 (Alternate), 01-080-2778 (Alternate), 01-060-6531

 (Alternate), 01-080-2790 (Alternate),
 04-006-5421 (Primary),
 04-012-0488 (Alternate),
 04-014-1837

 (Alternate), 01-080-2790 (Alternate),
 04-017-9180 (Alternate),
 04-012-0488 (Alternate),
 04-016-5531

 (Alternate),
 04-017-0148 (Alternate),
 04-017-9180 (Alternate)
 04-012-0488 (Alternate),
 04-014-1837

 (Alternate),
 04-017-9180 (Alternate)
 04-012-0488 (Alternate),
 04-014-1837

 Cross-Ref PDF #'s: Last Modification Date: 09/01/2011 Last Modifications: Reflections Entry Date: 09/01/2009 References: Туре DOI Reference Primary Reference Calculated from ICSD using POWD-12++. Crystal Structure Crystal Structure Source: LPF. "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). Structure

 Jun 9, 2020 12:05 PM (fal-sharji2

 ANX: ABX3. Analysis: C1 Ca1 03. Formula from original source: Ca (C 03). 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.

20 (°)	d (Å)	I	h	k	1 *	20 (°)	d (Å)	1	h	k	*	20 (°)	d (Å)	1	h	k	1
0.0249	4.660960	2	0	1	1	76.5331	1.243750	m	3	4	1	106.7505	0.959779	19	1	7	3
1.0679	4.213370	18	1	1	0	76.7109	1.241310	55	4	0	0	107.0264	0.958067	23	0	0	6
2.3085	3.981790	8	0	2	0	77.0036	1.237320	86	3	1	3	107.8887	0.952791	1	3	4	4
6.2019	3.398280	999	1	1	1	77,9437	1.224730	58m	0	5	3	108.1511	0.951208	1	0	1	6
7.2218	3.273230	544	0	2	1	77.9437	1.224730	m	1	3	4	109.9345	0.940715	2m	0	8	2
1.0903	2.874200	45	0	0	2	78.6950	1.214910	12	2	5	2	109.9345	0.940715	m	1	0	6 2
2.7426	2,732840	86	1	2	1	79,3459	1.206570	56	2	4	3	110,3028	0.938605	10	5	0	2
3.1080	2.703510	510	0	1	2	79.4706	1.204990	21	0	6	2	110.4690	0.937659	13m	3	1	5
6.0775	2.487500	322m	1	0	2	80.2846	1,194810	3	3	2	3	110,4690	0.937659	m	3	7	0
6.0775	2.487500	m	2	0	0	80,7421	1,189190	44	1	5	3	111.3110	0.932926	13	4	1	4
7.2800	2,409980	129	Ō	3	1	82.3077	1,170490	57m	1	6	2	111,4502	0.932153	21m	0	2	6
7.8604	2.374360	407	1	1	2	82.3077	1.170490	m	2	6	0	111.4502	0.932153	m	5	1	2
8.4212	2,340980	241	1	3	0	82.7598	1.165240	5	ō	4	4	111.8229	0.930096	10	5	3	ō
8.6012	2,330480	190	Ó	2	2	83,1596	1.160650	28	4	2	1	112,7045	0.925306	5	3	7	1
1.1627	2 191180	125	2	1	ĩ	84.3798	1,146950	1m	2	6	1	112,9362	0.924064	8m	2	4	
1.6213	2,168090	5	ĩ	3	-1	84.3798	1.146950	m	ŝ.	Š	ò	112.9362	0.924064	m	ĩ	8	5 0
2.8936	2.106680	193m	1	2	ż	85.0542	1,139570	7	4	õ	2	114.0574	0.918155	1m	3	2	5
2.8936	2.106680	m	ż	2	õ	85.2104	1,137880	3	ó	ĭ	5	114.0574	0.918155	m	š	ã	Ĩ.
5.5238	1.990890	35	Ō	4	ŏ	85.5323	1.134420	2	1	4	4	114,4380	0.916186	12m	ĭ	2	6
5.8366	1.978030	648	2	2	ĭ	85.6877	1.132760	4	3	3	3	114,4380	0.916186	m	- î -	5	5
6.5318	1.950080	5	õ	3	2	86.1294	1.128080	14	4	1	2	114.8072	0.914294	9	4	2	4
8.3405	1.881260	290m	ŏ	4	ĩ	86.3828	1.125420	24m	2	3	4	115,2132	0.912233	9	2	8	1
8.3405	1.881260	m	2	0		86.3828	1.125420	m	3	5	1	115.6329	0.910124	1	2	7	3
8.8461	1.862960	6	ô	ĭ	2 3	87.2933	1.116010	1	ŏ	7	4	116.1508	0.907552	3	ź	6	4
9.8261	1.828590	22	2	1	2	87.9732	1.109130	25m	1	1	5	116.3436	0.906603	8	4	6	0
0.2220	1.815100	259	1	3	2	87.9732	1.109130	m	1	ż	õ	117,4657	0.901169	š	ō	3	6
1.9340	1,759220	32	4	4	í	88.4317	1.104560	11m	Ó		5	118,3968	0.896774	9			4
24141	1.744230	298	1	1	3	88,4317	1.104560	m	4	23	1	119.0352	0.893819	9	32	5 0	4 6
	1.729220				1	89.0556	1.098430				3	119.5850	0.891312	7		7	2
2.9042		84	2	3				1.	2	5	2				3		2
2.9904	1.726610	139 20	02	22	3 2	89.3482	1.095590	14	4	27	1	119.9598 120.2689	0.889623	12	32	3	5 6
3.9157	1.699140					90.0527		6					0.888242				
6.1537	1.636610	22 9	0	42	23	90.5617	1.084040	7	2	6	2 5	120.6207	0.886683	17	1	33	62324
6.3709	1.630820		1	4	3	91.1902	1.078200	1	1	2		121.0232	0.884916	16	5		2
6.7642	1.620450	17	3	1	0	91.5182	1.075190	10	3	1	4	121.3823	0.883355	1	0	8	3
9.1910	1.559670	57	3	1	1	92.5587	1.065810	10m	1	6	3	122.2571	0.879611	3	2	8	4
9.4640	1.553160	10m	0	3	3	92.5587	1.065810	m	3	5	2	122.6554	0.877934	8m	1	7	
9.4640	1.553160	m	2	4	0	93.1980	1.060170	1	3	4	3	122.6554	0.877934	m	5	4	1
0.2445	1.534890	18m	0	5	1	93.4698	1.057800	1	0	7	2	123.0418	0.876323	15	5	1	3
0.2445	1.534890	m	2	3	2	93.8132	1.054830	13m	0	3	5	123.4734	0.874542		0	9	1
1.0480	1.516600	1	1	5	0	93.8132	1.054830	m	2	4	4	124.0692	0.872116	10m	2	2	6
1.8246	1.499400	47	22	4	1	93.9866	1.053340	4	4	4	0	124.0692	0.872116	m	4	5	3
2.2543	1.490080	2	2	1	3	94.7141	1.047160	1m	3	2	4	124.3170	0.871118	3	1	9	0
2.5962	1.482760	1	1	3	3	94.7141	1.047160	m	4	3	2	124.6721	0.869699	1	1	8	3
2.8681	1.477000	30	3	2	1	95.1923	1.043160	9	1	5	4	125.9726	0.864611	11	4	6	326
3.3741	1.466420	44	1	5	1	96.0521	1.036090	32	4	4	1	126.3130	0.863307	3	0	4	6
1.8230	1.437100	3	0	0	4	96.2592	1.034410	23m	1	7	2	126.9691	0.860827	1m	1	9	1
4.9661	1.434280	5	3	0	2	96.2592	1.034410	m	2	1	5	126.9691	0.860827	m	5	2	355
5.0018	1.414260	40	0	1	4	98.2060	1.019040	1	3	6	1	128.2823	0.855989	1	1	6	5
5.1437	1.411570	29	33	1	2	98.3556	1.017890	2	2	7	1	129.0776	0.853140	2	3	4	5
5.5219	1.404460	28	3	3	0	99.5072	1.009180	30	2	2	5	130.0984	0.849570	5	4	4	4
7.8346	1.380440	2m	0	4	3	99,6820	1.007880	24	4	2	3	130.8250	0.847088	5	2	3	6
7.8346	1.380440	m	1	0	4	100.1482	1.004440	28	3	3	4	131.2455	0.845674	1	0	9	2
8.6271	1.366420	26	2	4	2	100.9151	0.998868	4	2	6	3	131,8092	0.843803	1	3	8	1
3.9874	1.360160	50	1	1	4	101.3716	0.995601	14m	ō	4	5	132.3202	0.842132	14m	3	7	3
4780	1.351750	19	Ó	2	4	101.3716	0.995601	m	Ó	8	0	132,3202	0.842132	m	5	5	0
6165	1.349400	6	3	2	2	102,3080	0.989016	6	4	4	2	133,1560	0.839449	5	2	57	4
0.0971	1.341320	20	1	5	2	102.9554	0.984552	12	3	5	3	133.3642	0.838790	ă	ž	1	
0.7753	1.330120	5	i	4	23	103.5861	0.980272	10m	õ	8	1	134.0228	0.836731	ž	5	3	532
0.9508	1.327260	12	ó	6	ŏ	103.5861	0.980272	m	2	5	4	135.0252	0.833669	13m	ĩ	9	ž
1.5870	1.317020	12	2	2	3	104.3710	0.975038	8		6	4	135.0252	0.833669	m	5	5	í
2.3159	1.305530	6	22	35	1	104.5050	0.975038	10	03	6	2	135.50232	0.832242	4	2	8	3
2.3962	1.304280			3	4	104.6579	0.973150	6					0.829912	1		7	1
2.3902	1.293240	5	1	26	1	104.6579	0.973150	18m	22	73	25	136.2954 136.5533	0.829912	1	43	6	6
5.2415	1.293240	58	3	3	2	104.9489	0.971249		5	1	5	130.0033	0.829166	6	5	0	0
5.9751	1.251490	58 1	12	5 6 0	1	104.9489	0.965177	m 2 2	э 4	58	4	137.1219	0.827540	13m	3	12	65

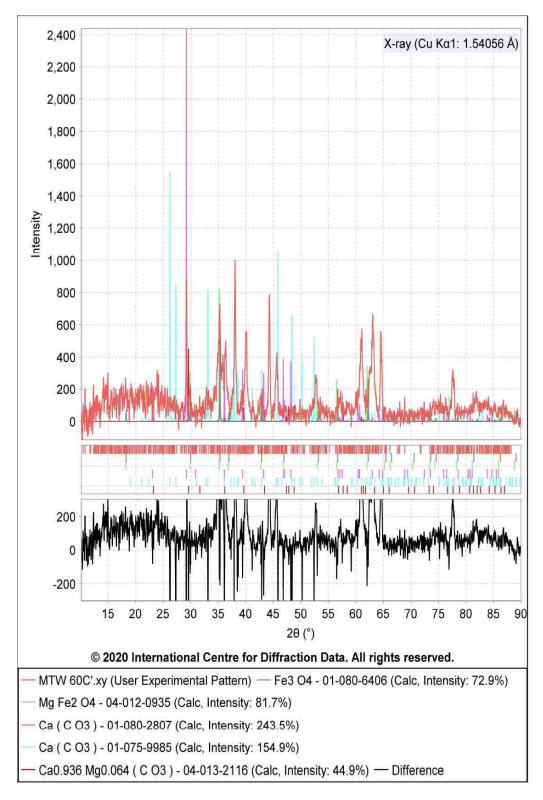


Figure E.4 XRD patterns of substances precipitated from Magnetically treated Water (MTW) tank at 60 °C from experiment with a tank with little exposure of iron.

SIeve+ Report

Experiment

Search Line: 2	.365239 Å	D1 Range:	2.356 Å - 2.374 Å
Search Line: 2	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	5 <mark>16</mark> 107 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	2.253650 Å	D1 Range:	2.246 Å - 2.262 Å
Search Line: 2	2.245449 Å	D1 Range:	2.237 Å - 2.253 Å
Search Line: 1	4694 <mark>3</mark> 1 Å	D1 Range:	1.466 Å - 1.473 Å
Rotation: All 8	Rotations		

Preferences

Radiation: X-rayWavelength: Cu Ka1 1.54056 ÅSearch Method: HanawaltSearch Window: 0.15°Match Window: 0.15°2nd Pass Filter: Yesd-Spacings: WeightedLowest 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 Empirical Formula Compound Name	1: Fe3 O4 Weight %: Fe72.36 O27.64 Atomic %: Fe42.86 O57.14 ANX: A3X4
Radiation: CuKat	A: 1.5406 Å d-Spacing: Calculated Intensity: Calculated Vic: 4.8 Vic - ND: 1.31
Density [Dcalc: 5	'GR: Fd-3m (227) thCell a: 8.4324(5)Å AuthCell Vol: 599.59Å ^a AuthCell Z: 8.00 AuthCell MolVol: 74.95] 5.13 g/cm ² Dstrue: 5.13 g/cm ²] SS/FOM: F(30) = 999.9(0.0001, 30) uhor provided temperature) R-factor: 0.026
Crystal Data [XtlC XtlCell γ: 90.00° Crystal Data Axial Reduced Cell [Re RedCell β: 60.00°	3m (227) Molecular Weight: 231.54 zell a: 8.432 Å XtiCell b: 8.432 Å XtiCell c: 8.432 Å XtiCell a: 90.00° XtiCell β: 90.00° XtiCell Vol: 599.59 Å* XtiCell 2: 8.00] Ratio [a/b: 1.000 c/b: 1.000] dCell a: 5.963 Å RedCell b: 5.963 Å RedCell c: 5.963 Å RedCell a: 60.00° RedCell y: 60.00° RedCell Vol: 149.90 Å*]
COL MEA	y Allowed): Centrosymmetric
	on Phase, Forensic, Inorganic, Metais & Alloys, Micro & Mesoporous, Mineral Related (Mineral , Natural) re [Formula Order]: Mg Al2 O4 Prototype Structure [Alpha Order]: Al2 Mg O4 cF56.00
	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), 01-075-1809 (Alternate), 01-075-1809 (Alternate), 01-075-1809 (Alternate), 01-075-1810 (Alternate), 01-075-0710 (Alternate), 01-076-1849 (Alternate), 01-075-0710 (Alternate), 01-076-1849 (Alternate), 01-075-0710 (Alternate), 01-080-6403 (Alternate), 01-080-6402 (Alternate), 01-080-6402 (Alternate), 01-080-6403 (Alternate), 01-080-6403 (Alternate), 01-080-6403 (Alternate), 01-080-6403 (Alternate), 01-080-6409 (Alternate), 01-080-6403 (Alternate), 01-080-640

	01-089-4319	(Alternate), J	03-065-3107	(Alternate), v	04-001-7822	(Alternate), V	04-001-7909	(Alternate),	ÿ.
		(Alternate), V							
		(Alternate), .							
		(Alternate), J							
		(Alternate), J							
		(Alternate), 🗸							
	04-002-8629	(Alternate), J	04-002-9019	(Alternate), V	04-002-9635	(Alternate), V	04-003-1446	(Alternate),	4
		(Alternate), /							
		(Alternate), J							
		(Alternate),							
Cross-Ref PDF #'s:	04-006-0425	(Alternate), V	04-000-1058	(Alternate), V	04-005-2406	(Alternate), V	04-006-2467	(Alternate),	ξ.
	09-000-2702	(Alternate), /							
		(Alternate),							
	04-007-0010	(Alternate), / (Alternate), /	04-007-8307	(Alternate),	04-007-89/0	(Alternate), -	04-007-9093	Alternate),	б.
		(Alternate),							
		(Alternate),							
		(Alternate),							
		(Alternate),							
		(Alternate),							
		(Alternate),							
	04-009-8435	(Alternate),	04-009-8436	(Alternate)	04-009-8437	(Alternate)	04-009-8438	(Alternate)	ä.
		(Alternate), J							
		(Alternate),							
	04-013-9806	(Alternate), J	04-013-9807	(Alternate), J	04-013-9808	(Alternate), V	04-013-9809	(Alternate)	Я.
	04-013-9810	(Alternate), /	04-013-9811	(Alternate), V	04-014-1396	(Alternate), V	04-014-9664	(Alternate),	4
	04-015-3100	(Alternate), J	04-015-3101	(Alternate), /	04-015-3102	(Alternate), J	04-015-8200	(Alternate),	2
	04-015-8203	(Alternate), V	04-015-8204	(Alternate), J	04-015-8207	(Alternate), J	04-015-8209	(Alternate),	1
	04-015-8211	(Alternate), J	04-015-8213	(Alternate), J	04-015-8214	(Alternate), V	04-017-1024	(Alternate)	

Entry Date: 09/01/2013

References: Type D	I 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).

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1/2

01-080-6406

Jun 9, 2020 12:22 PM (fal-sharji2) ANX: A3X4. Analysis: Fe3 O4. Formula from original source: Fe3 O4. ICSD Collection Code: 183973. Sample Source of 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.

Database Comments:

20 (*)	d (Å)	3 I -	h	k	1	28 (*)	d (Å)	I	h	k	1	•	28 (*)	d (Å)	1	h	k	E	1
16,2070	4 868450	96	1	1	1	73.6975	1.285930	60	5	3	3		109.5788	0.942771	15	8	4	õ	
29.9468	2.981300	295	2	2	0	74.5920	1.271230	24	6	2	2		112.6543	0.925576	1	8	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	
6.8953	2.434220	75	2	2	2	81.4385	1.180770	3	5	5	1		117.9443	0.898897	4	6	6	4	
2.8633	2.108100	201	4	0	0	86,2483	1.126830	24	б	4	2		121.2437	0.883956	27	9	3	1	
6 9282	1,934530	4	3	3	1	89,1203	1.097800	78	7	3	1		127.0222	0.860628	54	8	4	- 44	
3,1680	1.721260	83	4	2	2	93,9039	1.054050	29	8	0	0.		130,7070	0.847488	1	9	3	3	
6.6738	1.622820	264	5	1	1	96,7855	1.030180	1	7	3	3		137.3608	0.826865	11	10	2	0	
52 2278	1,490650	341	4	4	0	97,7491	1.022580	1	6	4	4		141,7855	0.815191	32	9	52	1	
55.4243	1.425340	7	5	3	1	101.6301	0.993768	10	8	2	2		143.3589	0.811408	6	10	2	2	
56.4716	1.405400	1	4	4	2	104.5757	0.973690	39	7	5	1								
70.5825	1.333280	25	6	2	Ū	105.5659	0.967263	7	6	б	2								

04-012-0935 Jun 9, 2020 12:22 PM (fal-sharji2) Chemical Formula: Mg Fe2 O4 QM: Star Pressure/Temperature: Temperature (Non-ambient) Status Alternate 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: CuKa1 A: 1,5406 Å d-Spacing: Calculated Intensity: Calculated I/Ic: 4.01 I/Ic - ND: 1.38 SYS: Cubic SPGR: Fd-3m (227) AuthCell Vol: 604.87 Å3 Author's Cell [AuthCell a: 8.45708(4) Å 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 [XtiCell a: 8.457 Å XtiCell b: 8.457 Å XtlCell c: 8,457 Å XtlCell α: 90.00° XtlCell β: 90.00° XtlCell y: 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 a: 60.00° RedCell 8: 60.00° RedCell y: 60.00° RedCell Vol: 151.22 Å3] ADP: U Origin: O2 Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: Seq Operator Seg Operator Sea Operator Operator Seq Operator Seq 2,-x+1/4,-y+1/4 -z,x+3/4,y+3/4 -z+1/4,-x,y+3/4 +z+3/4,-x,y+3/4 -z+1/4,-x+1/4,y z+3/4,x+3/4,-y x,y,z x,y,z x,y+1/4,-z+1/4 -x,y+3/4,z+3/4 -x+1/4,y,z+1/4 x+3/4,y,z+1/4 x+3/4,y+1/4,z x+3/4,y+3/4,-z z,x,y -z,-x,-y Z,y,x z,-y+1/4,-x+1/4 -z,+1/4,y+3/4 -z+1/4,y-x+1/4 z+3/4,-y,x+3/4 -z+1/4,y+1/4,x z+3/4,y+3/4,-x -y+1/4,z,-x+1/4 y+3/4,-z,x+3/4 -y+1/4,-z+1/4,x y+3/4,z+3/4,-x 21 22 23 24 25 26 27 28 29 30 -x+1/4,-z+1/4,y x+3/4,z+3/4,-y 31 32 33 4 355 37 38 39 40 1121314156 1781920 41 42 43 44 45 46 47 48 x+3/4,z+3/4,-y y,x,z -y,-x+1/4,-z+1/4 -y,x+3/4,z+3/4 -y+1/4,x,-z+1/4 y+3/4,-x,z+3/4 -y+1/4,-x,+1/4,z y+3/4,x+3/4,-z 45678910 x,z,y -x,-z,-y x,-z+1/4,-y+1/4 -x,z+3/4,y+3/4 -x+1/4,z,-y+1/4 x+3/4,-z,y+3/4 y,z,x -y,-z,-x y,-z+1/4,-x+1/4 -y,z+3/4,x+3/4 Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Uiso AET 0.125 0.125 0.5 0.5 0.2543 0.125 0.125 0.5 0.5 0.2543 8a 8a 16d 16d 32e 0.125 0.125 0.5 0.5 0.2543 0.0082 0.0082 0.0108 0.0108 0.0108 Fe Mg Fe Mg O -43m -43m -3m -3m .3m 0.826 0.174 0.587 0.413 12345

Subfile(s): Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural) Former PDF's #: 01-076-9752

10

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-sharji
	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 (Alternat
	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), < 04-005-7127 (Alternate), < 04-005-0223 (Alternat
	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), < 04-012-0910 (Alternate), < 04-012-0917 (Alternate), < 04-012-0920 (Alternate), < 04-012-0922 (Alternate), < 04-012-0922 (Alternate), < 04-012-0920 (Alternat
	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),
Cross-Ref PDF #'s:	
	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), < 04-012-0949 (Alternate), < 04-012-0949 (Alternate), < 04-012-0951 (Alternat
	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),
	04-012-1070 (Alternate), < 04-012-1071 (Alternate), < 04-012-1072 (Alternate), < 04-012-1073 (Alternate), < 04-012-1077 (Alternat
	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), v 04-014-3733 (Alternate), v 04-014-3734 (Alternate), v 04-015-7027 (Alternate)
Entry Date: 09/01/2	2009 Last Modification Date: 09/01/2011 Last Modifications: Reflections
References:	
	DI Reference
Primary Reference	Calculated from LPF using POWD-12++.
Structure	"Cation ordering in magnesic/errite, 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).

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.

28 (°)	d (Å)	1	h	k	1	1	28 (°)	d (Å)	I	h	k	1	*	20 (°)	d (Â)	1	h	k	1	*
18 1535	4.882700	36	11	1	1		73 3478	1.289690	69	5	3	3	7.5	109 1064	0.945530	17	8	4	0	
9.8573	2,990030	345	2	2	0		74.3375	1.274950	17	5	2	2		112 1540	0.928285	1	9	1	1	
5.1653	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	69	6	4	
2,7320	2.114270	204	4	ō	ō		85,9362	1.130120	33	6	4	2		120,6524	0.886543	35	9	3	1	
6,7831	1.940190	1	3	3	1		88,7908	1.101020	96	7	3	1		126,3550	0.863147	75	8	4	4	
3.0010	1.726290	105	4	2	2		93.5470	1.057130	37	8	Ō	0		129 9829	0.849969	1	9	3	3	
6.4935	1.627570	280	5	1	1		96,4090	1.033200	1	7	3	3		136,5120	0.829285	19	10	2	0	
2.0262	1.495010	395	4	4	0		97.3672	1.025570	1	6	4	4		140,8316	0.817577	44	9	5	1	
5.2097	1.429510	3	5	3	1		101,2208	0.996676	15	8	2	2		142.3620	0.813783	6	10	2	2	
6.2528	1.409510	1	4	4	2		104.1444	0.976539	50	7	25	1		10/2229/14224	0.53501356587577	98.7	0.020		1.2	
70.3461	1.337180	34	6	2	0		105.1267	0.970094	6	6	6	2								

Empirical Formula:	QM: Star Pressure/Temperature: Temperature (Non-ambient) Chemical Formula: Ca (CO3) C Ca O3 Weight %: C12.00 Ca40.04 O47.95 Atomic %: C20.00 Ca20.00 O60.00 npound Name: Calcium Carbonate Mineral Name: Calcite
Radiation: CuKa1	A: 1.5406 Å d-Spacing: Calculated Intensity: Calculated I/Ic: 2.93 I/Ic - ND: 0.79
AuthCell MolVol: 6 Density [Dcalc: 2.6	ICell a: 4.9764(1)Å AuthCell c: 17.3886(5)Å AuthCell Vol: 372.93Å ^s AuthCell Z: 6.00 2.16] Author's Cell Axial Ratio [c/a: 3.494]
Space Group: R-3c Crystal Data [XtiCe XtiCell γ: 120.00° Crystal Data Axial R Reduced Cell [Red RedCell β: 67.38°	il a: 4,976 Å XtlCell b: 4,976 Å XtlCell c: 17,389 Å XtlCell α: 90.00° XtlCell β: 90.00° XtlCell Vol: 372,93 Å* XtlCell Z: 6,00] Ratio [c/a: 3,495 a/b: 1.000 c/b: 3,495]
Crystal (Symmetry	Allowed): Centrosymmetric
Prototype Structure	and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Pharmaceutical (Excipient), Superconducting Material [Formula Order]: Ca C O3 Prototype Structure [Alpha Order]: C Ca O3 n: Calcite (Supergroup), calcite (Group) Pearson Symbol: hR10.00
	(Deleted) (0-003-0670 (Deleted), 0-004-0636 (Deleted), 0-004-0637 (Deleted), 0-005-0586 (Primary)
Cross-Ref PDF #'s: Entry Date: 09/01/2	01-030-200 (Alternate), 01-030-200 (Alternate), 01-030-2009 (Alternate), 01-030-200 (Alternate), 01-030-200 (Alternate), 01-030-0577 (Alternate), 01-000-05659 (Primary), 01-030-0598 (Alternate), 01-000-0586 (Alternate), 01-000-0586 (Alternate), 01-000-0586 (Alternate), 01-000-0586 (Alternate), 01-001-0507 (Alternate), 01-001-0578 (Alternate), 01-012-0072 (Alternate), 01-001-0578 (Alternate), 01-012-0072 (Alternate), 01-010-0713 (Alternate)), 01-010-0713 (Alternate), 01-001-0578 (Alternate), 01-012-072 (Alternate), 01-010-0713 (Alternate), 0
Entry Date: 09/01/2 References:	01-072-4582 (Alternate), 01-075-6049 (Alternate), 01-08-3252 (Alternate), 01-078-4614 (Alternate), 01-078-4615 (Alternate), 01-080-2795 (Alternate), 01-080-2804 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2810 (Alternate), 01-090-2810 (Alternate), 01-090-2810 (Alternate), 01-090-2810 (Alternate
Entry Date: 09/01/2 References: Type DO	01-072-4582 (Alternate), 01-075-6049 (Alternate), 01-08-3252 (Alternate), 01-080-2793 (Alternate), 01-080-2804 (Alternate), 01-080-2804 (Alternate), 01-080-2804 (Alternate), 01-080-2803 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2810 (Alternate), 01-090-0810 (Alternate), 01-080-2810 (Alternate), 01-080-2810 (Alternate), 01-080-2810 (Alternate), 01-080-2810 (Alternate), 01-080-2810 (Alternate), 01-080-2810 (Alternate
Entry Date: 09/01/2 References:	01-072-4582 (Alternate), 01-075-6049 (Alternate), 01-08-3252 (Alternate), 01-078-4614 (Alternate), 01-078-4615 (Alternate), 01-080-2795 (Alternate), 01-080-2804 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2810 (Alternate), 01-090-2810 (Alternate), 01-090-2810 (Alternate), 01-090-2810 (Alternate
Entry Date: 09/01/2 References: <u>Type D(</u> Primary Reference	01-072-4582 (Alternate), 01-075-6049 (Alternate), 01-078-3252 (Alternate), 01-078-4615 (Alternate), 01-080-2795 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2816 (Alternate), 01-086-2340 (Alternate), 01-086-2340 (Alternate), 01-086-2340 (Alternate), 01-086-2340 (Alternate), 01-086-2340 (Alternate), 01-086-2340 (Alternate), 01-086-2346 (Alternate), 01-086-2340 (Alternate), 01-086-2348 (Alternate), 01-086-2340 (Alternate), 04-007-2658 (Alternate), 01-086-2340 (Alternate), 04-007-2658 (Alternate), 04-007-2658 (Alternate), 04-007-2659 (Primary), 04-007-049 (Alternate), √ 04-007-7246 (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), √ 04-017-2458 (Alternate), 04-008-0213 (Alternate), √ 04-016-0198 (Alternate), √ 04-016-7113 (Alternate) 01 Reference Calculated from ICSD using POWD-12++, "Temperature dependence of the structural parameters in the transformation of aragonite to calcite, as determined from in situ sindrotron powder x-ray-diffraction data". Antao, S.M., Hassan, I. Can. Mineral, 48, 1225 (2010). ANX: ABX3, Analysis: C1 Ca1 O3, Formul
Entry Date: 09/01/2 References: Type DO Primary Reference Structure Database Comment	01-072-4582 (Alternate), 01-075-6049 (Alternate), 01-08-3252 (Alternate), 01-078-4613 (Alternate), 01-078-4615 (Alternate), 01-080-2793 (Alternate), 01-080-2804 (Alternate), 01-080-2804 (Alternate), 01-080-2804 (Alternate), 01-080-2804 (Alternate), 01-080-2803 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2803 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2804 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate

20 (°)	d (Å)	I	h	k	1	20 (°)	d (Å)	I	h	k	1	*	20 (°)	d (Â)	I	h	k	*
94.2851	1.050790	1	1	1	15	108,1817	0.951024	1	2	32	5		131,3038	0.845479	1m	0	5	4
94 6892	1.047370	9	3	1	8	109.3798	0.943929	3	22	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	33	33	3
98.0570	1.020190	7	Ū.	3	12	116.8679	0.904045	2	2	1	16		142,3232	0.813877	1m	Ó.	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	10	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	3	2	3	2	125 5524	0.866236	1	- 313	2	17		146 6447	0.804105	2	ΞŤ.	3	16
105,0859	0.970359	2	õ	2	16	126,8556	0.861253	- ii -	3	ĩ	14		147.8428	0.801638	1	3	ŏ	18
105,8679	0.965334	4m	õ	õ	18	127,3283	0.859487	ź	3	ż	10		148.0418	0.801238	- i -	5	õ	8
105.8679	0.965334	m	ŏ	4	8	127,8037	0.857733	1	35	õ	2		148.3997	0.800526	1	52	4	4
106.0641	0.964089	3	3	2	4	129.3266	0.852260	1	ō	Ť	20		149,7712	0.797881	31	2	31	19

01-075-9985

Status Alternate QM: Star Pressure/Temperature: Ambient Chemical Formula: Ca (CO3) 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: CuKa1 λ: 1.5406 Å d-Spacing: Calculated Intensity: Calculated 1/lc: 1.14 I/Ic - ND: 0.58 SYS: Orthorhombic SPGR: Pmcn (62) Author's Ceil [AuthCell a: 4.96937(27) Å AuthCeil b: 7.9591(4) Å A AuthCeil Vol: 227.53 Å³ AuthCeil Z: 4.00 AuthCeil MolVol: 56.88] AuthCell c: 5.75278(17) Å 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 [XtiCell a: 5.753 Å XtiCell b: 7.959 Å XtiCell y: 90.00° XtiCell Vol: 227.53 Å3 XtiCell 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 a: 90.00° RedCell y: 90.00° RedCell Vol: 227.53 Å3] RedCell 6: 90.00° Atomic parameters are cross-referenced from PDF entry 04-008-5421 ADP: B Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: Seg Operator Seq Operator Seg Operator Seg Operator -x+1/2,-y+1/2,z+1/2 x+1/2,y+1/2,-z+1/2 3 56 x+1/2,-y,-z -x+1/2,y,z -x,y+1/2,-z+1/2 x,-y+1/2,z+1/2 X,Y,Z -X,-V,-Z 8 Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Biso AET Ca C O O 0.25 0.41508 0.25 0.76211 0.25 0.92224 0.47347 0.68065 0.24046 0.08518 0.09557 0.08726 1.0 1.0 1.0 1.0 0.61095 0.43867 0.77616 0.70856 9-a 3#a 1#a 1#a 4c 4c m., m... m... 1 34 4c 8d Anisotropic Displacement Parameters: Bani22 Atom Num Bani11 Bani33 Bani12 Bani13 Bani23 Ca 0.665479 0.442997 1.13407 0.670266 0.573788 0.540783 0.926694 0.497141 0.299269 0.653666 0.689106 0.0 0.0 0.0 0.180227 0.0 0.0201231 0.0 0.0073175 0.0 -0.05854 -0.0136696 0.0841512 34 1.13407 Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material Subfile(s): Prototype Structure [Formula Order]: Ca C O3 Prototype Structure [Alpha Order]: C Ca O3 Mineral Classification: Aragonite (Group), carbonate (Subgroup) Pearson Symbol: oP20.00 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), 01-078-0980 (Alternate), 01-078-438 (Alternate), 01-078-4339 (Alternate), 01-080-2778 (Alternate), 01-080-2779 (Alternate), 01-080-2779 (Alternate), 01-080-2778 (Alternate), 01-080-2779 (Alternate), 01-080-2778 (Alternate), 01-080-2779 (Alternate), × 04-006-5421 (Alternate), × 04-007-5048 (Alternate), × 04-014-1837 (Alternate), × 04-017-9180 (Alternate), × 04-012-0488 (Alternate), × 04-014-1837 (Alternate), × 04-015-4109 (Alternate), × 04-017-9180 (Alternate) Cross-Ref PDF #'s: Entry Date: 09/01/2009 Last Modification Date: 09/01/2015 Last Modifications: Update References: Туре DOI Reference Primary Reference Calculated from ICSD using POWD-12++. Crystal Structure Crystal Structure Source: LPF. "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). Structure

01-075-9985

Database Comments:

Jun 9, 2020 12:23 PM (fal-sharji2) 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.

20 (°)	d (Å)	I	h	k	1	20 (°)	d (Â)	I	h	k	1 *	28 (*)	d (Â)	I	h	k	1
19.0190	4.662400	1	0	1	1	76.6357	1.24234) m	4	0	0	111.1798	0.933657	15	4	1	4
21.0585	4.215220	11	1	1	0	76.9337	1.23827	91	3	1	3	111.3151	0.932903	20m	0	5	5
22.3212	3.979550	12	0	2	0	77.8983			0	5	3	111.3151	0.932903	m	55	1	20
26.1872	3.400160	999	1	1	1	77.8983			1	3	4	111.7113	0.930710	11	5	3	0
27.2256	3.272790	529	0	2 0 2	1	78.6942			220	5	2	112.3708	0.927107	1	4	5 8	225
31.0661	2.876390	40	0	0	2	79.3184	1.20692		2	4	32	112.8523	0.924513	6m	1	8	2
32.7373	2.733270	89	1	2	1	79.5022				6	2	112.8523	0.924513	m	2	4	5
33.0873	2.705150	520	0	1	220	80.2192			3	2	3	113.9404	0.918764	1m	3	2325	5
36.0484	2.489440	307	1	0	2	80.7396			1	5	3	113.9404	0.918764	m	5	3	1
36.1199	2.484680	236	120	0		82.3334			1	6	2	114.3802	0.916484	10m	1	2	6 5
37.2928	2.409180	117	0	3	1	82.3334			20	6	0	114.3802	0.916484	m	1	2	5
37.8344 38.4315	2.375930 2.340380	417	1	3	20	82.7286			4	4	4	114.6765 115.2748	0.914962 0.911922	10 5	42	28	4
		171		2	2	84,3065					ò				4	7	3
38.5888 41.1319	2.331200 2.192750	126	02	2	1	84.4015			324	5 6	1	115.6469 116.1228	0.910054 0.907690	12	2	6	4
41.6261	2.167850	7	1	2	1	84,9677			4	õ	2	116.3102	0.906767	6	4	6	0
42.8737	2.107610	192m		3224	2	85,1327			ő	1	5	117.3509	0.900707	2	õ	3	6
42.8737	2.107610	192m	12	2	ő	85.6287			3	3	53	118.3272	0.897099	6	3	5	4
45.5506	1.989780	33	õ	ā	ŏ	86.0441	1.12898		4	ĩ	2	118.8855	0.894508	10	32	ŏ	6
45.8133	1.978980	630	ž		1	86.2454			3	3	4	119,5912	0.891284	4	3	ž	3
46.5296	1.950170	5	20	2 3 4	2	86.3685	1.12557		23	5	1	120.1186	0.888912	1	2	Ť	26
48.3621	1.880470	387m	ň	Ă	ĩ	87.3492			õ	5 7	ł.	120,4969	0.887230	16	1	3	6
48.3621	1.880470	m	020	ö	3	87,8915			ĭ	1	5	120.8877	0.885509	19m	à.	ã	
48.8101	1.864250	6	õ	ĭ	3	88.3581	1.10529		Ó		5	120.8877	0.885509	m	5	ă	2
49.7874	1.829920	22	2	1	232	89.2676			4	2	52	121.4397	0.883107	3	ŏ	338	423
50.2137	1.815380	244	1	3	2	90,1033			1	7	1	122,4739	0.878696	5	5	4	1
51.9486	1,758760	35	4	4	1	90.3551	1.08598			ó	4	122.6606	0.877912	6		7	4
52.3740	1.745470	303	1	1	133	90.5734			32	6	2	122.8732	0.877024	20	152	÷	3
52.9610	1.727500	138m	ò		ă	91.1122			1	2	5	123,9169	0.872733	10m	2	2	6
52.9610	1.727500	m	2	232	1	91.4286	1.07601		3	ĩ	4	123.9169	0.872733	m	4	5	3
53,8835	1,700080	15	22	2	2	92,5351	1.06602		1	6	3	124,4300	0.870665	1	1	ğ	õ
56.1616	1,636400	20	õ	Ā	2	92.5351	1.06602			5		124,8058	0.869168	1m	0	6	
56.3370	1.631720	7	Ť	42	23	93.1477	1.06061		33	4	235	124.8058	0.869168	m	ĩ	ě.	5326
56,7161	1.621710	16	3	1	õ	93.7644			õ	3	5	125,9203	0.864812	7	4	6	2
59.1410	1.560870	66	3	1	1	93.7644) m	2	4	4	126.1973	0.863749	3	Ó	4	6
59,4648	1.553140	11m	02	3	3	93,9318			4	4	0	126,7968	0.861474	1	5	2	3
59,4648	1.553140	m	2	3 4	0	94,6393			3	2	4	128.2321	0.856171	1	1	6	5
60.2758	1.534170	23m	0	5	1	94.6393			4	3	2	128.9486	0.853598	1	3	4	5
60.2758	1.534170	m	2	53541	2	95.1683	1.04336) 6	1	54	4	129,9627	0.850039	6m	4	4	- 4
61.0774	1.515940	1	1	5	201	95,9943	1.03656	30	4	4	1	129.9627	0.850039	m	5	4	26
61.8223	1.499450	38	2	4		96.1641	1.03518	18	2	- 1	5	130,6663	0.847626	4	20	3	6
62.2028	1.491190	3	223	1	3	98.2047			232	6	1	131.3587	0.845296	1		98	2
62.8235	1.477940	27		2	1	98.3934			2	7	1	131.8536	0.843657	1	3	8	
63.3992	1.465900	30	1	5	1	99.4134		35	24	2	5	132.3060	0.842178	9	3	7	3
64.7678	1.438190	4	0	0	4	99.5838			4	2	3	132.8878	0.840303	2	332	67	4
64.9066	1.435450	7	nonn	0	24	100.066			32	З	4	133,1575	0.839444	5m	2	7	4
65.9487	1.415270	42	0	1	4	100.912	0 0.99889		- 2	6	3	133.1575	0.839444	m	4	1	453
66.0861	1.412660	35	3	1	20	101.311	5 0.99602		0	4	5	133.8396	0.837300	1	5	3	3
66.4892	1.405070	28		3	0	101.472	0 0.99488		0	8	0	134.8708	0.834135	6	5	5	1
67.1539	1.392770	1	0	54	234	102.239			4	4	2	135.1393	0.833326	4	1	9	236
67.7755	1.381500	Зm	0	4	3	102.915		12	3 0	5 8 5 7	3	135.5461	0.832112	1	23	8	3
67.7755	1.381500	m	1	0	4	103.546	8 0.98053		0	8	1	136.3299	0.829812	2m	3	0	6
68.6151	1.366630	23	2	4	24	103.546	8 0.98053		20	5	4	136.3299	0.829812	m	4	7	1
68.9302	1.361150	51	1	1	4	103.922			0	7	3	136.8802	0.828228	8	6	0	0
59.4293	1.352580	18	0	2	4	104.364			0	6	4	137.7490	0.825778	16m	3	1	6
69.5640	1.350290	5	3	2 5 4	2	104.494		5 9	325	6 3	25	137.7490	0.825778	m	4	2 5	5
70.1109	1.341090	14	1	5	2	104.828			2	3	5	139.3903	0.821317		0	5	6
70.7606	1.330360	4	1	4	22303	104.828			5	1	1	139.7303	0.820420	1	2052	6	5 6 5 7
70.9964	1.326520	9	0	6325	õ	105.844		3	4	5	1	140.8702	0.817479	3m	0	1	
71.5500	1.317610	1	2	3	3	106.427			1	8	1	140.8702	0.817479	m	5	0	4
72.3435	1.305100	7m	1	2	4	106.778			1	7	3	141.5159	0.815858	4m		4	6
72.3435	1.305100	m	2	5	1	106.908	5 0.95879		0	0	6	141.5159	0.815858	m	6	1	1
73.1558	1.292600	1	0	6	1	107.813	2 0.95324		3	4	4	142.5401	0.813353	18	5	1	4
	1.262500	58	3	3	2	108.033	9 0.95191	1	0	1	6	142.8651	0.812575	13m	3	2	6
75.1968					· .					22							- A E A
76.0123	1.250970	2		6	2	109.809	7 0.94143		1	Ó	6	142.8651	0.812575	m	3	2 5	6 5
			123		14	109.809 110.167 110.342	7 0.94143 3 0.93937	1 10	153	0					3	5	5

04-013-2116	

Empi Atom	ic %:	ormula:	Ca18	a0.93 .72 N	36 Mg0 Ag1.28	ssure/Ter .064 O3 O60.00	Wei		C12.12	Ca3	7.86 Mg1	.57 048	: Ca0.936 Mg 44 um Magnesiu			
Radia	ition:	CuKa1	λ:	1.54	06 Å	d-Spac	ing: (Calculate	ed In	tens	ity: Calc	ulated	VIc: 3.05	l/lc - l	ND: (.88
Auth Auth Dens	or's Ce Cell Mo ity [Do	bohedin II [Auti olVol: (alc: 2 0 K (Au	hCell 50.41 723 g	a: 4] Vcm ³	.9673(. Autho Dst	c (167) 3) Â A or's Cell / truc: 2.72 iperature)	Axial F 2 g/cm		la: 3.4 SS/FON	15]	AuthC 30) = 999		362.47 ų 0, 30)	AuthC	ell Z:	6.00
Cryst XtiCe Cryst Redu	al Data II y: 12 al Data	Axial all [Red	ell a: Xti Ratio ICell	4.96 Cell [c/a a: 4,	7Å Vol: 3 1: 3.41	RedCo	: 4.96 Xti 1.000 all b:	57 Å Cell Z:	6.00] 3.415 Rec] iCell	6.963 Å c: 6.340	6	ll α: 90.00* edCell α: 66		ell β:	90.00*
ADP:	U	Crystal	(Syn	nmet	ry Allo	wed): Ce	entrosy	/mmetrix	c							
5eq 1 2	Operati x.y.z -xyz	y Opera' or linates:	<u>Seq</u> 3 4	-y.x	erator -y.z +yz	<u>5</u> 5	Oper -x+y, x-y,x		<u>5en</u> 7 8	-y	erator 1,z+1/2 -z+1/2	<u>Seq</u> 9 10	Operator #,x+y,z+1/2 -x,-x+y,-z+1/2	<u>Seq</u> 11 12	-x+y	rator .y.z+1/2 y,-z+1/2
Atom Ca Mg C O	1234	Wycks 6b 6b 6a 18e	N M M M	8. 2. 2.	0000	0 0.0 0 0.0 0 0.0 0 0.0 2575 0.0	0.0	SOF 0.936 0.064 1.0 1.0	Uiso 0.01473 0.01473 0.01426 0.02852		I					
Aniso Atom Ca Mg C O	P	Displace Uani1 0.0151 0.0151 0.0128 0.0161	1 Ua 0.0 0.0 0.0	Parai ni22 1151 1151 1128 1336		0.0075 0.0075 0.0075 2 0.0064	5 0.0 5 0.0 2 0.0	0. 0. 0.	0							
LPF F LPF F Miner Cross	Prototy Prototy ral Clas s-Ref P	pe Stru pe Stru sificati	icture icture ion: 01-0	e (For Alp Calcil 389-1	rmula (oha Oro te (Sup 304 (R	d (Minera Order]: C der]: C C lergroup), lelated Ph Last I	a (C) a O3,1 calcite ase), (03),hR hR30,16 e (Group	30,167 7) Pe 1305 (Re	arso elate		I: hR10		/2010		
Refer Type	encesi	5	01_F	Inform												
	y Refere		C S	Calcula Single	ated from e-crystal	m LPF usin X-ray struc 151,1158 (1	ture rel		s of two is	ioger	ic magnesi	ian calcite	crystals*. Paqu	ette J., F	Reeder	RJ.Am.
Datat	oase Co	ommen											ginal Remarks . (1985) 70, 58			
d-Spa	cings (77) - Ca	0.936	MgC	.064 (C (03) - 04	-013-	2116 (S	tick, Fix	ed Si	it Intensil	ty) - Cu H	(o1 1.54056 Å	ł		
28 (*)		(Å)	1	h J	<u>s I</u>	* 28 (d (Å)	1	h	<u>1 *</u>	28 (=		1	hk	
23.164 29.553 31.620	9 3.0 8 2.8	336550 120030 327180	89 999 20	0 0	0 4	48.7 55.8 57.6	384 812	1.865910 1.618510 1.596850) 29) 85	2	1 6	64.983 66.031 69.570	71 1.413590 04 1.350180	56 30 9	3 0 0 1	0 12 7
36.135 39.600 43.364	4 2.2	183650 273950 084910	143 181 148	3 3	1013	58.4 60.9 61.3	781	1.578050	53	2	0 10 1 4 0 8	70.664 73.310 74.073	1.290260	18 27 6	0 2 2 3 0	10 8 6
47.350	1 1.9	018270	67 188	0 2	2 4	61_7 63_3	328	1.501410		1	9	76.67	36 1.241820	11 19	2 2	0 12

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1/2

04-013-2116 22(5) d(A) 784492 1.212900 80.6519 1.190170 81.3022 1.181470 82.0256 1.173800 82.2055 1.173800 85.2039 1.136840 85.2039 1.136840 85.2039 1.136840 85.05239 1.136840 87.0123 1.118880 87.0123 1.118880 87.0123 1.118880 87.0123 1.056510 95.2778 1.056510 95.2778 1.042450 95.5786 1.039800 95.68846 1.022930 96.8846 1.022930 99.84864 1.027650 99.9440 1.007660 * 20 (*) 102.8556 103.5836 104.2421 104.9024 106.5202 106.8537 108.1942 108.7518 109.4280 110.2807 111.3060 112.5652 114.8627 116.0013 118.8360 119.6750 120.3057 d (Å) II. h 321130023042434212 ٠ 2 1 2 1 1 4 6 5 1 7 2 4 4 8 16 15 12 2 3 1 2 1 3 2 1 2 3 4 0 0 1 8 16 15 12 2 1 1 1 2 3 1 1 0 2 4 3 1 0 1 1 1 1 2 0 0.985236 0.980289 0.975891 0.971652 0.961217 0.959137 0.959137 0.959137 0.947622 0.943648 0.942394 0.942394 0.932954 0.932954 0.926056 0.914011 0.908291 0.994736 0.894736 0.88078 12114 8 15 118 0 12 37 10 8 6 16 293881421118121667 152033516 1411720412 m221

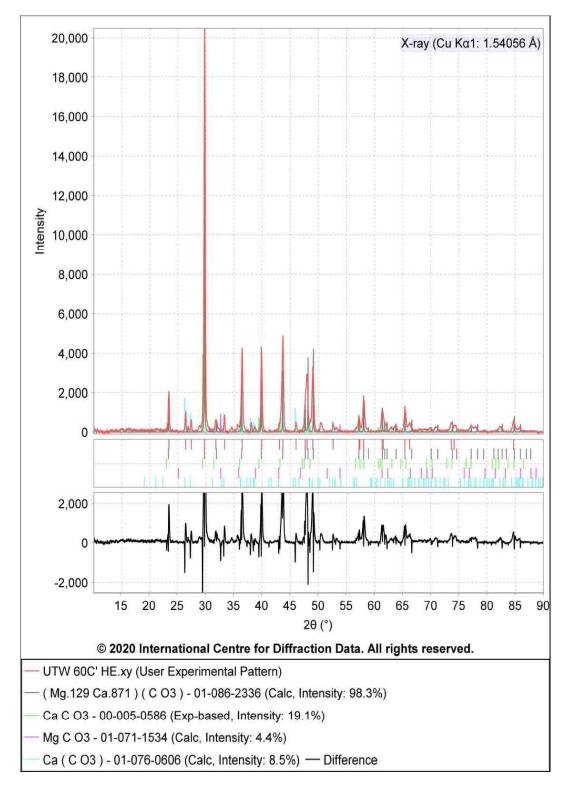


Figure E.5 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 60 °C from experiment with a tank with little exposure of iron.

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 <mark>Å</mark>	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 <mark>Å</mark>	D1 Range:	3.772 Å - 3.820 Å
Rotation: All	8 Rotations		

Preferences

Radiation: X-rayWavelength: Cu Ka1 1.54056 ÅSearch Method: HanawaltSearch Window:0.15°Match Window:0.15°2nd Pass Filter: Yesd-Spacings:WeightedLowest 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

 Status
 Primary
 QM: Star
 Pressure/Temperature: Ambient
 Chemical Formula: (Mg.129 Ca.871)(CO3)

 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
 Compound Name: Magnesium Calcium Carbonate

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 ų
 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 a: 90.00° XtlCell β: 90.00° XtlCell γ: 120.00° XtiCell Vol: 355.47 Å³ XtlCell Z: 6.00] Crystal Data Axial Ratio [c/a: 3.409 a/b: 1.000 c/b: 3.409] RedCell c: 6.293 Å RedCell a: 66.90° Reduced Cell [RedCell a: 4.938 Å RedCell b: 4.938 Å RedCell β: 66.90° RedCell y: 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:

Туре	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).

ANX: ABX3. Analysis: C1 Ca0.871 Mg0.129 O3. Formula from original source: (Mg.129 Ca.871) (C O3). Database Comments: 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.

20 (°)	d (Å)	I	h	k	1	*	20 (°)	d (Å)	I	h	k	1	*	20 (°)	d (Å)	I	h	k	1	*
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 03 Atomic %: C20.00 Ca20.00 O60.00 Empirical Formula: C Ca O3 Weight %: C12.00 Ca40.04 O47.95 Compound Name: Calcium Carbonate Mineral Name: Calcite, syn Filter: Ni Beta Intensity: Diffractometer Radiation: CuKa1 A: 1.5405 Å 1/lc: 2 SYS: Rhombohedral SPGR: R-3c (167)
 STS.
 Kholinoinadiai
 Group, Kall
 Kall Temp: 299.0 K (Author provided temperature) Color: Colorless Space Group: R-3c (167) Molecular Weight: 100.09 Space Group: Resc (107) molecular weight: 4,089 Å XtlCell c: 17.062 Å XtlCell α: 90.00° Xtl Crystal Data Atial [XtlCell vi: 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] XtiCell c: 17.062 Å XtiCell a: 90.00° XtiCell 6: 90.00° εα: =1.487 πωβ: =1.659 Sign: =-Atomic parameters are cross-referenced from PDF entry 04-012-8072 ADP: U Crystal (Symmetry Allowed): Centrosymmetric 5G Symmetry Operators: Seq Operator Seg Operator Seg Operator Sea Operator Seg Operator Seq Operator . 1 x,y,z 2 -x,-y,-z 5 -x+y,-x,z 6 x-y,x,-z 7 -y,-x,z+1/2 8 y,x,-z+1/2 9 x,x-y,z+1/2 11 -x+y,y,z+1/2 10 -x,-x+y,-z+1/2 12 x-y,-y,-z+1/2 34 -y,x-y,z y,-x+y,-z Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Uiso AET 0.0 0.0 0.0 1.0 0.01525 0.0 0.0 0.25 1.0 0.02084 0.25 0.0 0.25 1.0 0.02084 Ca 6b 6a 18e -3. 227 õ Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Educational Pattern, Forensic, Inorganic, Subfile(s): 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: 04-006-6528 (Alternate), < 04-007-2499 (Alternate), < 04-007-8659 (Primary), < 04-008-0788 (Alternate), < 04-007-2088 (Alternate), < 04-007-8659 (Primary), < 04-012-0489 (Primar CAS Number - PR: 13397-26-7 Entry Date: 09/01/1955 References: Type **DOI** Reference Primary Reference Crystal Structure Optical Data Swanson, Fuyat. Natl. Bur. Stand. (U. S.), Circ. 539 II, 51 (1953). Crystal Structure Source: LPF. Dana's System of Mineralogy, 7th Ed. II, 142. 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: Colortes. 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 form 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 Ku1 1.54056 Å
 33 - 00-005-0586 (5ttck, Fixee Jmt II

 h
 I
 *
 28 (°)
 d (Å)

 0
 1
 2
 48.6122
 18.7500

 0
 1
 2
 48.6122
 1.87500

 0
 0
 6
 57.4001
 1.6040

 1
 0
 58.0733
 1.58700

 1
 1
 50.6752
 1.52500

 2
 0
 2
 60.9675
 1.51600

 0
 2
 4
 61.3435
 1.51000

 0
 1
 8
 63.0548
 1.4730
 28 (°) d (Ā) I I hkl 28 (°) d (Å)
 d (A)
 1

 1.875000
 17

 1.626000
 4

 1.604000
 8

 1.587000
 2

 1.525000
 5

 1.518000
 4

 1.510000
 3

 1.473000
 2
 d (A) 3.860000 3.035000 2.845000 2.495000 2.285000 2.095000 1.927000 1.913000 d (A) 1.440000 1.422000 1.356000 1.339000 1.297000 1.284000 1.284000 23.0218 29.4049 31.4176 35.9654 12 100 3 14 18 18 0 1 0 0 1 1 0 0 1 1 1 2 0 2 1 0 0 1 64.6765 65.5972 69.2291 70.2364 72.8676 73.7264 76.2977 77.1749 3 0 0 1 2 2 0 2 1 3 2 1 1 1 1 6 2 1 1 2 1 2 10 2 10 2 10 4 2 1 2 5 0 12 7 10 8 6 0 53122112 39.4009 43.1447 47.1226 5 1.247000 1.235000 Page 1 / 2 63.0584 1.473000 © 2020 International Centre for Diffraction Data. All rights reserved.

00-005	-0586												Jun	9.2020	12:	27 1	PM	(fal-sharii2)
28 (°)	d (Å)	I	h	k	1		28 (°)	d (Å)	I	h	k	1	28 (°)	d (A)	1	h	k	1
80.9302	1.186900	<1	3	1	2	Ε	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	ō	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	D	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)
 Pressure/Temperature:
 Ambient
 Chemical Formula:
 Mg C 03

 Weight %:
 C14.25 Mg28.83 056.93
 Atomic %:
 C20.00 Mg20.00 060.00
 OM: Star Status Alternate Empirical Formula: C Mg O3 ANX: ABX3 Compound Name: Magnesium Carbonate Mineral Name: Magnesite, syn Radiation: CuKo1 A: 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: 279.7

 AuthCell MolVol: 46.62]
 Author's Cell Axial Ratio [c/a: 3.240]
 3.003 g/cm³
 Dstruc: 3 g/cm³]
 SS/FOM: F(30) = 599.5(0.0014, 36)
 AuthCell Vol: 279.74 Å3 AuthCell Z: 6.00 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 [XtiCell a: 4.637 Å XtiCell b: 4.637 Å XtiCell c: 15.023 Å XtiCell α: 90.00° XtiCell β: 90.00° XtiCell y: 120.00° XtiCell Vol: 279.74 Å3 XtlCell Z: 6.00] Atomic parameters are cross-referenced from PDF entry 04-009-2317 ADP: 8 Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: Seq Operator Seq Operator Seg Operator Seg Operator Seq Operator Seq Operator 12 X,Y,Z -X,-Y,-Z 34 -y,x-y,z y,-x+y,-z 5 -x+y,-x,z 6 x-y,x,-z 7 -y,-x,z+1/2 8 y,x,-z+1/2 9 x,x-y,z+1/2 10 -x,-x+y,-z+1/2 11 -x+y,y,z+1/2 12 x-y,-y,-z+1/2 Atomic Coordinates: Atom Num Wyckoff Symmetry x AET SOF Biso Z 0.2775 0.0 0.0 0.0 0.25 1.0 0.0 0.25 1.0 0.0 0.0 1.0 0.36879 1#a 0.34715 3#b 0.35475 6-a 18e 6a 6b 2323 C Mg -cum Anisotropic Displacement Parameters:
 Bani33
 Bani12
 Bani13
 Bani23

 0.0496549
 0.323079
 -0.0386154
 -0.0772308

 0.023177294
 0.2553433
 0.0
 0.0

 0.034178
 0.257947
 0.0
 0.0
 Bani22 Atom Num Bani11 0.469464 0.506867 0.51525 0.646158 0.506867 0.51525 Mg 23 Subfile(s): Cement and Hydration Product, Common Phase, Forensic, Inorganic, Mineral Related (Mineral , Synthetic) Mineral Classification: Calcite (Supergroup), calcite (Group) Pearson Symbol: hR10.00 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), Cross-Ref PDF #'s: Entry Date: 09/01/1998 Last Modification Date: 09/01/2011 Last Modifications: Reflections References: Type DOI Reference Calculated from ICSD using POWD-12++. Crystal Structure Source: LPF "The crystal Structure of magnesite". Oh, K.D., Morikawa, H., Iwai, S.I., Aoki, H. Am. Mineral. 58, 1029 (1973). Primary Reference Crystal Structure Structure 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 Ka1 1.54056 Å 20 (°) 28 (%) d (Å) hkl d (Å) I. h k l 28 (0) d (Å) I h 28 (°) 66 3734 66 3734 69 3074 69 3074 69 3074 70 2611 75 9444 76 8639 79 6378 81 4662 81 4662 20 (C) 83.2625 86.0062 87.8150 88.7338 88.7338 88.7338 92.3345 25.1251 32.6175 35.8342 38.8086 42.9522 46.7938 51.5718 3.541430 2.743030 2.503830 2.318500 1.407240 1.407240 1.371520 1.354660 1.159250 1.129380 1.110720 1.101580 1.101580 5 999 123 62 480 131 49 0101 58m 10 4 8 9 5 0 12 7 10 01010001000 881 22311312112 031122410 2460324 1001 m 18 83m 1221 10m m 114 39 16 16 28m m 70m 70m 21 1 1 6 2.103940 1.939770 1.770720 1.354660 12001 1.001580 1.067810 1.067810 1.051970 1.044330 1.036700 1.015240 0211 1.338590 1.251920 3020 53.8459 53.8459 61.3377 62.3627 1.701180 1.701180 1.510130 1.487750 389m m 47 70 1.239220 1.202880 1.180440 1.180440 86 2 6 1 14 2 11 21 1 1 2 2 13 86 © 2020 International Centre for Diffraction Data. All rights reserved. Page 1/2

01-071	-1534							255					Jun 9.	2020 12	27 P	M	fal	-sharii2)
20 (°)	d (Å)	I	h	k		<u>+</u>	20 (°)	d (Å)	1	h	k	1	 28 (°)	d (Å)	1	h	k	1 4
101,4432	0.995092	2	0	4	2	121	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	Ō	2	16	149.4430	0.798502	m	5	0	2

01-076-0606

Page 1/2

Pressure/Temperature: Ambient Chemical Formula: Ca (CO3) Status Alternate QM: Star 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: CuKa1 Intensity: Calculated I/Ic - ND: 0.57 **λ**: 1.5406 Å d-Spacing: Calculated I/Ic: 1.14 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]

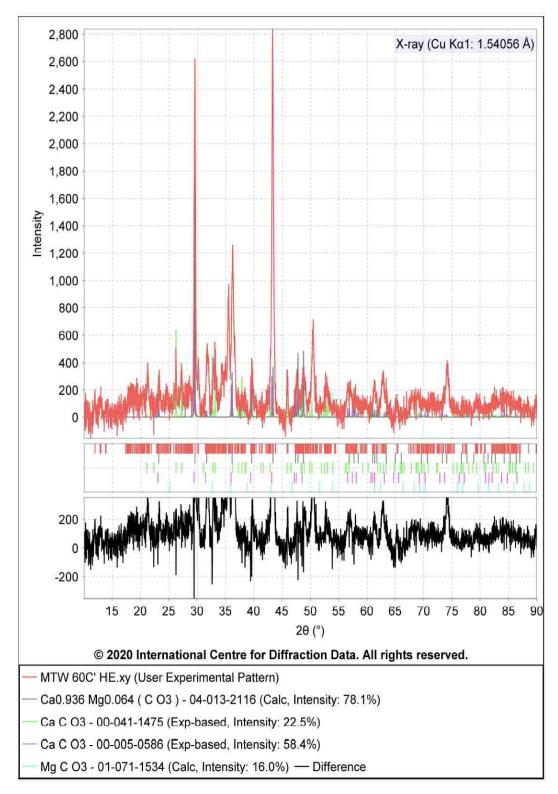
 Density [Dcalc:
 2.933 g/cm³
 Dstruc:
 2.93 g/cm³]
 SS/FOM:
 SS/FOM: F(30) = 306.0(0.0031, 32) Temp: 298.0 K (Author provided temperature) R-factor: 0.03 Space Group: Pnam (62) Molecular Weight: 100.09 Crystal Data [XtlCell a: 5.738 Å XtlCell b: 7.964 Å XtiCell c: 4.960 Å XtiCell α: 90.00° XtlCell β: 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 a: 90.00° RedCell y: 90.00° RedCell Vol: 226.65 Å3] RedCell 6: 90.00° Atomic parameters are cross-referenced from PDF entry 04-008-5421 ADP: B Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: Seg Operator Seq Operator Seq Operator Seg Operator -x+1/2,-y+1/2,z+1/2 x+1/2,y+1/2,-z+1/2 x+1/2,-y,-z -x+1/2,y,z x,y,z -x,-y,-z 3 4 56 -x,y+1/2,-z+1/2 x,-y+1/2,z+1/2 12 8 Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Biso AET x 0.25 0.25 0.25 0.24046 0.08518 0.09557 0.61095 0.43867 0.77616 Ca C O O 0.41508 0.76211 1.0 1.0 1.0 4c 4c 4c 9-a 3#a m... m. 3 m. 0 92224 1#2 ă 8d 0 47347 0.68065 0.08726 1.0 0.70856 1#2 Anisotropic Displacement Parameters: Bani22 Bani33 Atom Num Bani11 Bani12 Bani13 Bani23 0.665479 0.442997 1.13407 0.670266 0.573788 0.540783 0.497141 0.299269 0.653666 0.0201231 0.0073175 -0.05854 0.0 0.0 0.0 0.0 Ca 0.0 23 ö õ ň 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 Aragonite (Goup), Carbonate (Subgroup)
 Petrson Symbol: 0P2/001
 00-001-0628 (Deleted), 00-003-0405 (Deleted), 00-003-0425 (Deleted), 00-003-1067 (Deleted), 00-005-0453 (Alternate), 00-011-1475 (Primary), √0-061-0390 (Primary), 01-071-2392 (Alternate), 01-071-3206 (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), 01-075-9987 (Alternate), 01-078-4337 (Alternate), 01-078-4338 (Alternate), 01-078-4339 (Alternate), 01-080-2768 (Alternate), 01-080-2769 (Alternate), 01-080-2774 (Alternate), 01-080-2771 (Alternate), 01-080-2772 (Alternate), 01-080-2773 (Alternate), √04-006-5441 (Alternate), 01-080-2778 (Alternate), 01-080-2779 (Alternate), √04-006-5441 (Alternate), √04-006-6531 (Alternate), √04-007-048 (Alternate), √04-006-5421 (Primary), √04-012-0488 (Alternate), √04-014-1837 (Alternate), √04-017-9180 (Alternate), √04-0014-014 Cross-Ref PDF #'s: 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. "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). Structure © 2020 International Centre for Diffraction Data. All rights reserved.

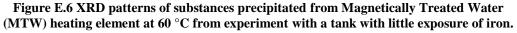
01-076-0606

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-Spacin	gs (199) - (Ca (C C)3)	- 0	1-076-0	506 (Stick,	Fixed Slit	Intensi	y)	Cu	Ka1 1.5	4056 Å						
20 (°)	d (Å)	I	h	k	*	20 (°)	d (Å)	1	h	k	*	20 (°)	d (Å)	I	h	k	1	*
19.0476	4 655460	2	0	1	1	78 0719	1 223040	61m	0	5	3	107 3104	0 956317	m	1	6	4	_
21.0843	4.210120	16	1	1	0	78.0719	1.223040	m	1	3	4	108.0705	0.951693	2	3	4	4	
22.3070	3.982050	6	0	2	0	78.7469	1.214240	13	2	5	2	108.4368	0.949496	1m	0	1	6	
26.2324	3.394400	999	1	1	1	79.4374	1.205410	66m	0	6	2	108.4368	0.949496	m	5	2	1	
27.2371	3.271430	562	0	2	1	79.4374	1.205410	m	23	4	3	109.9717	0.940501	1	0	8	2	
31.1487	2.868950	47 80	0	0	2	80.4086 80.8134	1.193280	3 48	3	2 5	3	110.4965	0.937503	10m	35	7	0	
32.7667 33.1629	2.730880 2.699160	504	ò	2	1	81.0531	1.188320	5	2	2	4	110.4965 110.7283	0.937503 0.936191	m 13	3	1	25	
36,1390	2.483410	341m	1	ò	2	82.3274	1.170260	63m	1	6	2	111.6453	0.931074	22m	õ	5	5	
36,1390	2,483410	m	2	õ	õ	82.3274	1,170260	m	2	6	õ	111.6453	0.931074	m	5	1	2	
37.2904	2,409330	134	ō	3	1	82.8786	1.163870	5m	õ	4	4	111.9847	0.929209	11m	0	2	6	
37.9191	2.370820	404	1	1	2	82.8786	1.163870	m	3	4	2	111.9847	0.929209	m	5	3	0	
38.4291	2.340520	256	1	3	0	83.2640	1.159460	30	4	2	1	112.7645	0.924984	7	3	7	1	
38.6486	2.327730	191	0	2	2	84.4061	1.146660	1m	2	6	1	113.1648	0.922846	9	2	4	5	
41.2106 41.6400	2.188740 2.167160	129	2	13	1	84.4061 85.1817	1.146660	m 7	3 4	5 0	0	114.2302 114.2302	0.917259	2m	3 5	23	5	
42.9282	2.105060	5 196m	1	2	2	85.3989	1.138190	2	0	1	5	114.2302	0.917259 0.915107	m 13	1	5	5	
42.9282	2.105060	m	2	2	ō	85.6568	1.133090	2	1	4	4	115.0462	0.913078	10	4	2	4	
45.5204	1,991030	36	õ	4	ŏ	85,8090	1,131470	4	3	3	3	115.2383	0.912106	13m	2	8	1	
45.8799	1.976260	665	2	2	1	86,2559	1,126750	15	4	1	2	115,2383	0.912106	m	5	2	2	
46.5718	1.948500	5	0	3	2	86.4412	1.124810	31m	2	3	4	115.7275	0.909652	1	2	7	3	
48.3476	1.881000	268	0	4	1	86.4412	1.124810	m	3	3 5 7	1	116.4459	0.906101	10	4	6	0	
48.4808	1.876140	204	2	0	2	87.2943	1.116000	1	0	7	1	117.7705	0.899719	2	0	3	6	
48.9360	1.859750	4	0	1	3 2	87.9932	1.108930	4	1	7	0 0	118.5919	0.895866	10	3	5	4	
49.8970 50.2673	1.826160	22 271	2	13	2	88.1672 88.6200	1.107190	25 13m	1	12	5 5	119.3738 119.6744	0.892271	9 8m	20	07	64	
51.9482	1.758770	30	1	4	1	88.6200	1.102700	m	4	3	1	119.6744	0.890908	m	3	7	2	
52,5071	1.741360	298	1	1	3	89.1450	1.097560	1	2	5	3	120.2392	0.888374	1	3	3	5	
52.9425	1.728060	69	2	3	ĩ	89.4746	1.094370	14	4	2	2	120.6116	0.886723	ż	2	Ť.	6	
53.0746	1.724070	135	0	2	3	90.0590	1.088780	9	1	7	1	120.9420	0.885271	19	1	3	6	
53.9824	1.697200	22	2	2	2	90.6108	1.083580	11m	2	6	2	121.2338	0.883999	18m	4	3	4	
56.1870	1.635720	24	0	4	2	90.6108	1.083580	m	3	0	4	121.2338	0.883999	m	5	3	2	
56.4588	1.628490	9	1	2	3	91.3838	1.076420	1	1	2	5	122.3108	0.879384	4	2	8	2	
56.8289 59.2633	1.618760 1.557940	18 58	3	1	0	91.6937 92.6397	1.073590 1.065090	10 12m	3	1 6	4	122.7979 122.7979	0.877338	10m	15	7	4	
59.4893	1,552560	11m	õ	3	3	92.6397	1.065090	1210 m	3	5	2	123,3035	0.875241	m 16	5	1	3	
59,4893	1.552560	m	2	4	ŏ	93,3182	1.059120	1	3	4		124.4260	0.870681	11m	52	2	ő	
60,2493	1.534780	16	õ	5	1	93,4929	1.057600	1	ŏ	Ż	3	124,4260	0.870681	m	4	5	3	
61.0507	1.516540	1	1	5	0	93.9563	1.053600	13m	0	3	5	124.7511	0.869385	1	1	8	3	
61.8580	1.498670	54	2	4	1	93.9563	1.053600	m	2	4	4	125.0720	0.868116	1	0	6	5	
62.3580	1.487850	1	2	1	3	94.8403	1.046100	1m	3	2	4	126.1234	0.864032	14	4	6	2	
62.6781	1.481020	1	1	3	3	94.8403	1.046100	m	4	3	2	126.6479	0.862036	2	0	4	63	
62.9369 63.3852	1.475550 1.466190	29 54	3 1	25	1	95.3164 96.1543	1.042130 1.035260	10 35m	1	5 7	4	127.2433 128.5242	0.859803 0.855116	1	5	26	5	
64,9564	1.434470	3	ò	õ	4	96.1543	1.035260	m	4	4	1	129,3883	0.852043	- á	3	4	5	
65.0593	1.432450	5	ž	ŏ	2	96.4736	1.032680	16	2	1	5	130,3804	0.848601	5m	4	4	ž	
65.9319	1,415590	5	2	2	3	98,3804	1.017700	2	22	7	1	130.3804	0.848601	m	5	4		
66.1336	1.411760	41	0	1	4	99.7224	1.007580	32	2	2	5	131.2150	0.845776	4m	0	9	22	
66.2363	1.409820	32	3	1	2	99.8494	1.006640	27	4	2	3	131.2150	0.845776	m	2	3	6	
66.5803	1.403370	32	3	3	0	100.3244	1.003150	29	3	3	4	131.8804	0.843569	1	3	8	1	
67.9711	1.378000	2m	0	4	3	101.0037	0.998231	4	2	6	3	132.4764	0.841626	16m	3	7	3	
67.9711 68.6832	1.378000	m 29	12	04	4	101.3840 101.5617	0.995513 0.994252	4	00	8	0	132_4764 133_3452	0.841626 0.838850	m 5m	52	57	04	
69.1232	1.357820	50	í	1	4	102.4357	0.994232	7	4	4	2	133.3452	0.838850	m	3	6	4	
69.6058	1,349580	19	ò	2	4	103.0774	0.983719	15m	3	5	3	133,7578	0.837555	2	4	1	5	
70,1318	1.340740	22	1	5	2	103.0774	0.983719	m	5	5 1	ŏ	134,3266	0.835794	2	5	3	3	
70.9453	1.327350	15	0	6	0	103.4990	0.980859	10	0	8	1	135.0605	0.833563	13m	1	9	32	
71.6832	1.315490	1	2	3	3	103.7316	0.979294	7	2	5	4	135.0605	0.833563	m	5	5	1	
72.3461	1.305060	5	2	5	1	104.4904	0.974251	11m	0	6	4	135.6210	0.831890	7	2	8	3	
72.5282	1.302230	3	1	2	4	104.4904	0.974251	m	1	4	5	136.4369	0.829502	1	4	7	1	
73.1164	1.293200	1 61	0	6	1	104.5872	0.973614 0.970181	11 17m	3	6	2	137.0293	0.827803	1	3	0	6	
75.3277 75.9844	1.260630 1.251360	1	3 1	36	2	105.1133 105.1133	0.970181	17m	2 5	3	5 1	137.4433 138.3947	0.826633 0.823997	6 12	64	02	05	
76.6817	1.241710	34m		0	4	105.9975	0.964511	2	4	5	1	139.9316	0.819893	1m	0	5	6	
76.6817	1.241710	m	2 3	4	1	106.3597	0.962224	2	1	8	1	139.9316	0.819893	m	2	6	5	
76.8104	1.239950	57	4	Ó	0	106.8204	0.959344	21	1	ž	3				~			
77.1290	1.235620	87	3	1	3	107.3104	0.956317	22m	0	0	6							

© 2020 International Centre for Diffraction Data. All rights reserved.





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 W	avelength: Cu Kal 1.54056 Å	Search Method: Hanawalt
Search Window: 0.15	Match Window: 0.15°	2nd Pass Filter: Yes
d-Spacings: Weighted	Lowest Allowable GOM: 2	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

Atomi	c %: (a18.7).936 2 Mg	Mg0.0			t %: (C12.12	2 Ca3	7.86 Mg	Formula 1.57 O48 ne: Calc	.44		525 C 4		
Radia	tion: (CuKa1	A: 1	.540	6 Å	d-Spaci	ng: Cai	culate	d lı	ntens	ity: Cal	culated	l/lc:	3.05	l/lc -	ND: 0	88
Autho AuthC Densi	r's Cel iell Mo ly [Dc	bohedra II [Auth IVol: 6i alc: 2.7 D K (Auti	Cell a: 0.41] 23 g/c	4.9 m ³	Author' Dstru	Å Au s Cell A c; 2.72	g/cm ³]	lo [c/	/a: 3.4 SS/FOM	115]		Cell Vol: 9.9(0.000			AuthO	cell Z:	6.00
Crysta (tiCel Crysta Reduc Reduc	al Data Iγ: 12 al Data ced Cel all β: 6	Axial R II [Red 6.94*	II a: 4 XtlCo atio [Cell a: Red0	.967 ell Vo c/a: 4.90 Cell y	Å X 3.415 57 Å 7: 60.0	a/b: RedCe 0° Re	4.967 XtiCe 1.000 II b: 4.9 dCell V	Å : c/b: 67Å ol: 13	6.00] 3.415 Re 20.82 /] dCell	5.963Å ⊄: 6.34	3	ell a: RedCel	90.00* Ila: 66		ell β:	90.00*
ADP:		Operation Operation		ietry	Allowe	ad): Cer	ntrosym	netric									
<u>Seg (</u> 1) 2 -	Dperato Ly.z XYZ	<u>.</u>	<u>Seg </u> 3 -	<u>Opers</u> -y, x-y, y, -x+y	z	<u>5</u> 5	Operat -x+y,-x,: x-y,x,-z		<u>5eg</u> 7 8	-y,-)	zator z+1/2 z+1/2	9 10	Oper: x,x-y,z -x,-x+		<u>Seq</u> 11 12		ator /.z+1/2 z+1/2
Atom	Num	Wyckol	f Syn	met	ту х	v	z s	OF	Uiso	AE	L						
a Ig	123	6b 6b 6a	333		0.0 0.0 0.0	0.0 0.0 0.0	0.0 0	.064	0.0147 0.0147 0.0142	3 6							
) Anisot	4 ropic D	18e Isplacen	.2 sent Pa	arəm		75 0.0	0.25 1	.0	0.0285	2							
	Num 1 2 3 4	Uani11 0.0151 0.0151 0.0128 0.0161		22	Vani33 0.014 0.014 0.0172 0.0306	Uani12 0.00755 0.00755 0.00642 0.00849	0.0 0.0 0.0	0.0	9 (
LPF P LPF P Miner Cross Last N Refere	rototy rototy al Clas -Ref Pi lodific	pe Struc sificatio DF #'s: ation D	ture [ture [on: Ca 01-08 ate: 0 01-08 ate: 0 Cal	Form Alph alcite 9-13(9/01/ feren iculate	a Orde (Super 04 (Rela 2011	.PF using	a (C O3 i O3,hR alcite (0 se), 01- lodifica),hR3 30,167 Group) 089-1 Lions: 2++.	80,167 7 305 (R Refle	elarso elatec	n Symbo I Phase) I) 00 y Date	: 09/01			
Structu	re		"Sir Min	ngle-o	rystal X- 75 1151	ray struct 1158 (19	are refine	ments	of two k	biogen	c magnes	sian calcit	e crysta	is". Paqı	ette J., i	Reeder	R.J. Am.
Datab	ase Co	omment	AN s: Am	X: Al	BX3. LF heral. (1	F Collec	tion Co 1183. s	ame s	sample	studi	ed in Am	attern Or Minera	iginal I I. (198	Remark 5) 70, 5	s: same 81. Ten	e samp Iperati	le studied ire of Data
d-Spac	ings (7	77) - Cat	.936 M	lg0.0	164 (C I	33)-04	013-21	16 (S t	ick, Fir	ced Sl	t Intensi	ity) - Cu	Ka1 1.	54056 A			
28 (*)	9 3.0	36550 20030 27180	L h 89 0 999 1 20 0	0	24	28 (* 48.76 56.83 57.68 58.43	39 1.8 84 1.6 12 1.5	A) 65910 18510 96850 78050	29	h 1 2 2 2		20 (9 64.98 66.03 69.57 70.66	134 1 171 1 104 1	433940 413590 350180 331940	1 56 30 9 18	h k 3 0 0 0 2 1 0 2	0 12 7 10
23.164 29.553 31.620 36.135 39.600 43.364 47.350 47.350	4 2.4 4 2.2 0 2.0 1 1.9	73950 84910 18270	143 1 181 1 148 2 57 0 188 0	1	0 3 2 4 8	60.97 61.34 61.73 63.38	81 1.5 31 1.5 28 1.5	18170 10010 01410 66240	53 22 22 17	2211	4 8	73.31 74.07 76.67 77.65	28 1 36 1	290260 278850 241820 228540		0 2 2 0 2 1 1	8 6 0 12

04-013-2116 26(5) d(Å) 78.8492 80.6619 11.90170 81.3002 82.0256 11.90170 82.20256 11.91470 82.20256 11.73800 82.20256 11.73800 82.20256 11.73800 85.2039 11.25530 85.2039 11.25530 85.2039 11.25530 85.2785 10.056910 93.7158 10.056910 93.7158 10.056910 95.2788 10.024502 95.5986 10.023500 96.8846 10.023500 96.8846 10.023500 96.8846 10.023500 96.8846 10.023500 96.8846 10.023500 96.8846 10.023500 96.8846 10.023500 96.8846 10.023500 96.8846 10.023500 96.8846 10.075600 99.84400 10.076600 99.84400 10.076600 99.84400 10.076600 99.84400 10.076600 99.84400 10.076600 99.84400 10.076600 99.84400 10.076600 99.84400 10.076600 99.84400 10.076600 99.84400 10.076600 99.84400 10.0766000 10.0766000 10.0760

I

 d (Å)
 I

 0.985/236
 2

 0.800/289
 9

 0.975/891
 3

 0.9775/821
 8

 0.9672/17
 8

 0.9672/17
 8

 0.9509/09
 4

 0.945644
 1

 0.9436448
 1

 0.9282544
 1

 0.9387311
 14

 0.9329541
 8

 0.943645
 1

 0.9260565
 1

 0.9436443
 1

 0.9387311
 14

 0.9329541
 8

 0.943645
 1

 0.943646
 1

 0.943645
 1

 0.9387311
 14

 0.9329541
 8

 0.890905
 6

 0.884078
 7
 28 (°) 102.8556 103.5835 104.2421 104.9024 106.5202 108.1942 108.7518 109.4280 109.6438 110.2807 111.3060 112.5662 114.8627 116.0013 118.8560 119.6750 119.6750 . h k l
 k
 I

 1
 21014

 32114
 30023014

 48151118
 0123708

 616
 112034
 .

00-005-0586 Jun 9, 2020 12:39 PM (fal-sharji2)
 Status Primary
 QM: Star
 Pressure/Temperature: Ambient
 Chemical Formula: Ca C03

 Empirical Formula:
 C Ca O3
 Weight %: C12.00 Ca40.04 O47.95
 Atomic %: C20.00 Ca20.0

 Compound Name:
 Calcium Carbonate
 Mineral Name: Calcite, syn
 Atomic %: C20.00 Ca20.00 O60.00 Radiation: CuKo1 A: 1.5405 Å Filter: Ni Beta Intensity: Diffractometer 1/1c: 2 SYS: Rhombohedral SPGR: R-3c (167) AuthCell Vol: 367.78 Å³ AuthCell Z: 6.00 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 γ: 120.00° XtlCell Vol: 367.78 Å³ XtlCell XtiCell c: 17.062 Å XtiCell α: 90.00° XtiCell β: 90.00° XtiCell Z: 6.00]
 KitCell γ:
 120:00
 AltCell vol. 307/76 A*
 Autoritz.
 0.000 [
 2
 3
 7
 Autoritz.
 0.000 [
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 B
 A
 C
 O
 O
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 D
 <thD</th>
 <thD</t 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 2 -x,-y,-z 34 -y,x-y,z y,-x+y,-z 5 -x+y,-x,z 6 x-y,x,-z 7 -y,-x,z+1/2 8 y,x,-z+1/2 9 x,x-y,z+1/2 10 -x,-x+y,-z+1/2 11 -x+y,y,z+1/2 12 x-y,-y,-z+1/2 Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Uiso AET Ca 6b 6a 18e 0.0 0.0 0.0 1.0 0.0 0.0 0.25 1.0 0.25 0.0 0.25 1.0 0.01525 0.02084 0.02084 -322 23 Cement and Hydration Product, Ceramic (Bioceramic), Common Phase, Educational Pattern, Forensic, Inorganic, Subfile(s): 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 01-072-1937 (Alternate), 01-083-0577 (Alternate), 01-083-0578 (Alternate), \checkmark 04-001-7249 (Alternate), \checkmark Cross-Ref PDF #'s: 04-006-6528 (Alternate), \checkmark 04-007-2808 (Alternate), \checkmark 04-007-4388 (Alternate), \checkmark 04-007-8659 (Primary), \checkmark 04-008-0788 (Alternate), \checkmark 04-012-0489 (Primary), \checkmark 04-012-8072 (Alternate) CAS Number - PR: 13397-26-7 Entry Date: 09/01/1955 References: Type DOI Reference Primary Reference Crystal Structure Optical Data Swanson, Fuyat. Natl. Bur. Stand. (U. S.), Circ. 539 II, 51 (1953). Crystal Structure Source: LPF. Dana's System of Mineralogy, 7th Ed. II, 142. 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. Database Comments: d-Spacings (45) - Ca C O3 - 00-005-0586 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å 28 (°) 48 5122 56 5530 57 4001 58 0733 60 6762 60 9857 61 3435 63 0584 J 0 0 12 1 7 1 2 10 1 2 2 1 2 10 1 2 8 3 0 6 2 0 1 12 Page 1 / 2 28 (*) d (Å) d (Å) 28 (°) Т hkl + 174825432 h k 1 d (Å) 23.0218 29.4049 31.4176 35.9654 39.4009 43.1447 47.1226 47.4886 3.860000 3.035000 2.845000 2.495000 2.285000 2.095000 1.927000 1.913000 12 100 3 14 18 18 5 17 1.875000 1.626000 1.604000 1.587000 1.525000 1.518000 1.510000 1.473000 20 C1 64 6765 65 5972 69 2291 70 2364 72 8676 73 7264 76 2977 77 1749 1.440000 1.422000 1.356000 1.339000 1.297000 1.284000 1.247000 1.235000 01011200 10011021 24603248 61210 4895 30201321 11201010 53122112 1221 © 2020 International Centre for Diffraction Data. All rights reserved. Jun 9, 2020 12:39 PM (fal-sharji2) 00-005-0586 d (Å) 20 (°) d (Å) 28 (* 20 (°) h k 94.6975 95.0075 96.1617 97.6440 99.1573 102.2384 102.9484 103.8950 104.1201 105.8419 106.1414 107.3295 109.5566 110.4794 0.978200 0.976700 0.965500 0.963600 0.956200 80.9302 81.5449 82.1106 83.7646 84.7850 1 186900 1 179500 1 172800 1 153800 1 142500 2 E 10 14 E 4 6 11 14 Ε 1.047300 1.044700 1.035200 TW1401 342727 4312332 0101023 4 8 16 13 12 1 2 3224212 10 14 4 8 16 0 12 3201212 1113220 324<122 100042 1.023400 1.011800

0.989500

0.942900 0.937600

86.4804 93.0691

Compo	Primary al Formul und Name	a: CO	Ca O3	Pressure/Ten Weight %: (onate Min		0.04 04	7.95			la: Ca C C 20.00 Ca20		60.00	1	
Radiatic	on: CuKa	1 A:	: 1.5406	4-Spac	ing: Diff.	Intens	ity: I	Diffractor	neter	1/lc: 1				
Author's AuthCe Author's Density	orthorhomb s Cell [Au II Vol: 22] s Cell Axia [Dcalc: 298.0 K (A	thCel 7.11 Å al Rati 2.927	ª Auth o[c/a:1 g/cm³ [23(3) Å A Cell Z: 4.00	0.623 (g/cm ³]	eli Mol\ :/b: 0.7 SS/F	/ol: 5 21] 2M: 1		20.6(0.0	7439(3) Å 040, 34)				
rystal tlCell rystal leduce	Group: Pn Data [Xtif γ: 90.00 ⁻ Data Axia d Cell [Re β: 90.00 ⁻	Cell a: Xtil I Ratic edCell	5.744 Å Cell Vol: o[c/a: 0	227.11 Å* 864 a/b: Å RedCo	: 7.968 Å XtiCell Z:	4.00] /b:0.62 Å R	3] edCe	4.962 Å II c: 7.9		ell a: 90.0 RedCell a			H B :	90.00°
a: =1.5	5300 π	ωβ: =	1.6810	ε γ: =1.685	4 Sign:	- 2	V: =1	8(calc.)*						
Crystal G Symr	(Symmetr netry Oper	y Allo	wed): Ce	erenced from entrosymmetr	ic.	- Cherroretter			DP: U	10.00				
eq Op				perator		Operato				rator +1/2,-z+1/2	-			
×.¥	-yz		4 x+	+1/2,-y+1/2,z+1 1/2,y+1/2,-z+1/	2 6	x+1/2,-y. -x+1/2,y,	z		- , y x, -y	1/2,2+1/2				
tomic (Coordinate	5.¢												
			Symmetry		z	SI		SO AET						
a 1	4c 4c		m		41502 0.75 76194 -0.08									
234	4c		m		02238 -0.09	453 1.	0							
ubtile(and a growth as	Carl I Construction of): CCaO				
rototy PF Pro PF Pro Ineral Ineral	Materi pe Structu ototype Str ototype Str Classifica Ref PDF #1	ructur ructur ructur ation: s: 00- 04-	e (Formu e (Alpha Aragonite 005-0453 -007-0048	der]: Ca C (la Order]: C Order]: C C (Group), car (Alternate), ((Alternate), S	a [C O3],o a O3,oP20, bonate (Su)1-071-239 / 04-008-54	P20,62 62 bgroup) 2 (Altern 121 (Prir	Pe ate), f	earson 8 01-076-0	iymbol: 606 (Allı	oP20:00 emate), ∉ (Alternate)	04-006	-5441	(Alte	rmate), √
PF Pro PF Pro PF Pro lineral ross-F	Materi pe Structu ototype Str ototype Str Classifica Ref PDF # mber - PR	ructur ructur ructur ation: s: 00- 04-	e (Formu e (Alpha Aragonite 005-0453 -007-0048	la Order]: C Order]: C C (Group), car (Alternate), ((Alternate), (a [C O3],c a O3,oP20, bonate (Su)1-071-239	P20,62 62 bgroup) 2 (Altern 121 (Prir	Pe ate), f	earson 8 01-076-0	iymbol: 606 (Allı	ernate), 🗸 (04-006	-5441	(Alte	ernate), 🗸
Prototy PF Pro PF Pro Mineral Cross-F CAS Nu	Materi pe Structu ototype Str Classifica Ref PDF #1 mber - PR	re [For ructur ructur s: 00- s: 04- t: 147	e (Formu e (Alpha Aragonite 005-0453 007-0048 91-73-2	la Order]: C Order]: C C e (Group), can (Alternate), ((Alternate), Entry Date	a [C O3],o a O3,oP20, bonate (Su)1-071-239 / 04-008-54	P20,62 62 bgroup) 2 (Altern 121 (Prir	Pe ate), f	earson 8 01-076-0	iymbol: 606 (Allı	ernate), 🗸 (04-006	-5441	(Alte	rmate), √
.PF Pro .PF Pro Mineral Cross-F CAS Nu Reference	Materi pe Structu ototype Structu totype Structure Classifica Clas	re [For ructur ructur s: 00- s: 04- t: 147	e (Formu e (Alpha Aragonite 005-0453 007-0048 91-73-2 Reference Keller, L., F Crystal Stm Dana's Sys	la Order]: C Order]: C C e (Group), can (Alternate), ((Alternate), Entry Date	a [C O3], c a O3, oP20, bonate (Su)1-071-239, 04-008-54 ; 09/01/19 ; 09/01/19	P20,62 62 bgroup) 2 (Altern 121 (Prir 91 State Ur 1, 182 (15	Pr ate), nary), niv_ Te 61).	mpe, AZ,	iymbol: 606 (Alt 2-0488 (USA. ICE	ernate), ∠ (Alternate)			(Alte	emate), ↓
Prototy PF Pro PF Pro Aineral Cross-F CAS Nu CaS Nu Ceferency Primary F Crystal S Optical D Structure	Materi pe Structu ototype Structu totype Structure Classifica Clas	ents:	e (Formu e (Alpha (Aragonite 005-0453 007-0048 91-73-2 Reference Keller, L., F Crystal Str. Dana's Sys- Jarosch, D. Additional 01-071-23 Colorless. Bilin, Bohe	la Order]: C Order]: C C e (Group), cai (Alternate), ((Alternate), Entry Date Rask, J., Bused acture Source: term of Mineral , Heger, G. Tsi Patterns: To	a [C 03],c a 03,0P20, bonate (Su)1-071-239; 04-008-5; ; 09/01/19 c, P, Arizona PF, gy, 7h Ed I thermaks Mir replace 00- 6-0606. An rmments: An stovakia. St	P20,62 62 bgroup) 2 (Altern 121 (Prir 91 state Ur 1, 182 (15 heral, Pet -005-04 alysis; O alysis; O	Pr ate), (nary), niv., Te 51), rogr. N 53 and Microp ptical	mpe, AZ, itt. 35, 12 itt. 35, 12 itt. 35, 12	iymbol: 606 (Alti 2-0488) USA. ICE 7 (1986). ad by cal liyses (w scimen I	D Grant-in-/	tiern OC r Ca, au	9).)-024- nd tra ata on	0025 ce Si sper	i. See PDF r(<<1). Color. simen from
Prototy PF Pro Mineral Cross-F CAS Nu Ceference VPC Cross-F CAS Nu Ceference VPC Cross-F Case Cose Cose Cose Cose Cose Cose Cose Co	Materi pe Structu pototype Str Classifica Ref PDF #' mmber - PR cessi Reference tructure ata	rre [Fc ructur ructur ructur s: 00- 04- t: 147 DOI	e (Formu e (Alpha t Aragonite 005-0453 007-0048 91-73-2 Reference Ketter, L., R Crystal Str. Dana's Sys Jarosch, D. Additiorial 01-071-23 Colorless, Bilin, Bohe Data Sour	la Order]: C Order]: C C (Group), car (Alternate), (Alternate), (Alternate), (Alternate), (Bask, J, Busee Atoms Sonroe, Stars Gonroe, Stars Gonroe, Star	a [C 03], d a 03,0P20, bonate (Su)1-071-239; r 04-008-5; r 04-008-5; r 04-008-5; r 04-008-5; r 09/01/19 c, P, Atizona LPF replace 00- 6-0606. An mentis: An slovakia. S liftraction. Fixed Sitt I	P20,62 62 bgroup) 2 (Altern 121 (Prir 91 state Ur 1, 182 (19 ers). Pet 005-04 alysis: 1 tacid. O ample S	P(ate), mary), niv_Te 61) rogr M 53 ann ficrop ptical ource	mpe, AZ, int. 35, 12 int. 35, 12 ivalidate robe and Data Spi or Loca	USA ICE 7 (1986). Hyses (v ecimen li ity: Spec	D Grant-in-A Culated part t.%), majo cation: Op imen from	tiern OC r Ca, au	9).)-024- nd tra ata on a, Mor	0025 ce Si sper	i. See PDF r(<<1). Color. simen from
rototy; PF Pro PF Pro Uneral (ross-Fi (AS Nu eferent rystal S S phical D phical D phical D phical D atabas	Materi pe Structu tototype Str Classifica Ref PDF #' imber - PR ces: Reference tructure ata	rre (Fc ructur ructur s: 00- t; 147 DOI	e (Formu e (Alpha I Aragonite 005-0453 007-0048 91-73-2 <u>Reference</u> Keller, L., R Crystal Str., L., R Colorless, Bilin, Bohe Data Sour 3 - 00-041 b. k. L	la Order]: C Order]: C C (cfoup), ca (cfoup), ca (Alternate), (Alternate), (Atternate), (Entry Date Market, J., Busec Latters Source, term of Mineral, Market, S. To Santo, Caller, Santo, Call General Cor General Cor General Cor Call Orlo, Call General Cor Call Collector, Call Call Collector, Call Call Collector, Call Call Collector, Call Call Collector, Call Collector, Call Collector, Call Call Collector, Call Collector, Call Collector, Call Collector, Call Call Collector, Call Call Call Call Call Call Call Call	a [C 03], c a (C 03], c a 03,0P20, bonate (Su 04-008-54 ; 09/01/19 c, P, Arizona P, PF replace 00 6-0606. An rmments: An slovakia. S liftraction. Fixed Sit I d (A)	P20,62 62 bgroup) 2 (Altern 121 (Prir 91 State Un 1, 182 (15 seral, Pet 005-04; alysis; 1 alysis; 1 tacid, O ample S	Pri ate), nary), niv_ Te 61). rogr. N 53 anti Aicrop Aicrop Ource ource	mpe, AZ, int 35, 12 int 35, 12 ivalidate robe and Data Spy or Loca Kol 1.5-	ymbol: 606 (Alt 2-0488 (USA. ICE 7 (1986). ad by cal lyses (w cimen li ity: Spec 1056 Å 29 (=)	amate), Alternate) D Grant-in-A culated pair (%); majo cation: Op imen from d (Å)	Nor (198 Item 00 r Ca, a Sefrou I	9).)-024- nd tra ata on a, Mor b k	0025 ce Si sper occo	i. See PDF r(<<1). Color. simen from
rototy PF Pro PF Pro lineral cross-F cAS Nu eference vpe rimary F rystal S prical D tructure	Materi pe Structu pototype Str Classifica Ref PDF #' mmber - PR cessi Reference tructure ata	rre [Fc ructur ructur ructur s: 00- 04- t: 147 DOI	e (Formu e (Alpha t Aragonite 005-0453 007-0048 91-73-2 Reference Ketter, L., R Crystal Str. Dana's Sys Jarosch, D. Additiorial 01-071-23 Colorless, Bilin, Bohe Data Sour	la Order]: C Order]: C C (Group), car (Alternate), (Alternate), (Alternate), (Alternate), (Alternate), (Alternate), (Alternate), (Alternate), (Bask, J, Busee Attace Source, (Alternate), (Bask, J, Busee Attace Source, (Alternate), (Bask, J, Busee Attace Source, (Bask, J, Bask, J	a [C 03], c a (C 03], c a 03,0P20, bonate (Su 04-008-54 ; 09/01/19 c PF c galace 00 c 6-0606 An replace 00 c 6-0606 An replace 00 c 6-0606 An replace 00 c 6-0606 An replace 00 c f of 0-0606 Sit I d () 3,274000 3,274000	P20,62 62 bgroup) 2 (Attern 421 (Prir 91 state Ur 1, 182 (15 seral, Pet 005-04: alysis: 1 tacid, O ample S so 50 6	P(ate), mary), niv_Te 61) rogr M 53 ann ficrop ptical ource	mpe, AZ, int. 35, 12 int. 35, 12 ivalidate robe and Data Spi or Loca	USA ICE 7 (1986). Hyses (v ecimen li ity: Spec	D Grant-in-A Culated part t.%), majo cation: Op imen from	tiern OC r Ca, au	9).)-024- nd tra ata on a, Mor	0025 ce Si sper	i. See PDF r(<<1). Color. simen from

28 (*)	d (Å)	I	h	k	1 *	26 (*)	d (Å)	1		k	1 *	28 (*)	d (Å)	1	h	k	1 *
37,8829	2.373000	45	1		2	62 2998	1.489100	1	23	1	3	77.9611	1.224500	3m	0	5	3
38.4039	2.342000	25	1	132	0	62,8965	1.476400	2	3	2	1	77.9611	1.224500	175	1202	500	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	3	64.8787	1.436000	4	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	11	5	3
42.8654	2.108000	m	2	2	0	66.1897	1.410700	4	03	11	2	80.9714	1.186400	2	2	52	4
45.8520	1.977400	55	2	23	1	66.5465	1.404000	3	30	3	0	82,2555	1.171100	3m	1	6	2
46,5339	1,950000	1	0	3	2	67.8369	1.380400	<1	Ö.	4	3	82,2555	1.171100	m	2	6	ō
48.3175	1.882100	25	0	4	1	68.6339	1.365300	2	2	4	2	82.8500	1.164200	1m	0	4	4
48,4435	1.877500	25	0	0	2	68,7716	1.363900	2	3	3	1	82,8500	1,154200	m	1004	4	2
48.8842	1.851500	2	02	1	23	69.0430	1.359200	5	1	1	4	83.2166	1_160000	2	- 4	20	1
49.8579	1,827500	4	2		2	69.5398	1.350700	2	0	2	4	85,1161	1.138900	1	- 4	ō	2
50.2279	1.814900	20	1	3	2	69.6578	1.348700	3	03	22	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	03423	3	3
52,4539	1.743000	25	1	1	3	70.8439	1.329000	1m	0	6	0	86,1940	1.127400	1	4	4	2
52.9114	1.729000	12	2	3	ii -	70.8439	1.329000	m	1	4	3	86,3655	1.125600	2m	2	3	4
53.0205	1.725700	16	0	2	3	72.2986	1.305800	1	2	5	1	86.3655	1.125500	m	3	3517	4
53,9411	1.698400	2	20	2	2	72,4464	1.303500	1	1	23	4	87,9962	1.108900	2m	- 3	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		3	76.6095	1.242700	3m	2	G	4	88,5389	1.103500	m	04	232	1
59.2273	1.558800	4	3	4	3	76.6095	1.242700	m	3	4		89.4092	1.095000	<1	4	2	2
60.2095	1.535700	2	0	5	1	76.7628	1,240600	4	4	0	0	1-22-02-547-51					
61.8292	1,499300	4	2	4	3	77.0640	1 236500	6	3	1	3						

```
01-071-1534
                                                                                                                                                                                                                                                                                           Jun 9, 2020 12:39 PM (fal-sharii2)

        Status Alternate
        QM; Star
        Pressure/Temperature: Ambient
        Chemical Formula: Mg C 03

        Empirical Formula:
        C Mg 03
        Weight %: C14.25 Mg28.83 056.93
        Atomic %: C20.00 Mg20.00 060.00

ANX: ABX3 Compound Name: Magnesium Carbonate Mineral Name: Magnesite, syn
Radiation: CuKa1 A: 1.5406 Å d-Spacing: Calculated Intensity: Calculated Vic: 1.83 Vic - 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:
        279.7

        AuthCell MolVol:
        46.62 ]
        Author's Cell Axial Ratio [c/a:
        3.240 ]
        Density [Decid:
        3.003 g/cm<sup>2</sup>
        Density [Decid:
        3.003 g/cm<sup>2</sup>
        SKFOM:
        F(30) = 599.5(0.0014, 36)

        Temp:
        298.0 K (Ambient temperature assigned by ICDD editor)
        R-factor:
        0.037

                                                                                                                                                                                                                                        AuthCell Vol: 279.74 Å* AuthCell Z: 6.00
 Space Group: R-3c (167) Molecular Weight: 84.31
Space Group: N-30 (167) Molecular Weight: 64-31
Crystal Data (XtiColl a: 4,637 Å XtiColl b: 4,637 Å XtiColl c: 15.023 Å XtiColl α: 90.00° XtiColl β: 90.00°
XtiColl γ: 120.00° XtiColl Vol: 279.74 Å<sup>3</sup> XtiColl 2: 6,00 ]
Crystal Data Axial Ratio [c/a: 3.240 a/b: 1.000 c/b: 3.240 ]
Reduced Coll [RedColl 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 Å<sup>3</sup> ]
 Atomic parameters are cross-referenced from PDF entry 04-009-2317
                                                                                                                                                                                                                                                      ADP: B
 Crystal (Symmetry Allowed): Centrosymmetric
SG Symmetry Operators:
                                                                                                                                                                                                                                                                                                                                                Seg Operator
Seg Operator Seg Operator Seg Operator Seg Operator Seg Operator
                                                                                                                                       5 -x+y,-x,z
6 x-y,x,-z
                                                                                                                                                                                                            7 -y,-x,z+1/2
B y,x,-z+1/2
                 x.y.z
-x.-y,-z
                                                                   3 -y,x-y,z
4 y,-x+y,-z
                                                                                                                                                                                                                                                                                   9 x,x-y,z+1/2 11 -x+y,y,z+1/2
10 -x,-x+y,-z+1/2 12 x-y,-y,-z+1/2
 Atomic Coordinates:
 Atom Num Wyckoff Symmetry x

        x
        y
        z
        SOF
        Biso
        AET

        0.2775
        0.0
        0.25
        1.0
        0.36879
        1#a

        0.0
        0.0
        0.25
        1.0
        0.34715
        3#b

        0.0
        0.0
        0.0
        1.0
        0.35475
        6-a

                                                                                                                                                                              SOF Biso
                                                                                                                                                                                                                              AET
                                           18e
6a
6b
 0
                                                                            2 32 3
                      23
 C
Mg
 Anisotropic Displacement Parameters:

        Banil1
        Bani22
        Bani33
        Bani12
        Bani23
        Bani23

        0.469464
        0.646158
        0.0495549
        0.232079
        -0.0386154
        0.0772308

        0.50687
        0.50687
        0.5077294
        0.23433
        0.0
        0.0

        0.51525
        0.51525
        0.034178
        0.257947
        0.0
        0.0

 Atom Num Bani11 Bani22 Bani33
 0
                      123
 Mg
 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: Alternate), 00-002-0875 (Deleted), 00-003-0773 (Deleted), 00-003-0788 (Deleted), 00-009-0479 (Primary), 00-036-0383 (Primary), 01-071-3698 (Alternate), 01-071-6263 (Alternate), 01-086-0042 (Alternate), 01-086-2344 (Alternate), < 04-009-2317 (Primary), < 04-010-3138 (Alternate), < 04-012-1188 (Alternate), < 04-012-1189 (Altern
 Entry Date: 09/01/1998 Last Modification Date: 09/01/2011 Last Modifications: Reflections
 References
                                                                             Reference
Calculated from ICSD using POWD-12++.
Crystal Structure Source: LPF.
"The crystal structure of magnesite". Oh, K.D., Morikawa, H., Iwai, S.I., Aoki, H. Am. Mineral. 56, 1029 (1973).
"The crystal structure of magnesite". Oh, K.D., Morikawa, H., Iwai, S.I., Aoki, H. Am. Mineral. 56, 1029 (1973).
 Type
Primary Reference
Crystal Structure
Structure
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 03 - 01-071-1534 (Stick, Fixed Slit Intensity) - Cu Ku1 1.54056 Å
 28 (*)
                               d (Å)
                                                                                       hki
                                                                                                                                          28 (*)
                                                                                                                                                                            d (Å)
                                                                                                                       .
                                                                                                                                                                                                             1
                                                                                                                                                                                                                                   hkl
                                                                                                                                                                                                                                                                                        28 (*)
                                                                                                                                                                                                                                                                                                                            d (Å)
                                                                                n K 245
0100113248
011021122
n 122
n 122

        n
        k
        l

        1
        0
        10
        10

        2
        0
        8
        9

        1
        2
        0
        8

        1
        1
        2
        0
        9

        1
        2
        0
        9
        1
        2
        0

        3
        0
        0
        12
        2
        1
        7
        0
        2
        8
        3
        0
        1
        2
        8
        3
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
        5
25.1251
32.6175
35.8342
                                3.541430
2.743030
2.503830
                                                                                                                                            66.3734
66.3734
68.3365
                                                                                                                                                                             1.407240 58m
1.407240 m
1.371520 18
1.354550 83m
1.254550 m
                                                                                                                                                                                                                                                                                        83.2825
86.0062
87.8150
                                                                                                                                                                                                                                                                                                                        1.159250
1.129380
1.110720
                                                                                                                                                                                                                                                                                                                                                                                2 2 0 3 1
                                                                 5
999
123
62
480
131
49
389m
47
70
                                                                                                                                                                                                                                                                                                                                                         881
                                                                                                                                            68.3365
69.3074
69.3074
70.2611
75.9444
76.8639
79.6378
81.4662
81.4662
                                                                                                                                                                            1.371520 18
1.354650 m
1.354650 m
1.338590 114
1.251920 39
1.239220 16
1.202880 16
1.202880 16
1.180440 28m
1.180440 m
                                                                                                                                                                                                                                                                                        87.8150
88.7338
92.3345
92.3345
94.1457
95.0518
95.9772
98.7025
                                                                                                                                                                                                                                                                                                                        1.110720 1
1.101580 m
1.067810 70m
1.067810 m
1.057810 70m
1.051970 21
1.04330 1
1.04330 1
1.036700 1
1.015240 6
                                                                                                                                                                                                                                                                                                                                                                                       3 1 12
1 2 4
1 2 4
1 2 5
1 10
1 5
1 11
2 11
35.8342
38.8086
42.9522
46.7938
51.5718
53.8459
53.8459
61.3377
62.3627
                                 2.318500 2.103940
                                                                                                                                                                                                                                                                                                                                                                                13122
                                 1.939770
1.770720
1.701180
1.701180
                                  1.510130
```

28 (°)	d (A)	I	h	k	10.1	* 28 (°)	d (Å)	I	h	k		28 (°)	d (A)	1	- h	k	1 4
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	4	1	3	7	118.8323	0.894753	m	3	2	4	130.9773	0.846574	6	3	2	7
105.1587	0.959887	36	4	0	4	120.9221	0.885358	29	0	4	8	134.5809	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	O	14	123.0447	0.876311	-	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	147.5934	0.801940	1	1	3	13
113.8151	0.919418	m	2	- #3	13	126.3427	0.863194	m	3	3	11	149.4430	0.798502	12m	2	1	16
114,7974	0.914344	73	O.	3	12	129,8042	0.850589	10m	0	2	16	149,4430	0.798502	-	5	0	2

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1/2

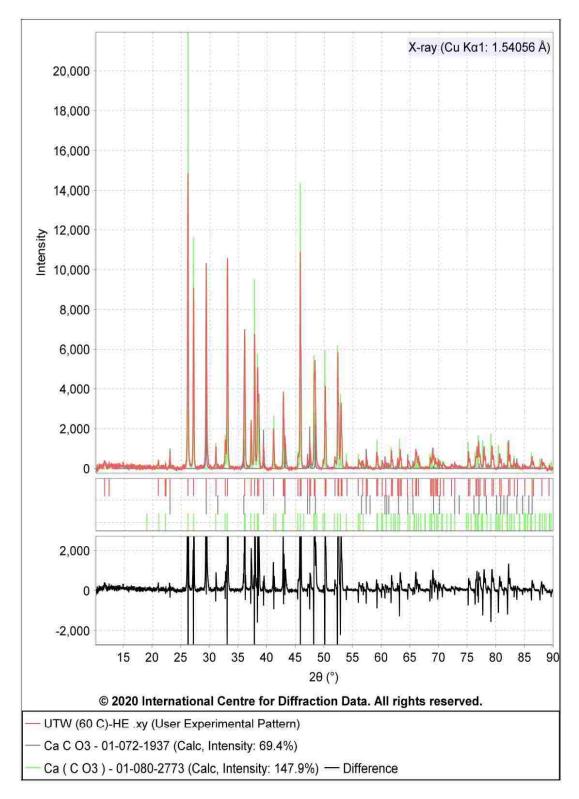


Figure E.7 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 60 °C from accelerated scale simulation study

SIeve+ Report

Experiment

Search Line:	1.974036 Å	D1 Range:	1.968 <mark>Å -</mark> 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 <mark>Å</mark> - 1.885 Å
Rotation: All	8 Rotations		

Preferences

Radiation: X-rayWavelength: Cu Ka1 1.54056 ÅSearch Method: HanawaltSearch Window: 0.15°Match Window: 0.15°2nd Pass Filter: Yesd-Spacings: WeightedLowest 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

QM: Star Pressure/Temperature: Temperature (Non-ambient) Status Alternate Chemical Formula: Ca (CO3) Weight %: C12.00 Ca40.04 O47.95 Atomic %: C20.00 Ca20.00 O60.00 Empirical Formula: C Ca O3 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 c: 5.7629(5) Å AuthCell b: 7,9925(6) Å AuthCell Vol: 228.48 Å3 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/cm³ Dstruc: 2.91 g/cm³] 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 c: 4,960 Å XtlCell α: 90.00° XtlCell β: 90.00° XtlCell b: 7,992 Å XtlCell v: 90.00° XtiCell Vol: 228.48 Å3 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 RedC RedCell c: 7.992 Å RedCell a: 90.00° RedCell β: 90.00° RedCell γ: 90.00° RedCell Vol: 228.48 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 -x+1/2,-y+1/2,z+1/2 x+1/2,y+1/2,-z+1/2 -x,y+1/2,-z+1/2 x,-y+1/2,z+1/2 x+1/2,-y,-z -x+1/2,y,z x,y,z -x,-y,-z 56 34 78 Atomic Coordinates: Atom Num Wyckoff Symmetry SOF Biso AET 0.25 0.25 0.25 0.41508 0.76211 0.92224 0.24046 0.08518 0.09557 1.0 1.0 1.0 1.0 0.61095 0.43867 0.77616 0.70856 Ca C O O 9-a 3#a 1#a 4c 4c 4c 8d m. m. m. 1 234 0.47347 0.68065 0.08726 1#a Anisotropic Displacement Parameters: Atom Num Bani11 Bani22 Bani33 Bani12 Bani13 Bani23 0.665479 0.442997 1.13407 0.509938 0.670266 0.573788 0.540783 0.926694 0.497141 0.299269 0.653666 0.689106 0.0 0.0 0.0 0.0 0.0 0.0 0.180227 -0.0136696 0.0201231 0.0073175 -0.05854 0.0841512 Ca C O O 34 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 on: Aragonite (Group), carbonate (Subgroup) Pearson Symbol: 0F20.00 00-001-0628 (Deleted), 00-003-0405 (Deleted), 00-003-0425 (Deleted), 00-003-1067 (Deleted), 00-005-0453 (Alternate), 00-041-1475 (Primary),

 0.0.001-0628 (Deleted), 00-003-0405 (Deleted), 00-003-0425 (Deleted), 00-003-1067 (Deleted), 00-05-0453 (Alternate), 01-071-3700 (Alternate), 01-071-4891 (Alternate), 01-075-9982 (Alternate), 01-075-9987 (Alternate), 01-075-984 (Alternate), 01-075-9985 (Alternate), 01-075-9987 (Alternate), 01-075-0606 (Alternate), 01-075-9985 (Alternate), 01-078-4338 (Alternate), 01-078-4339 (Alternate), 01-080-268 (Alternate), 01-080-2779 (Alternate), 01-080-2771 (Alternate), 01-080-2786 (Alternate), 01-080-2776 (Alternate), 01-080-27771 (Alternate), 01-080-2778 (Alternate), 01-080-2774 (Alternate), 01-080-2775 (Alternate), 01-080-2789 (Alternate), 01-080-2789 (Alternate), 01-080-2774 (Alternate), 01-080-2775 (Alternate), 01-080-2789 (Alternate), 01-080-2789 (Alternate), 01-080-2774 (Alternate), 01-080-2775 (Alternate), 01-080-2789 (Alternate), 01-080-2789 (Alternate), 01-080-2778 (Alternate), 01-080-2789 (Alternate), 01-080-2789
 Cross-Ref PDF #'s: Entry Date: 09/01/2013 References: DOI Reference Type Primary Reference Calculated from ICSD using POWD-12++. Crystal Structure Crystal Structure Source: LPF "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). Structure

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1/2

Jun 9, 2020 1:46 PM (fal-sharji2) 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.

20 (°)	d (Å)	I	h	k	*	20 (°)	d (Å)	I	h	k	1 *	20 (°)	d (Å)	I	h	k	1	- 3
8,9693	4.674490	4	0	1	1	77,7084	1.227850	m	1	3	4	108,4014	0,949707	1	5	2	1	
1.0610	4 214730	16	1	1	Ó	78 4768	1 217740	8	2	5	2	109,3790	0.943934	1	0	8	2	
2267	3.996250	16	Ó	2	ō	79.1464	1.209110	73m	ō	6	2	109.5447	0.942969	1	1	õ	2 6	
1729	3.401980	999	1	1	1	79.1464	1.209110	m	2	4	3	110.0783	0.939889	6	4	0	4	
1313	3.283940	525	0	2	1	80.4573	1,192680	50	21	5	3	110,2355	0.938989	12m	3	1	5	
.0102	2.881450	56	0	0	2	80.7298	1.189340	3	2	2	4	110.2355	0.938989	m	3	7	0	
.6759	2.738260	79	1	2	1	81.1359	1.184410	1.	4	2	0	110.3993	0.938055	4	5	0	2	
3.0180	2.710670	494	0	1	2	82.0477	1.173540	56	2	6	0	110.6782	0.936474	2	1	1	6	
5.0163	2.491590	184	1	0	2	82.4681	1.168620	5	0	4	4	110.9580	0.934898	3	0	5	5	
5.1866	2.480250	171	2	0	0	83.2026	1.160160	27	4	2	1	111.2157	0.933457	4m	0	2	6	
7.1477	2.418260	96	0	3	1	84.1100	1.149940	1m	2	6	1	111.2157	0.933457	m	4	1	4	
7.7888	2.378690	423	1	1	2	84.1100	1.149940	m	34	5	0	111.5392	0.931660	9	5	1	2	
8.3175	2.347080	275	1	3	0	85.0967	1.139110	8		Ō	2	111.8900	0.929728	10	5	3	0	
8.4851	2.337240	167	0	2	2	85.5725	1.133990	3	3	3 5	3	112.3339	0.927307	9m	1	8	2	
1.1674	2.190940	116	2	1	1	86.2254	1.127070	33m	3	5	1	112.3339	0.927307	m	3	7	1	
1.5087	2.173710	6	1	3	1	86.2254	1.127070	m	4	1	2	112.5444	0.926168	12m	2	4	5	
2.8790	2.107360	175	2	2	0	86.9036	1.120010	1	0	7	1	112.5444	0.926168	m	2	8	0	
5.3499	1.998120	35	0	4	0	87.7119	1.111760	20m	1	1	5	112.9799	0.923831	4	4	4	3	
5.8084	1.979180	626	2	2	1	87.7119	1.111760	m	1	7	0	113.9483	0.918723	14	1	5	5	
5.3788	1.956160	4	0	3	2	88.1421	1.107440	14	0	23	5	114.6784	0.914952	23m	2	8	1	
8.1605	1.887870	266	0	4	1	88.5399	1.103490	2	4	3	1	114.6784	0.914952	m	4	2	4	
8.3809	1.879780	134	2	0	2	88.7908	1.101020	1	2	5	3	115.6804	0.909887	8	24	6	4	
8.7119 9.7895	1.867780 1.829850	4 22	02	1	3 2	89.3606	1.095470	10m	04	62	3	116.1267 116.9687	0.907671	10 1	0	63	6	
0.0842	1.819770	260	1	3	2	89.3606	1.095470	m 13	1	7	1	118.0432	0.903557	5	3	5	4	
1.7699	1.764410	19	1	4	2	89.6680 90.2618	1.092510	15m	2	6	2	118,6343	0.895669	8	2	ő	6	
2.2934	1.747970	267	1	1	2	90,2618	1.086860	m	3	0	4	119,1565	0.893263	9	3	7	2	
2.8347	1.731330	161m	ó	2	3 3	90,9059	1.080830	1	1	2	5	120,1146	0.888930	15	1	3	6	
2.8347	1.731330	m	2	3	1	91.3926	1.076340	5	3	1	4	120.6951	0.886355	4m	ò	8	3	
3.8524	1,700990	31	2	2	2	92.0693	1.070190	1	õ	5	4	120.6951	0.886355	m	4	3	4	
5.9543	1.641970	30	ō	4	2	92.3703	1.067490	9	3	5	2	121.0475	0.884810	15	5	3	2	
3.2278	1.634630	1	1	2	3	93.0474	1.061490	1m	ŏ	7	2	121,6492	0.882204	4	2	8	2	
5.8116	1,619210	17	3	1	ŏ	93.0474	1.061490	m	3	4	23	122.0166	0.880632	6	1	7	4	
9.2253	1.558850	62m	ŏ	3	3	93,5447	1.057150	8m	ŏ	3	5	122,5876	0.878218	2m	ò	9	1	
9.2253	1.558850	m	3	ĭ	ĭ	93,5447	1.057150	m	2	4	4	122.5876	0.878218	m	5	4	1	
9.3446	1.556000	22	2	4	Ó	93.9469	1.053680	4	4	4	Ó	123.0789	0.876169	13	5	1	3	
0.0094	1.540340	18	õ	5	1	94.8379	1.046120	6	1	5	4	123,6092	0.873986	11m	1	9	õ	
0,1991	1.535940	9	2	3	ż	95.8192	1.037990	13	1	5 7	2	123,6092	0.873986	m	2	2	6	
0.8327	1.521450	2	1	5	0	96.0017	1.036500	32m	2	1	5	125.6817	0.865734	15m	0	4	6	
1.6963	1.502210	46	2	4	1	96.0017	1.036500	m	4	4	1	125.6817	0.865734	m	4	6	2	
2.8747	1.476860	20	3	2	1	97.9833	1.020760	3m	2	7	1	127.6078	0.858453	1	1	6	5	
3,1516	1.471050	63	1	5	1	97,9833	1.020760	m	3	6	1	128,6476	0.854673	1	3	4	5	
1.6403	1.440720	4	0	0	4	99.2345	1.011220	21	2	2	5	129.8309	0.850496	4	4	4	4	
4.9727	1.434150	1	3	0	2	99.6416	1.008180	19	4	2	3	130.2710	0.848976	2m	0	9	2	
5.8124	1.417870	19m	0	1	4	99.9578	1.005840	29	3	3	4	130.2710	0.848976	m	2	3	6	
5.8124	1.417870	m	2	2	3	100.5579	1.001450	4	2	6	3	131.1970	0.845836	1	3	8	1	
5.1421	1.411600	32	3	1	2 0	100.9818	0.998388	9m	0	4	5	131.7477	0.844006	16	3	7	3	
6.4978	1.404910	29	3	3	0	100.9818	0.998388	m	0	8	0	132.4417	0.841738	3m	2	7	4	
7.6615	1.383550	5m	0	4	3 4	102.2252	0.989592	7	4	4	2	132.4417	0.841738	m	3	6	4	
7.6615	1.383550	m	1	0	4	102.7101	0.986235	15	3	5	3	133.1144	0.839581	1	4	1	5	
3.4723	1.369130	30	2	4	2	102.9806	0.984380	12m	0	8	1	134.0942	0.836510	16m	1	9	2	
3.8073	1.363280	35	1	1	4	102.9806	0.984380	m	5	1	0	134.0942	0.836510	m	5	3	3	
9.2677	1.355340	17	0	2	4	103.2387	0.982621	3	2	5	4	134.6980	0.834659	10	25	8	3	
.5899	1.349850	3	3	2	2	103.9130	0.978080	12m	0	6	4	134.8923	0.834070	10		5	1	
.8523	1.345420	23	1	5	2	103.9130	0.978080	m	1	4	5	135.8551	0.831199	1	4	7	1	
0.6556	1.332080	16	0	6	0	104.2451	0.975871	8m	2	7	2	136.0830	0.830531	1	3	0	6	
.4380	1.319400	1	2	3	3 4	104.2451	0.975871	m	32	6	2 5	137.4016	0.826750	6	6	0	0	
2.1240	1.308530	4m	1	2		104.6767	0.973027	3	2	3	0	137.6621	0.826020	16m	3	1	6	
2.1240	1.308530	m	2	5	1	105.0668	0.970483	14m	4	3	3	137.6621	0.826020	m	4	2	5	
2.8116	1.297860	2	0	6	1	105.0668	0.970483	m	5	1	1	139.0191	0.822307	1	2	6	5	
5.1758	1.262800	57	3	3	2	105.7684	0.965968	2m	1	8	1	139.5161	0.820984	1m	0	8	4	
6825	1.255600	1	1	6	1	105.7684	0.965968	m	4	5 7	1	139.5161	0.820984	m	4	6	3	
5.3844	1.245800	36	2	0	4	106.2631	0.962832	20	1	1	3	139.9823	0.819761	1	3	8	2	
5.7979	1.240120	43	4	0	0	106.6376	0.960483	12	03	04	6 4	140.2997	0.818938	1	02	1	7	
3,9491	1.238060	70	3	1	3	107.6348	0.954333	1				140,9357		4m				

 O1-072-1937
 Jun 9, 2020 1:46 PM (fal-sharji2)

 Status Alternate
 QM: Star
 Pressure/Temperature: Ambient
 Chemical Formula: Ca C 03 Atomic %: C20.00 Ca2000 060.00 AX: ABX3

 AX: ABX3
 Compound Name: Calcium Carbonata
 Mineral Name: Calciut
 Calcius

 Radiation:
 CuKo1
 A: 1,5406 Å
 d-Spacing: Calculated
 Intensity: Calculated
 Mic: 3.23
 Mic - ND: 0.89

 SYS:
 Rhombohedral
 SPGR: R-3c (167)

 AuthCell MolVol:
 51.49
 AuthCell C: 17.081(5) Å
 AuthCell Vol: 368.93 Å
 AuthCell Z: 6.00

 AuthCell MolVol:
 51.49
 AuthCell C: 17.081(5) Å
 AuthCell Vol: 368.93 Å
 AuthCell Fig. 6.00

 Sysce Group: R-3c (167)
 Mulceular Weight: 100.09
 Crystal Data Kail Ratio (cai: 34.20]
 Space Group: R-3c (167)
 Molecular Weight: 100.09

 Crystal Data Kail Ratio (cai: 34.20 abb: 1.000 Gb: 34.20]
 Redcell c: 6.302 Å
 RedCell g: 90.00°
 XtiCell β: 90.00°

 Redcell y: 120.00°
 XtiCell Vol: 368.93 Å
 XtiCell Vol: 122.97 Ű]
 Redcell c: 6.37*

 Redcell B: 66.97°
 RedCell Y: 4.994 Å
 RedCell Vol: 122.97 Ű]
 Song Operator
 Sog Operator
 Sog Operator
 Sog Operator</t

0 Cross-Ref PDF #'s: 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	0-024-0027 (Deleted), 00-047-1743 (Primary), 01-071-3699 (Alternate), 01-072-4582 (Alternate), 1-075-6049 (Alternate), 01-078-3252 (Alternate), 01-078-614 (Alternate), 01-078-6165 (Alternate), 1-080-2795 (Alternate), 01-080-2792 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 1-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 1-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2801 (Alternate), 01-080-2802 (Alternate), 1-080-2807 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2806 (Alternate), 1-080-2807 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2806 (Alternate), 1-080-2807 (Alternate), 01-080-780 (Alternate), 01-080-7876 (Alternate), 01-080-277 (Alternate), 1-080-2807 (Alternate), 01-080-7876 (Alternate), 01-080-2781 (Alternate), 1-080-2807 (Alternate), 01-080-7876 (Alternate), 01-080-2344 (Alternate), 01-080-2334 (Alternate), 1-088-2340 (Alternate), 01-006-2941 (Alternate), 01-080-2342 (Alternate), 01-080-2334 (Alternate), 4-007-2808 (Alternate), <0-007-4388 (Alternate), 01-080-2344 (Alternate), 01-080-2334 (Alternate), 4-007-2808 (Alternate), <0-007-4389 (Alternate), 01-080-2344 (Alternate), 01-080-2334 (Alternate), 4-007-2808 (Alternate), <0-007-4389 (Alternate), <0-007-6358 (Alternate), 01-080-2334 (Alternate), 4-007-2808 (Alternate), <0-007-4389 (Alternate), <0-007-6358 (Alternate), <0-080-080-0389 (Alternate), 4-007-2808 (Alternate), <0-007-4389 (Alternate), <0-007-6358 (Alternate), <0-080-0389 (Alternate), 4-007-2808 (Alternate), <0-007-4389 (Alternate), <0-007-6358 (Alternate), <0-080-0389 (Alternate), 4-007-2808 (Alternate), <0-007-4389 (Alternate), <0-007-6358 (Alternate), <0-008-0389 (Alternate), 4-007-2808 (Alternate), <0-007-3489 (Alternate), <0-007-6358 (Alternate), <0-012-00489 (Primary), <4-012-02489 (Primary), <4-012-015-9713 (Alternate), <0-015-9713 (Alternate), <0-015-9713 (Alternate), <0-015-9713 (Alternate), <0-015-9713 (Alternate), <0-015-9713 (Alternate)
	- 방법에 가격 바람이 가입니다. 가격 방법에 가격하게 많은 것이다. 알려 가 있는 것이다. 이렇게 가장 말할 것이다. ㅠㅠ ㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋㅋ
CAS Number - PR: 13 Last Modifications: F	2202201 - Have Manuel Contract Wilson - Additional Additional Addition (1999)
Last Modifications: F References:	eflections
Last Modifications: F References: Type DOI	effections Reference
Last Modifications: F References:	eflections
Last Modifications: F References: Type DOI	effections Reference
Last Modifications: F References: Type DOI Primary Reference	Reference Calculated from ICSD using POWD-12++ (2004).

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1/2

28 (°)	d (Å) b	1	h	k	1	•	20 (°)	d (Å)	1	h	k	1	28 (*)	d (Å)	1	h	k	1	+
23.0315	3,856400	95	Ð	1	2		80.8512	1.187860	5	3	1	2	109,4059	0.943777	18	4	1	O.	
20 3686	3.038670	000	14	0	4		81.4203	1,180990	24	2	1	10	110,3023	0.938508	10	2	2	12	
31.3969	2.846830	19	0	0	6		81.9883	1.174240	3	a	े हैं।	14	111,6455	0.931073	1	4	1	3	
35.9356	2,497000	144	1	- T	G	- 3	83.6739	1.154820	43	1	3	4	113.8704	0.919129	2	3	2	7	
9.3693	2.285760	183		11	3		84,7045	1,143380	20	2	2	6	114,9470	0.913582	1	4	0	10	
3,1163	2.096310	155	2	0	2		85.7798	1,131780	1	3	1	5	117,7542	0.899796	8	2	3	8	
7.0656	1.929200	68	20	2	4		85.3436	1.125830	-4	1	2	11	118 5992	0.896832	8	2	4	6	
7.4483	1,914530	196	0	1	8		91.3762	1.076490	1		3	7	119,0322	0.893833	9	2	1	16	
18.4512	1.877220	205		1	6		91.7950	1.072670	1	0	4	2	120,5380	0.887048	9	1	- 12	18	
56.5060	1.627240	33	2	1	1		92 9201	1.062610	8	0114	0	14	127,0340	0.860584	2	5	0	2	
57.3403	1.605530	.94	1	2	2		94.5955	1.048160	25	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	22	17	
50.6042	1.526640	55	2	1	4		96.0079	1.036450	14m	1	0	16	128,4559	0.855362	3	3	-10	14	
50.9262	1.519340	24	2	0	8	- 3	96.0079	1.036450	m	1	1	15	130.6242	0.847769	7	04	5	4	
51,2995	1.510980	25	1	1	9	- 18	97.5532	1.024110	2	2	1	13	131,4301	0.845055	1	- 4	1	9	
52.9845	1.474550	20 62	13	120	5	- 3	99.0126	1.012890	26	03	32	12	132.5646	0.841341	10	20	2	15	
4.5940	1.441640				G		102.0898	0.990537	3			1	133.6570	0.837870	8	0		20	
55.5236	1,423420	34	0	0	12		102.8057	0.985578	12	2	3	2	134.2277	0.836098	1	2	3	11	
59.1075	1.358090	11	2	1	7		103.3829	0.981644	4	1	3	10	135.47.17	0.832333	4	NWWN	33	0	
70.1529	1.340390	20	0	2	10		103.9514	0.977757	10	1	2	14	138.5477	0.823580	1	3	3	3	
2.8057	1.297950	29	St.,	2	8		105.6912	0.966461	10	3	2	4	141.2982	0.816401	5	2	4	1	
3.5842	1,286130	7	32	02	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	0000	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	
8.3403	1.219520	1	2	2.3	3		108.4735	0.949276	1m		0	18	147.8140	0.801595	6	0250	0	8	
30.1425	1.196570	1	18	3	1		108,4736	0.949276	100	3	1	11	149,2409	0.798888	8	3	3	6	

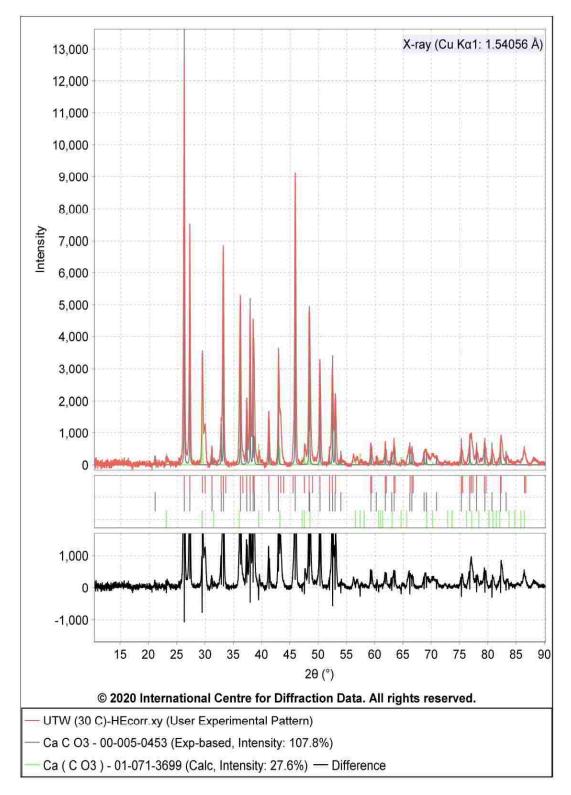


Figure E.8 XRD patterns of substances precipitated from Untreated Water (UTW) heating element at 30 °C from accelerated scale simulation study

SIeve+ Report

Experiment

Search Line: 2.330781 Å D1 Range: 2.322 Å - 2.339 Å D1 Range: 2.080 Å - 2.094 Å Search Line: 2.086682 Å D1 Range: 2.969 Å - 2.999 Å Search Line: 2.983988 Å Search Line: 1.170193 Å D1 Range: 1.168 Å - 1.172 Å D1 Range: 1.235 Å - 1.239 Å Search Line: 1.236700 Å D1 Range: 2.471 Å - 2.491 Å Search Line: 2.481368 Å Search Line: 1.992372 Å D1 Range: 1.986 Å - 1.999 Å D1 Range: 1.550 Å - 1.557 Å Search Line: 1.553837 Å Rotation: All 8 Rotations

Preferences

Radiation: X-rayWavelength: Cu Ka1 1.54056 ÅSearch Method: HanawaltSearch Window: 0.15°Match Window: 0.15°2nd Pass Filter: Yesd-Spacings: WeightedLowest Allowable GOM: 2000

Phases (2)

#	Accepted	PDF #	QM	Compound Name	I Ratio	I %	I/Ic	Est Wt %
1	true	00-005-0453		Calcium Carbonate	1.078	79.593	*1.14	92
2	true	01-071-3699		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 03

 Empirical Formula:
 C Ca O3
 Weight %:
 C12.00
 Ca40.04 O47.95
 Atomic %:
 C20.00
 Ca00.00
 000.00
 Ca Co3
 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 Space Storp, Friam (02) 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° Xtl 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 cb: 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] XtlCell c: 4 959 Å XtlCell α: 90 00° XtlCell β: 90 00° εα: =1.530 πωβ: =1.6810 εγ: =1.6854 Sign: =- 2V: =18° ADP: B Atomic parameters are cross-referenced from PDF entry 04-008-5421 Crystal (Symmetry Allowed): Centrosymmetric SG Symmetry Operators: Seq Operator Seq Operator Seq Operator Seq Operator x+1/2, y+1/2,z+1/2 x+1/2,y+1/2, z+1/2 -x,y+1/2,-z+1/2 x,-y+1/2,z+1/2 34 5 6 x+1/2,-y,-z -x+1/2,y,z x,y,z -x,-y,-z 2 8 Atomic Coordinates: Atom Num Wyckoff Symmetry x SOF Biso AET 0.25 0.25 0.25 0.47347 0.41508 0.76211 0.92224 0.68065 0.24046 0.08518 0.09557 0.08726 1.0 1.0 1.0 1.0 0.61095 0.43867 0.77616 0.70856 9-a 3#a 1#a 1#a Ca C O O 4c 4c 4c 8d m.. m.. m.. 234 otropic Displace ent Para ters: Bani22 Atom Num Bani11 Bani33 Bani12 Bani13 Bani23 0.665479 0.670266 0.442997 0.573788 1.13407 0.540783 0.509938 0.926694 0.497141 0.299269 0.653666 0.689106 0.0 0.0 0.0 0.180227 0.0 0.0 0.0 -0.0136696 0.0201231 0.0073175 -0.05854 0.0841512 Ca C O O 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 P20.00
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), 01-075-9887 (Alternate), 01-075-0987 (Alternate), 01-075-9887 (Alternate), 01-080-2776 (Alternate), 01-080-2776 (Alternate), 01-080-2777 (Alternate), 01-080-2776 (Alternate), 01-080-2778 (Alternate), 01-080-2776 (Alternate), 01-080-2777 (Alternate), 01-080-2776 (Cross-Ref PDF #'s: CAS Number - PR: 14791-73-2 Entry Date: 09/01/1955 **References:**

190	e	DOI	Reference
Crys	nary Reference stal Structure ical Data		Swanson, Fuyat. Natl. Bur. Stand. (U. S.), Circ. 539 3, 53 (1954). Crystal Structure Source: LPF. Winchell. Elements of Optical Mineralogy (1951).

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1 / 2

00-005-0453

Jun 9, 2020 2:05 PM (fal-sharji2) 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. Database Comments:

20 (°)	d (Å)	I	h	k	*	20 (°)	d (Å)	I	h	k	1	*	20 (°)	d (Å)	I	h	k	1	*
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					J	un 9, 2020	2:05	PM (fal-sharji
Status Alternate Empirical Formula: ANX: ABX3 Cor		ssure/Temperat ght %: C12.00 (calcium Carbonat	Ca40.04 O47		%: C20.	i: Ca (C O3) 00 Ca20.00 C		
Radiation: CuKa1	λ: 1,5406 Å	d-Spacing: Ca	Iculated I	ntensity: Calc	ulated	l/lc: 3.23	l/lc - N	I D : 0.9
SYS: Rhombohedra Author's Cell [Auth AuthCell MolVol: 6 Density [Dcalc: 2. Femp: 298.0 K (Am	nCell a: 4.991(2) 1.34] Author 709 g/cm³ Dstr	Å AuthCell c r's Cell Axial Ra uc: 2.71 g/cm³]	SS/FO		.9(0.0000		uthCell	Z : 6.00
Space Group: R-3c Crystal Data [XtlCc (tlCell γ: 120.00° Crystal Data Axial F Reduced Cell [Red RedCell β: 66.96° Atomic parameters	ili a: 4,991 Å XtiCell Vol: 36 Ratio [c/a: 3.419 Cell a: 4,991 Å RedCell γ: 60.0	a/b: 1.000 RedCell b: 4 00° RedCell V	Å XtlCell ell Z: 6.00] c/b: 3.419 991 Å Re /ol: 122.69 /	dCellc: 6.376 ų]		lα: 90.00° dCellα: 66.9		Η β: 90.00°
Crystal (Symmetry G Symmetry Operat	,	symmetric						
eq Operator	Seq Operator	Seq Opera				Operator	Seq	Operator
x,y,z -x,-y,-z	3 y,x-y,z 4 y, x+y, z	5 -x+y,-x 6 x-y,x,-z		-y,-x,z+1/2 y,x,-z+1/2	9 10	x,x-y,z+1/2 -x,-x+y,-z+1/2	11 12	-x+y,y,z+1/2 x-y,-y,-z+1/2
tomic Coordinates:								
<u>tom Num Wycko</u> a 1 6b	ff Symmetry x -3. 0.0			<u>ET</u> -a				
2 6a 3 18e	32 0.0 2 0.2			#b #a				
Subfile(s): Serifier Mineral Classificati	00-001-0837 (De (Deleted), 00-003 00-024-0027 (De 01-075-6049 (Alt 01-080-2795 (Alt 01-080-2795 (Alt 01-080-2803 (Alt 01-080-2807 (Alt 01-080-2811 (Alt 01-080-2811 (Alt 01-083-0578 (Alt	I (Excipient), Pig rgroup), calcite (leted), 00-002-00 leted), 00-047-11 ernate), 01-078-3 ernate), 01-080-3 ernate), 01-080-3 ernate), 01-080-3 ernate), 01-080-3 ernate), 01-080-3 ernate), 01-080-3 ernate), 01-085-6	ment/Dye, SL Group) P (323 (Deleted) 00-004-0633 (433 (Primary) 262 (Alterna 2796 (Alterna 2800 (Alterna 2804 (Alterna 2808 (Alterna 775 (Alterna 2849 (Alterna	perconducting earson Symbo , 00-002-0629 () (Deleted), 00- 01-072-1937 (te), 01-078-461 te), 01-080-279 te), 01-080-280 te), 01-080-280 te), 01-080-280 te), 01-080-280 te), 01-080-280 te), 01-080-283 te), 01-080-280 te), 01-080-	Material I: hR10.0 (Deleted). 004-0637 (Alternate 4 (Alterna 1 (Alterna 9 (Alterna 9 (Alterna 6 (Alterna 4 (Alterna)	00 00-003-0569 (Deleted), 00), 01-072-458 ate), 01-078-4 ate), 01-080-2 ate), 01-080-2 ate), 01-080-2 ate), 01-080-2 ate), 01-080-2 ate), 01-083-2 ate), 01-088-2	0 (Delet 0-005-0 2 (Alte 615 (A 2794 (A 2798 (A 2806 (A 2806 (A 2806 (A 2810 (A 2339 (A	ed), 00-003-0596 586 (Primary), rnate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate), Iternate),
	01-086-2340 (Alt 04-001-7249 (Alt 04-007-2808 (Alt 04-008-0212 (Alt 04-016-9713 (Alt	ernate), ✓ 04-00 ernate), ✓ 04-00 ernate), ✓ 04-00 ernate)	2-9082 (Alteri 7-4388 (Alteri 8-0213 (Alteri	nate), √ 04-006 nate), √ 04-007 nate), √ 04-008	6528 (A 7-8659 (P 8-0788 (A	Iternate), √ 04 rimary), √ 04- Iternate), √ 04	2343 (A 4-007-0 -008-01 4-012-8	Iternate), √ 1049 (Alternate), 98 (Alternate), √ 1072 (Alternate),
CAS Number - PR: _ast Modifications:		ntry Date: 09/07	/2005 La :	st Modificatior	Date: 0	9/01/2011		
References:	DOI Boferere							
	DOI Reference	1000	ND 10.					
rimary Reference		m ICSD using POV						
dditional Reference	Pilati, T., Dem	artin, F., Gramacci	oli, C.M. Golde	n Book of Phase	Transitions	s, Wroclaw 1, 1	(2002).	
Crystal Structure	Crystal Struct	ure Source: LPF.						
Structure	"Lattice-dynar dolomite Ca M Struct, Sci. 54	nical estimation of Ag (C O3)2, and ma , 515 (1998).	atomic displace agnesite Mg C (ement parameters O3". Pilati, T., Der	in carbon martin, F.,	ates: Calcite an Gramaccioli, C	d aragor M. Acta	nite Ca C O3, Crystallogr., Sec. E
© 2020 Internatio	nal Centre for F	Diffraction Dat	a. All rights	reserved				Page 1/

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1 / 2

01-071-3699

Jun 9, 2020 2:05 PM (fal-sharji2)

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: Database Comments: .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.

20 (°)	d (Å)	I	h	k	1	*	20 (°)	d (Å)	I	h	k	1	*	20 (°)	d (Å)	I	h	k	1	*
3.0480	3.855680	95	0	1	2		80.9104	1.187140	5	3	1	2		109.5033	0.943210	17	4	1	0	
9.3944	3.036060	999	1	0	4		81.5038	1.179990	23	2	1	10		110,4380	0.937835	9	2	2	12	
1.4327	2.843670	20	0	0	6		82.0953	1.172980	3	0	1	14		111.7493	0.930501	1	1	4	3	
5.9579	2.495500	143	1	1	0		83.7388	1.154090	43	1	3	4		113.9892	0.918510	3	3	2	7	
9.3975	2.285190	190	1	1	3		84.7758	1.142600	20	2	2	6		115.0813	0.912900	1	4	0	10	
3.1449	2.094990	152	2	0	2		85.8495	1.131040	1	3	1	5		117.8856	0.899174	7	2	3	8	
7.1008	1.927840	66	0	2	4		86.4373	1.124850	5	1	2	11		118.7250	0.895249	6	1	4	6	
7.4994	1.912590	195	0	1	8		91.4592	1.075730	1	1	3	7		119.2195	0.892975	8	2	1	16	
8.4938	1.875670	202	1	1	6		91.8667	1.072020	1	0	4	2		120,7489	0.886118	9	1	1	18	
6.5435	1.626250	34	2	1	1		93.0395	1.061560	8	2	0	14		127.1737	0.860062	2	5	0	2	
7.3794	1.604530	94	1	2	2		94,6749	1.047490	26	4	0	4		127,9124	0.857335	8	3	2	10	
8.0720	1.587030	10	1	0	10		94.9680	1.045030	29	3	1	8		128.5117	0.855161	2	1	2	17	
0.6489	1.525620	53	2	1	4		96.1456	1.035330	14m	1	0	16		128.6587	0.854633	2	3	1	14	
0.9844	1.518030	24	2	0	8		96.1456	1.035330	m	1	1	15		130.7795	0.847242	7	0	5	4	
1.3625	1.509580	26	1	1	9		97.6734	1.023170	2	2	1	13		132.7947	0.840601	1	2	2	15	
3.0331	1.473530	21	1	2	5		99.1280	1.012020	25	0	3	12		133.9509	0.836954	7	0	1	20	
4.6372	1.440780	63	3	0	0		102.1752	0.989941	3	3	2	1		134.4319	0.835471	2	2	3	11	
5.6060	1.421830	34	0	0	12		102.8929	0.984980	12	2	3	2		135.6402	0.831833	4	3	3	0	
9.1674	1.357060	12	2	1	7		103.4946	0.980889	3	1	3	10		138.7335	0.823076	1	3	3	3	
0.2268	1.339160	20	0	2	10		104.0977	0.976849	10	1	2	14		141.4950	0.815910	1	2	4	1	
2.8728	1.296920	27	1	2	8		105.7860	0.965856	9	3	2	4		142.6350	0.813125	7	4	2	2	
3.6442	1.285230	6	3	0	6		106.0906	0.963921	18	0	4	8		144.6101	0.808533	1	0	4	14	
6.2436	1.247750	11	2	2	0		107.3138	0.956296	5	0	2	16		147.5330	0.802266	7	2	4	4	
7.1468	1.235380	20	1.	1	12		107.9828	0.952222	3	2	3	5		148.0828	0.801156	6	5	0	8	
8.3985	1.218760	1	2	2	3		108.5999	0.948524	1m	0	0	18		149.5093	0.798376	7	3	3	6	
0.2006	1.195850	1	1	3	1		108.5999	0.948524	m	3	1	11								

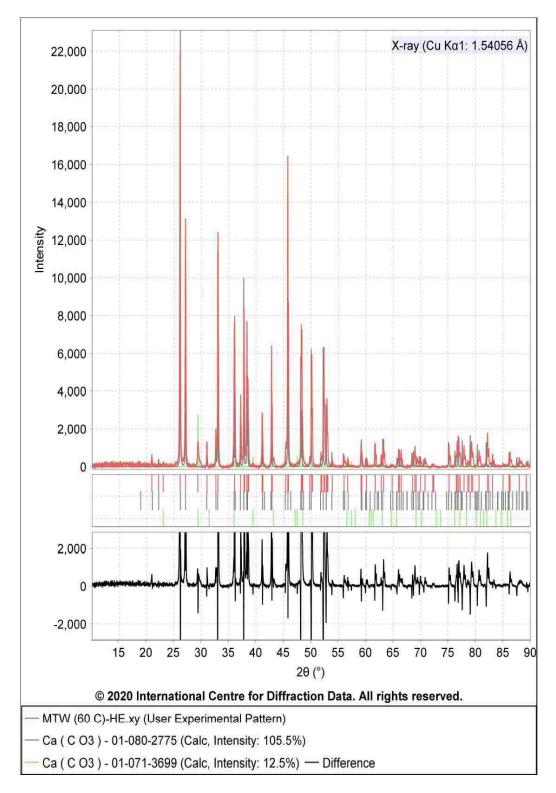


Figure E.9 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 60 °C from accelerated scale simulation study

SIeve+ Report

Experiment

Search Line: 1	1.976166 Å	D1 Range:	1.970 Å - 1.982 Å
Search Line: 1	1.880833 Å	D1 Range:	1.875 Å - 1.886 Å
Search Line: 2	2.372026 Å	D1 Range:	2.363 Å - 2.381 Å
Search Line: 1	1.728285 Å	D1 Range:	1.724 Å - 1.733 Å
Search Line: 1	1.741580 Å	D1 Range:	1.737 Å - 1.746 Å
Search Line: 1	1.813554 Å	D1 Range:	1.808 Å - 1.819 Å
Search Line: 2	2.489883 Å	D1 Range:	2.480 Å - 2.500 Å
Search Line: 2	2.195541 Å	D1 Range:	2.188 Å - 2.203 Å
Rotation: All 8	8 Rotations		

Preferences

Radiation: X-rayWavelength: Cu Ka1 1.54056 ÅSearch Method: HanawaltSearch Window: 0.15°Match Window: 0.15°2nd Pass Filter: Yesd-Spacings: WeightedLowest Allowable GOM: 2000

Phases (2)

#	Accepted	PDF #	QM	Compound Name	I Ratio	I %	I/Ic	Est Wt %
12	true	01-080-2775 01-071-3699		Calcium Carbonate Calcium Carbonate	1.055 0.125	89.416 10.584		96 4

	80-27	-											0 1:44 PM (fal-sharj
mpi	s Alter rical Fo ABX3	ormula: C	M: Star Ca O3 ound Nam	Weight %	: C12.00) Ca40.04	047.	rature (No 95 Ate Name: 7	omic %	: Ć20			ormula: Ca (C O3) O60.00
Radia	ation: (CuKa1	λ: 1.5406	Å d-Sj	oacing: (Calculated	d li	ntensity:	Calcu	ated	l/lc:	1.18	I/Ic - ND: 0.51
Autho Autho Autho Dens	or's Cel Cell Vol or's Cel ity [Dc	I: 229.09 II Axial Ra alc: 2.90	atio [c/a:	24(4) Å nCell Z: 4 1.163 a Dstruc: 2	1.00 A a/b: 0.62 2.9 g/cm ³) c/b :	0.722 /FOM	l: 57.27	-		•) Å	
Cryst Cryst Cryst Redu RedC	al Data IIγ: 90 al Data ced Ce cellβ: 9	0.00° X I Axial Ra II [RedCo 90.00°	a: 5.771 Å tlCell Vol: tio [c/a: 0 ella: 4.962 RedCellγ:	229.09 Å .860 a Å Re 90.00°	II b: 7.99 3 XtIC /b: 0.721 dCell b: RedCel	9 Å) ell Z: 4.(c/b: 5.771 Å I Vol: 22	00] 0.620 Re 9.09 /	dCell c: ` ∖₃]	7.999 /	R	α: 90 edCell).00° Ια: 90	XtiCell β: 90.00°
ryst	al (Syn		re cross-re lowed): C s:			entry 04	1-008-	5421	ADP:	В			
	Operato	or		perator			rator		Seq	Opera			
	x,y,z -x,-y,-z		3 -x 4 x+	+1/2, y+1/2 1/2,y+1/2,	,z+1/2 z+1/2	5 x+1/ 6 -x+1	2,-y,-z /2,y,z		7 8	-x,y+1 x,-y+1	/2, - z+1/ /2,z+1/2	2	
	ic Coord	linates:											
tom			Symmetry		V	Z	SOF	Biso	AET				
а	1 2	4c 4c	m. m.	0.25 0.25	0.41508 0.76211	0.24046 0.08518	1.0 1.0	0.61095 0.43867	9 - a 3#a				
)	3 4	4c 8d	m 1	0.25 0.47347	0.92224 0.68065	0.09557 0.08726	1.0 1.0	0.77616 0.70856	1#a 1#a				
niso	tropic D)isplaceme	nt Paramet	ers:									
tom	Num	Bani11	Bani22	Bani33	Bani12	Bani13		Bani23					
a	1 2 3 4	0.665479 0.442997 1.13407 0.509938	0.670266 0.573788 0.540783 0.926694	0.497141 0.299269 0.653666 0.689106	0.0 0.0 0.0 0.180227	0.0 0.0 0.0 -0.0136	(0.0201231 0.0073175 0.05854 0.0841512					
Proto Ainer	s-Ref P	Natural), F tructure [ssification (((DF #'s: (((((((((((((((((((Pharmaceut Formula O : Aragonit 0-001-0628 Alternate), (Alternate), (Alter	ical (Excip rder]: Ca e (Group), (Deleted) 00-041-14 01-071-37 01-075-99 01-076-06 01-080-27 01-080-27 01-080-27 01-080-27 / 04-007-1	ient), Sup C O3 carbonat , 00-003- 75 (Prima 00 (Altern 06 (Altern 68 (Altern 72 (Altern 90 (Altern 90 (Altern 90 (Altern	erconduc Prototyp e (Subgro 0405 (De ry), ✓ 00- ate), 01-0 ate), 01-0 ate), 01-0 ate), 01-0 ate), 01-0 ate), √ 04- ernate), ✓	ting M be Strip (061-0 (061-0 (071-48 (075-99) (075-99 (075-99) (075-	1aterial Deture [A Pearso , 00-003-(390 (Prim 91 (Altern 937 (Altern 73 (Altern 73 (Altern 5441 (Altern 5441 (Altern 5421 (Altern) 100 (Alt	Ipha O n Sym 0425 (E nary), 0 nate), 0 nate), 0 nate), 0 nate), 0 ernate), 0 Primary	rder]: bol: o leleted 1-071- 1-075- 1-075- 1-078- 1-080- 1-080- , √ 04-), √ 04-	C Ca P20.00), 00-0 2392 (9982 (9986 (4338 (2770 (2774 (006-54	O3 03-106 Alterna Alterna Alterna Alterna Alterna Alterna Alterna	Mineral Related (Mineral i7 (Deleted), 00-005-045 ite), 01-071-2396 ite), 01-075-9983 ite), 01-075-9987 ite), 01-080-2771 ite), 01-080-2771 ite), 01-080-2773 viernate), √ 04-006-655 iternate), √ 04-014-183
Refer	ences:		Reference										
ype rimar	y Refere			from ICSD	using POV	VD-12++							
	Structu			ucture Sour	-								
	. Judolu		5,,000,00										
Structu	Ino		"Temperat	ure depend otron powd	ence of the	structura	param	eters in the	transfo	mation	of arag	onite to	calcite, as determined from

© 2020 International Centre for Diffraction Data. All rights reserved.

Page 1 / 2

U1-U6U-2//5 Jun 9, 2020 1:44 PM (fal-sharji2) 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-Spacin	gs (199) -	Ca (C (D3)	- 01	1-080-2	775 (Stick,	Fixed Slit	Intensi	ty) -	Cu	Ka1 1.5	54056 Å						
20 (°)	d (Å)	I	h	k	*	20 (°)	d (Å)	I	h	k	*	20 (°)	d (Å)	I	h	k	1	*
18.9456 21.0504 22.2087 26.1505 27.1032 30.9633	4.680300 4.216830 3.999450 3.404840 3.287290 2.885700	3 15 17 999 515 55	010100	112120	1 0 1 1 2	78.4001 79.0549 79.0549 80.3567 80.6162 81.0953	1.218740 1.210280 1.210280 1.193920 1.190730 1.184900	7 69m 48 3 1	2021 24	564522	2 2 3 3 4 0	107.5222 108.3322 109.2380 109.2380 110.0530 110.0530	0.955020 0.950121 0.944758 0.944758 0.940034 0.940034	m 1 1m 11m 11m m	350133	4 2 8 0 1 7	412650	_
32.6482 32.9706 35.9716 36.1723 37.1124 37.7432 38.2893	2.740520 2.714460 2.494580 2.481200 2.420480 2.381460 2.348740	78 486 177 166 94 412 273	10120110	21003130	1 2 2 0 1 2 0	81.9772 82.3428 82.7009 83.1561 84.0337 84.0337 84.7896	1.174370 1.170080 1.165920 1.160690 1.150790 1.150790 1.150790	53 5 1 25 1m 1 	2034230	6442651	0 4 2 1 0 5	110.3172 110.3172 110.7513 110.8987 111.0742 111.4545 111.8164	0.938523 0.938523 0.936061 0.935231 0.934247 0.932129 0.930132	3m m 3 1 3 8 9	1500455	10521130	62564200	
38.4354 41.1426 41.4732 42.8566 45.3116 45.7786 46.3244 48.1157	2.340150 2.192200 2.175490 2.108410 1.999720 1.980400 1.958330 1.889520	168 112 6 170 34 609 4 259	02120200	21324234	2 1 0 0 1 2 1	85.0386 85.0386 85.4828 86.1579 86.1579 86.8135 87.5577 87.5577	1.139740 1.139740 1.134950 1.127780 1.127780 1.120940 1.113320 1.113320	8m m 3 31m m 1 20m m	14334011	40351717 7	4 2 3 1 2 1 5 0	112.2168 112.2168 112.3427 112.3427 112.8547 113.7347 114.0328 114.5427	0.927943 0.927943 0.927259 0.927259 0.924500 0.919839 0.918283 0.915648	9m m 12m m 4 13 1 20m	13224152	87484538	21503511	
48.3374 48.6376 49.7445 50.0299 51.7248 52.2198 52.7582	1.889320 1.881370 1.870460 1.831400 1.821620 1.765840 1.750260 1.733660	255 131 5 21 257 18 262 141m	02021110	40113412	2 3 2 2 1 3 3	87.9842 88.4853 88.6849 89.2955 89.2955 89.5764 90.1687	1.109020 1.104030 1.102060 1.096100 1.096100 1.093390 1.087740	13 2 1 10m m 13 14m	0 4 2 0 4 1	2356276	5 1 3 3 2 1 2	114.3427 114.9232 114.9232 115.4961 116.0209 116.7083 117.8643	0.915648 0.915648 0.913703 0.913703 0.910809 0.908194 0.904820 0.899275	2011 m 1m 7 9 1 5	44252403	02726635	4324064	
52.7582 53.8035 55.8925 56.1519 56.7868 59.1939 59.1939	1.733660 1.702420 1.643640 1.636660 1.619860 1.559600 1.559600	m 30 29 1 16 60m m	2201303	3 2 4 2 1 3 1	1 2 2 3 0 3 1	90.1687 90.7457 91.2749 91.9297 92.2853 92.9406 92.9406	1.087740 1.082320 1.077420 1.071450 1.068250 1.062430 1.062430	m 1 5 1 8 1m m	23130303	0215574	4 5 4 2 2 3	118.3779 118.3779 119.0117 119.8438 120.5055 120.5055 120.9397	0.896862 0.896862 0.893927 0.890144 0.887192 0.887192 0.885281	8m 8 13 4m m 14	2431045	0673833	6126342	
59.3031 59.9532 60.1438 60.7815 61.6490 62.8392 63.0947	1.556990 1.541650 1.537220 1.522610 1.503250 1.477610 1.472240	22 17 8 2 45 18 61	2021231	4535425	0 1 2 0 1 1	93.4123 93.4123 93.8852 94.6963 94.6963 95.7093 95.9342	1.058300 1.058300 1.054210 1.047310 1.047310 1.038890 1.037050	7m 4 5m 12 27m	0 2 4 1 4 1 2	3445371	5404225	121.4830 121.8023 122.4855 122.4855 122.9491 123.3306 123.3306	0.882920 0.881547 0.878647 0.878647 0.876708 0.875129 0.875129	4 6 2m 12 9m m	2105512	8794192	2411306	
64.5333 64.9254 65.7049 65.7049 66.0930 66.4604 67.5551 67.5551 68.4081	1.442850 1.435080 1.419930 1.419930 1.412530 1.405610 1.385470 1.385470 1.370260	4 19m 31 28 5m m 29	030233012	001213404	4 2 4 3 2 0 3 4 2	95.9342 97.8841 97.8841 99.0670 99.5461 99.8251 100.4314 100.8007 100.8007	1.037050 1.021530 1.021530 1.012480 1.008890 1.006820 1.002370 0.999692 0.999692	m 2m 19 17 26 3 10m m	423243200	476223648	1 1 1 5 3 4 3 5 0	125.5349 125.5349 126.8364 127.3380 128.3957 129.6263 129.9563 129.9563 130.1498	0.866304 0.866304 0.861325 0.859451 0.855579 0.851209 0.850061 0.850061 0.849393	12m m 1 1 1 4 1m m 1	045134250	462644349	623554622	
68.6999 68.6999 69.1575 69.5363 69.7792 70.5904 71.3557 72.0641	1.365150 1.365150 1.357230 1.350760 1.346650 1.333150 1.320720 1.309470	33m m 16 3 22 16 1 4m	1 3 0 3 1 0 2 1	13225632	4 1 4 2 2 0 3 4	102.1380 102.5914 102.8627 102.8627 103.0872 103.7505 104.1254 104.1254	0.990200 0.987053 0.985187 0.985187 0.983652 0.979167 0.976665 0.976665	7 14 11m 3 11 7m m	43052023	45815676	2 3 1 0 4 4 2 2	131.0192 131.5382 131.9422 132.1871 132.1871 132.8600 133.8659 133.8659	0.846433 0.844699 0.843366 0.842565 0.842565 0.842565 0.840392 0.837218 0.837218	1 14 3m m 1 14m m	33523415	87576193	1130445233	
72.0641 72.7407 75.1151 76.2768 76.7628 76.8720 77.5913 77.5913	1.309470 1.298950 1.263670 1.247290 1.240600 1.239110 1.229410 1.229410	m 2 54 34 45 67 55m m	20324301	56300153	1 1 2 4 0 3 3 4	104.4964 105.0040 105.6828 105.6828 106.1176 106.4112 107.5222	0.974211 0.970891 0.966515 0.966515 0.966515 0.963750 0.961900 0.955020	2 12m m 2m 18 11 1m	24514100	33185701	5 3 1 1 3 6 6	134.4570 134.7494 135.7438 135.7438 137.3789 137.3789	0.835394 0.834503 0.831527 0.831527 0.826814 0.826814	9 8 1m m 15m m	253446	850720	316150	

Status Alternate Empirical Formula: ANX: ABX3 Cor	QM: Star Pressure/Temperature: Ambient Chemical Formula: Ca (C 03) : C Ca 03 Weight %: C12.00 Ca40.04 O47.95 Atomic %: C20.00 Ca20.00 O60.00 mpound Name: Calcium Carbonate Mineral Name: Calcite, syn
Radiation: CuKa1	λ: 1,5406 Å d-Spacing: Calculated Intensity: Calculated I/Ic: 3.23 I/Ic - ND: 0.9
AuthCell MolVol: 6 Density [Dcalc: 2.	hCell a: 4.991(2) Å AuthCell c: 17.062(2) Å AuthCell Vol: 368.07 Å ³ AuthCell Z: 6.00 61.34] Author's Cell Axial Ratio [c/a: 3.419]
Space Group: R-3α Crystal Data [XtlCc KtlCell γ: 120.00° Crystal Data Axial I Reduced Cell [Red RedCell β: 66.96° Atomic parameters	ell a: 4,991 Å XtlCell b: 4,991 Å XtlCell c: 17,062 Å XtlCell α: 90,00° XtlCell β: 90,00° XtlCell Vol: 368.07 ų XtlCell Z: 6.00] Ratio [c/a: 3.419 a/b: 1.000 c/b: 3.419]
Crystal (Symmetry	Allowed): Centrosymmetric
G Symmetry Operation	Seg Operator Seg Operator Seg Operator Seg Operator 3 -y,xy,z 5 -xty-x,z 7 -y.x,z+1/2 9 x,xy,z+1/2 11 -xty,y,z+1/2 4 y,-xty,-z 6 x,y,x,z+1/2 8 y,x,z+1/2 10 -x,y-y,z+1/2 12 xy-y,z+1/2
tomic Coordinates: tom Num Wycko	off Symmetry x y z SOF IDP AET
Ca 1 6b C 2 6a D 3 18e	-3, 0,0 0,0 0,0 1,0 6-a 32 0,0 0,0 0,25 1,0 3#b .2 0,2593 0,0 0,25 1,0 1#a
Subfile(s): Cement	t and Hydration Product, Ceramic (Bioceramic), Common Phase, Forensic, Inorganic, Mineral Related (Mineral ic), Pharmaceutical (Excipient), Pigment/Dye, Superconducting Material
Mineral Classificati	ion: Calcite (Supergroup), calcite (Group) Pearson Symbol: hR10.00 00-001-0837 (Deleted), 00-002-0623 (Deleted), 00-002-0629 (Deleted), 00-003-0569 (Deleted), 00-003-0570 (Deleted), 00-004-0636 (Deleted), 00-004-0586 (Primary), 00-024-0637 (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), 01-073-3262 (Alternate), 01-078-4614 (Alternate), 01-078-4615 (Alternate), 01-078-4615 (Alternate), 01-080-2794 (Alternate), 01-070-4614 (Alternate), 01-080-2794 (Alternate), 01-080-2794 (Alternate), 01-070-4614 (Alternate), 01-080-2794 (Alternate), 01-070-4614 (Alternate), 01-070-4614 (Alternate), 01-080-2794 (Alternate), 01-080-2794 (Alt
	01-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2788 (Alternate), 01-080-2789 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2805 (Alternate), 01-080-2805 (Alternate), 01-080-2807 (Alternate), 01-080-2806 (Alternate), 01-080-2807 (Alternate), 01-080-2806 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2806 (Alternate), 01-080-2808 (Alternate), 01-080-2803 (Alternate), 01-080-2803 (Alternate), 01-080-2806 (Alternate), 01-080-2805 (Alternate), 01-080-2803 (Alternate), 01-080-2806 (Alternate), 01-080-2805 (Alternate), 01-080-2786 (Alternate), 01-080-2803 (Alternate), 01-080-2786 (Alternate), 01-080-2786 (Alternate), 01-080-2780 (Alternate), 01-086-2334 (Alternate), 01-086-2334 (Alternate), 01-086-2334 (Alternate), 01-086-2339 (Alternate), <04-007-2408 (Alternate), <04-007-4049 (Alternate), <04-007-2808 (Alternate), <04-007-4098 (Alternate), <04-007-2808 (Alternate), <04-007-4098 (Alternate), <04-007-2808 (Alternate), <04-007-4098 (Alternate), <04-007-2808 (Alternate), <04-007-4098 (Alternate), <04-007-2808 (Alternate), <04-007-3808 (Alternate), <04-007-3807 (Alternate), <04-007-3807 (Alternate), <04-007-3807 (Alternate), <04-007-3807 (Alternate), <04-007-3808 (Alternate), <04-007-3807 (Alternate),
CAS Number - PR:	10-80-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2788 (Alternate), 01-080-2899 (Alternate), 01-080-2809 (Alternate), 01-080-2805 (Alternate), 01-080-2805 (Alternate), 01-080-2805 (Alternate), 01-080-2805 (Alternate), 01-080-2807 (Alternate), 01-080-2808 (Alternate), 01-080-2811 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-2814 (Alternate), 01-080-2814 (Alternate), 01-080-2814 (Alternate), 01-080-2814 (Alternate), 01-080-2814 (Alternate), 01-080-2344 (Alternate), 01-080-2344 (Alternate), 01-080-2344 (Alternate), 01-080-2348 (Alternate), 01-090-2488 (Alterna
CAS Number - PR: .ast Modifications: References:	10-80-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 01-080-2899 (Alternate), 01-080-2809 (Alternate), 01-080-2809 (Alternate), 01-080-2805 (Alternate), 01-080-2805 (Alternate), 01-080-2805 (Alternate), 01-080-2807 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-2807 (Alternate), 01-080-2810 (Alternate), 01-080-2810 (Alternate), 01-080-2810 (Alternate), 01-080-2814 (Alternate), 01-080-2814 (Alternate), 01-086-2334 (Alternate), 01-086-2349 (Alternate), 01-086-2340 (Alternate), 01-086-2348 (Alternate), 01-086-2343 (Alternate), 01-086-2340 (Alternate), √ 04-007-2049 (Alternate), √ 04-007-2049 (Alternate), √ 04-007-2049 (Alternate), √ 04-007-2049 (Alternate), √ 04-006-6228 (Alternate), √ 04-007-0494 (Alternate), √ 04-006-0212 (Alternate), √ 04-008-0213 (Alternate), √ 04-008-0788 (Alternate), √ 04-008-0213 (Alternate), √ 04-008-0718 (Alternate), √ 04-008-0213 (Alternate), √ 04-008-0718 (Alternate), √ 04-008-0713 (Alternate), √ 04-008-0718 (Alternate), √ 04-008-0718 (Alternate), √ 04-008-0713 (Alternate), √ 04-008-0718 (Alternate), √ 04-008-07
CAS Number - PR: .ast Modifications: teferences: 'ype	10-80-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 01-080-2899 (Alternate), 01-080-2809 (Alternate), 01-080-2809 (Alternate), 01-080-2803 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2803 (Alternate), 01-080-2807 (Alternate), 01-080-2804 (Alternate), 01-080-2803 (Alternate), 01-080-2811 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-2814 (Alternate), 01-080-2819 (Alternate), 01-080-2819 (Alternate), 01-080-2819 (Alternate), 01-080-2839 (Alternate), 01-080-2349 (Alternate), 01-080-2349 (Alternate), 01-080-2349 (Alternate), 01-080-2349 (Alternate), 01-080-2349 (Alternate), <01-080-2349 (Alternate), 01-080-2348 (Alternate), 01-080-2349 (Alternate), <04-007-249 (Alternate), 01-080-2348 (Alternate), 01-080-2349 (Alternate), <04-007-249 (Alternate), 01-080-2348 (Alternate), 01-080-2349 (Alternate), <04-007-249 (Alternate), 04-007-2488 (Alternate), <04-007-248 (Alternate), 04-007-2488 (Alternate), <04-007-249 (Alternate), 04-007-2488 (Alternate), <04-007-249 (Alternate), 04-007-2488 (Alternate), <04-007-248 (Alternate), <04-007-249 (Alternate), <04-007-249 (Alternate), <04-007-248 (Altern
CAS Number - PR: .ast Modifications: References: Type	01-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2798 (Alternate), 01-080-2899 (Alternate), 01-080-2809 (Alternate), 01-080-2809 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2811 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2811 (Alternate), 01-080-2814 (Alternate), 01-086-2349 (Alternate), 01-086-2340 (Alternate), 01-086-2344 (Alternate), 01-086-2340 (Alternate), 01-086-2344 (Alternate), 01-086-2343 (Alternate), 04-007-7249 (Alternate), 01-080-2902 (Alternate), 01-086-2342 (Alternate), 01-086-2343 (Alternate), 04-007-7248 (Alternate), 04-007-388 (Alternate), 04-006-6528 (Alternate), 04-007-7249 (Alternate), 04-007-0049 (Alternate), 04-006-6528 (Alternate), 04-007-7249 (Alternate), 04-007-2048 (Alternate), 04-007-8659 (Primary), 04-007-7249 (Alternate), 04-007-388 (Alternate), 04-008-0788 (Alternate), 04-007-7249 (Alternate), 04-007-388 (Alternate), 04-007-7249 (Alternate), 04-007-388 (Alternate), 04-007-7249 (Alternate), 04-007-7249 (Alternate), 04-007-7249 (Alternate), 04-008-0231 (Alternate), 04-008-713 (Alternate) 13397-26-7 Entry Date: 09/01/2005 Last Modificati
CAS Number - PR: _ast Modifications: References: Fype Primary Reference Additional Reference	01-080-2795 (Alternate), 01-080-2706 (Alternate), 01-080-2797 (Alternate), 01-080-2789 (Alternate), 01-080-2809 (Alternate), 01-080-2809 (Alternate), 01-080-2809 (Alternate), 01-080-2803 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2811 (Alternate), 01-080-2805 (Alternate), 01-080-2816 (Alternate), 01-080-2816 (Alternate), 01-080-2805 (Alternate), 01-080-2813 (Alternate), 01-080-2813 (Alternate), 01-086-2334 (Alternate), 01-086-2334 (Alternate), 01-086-2334 (Alternate), 01-086-2334 (Alternate), 01-086-2334 (Alternate), 01-086-2343 (Alternate), 01-086-2343 (Alternate), 01-086-2343 (Alternate), 01-086-2348 (Alternate), 01-086-2343 (Alternate), 01-086-2348 (Alternate), 01-086-2343 (Alternate), 01-086-2348 (Alternate), 01-086-2343 (Alternate), 01-007-0498 (Alternate), 04-007-2049 (Alternate), 04-007-8088 (Alternate), 04-007-8048 (Alternat
Cross-Ref PDF #'s: CAS Number - PR: Last Modifications: References: Type Primary Reference Additional Reference Crystal Structure Structure	01-080-2795 (Alternate), 01-080-2796 (Alternate), 01-080-2797 (Alternate), 01-080-2788 (Alternate), 01-080-289 (Alternate), 01-080-2809 (Alternate), 01-080-2803 (Alternate), 01-080-2803 (Alternate), 01-080-2804 (Alternate), 01-080-2805 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2807 (Alternate), 01-080-2803 (Alternate), 01-080-2807 (Alternate), 01-080-2804 (Alternate), 01-080-2803 (Alternate), 01-080-2801 (Alternate), 01-080-2811 (Alternate), 01-080-2805 (Alternate), 01-080-2810 (Alternate), 01-080-2811 (Alternate), 01-080-9775 (Alternate), 01-080-2834 (Alternate), 01-080-2831 (Alternate), 01-080-2834 (Alternate), 01-086-2334 (Alternate), 01-086-2334 (Alternate), 01-086-2334 (Alternate), -/ 04-007-2049 (Alternate), -/ 04-007-2048 (Alternate), 01-080-2812 (Alternate), 01-086-2338 (Alternate), -/ 04-007-0489 (Alternate), -/ 04-006-6528 (Alternate), -/ 04-007-0489 (Alternate), -/ 04-006-0212 (Alternate), 04-007-2808 (Alternate), -/ 04-006-6528 (Alternate), -/ 04-012-8072 (Alternate), -/ 04-008-0212 (Alternate), -/ 04-008-0213 (Alternate), -/ 04-008-0718 (Alternate), -/ 04-012-8072 (Alternate), -/ 04-008-0213 (Alternate), -/ 04-008-0718 (Alternate), -/ 04-012-8072 (Alternate), -/ 04-018-018 (DITE) (Alternate), -/ 04-018-018 (DITE) (DITE) (Alternate), -/ 04-018-018 (DITE) (DITE) (Alternate), -/ 04-008-0218 (Alternate), -/ 04-008-018 (DITE) (DITE) (Alternate), -/ 04-018-018 (DITE) (DI

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.
--------------------	---

20 (°)	d (Å)	I	h	k	1	*	20 (°)	d (Å)	I	h	k	1	*	20 (°)	d (Å)	I	h	k	1	*
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	23	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	02	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	32	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	Ō		107.3138	0.956296	5	Ō	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	ō	õ	18		149.5093	0.798376	7	3	ž	6	
80.2006	1.195850	1	1	3	1		108.5999	0.948524	m	3	1	11				E.)			100	

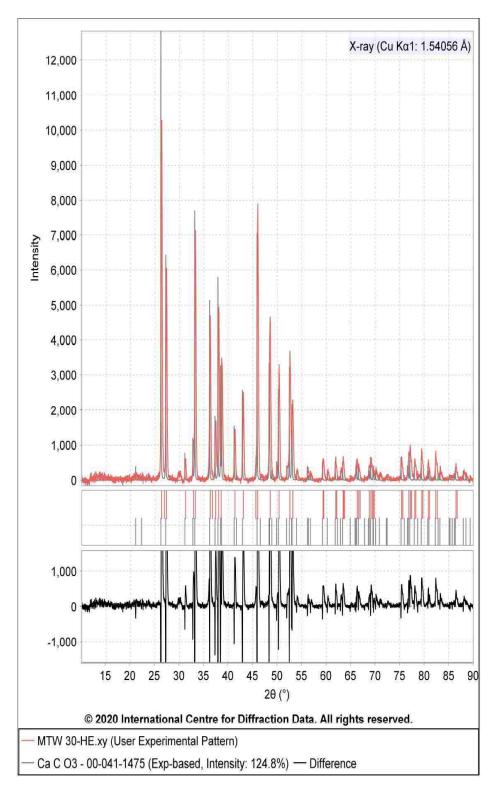


Figure E.10 XRD patterns of substances precipitated from Magnetically Treated Water (MTW) heating element at 30 °C from accelerated scale simulation study

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. 1 90 Å
Rotation: All	8 Rotations		

Preferences

Radiation: X-ray Wa	velength: Cu Ka1 1.54056 Å	Search Method: Hanawalt
Search Window: 0.15°	Match Window: 0.15°	2nd Pass Filter: Yes
d-Spacings: Weighted	Lowest Allowable GOM: 2	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

Jun 9, 2020 3:01 PM (fal-sharji2)

Status Primary QM: Empirical Formula: C	
Compound Name: Cal	-
Radiation: CuKα1 λ	λ: 1,5406 Å d-Spacing: Diff. Intensity: Diffractometer I/Ic: 1
Author's Cell [AuthCe AuthCell Vol: 227.11 Å Author's Cell Axial Rat Density [Dcalc: 2.927	ų AuthCell Z: 4.00 AuthCell MoÌVol: 56.78] atio [c/a: 1.158 a/b: 0.623 c/b: 0.721]
Crystal Data Axial Rati Reduced Cell [RedCel	a: 5.744 Å XtlCell b: 7.968 Å XtlCell c: 4.962 Å XtlCell α: 90.00° XtlCell β: 90.00° tlCell Vol: 227.11 Å ³ XtlCell Z: 4.00] tio [c/a: 0.864 a/b: 0.721 c/b: 0.623]
α: =1.5300 πωβ : :	=1.6810 εγ: =1.6854 Sign: =- 2V: =18(calc.)°
	re cross-referenced from PDF entry 04-012-0488 ADP: U lowed): Centrosymmetric s:
eq Operator	Seq Operator Seq Operator Seq Operator
x,y,z -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 4 x+1/2,y+1/2,-z+1/2 6 x+1/2,y,z 8 x,-y+1/2,z+1/2
tomic Coordinates: tom Num Wyckoff	Symmetry x y z SOF Uiso AET
Ca 1 4c C 2 4c	Ministry V<
Subfile(s): Mineral Rel Materials)	nd Hydration Product, Ceramic (Bioceramic), Common Phase, Educational Pattern, Forensic, Inorganic, slated (Mineral , Natural), Pharmaceutical (Excipient), Superconducting Material (Superconductor Related Formula Order]: Ca C O3 Prototype Structure [Alpha Order]: C Ca O3
PF Prototype Structu	ure [Formula Order]: Ca [C O3],oP20,62
	ure [Alpha Order]: C Ca O3,oP20,62 Aragonite (Group), carbonate (Subgroup) Pearson Symbol: oP20.00
00	0-005-0453 (Alternate), 01-071-2392 (Alternate), 01-076-0606 (Alternate), √ 04-006-5441 (Alternate), √
cross-Ref PDF #'s: 00	
04	4-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate)
CAS Number - PR: 14	4-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate)
CAS Number - PR: 14	4-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate) 4791-73-2 Entry Date: 09/01/1991
CAS Number - PR: 14 References: Type DOI Primary Reference Crystal Structure Dystical Data	4-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate) 4791-73-2 Entry Date: 09/01/1991
CAS Number - PR: 14: References: Type DOI Primary Reference Optical Data Structure	4-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate) 4791-73-2 Entry Date: 09/01/1991 Reference Keller, L., Rask, J., Buseck, P., Arizona State Univ., Tempe, AZ, USA. ICDD Grant-in-Aid (1989). Crystal Structure Source: LPF. Dana's System of Mineralogy, 7th Ed. II, 182 (1951). Jarosch, D., Heger, G. Tschermak Mineral. Petrogr. Mitt. 35, 127 (1986). 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). Co
CAS Number - PR: 14 References: <u>Vine</u> <u>DOI</u> 7/mary Reference 7/ystal Structure 2/ystal Structure 2/ystal Structure Structure Contabase Comments:	4-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate) 4791-73-2 Entry Date: 09/01/1991 Reference Keller, L., Rask, J., Buseck, P., Arizona State Univ., Tempe, AZ, USA. ICDD Grant-in-Aid (1989). Crystal Structure Source: LPF. Dana's System of Minerakogy, 7th Ed. II, 182 (1951). Jarosch, D., Heger, G. Tschermaks Mineral. Petrogr. Mitt. 35, 127 (1986). 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). Co Colorless. General Comments: Antacid. Optical Data Specimen location: Optical data on specimen from Blin, Bohemia, Czechosłovakia. Sample Source or Locality: Specimen from Sefrou, Morocco. Unit Cell
CAS Number - PR: 14 References: <u>Type Primary Reference</u> Crystal Structure Optical Data Structure Structure	4-007-0048 (Alternate), ✓ 04-008-5421 (Primary), ✓ 04-012-0488 (Alternate) 4791-73-2 Entry Date: 09/01/1991 Reference Keler, L., Rask, J., Buseck, P., Arizona State Univ., Tempe, AZ, USA. ICDD Grant-in-Aid (1989). Crystal Structure Source: LPF. Dana's System of Mineralexpy, 7th Ed. II. 182 (1951). Jarosch, D., Heger, G. Tschermaks Mineral. Petrogr. Mitt. 35, 127 (1986). 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 (Mt.%): major Ca, and trace Sr(<1). Co 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. 03 - 00-041-1475 (Stick, Fixed Slit Intensity) - Cu Ka1 1.54056 Å h k I * 20 (°) d(Å) I h k I * 20 (°) d(Å) I h k I * 20 (°) d(Å) I h k I * 1 0 2 0 311.1148 2.872000 60 0 0 2 38.1770 2.702000 60 0 1 2 0 2 0 0 1121

20 (°)	d (Å)	I	h	k	1 *	20 (°)	d (Å)	I	h	k	1	*	20 (°)	Jun 9, 2 d (Å)	I		k	
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
1.1858	2.190000	12	2	1	1	64.8787	1.436000	1	0	0	4		79.3988	1.205900	4m	0	6	2
1.6231	2.168000	2	1	3	1	65.8737	1.416700	1	2	2	3		79.3988	1.205900	m	2	4	3
12.8654	2,108000	20m	1		2	66.0576	1.413200	3	0	1	4		80,7577	1,189000	3	1	5	3
12.8654	2.108000	m	2	22	0	66.1897	1.410700	4	3	1	2		80.9714	1.186400	2	2	2	4
15.8520	1.977400	55	2	2	1	66.5465	1.404000	3	3	3	0		82.2556	1.171100	3m	1	6	2
6.5339	1.950000	1	0	3	2	67.8369	1.380400	<1	0	4	3		82.2556	1.171100	m	2	6	0
18.3175	1.882100	25	0	4	1	68.6339	1.366300	2	2	4	2		82.8500	1.164200	1m	0	4	4
18.4435	1.877500	25	2	0	2	68.7716	1.363900	2	3	3	1		82.8500	1.164200	m	3	4	2
18.8842	1.861600	2	0	1	3	69.0430	1.359200	5	1	1	4		83.2166	1.160000	2	4	2	1
19.8579	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	33	1	0	76.6095	1.242700	3m	23	0	4		88.5389	1.103500	m	4	3	1
59.2273	1.558800	4	3	1	1	76.6095	1.242700	m		4	1		89.4092	1.095000	<1	4	2	2
50.2095	1.535700	2	0	5	1	76.7628	1.240600	4	4	0	0							
51.8292	1.499300	4	2	4	1	77.0640	1.236500	6	3	1	3							