Quality control of *Calcarea carbonicum* 1X and 2X by FTIR

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Abstract

Background: Through this research work we determine the particle of calcium carbonate in 1X and 2X by FTIR

Methodology: prepared the *Calcarea carbonicum* 1x and 2x by the trituration with decimal scale, ex: 1 part of drug mixed in 9 parts of sugar of milk for preparing 1x, thereafter same procedure followed for prepare 2X Potency of *Calcarea carbonicum* by taking 1 part of previous potency 1X mixed with the sugar of milk. Afterwards take 1 part of each sample place over the FTIR (Fourier transform infrared spectroscopy) for determine the particle of calcium carbonate at different wavelength in 1X and 2X Potency.

Results: Identifying the calcium carbonate and calcite at 1431 nm, 869 nm, 307 nm (Wavlength) in 1X and 2X.

Key words: *Calcarea carbonicum*, FTIR, Trituration

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Introduction

One of the most adaptable analytical methods for the non-destructive, chemical characterization of geological samples, such as coal, is Fourier transform infrared spectroscopy (FTIR), which can offer essential information on the molecular structure of organic and inorganic components. Minerals, microfossils, silicate glass, fluid and melt inclusions, and shale are a few examples ([1-6]). The fundamental working principle of FTIR is transitions between quantized vibrational energy levels [7]. When a photon transfers to a molecule and excites it to a higher energy state, the molecule absorbs IR radiation during FTIR examination [8]. In the IR region of the light spectrum, the excited states cause molecular bonds to vibrate in a variety of ways, including stretching, bending, twisting, rocking, wagging, and out-of-plane deformation. The Each IR absorbance peak's wavenumber is unique to that particular functional group (such as C-H, O-H, C=O, etc.) and serves as a fingerprint for it thanks to its intrinsic physicochemical characteristics. An explanation of the core mechanism underlying this Griffiths and de Haseth [7] and Smith [9] both discuss technique. The bulk of inorganic and organic chemicals in the environment are IR active, and molecules having dipole moments can be detected using IR [7]. Mid-infrared (MIR) light (about 4000 to 400 cm'1) is the focus of much of the FTIR-related literature in geological sciences.

The abundance of the functional groups is inversely correlated with the absorbances of molecular vibrations under IR radiation. The greatest height or the integrated area between the peak and a baseline are frequently used to gauge the absorbance of each vibrational band. There are various baseline definition algorithms available. A linear line that is perpendicular to the minima on each side of the peak serves as the most often utilized baseline. [3].This kind of baseline is simple to establish and has excellent operator reproducibility [5]. As an alternative, baselines have been established using a French curve or flexi curve [10, 11], Gaussian combinations [12], and spectra of examined samples with the same composition but without the compounds of interest [13].

The Beer-Lambert Law (also known as Beer's Law) can be used to calculate the concentration of the component of interest from the IR absorbance:

Calcium carbonate

Widely found in nature, calcium carbonate is a mineral that develops from both biological sources and inorganic mineralogical processes.

CaCO3 is utilized in the manufacturing of civil construction materials as well as in food, cosmetics, pharmaceuticals, and agriculture. CaCO3 is used in biomedicine to create drug delivery systems for the treatment of cancer in the form of nanoparticles [16, 17]. A noteworthy application of CaCO3 is as a component in dietary supplements to prevent osteoporosis. A treatment created from the central layer of oyster shells is called calcarea carbonica, sometimes known as calcarea carb. Calcarea carbonica should be prepared through a process known as trituration because it is an impure carbonate, or CaCO3, as opposed to most homeopathic remedies, which are created from materials soluble in water or alcohol. [18]

Materials & Methodology

Type of study: Analytical method

Site of Study: PIHR (Parul Institute of Homoeopathy & Research) & CR4D (Centre of Research & Development of Parul University)

Tool used: FTIR (Fourier Transform Infrared spectroscopy)

Equipment's: Beaker, mortar, Pestle, Electronic balance, Spatula, Electric Potentizer machine

Procedure:

Sterilization: first sterilize all the laboratory equipment's under hot air oven for at least 10- 15 Minutes.

Weight: Measure the weight of calcium carbonate around 1 gm and sugar of milk around 9 gm by electronic balance.

(Preparation of 1X Potency)

Phase I: Take 1 part 1 gm of calcium carbonate in clean and dry mortar mixed with 1st part of sugar of milk such as (3 gm), thereafter starts trituration for 6 minutes, 3 minutes scrapping, 1 minutes mixing, repeat the same procedure for next 10 minutes. At the end of 20 minutes we will go for next phase.

Phase II: Add 2st part of sugar of milk i;e (3 gm) in mortar, thereafter starts trituration for 6 minutes, 3 minutes scrapping, 1 minutes mixing, repeat the same procedure for next 10 minutes. At the end of 20 minutes we will go for next phase.

Phase III: Add 3st part of sugar of milk i;e (3 gm) in mortar, thereafter starts trituration for 6 minutes, 3 minutes scrapping, 1 minutes mixing, repeat the same procedure for next 10 minutes. At the end of 20 minutes the whole procedure has finished. So at the end of total 60 minutes we get 1X Potency of *Calcium carbonate*.

(Preparation of 2X Potency)

Phase I: Take 1 part previous potency Calcium carbonate 1X in clean and dry mortar mixed with 1st part of sugar of milk i;e (3 gm), thereafter starts trituration for 6 minutes, 3 minutes scrapping, 1 minutes mixing, repeat the same procedure for next 10 minutes.

Phase II: Add 2st part of sugar of milk i;e (3 gm) in mortar, thereafter starts trituration for 6 minutes, 3 minutes scrapping, 1 minutes mixing, repeat the same procedure for 10 minutes.

Phase III: Add 3st part of sugar of milk i;e (3 gm) in mortar, thereafter starts trituration for 6 minutes, 3 minutes scrapping, 1 minutes mixing, repeat the same procedure for next 10 minutes. At the end of 20 minutes the whole procedure has finished. So as already told that at the end of 60 minutes we get 2X Potency of *Calcium carbonate*.

Storage:

All the drug material stored in a clean, dry, sterile, colourless bottle away from dampness, strong smelling bottles and sunlight.

Results

After analysis of *Calcium carbonate* 1X and 2X under FTIR (Fourier transform Infrared spectroscopy) Maximum transmission of functional groups are given below; such as see (Table. No.1. and Table.no.2)

Wavenumber	**Assignment**	**Ref**	**Wavenumber (cm$^{´1}$)**	**Assignment**	**Ref**
3300	OH stretch intermolecular bonding	[19, 21]	3698, 3652,1095, 1034, 908, 689, 528, 338	Kaolinite, $Al_2(Si_2O_5)(OH)_4$	[21,23]
3010	Aromatic C–H	[19–21]	1464, 705, 245	Aragonite, $CaCO_3$	[23
2950	Aliphatic CH_3	[19–21]	1450, 882, 729	Dolomite, $CaMg(CO_3)_2$	[23]
2920,	Aliphatic CH, CH_2, and CH_3	[19–21]	1431, 869, 307	Calcite, $CaCO_3$	[23]
1835	C=O, anhydride	[19]	3550, 3400,1615, 1155, 1132, 1106, 660	Gypsum, $CaSO_4$¨ $2H_2O$	[23]
1775–1765	C=O, ester with electron withdrawing group attached to single bonded oxygen	[19]	1115, 1148, 669	Anhydrite, $CaSO_4$	[23]
1735	C=O ester	[19]	1075, 790, 452	Quartz, SiO_2	[19,23]
1690–1720	C=O, ketone, aldehyde, and -COOH	[19]]	1052	Smectite, A D ¶	[24]
1650–1630	C=O highly conjugated	[19]]	1015	Oligoclase, [55] $(Na,Ca)[Al(Si,Al)Si_2O_8$]	
1600	Aromatic ring stretch	[19–21]	1006	Glauconite, 5] $(K,Na)(Mg,Fe)(Fe,Al)(Si, Al)_4O_{10}(OH)_2$	[5
~1600	High conjugated hydrogen bounded C=O	[19]	1001	Muscovite, $KAl_2(AlSi_3O_{10})(OH)_2$	[24]
1560–1590	Carboxyl group in salt from –COO´	[19]	984	Chlorite, $A_{5´6}T_4Z_{18}$ §	[24]
1490	Aromatic ring stretch	[19]	876, 727, 713	Ankerite, $Ca(Fe,Mg)(CO_3)_2$	[23]
1450	CH_2 and CH_3 bend, possibility of some aromatic ring modes	[19,20]	407, 396	Marcasite, FeS_2	[23]
1375	CH_3 groups	[19,21]	406, 340	Pyrite, FeS_2	[23]
1300–1100	C-O stretch and O–H bend in phenoxy structures, ethers	[19]			
1100–1000	Aliphatic ethers, alcohols	[19]			
900–700	Aromatic C–H out-of-plane bending modes	[19]			
860	Isolated aromatic H	[19]			
833	1,4-substituted aromatic groups	[19]			

815	Isolated H and/or 2 neighboring H	[19]
750	1,2-substituted, *i.e.*, 4 neighboring H	[19]

Table. No. 1. Maximum transmission of *Calcarea carbonicum* 1X

Wavenumber	**Assignment**	**Ref**	**Wavenumber (cm$^{´1}$)**	**Assignment**	**Ref**
3300	OH stretch intermolecular bonding	[19,21]	3698, 3652,1095, 1034, 908, 689, 528, 338	Kaolinite, $Al_2(Si_2O_5)(OH)_4$	[21,23]
3010	Aromatic C–H	[19–21]	1464, 705, 245	Aragonite, $CaCO_3$	[23]
2950	Aliphatic CH_3	[19–21]	1450, 882, 729	Dolomite, $CaMg(CO_3)_2$	[23]
2920,	Aliphatic CH, CH_2, and CH_3	[19–21]	1431, 869, 307	Calcite, $CaCO_3$	[23]
1835	C=O, anhydride	[19]	3550, 3400,1615, 1155, 1132, 1106, 660	Gypsum, $CaSO_4$¨ $2H_2O$	[23]
1775–1765	C=O, ester with electron withdrawing group attached to single bonded oxygen	[19]	1115, 1148, 669	Anhydrite, $CaSO_4$	[23]
1735	C=O ester	[19]	1075, 790, 452	Quartz, SiO_2	[19, 23]
1690–1720	C=O, ketone, aldehyde, and -COOH	[19]	1052	Smectite, A D ¶	[24]
1650–1630	C=O highly conjugated	[19]	1015	Oligoclase, [55] $(Na,Ca)[Al(Si,Al)Si_2O_8]$	
1600	Aromatic ring stretch	[19–21]	1006	Glauconite, [55] $(K,Na)(Mg, Fe)(Fe,Al)(Si,Al)_4O_{10}(OH)_2$	
~1600	High conjugated hydrogen bounded C=O	[19]	1001	Muscovite, $KAl_2(AlSi_3O_{10})(OH)_2$	[24]
1560–1590	Carboxyl group in salt from –COO´	[19]	984	Chlorite, $A_{5´6}T_4Z_{18}$ §	[24]
1490	Aromatic ring stretch	[19]	876, 727, 713	Ankerite, $Ca(Fe,Mg)(CO_3)_2$	[23]
1450	CH_2 and CH_3 bend, possibility of some aromatic ring modes	[19,20]	407, 396	Marcasite, FeS_2	[23]
1375	CH_3 groups	[19,21]	406, 340	Pyrite, FeS_2	[23]
1300–1100	C-O stretch and O–H bend in phenoxy	[19]			

	structures, ethers	
1100–1000	Aliphatic ethers, alcohols	[19]
900–700	Aromatic C–H out-of-plane bending modes	[19]
860	Isolated aromatic H	[19]
833	1,4-substituted aromatic groups	[19]
815	Isolated H and/or 2 neighboring H	[19]
750	1,2-substituted, *i.e.*, 4 neighboring H	[19]

Table. No. 2. Maximum transmission of *Calcarea carbonicum* 2X

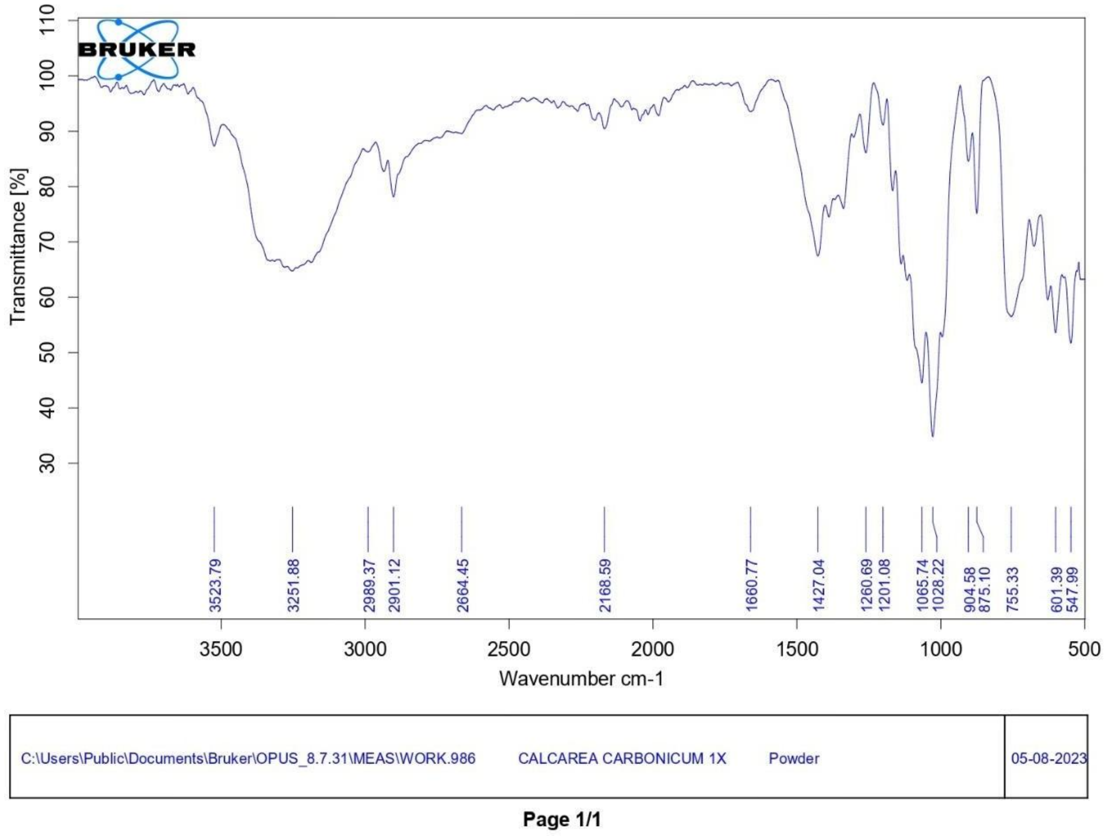

Figure no. 1. FTIR of *Calcarea carbonicum* 1X

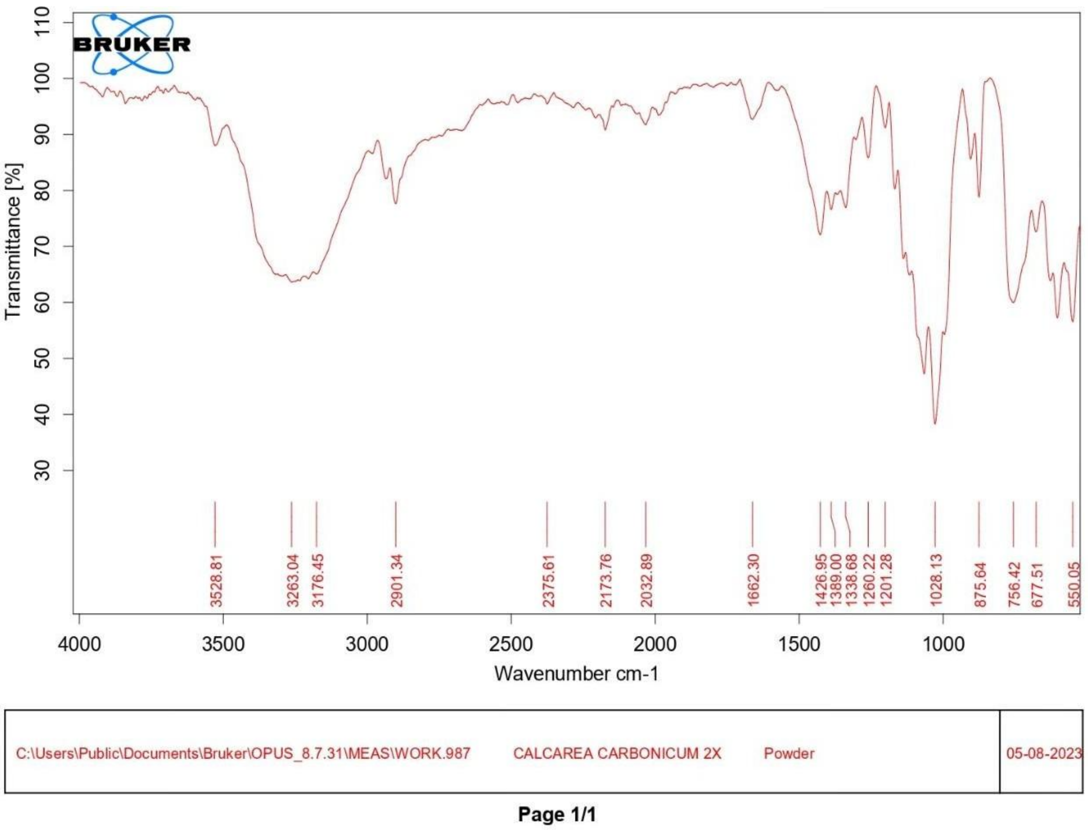

Figure no. 1. FTIR of *Calcarea carbonicum* 2X

Conclusion:

Through this research work, determination of drug particles of calcium carbonate and it's different functional groups at certain wavelength of *Calcium carbonicum* 1X and *Calcium carbonicum* 2X with the help of FTIR (Fourier transform infrared spectroscopy) is done and a good result has been obtained.

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