



Inorganic Composition and Crystal Structure of Zinc Phosphate

G. Patrick^{*1} and Mandava Sridhar²

^{1,2} Department of Physics, Gokaraju Rangaraju Institute of Engineering and Technology,
Hyderabad, Telangana, India.

*Corresponding Author: gratian.patrick@gmail.com

Abstract: Infrared spectroscopy is one of the most powerful analytical techniques which offer the possibility of chemical identification. The x-ray diffractogram reveals information regarding the inorganic constituent, crystallinity, and size distribution. X-ray diffractogram of zinc phosphate shows sharp peaks suggesting that it is highly crystalline in nature.

Introduction: Infrared spectroscopy is one of the most powerful analytical techniques which offer the possibility of chemical identification. This technique when coupled with intensity measurements can be used for quantitative analysis. Structure analysis of molecules can be carried out by infrared spectroscopy and x-ray diffraction among others. The x-ray diffraction pattern of a crystal is unique, and it is only necessary to measure diffraction angles and intensities of the peaks of the diffractogram of the sample concerned and to compare the results with those from a sample of the pure substance. Infrared spectroscopy and x-ray diffraction may be used as potential tools to provide valuable information in the study of biological systems.

Materials and methods

zinc phosphate (Harvard cement-Berlin) material was used for infrared spectroscopy analysis and x-ray diffraction studies. Infrared spectrum was recorded in K Br phase in a Perkin-Elmer FTIR-1605 spectrophotometer. The powdered dental samples mixed with K Br were pressed into a clear disc which were then mounted and examined directly. Shimadzu x-ray diffractometer XRD-6000 was used for x-ray analysis. X-rays were produced by a copper target at about 40,000 volts. The width of the receiving slit was 0.3 mm. General scan of the powder samples was taken with a scanning speed of 8 degree per minute for characterization whereas for the intensity measurements, diffractograms were taken with a slower scanning speed of 2 degree per minute.

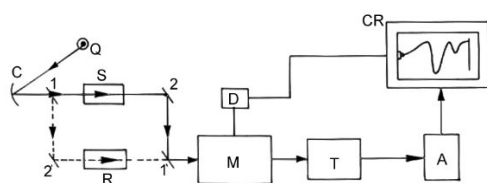


Figure 1. Schematic diagram for the measurement of IR spectrum

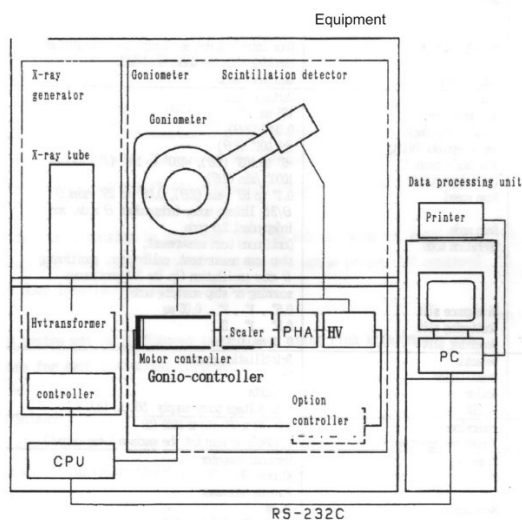


Figure 2. XRD-6000 system block diagram

Results and discussion

Infrared spectroscopy relies upon the interaction between electromagnetic radiation and oscillating dipoles caused by molecular vibrations. Functional groups have characteristic vibration frequencies and greater the force constant for a particular deformation, the higher the frequency of vibration. Stretching and bending vibrations may be observed but bending vibrations are only observed below 1500 cm^{-1} . The infrared spectra in the region $4000 - 200\text{ cm}^{-1}$ of zinc phosphate is shown in Fig. 3. The main aim of the infrared spectroscopic study is to analyze the principle constituent and its combination in the material.

The infrared spectrum can be divided into three regions.

1. The region 4000 to 3000 cm^{-1} is concerned with water and hydroxyl group. This region is of considerable interest, because it reveals the nature of hydrogen bonding.
2. The region 3000 to 1500 cm^{-1} , wherein bands for functional groups are seen. In this region the absorption bands pertaining to proteins occur.
3. The region 1500 to 200 cm^{-1} has significant importance in the context of biological minerals like the restorative dental material.

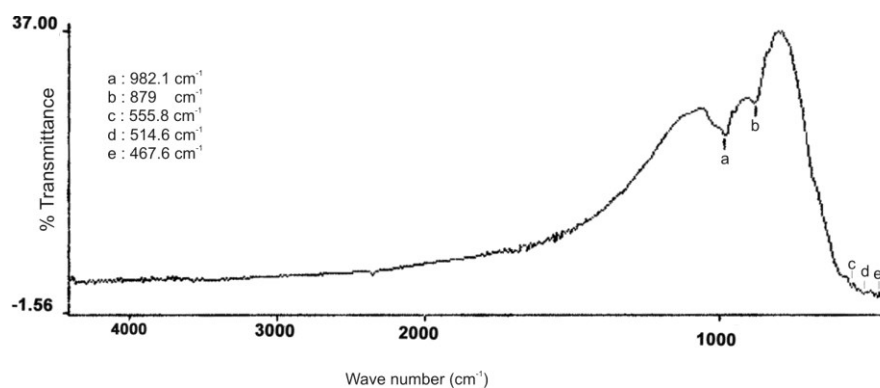


Fig 3. Infrared spectrum of Zinc Phosphate

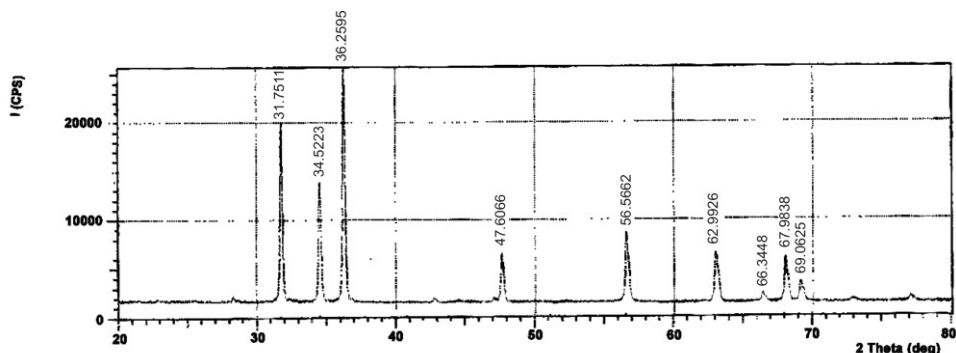


Fig 4. X ray diffractogram of Zinc Phosphate

The presence of H₂O in a mineral can be detected by the two characteristic bands in 3600 cm⁻¹ to 3200 cm⁻¹ region and in 1650 cm⁻¹ region. If water is present as lattice water, an additional band occurs in the region of 600 cm⁻¹ to 300 cm⁻¹. When H₂O is coordinated to a metal ion another band appears in the 880 cm⁻¹ to 650 cm⁻¹ regions. These peaks are due to combinations and overtones of the fundamental vibrational modes of the water molecule.

The bands 470 cm⁻¹ (P-O-symmetric bend), 560 cm⁻¹ (P-O anti symmetric bend) and 960 cm⁻¹ (P-O-symmetric stretch) are related to calcium phosphate. The significant difference in the intensity of the bands 560 cm⁻¹ and 600 cm⁻¹ speaks about the crystallinity of calcium phosphate. The bands 870 cm⁻¹ (C-O bend); 1410 cm⁻¹ and 1450 cm⁻¹ (C-O bend) are characteristic of carbonate ion. Zhang et al (2010) reported several sharp absorption bands from 900 to 1200 cm⁻¹ in zinc phosphate nanoparticles which were due to complex stretching of PO₄³⁻ group.

The x-ray diffractogram, figure 4, of zinc phosphates shows sharp peaks, suggesting that it is highly crystalline in nature and that the size distribution of crystallites is uniform. Jian Dong Wang et al (2011) reported strong peaks in zinc phosphate nanoparticles.

It can be concluded that zinc phosphate is crystalline in nature and that the nano sized particles would find wider use in medical field.

References

- [1] M. Zhang, J. K. Liu, R. Miao, G. M. Li and Y. J. Du, "Preparation and Characterization of Fluorescence Probe from Assembly Hydroxyapatite Nanocomposite," *Nano-scale Research Letters*, Vol. 5, 2010, pp. 675-679. doi:10.1007/s11671-010-9530-4
- [2] Jian Dong Wang, Da Li, Jin Ku Liu, Xiao Hong Yang, Jia Luo He and Yi Lu, "One-Step Preparation and Characterization of Zinc Phosphate Nanocrystals with Modified Surface," *Soft Nanoscience Letters*, 2011, 1, 81-85 doi:10.4236/sn.l.2011.13015