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Growth and Characterization of Glutamine Potassium Carbonate – New Semi Organic Crystal

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Abstract

A new semi organic crystal of Glutamine potassium carbonate (GPC) crystal has been grown by slow evaporation method by using water as solvent. The particle size of the GPC crystal was calculated by powder X-Ray diffraction method. Using UV-VIS-NIR spectral analysis, it was found that the crystal has good transparency in the expected region and the lower cut off wavelength is observed. The vibrational modes are assigned by recording the FT-IR spectrum. The Vickers hardness test has also been taken for experimental crystals. The NLO behavior of GPC crystal was tested by Kurtz-Perry powder technique.

Keywords: GPC - Glutamine potassium carbonate crystal, UV-Vis-NIR-Ultraviolet –visible - Near infrared, FT-IR-Fourier transform of Infrared, NLO-Non linear optic.

Introduction

Semi organic crystals play a vital role in the applications of optoelectronic communications, optoelectronic devices and in lasers also. In recent years organic nonlinear optical crystals have attracted much attention for their large non linear coefficient, high laser damage threshold. However, most of organic NLO materials have poor mechanical and thermal properties, resulting in the damage of crystal during processing. To avoid this drawback, a new type of NLO material has been grown from organic-inorganic complexes. These semi organic materials have high optical nonlinearity of a purely organic compound combined with the mechanical and thermal properties of inorganic materials. [1-3].

Experimental procedure Synthesis and growth

Single crystals of Glutamine potassium carbonate were grown at room temperature by slow evaporation of an aqueous solution containing Glutamine and potassium carbonate in the ratio 1:1 as per the reaction. Crystals have come to the shape in 90 days and shown in the Figure 1.



Figure 1. Photograph of GPC crystals

Characterization

Powder XRD analysis was done by using X-ray diffractometer with λ =1.5406X10⁻¹⁰m radiation to identify the size of the particle. By varying the position and height FWHM and d-spacing are determined. UV-Vis-NIR spectral analysis of GPC



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crystal was recorded in the range 200-1100 nm and the percentage of transmittance was also recorded. The FT-IR spectrum has also been taken in order to find the vibrational modes. The Vickers hardness test was also done to measure the physical strength of the crystal. SHG test was done to find out the NLO property of the crystal.

Results and discussion

Powder X ray diffraction

The particle size of Glutamine mixed potassium carbonate crystal was done by using XRD. The size of the particle was estimated using the formula of Scherer by monochromatic radiation.

 $D = 0.9 \lambda/\beta \cos\theta$

where, D stands for the size of the particle.

 $\lambda = 1.5406 \times 10^{\text{--}10} \text{ m}$

 θ = 30.0606 (observed diffracting angle)

 $D = 3.9042 \times 10^{-8} m$

By varying 2 θ , the (d-spacing) inter-planar spacings are noted.

FTIR spectral analysis

FT-IR spectrum was recorded by FT-IR spectrophotometer in the range 400- 4000cm⁻¹. By changing the wave numbers, the different assignments obtained are given in the following table.



Figure 2. FTIR spectrum of GPC crystal

From the FT-IR spectrum, (of the experimental crystal) assignments of vibrational modes are made and are tabulated. [4-5]

Wavenumber	Assignment
3199	N-H Symmetric Stretching
2528	S-H stretching
2239	N=C=O antisymmetric stretching
1879	C=C ring
1715	C=O stretching
1624	C=O stretching & NH2 deformation
1500	N-H Symmetric
1422	In plane OH bending
1310	COO ⁻ symmetric stretching
1125	C-O stretching
1019	C-O stretching
901	CH2 out of plane wagging
859	NH ₂ wagging
569	COO ⁻ Rocking
499	C-N-C bending



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UV-VIS spectrum analysis

From the spectrum, it is found that, the GPC is transparent in the region from 200nm-1100nm. It has good transmittance and the lower cut off wavelength is observed at 208.03nm. The large range of transmittance in the visible region enables the GPC to be good for optoelectronic applications. [6]



Figure 3. Transmission spectrum of GPC

Mechanical studies

The micro hardness of a substance is a key property to interpret the mechanical strength of the material which is basically related to the crystal structure and about the atomic package. This test affords useful details about the mechanical properties like elastic constants, yield strength etc., of materials. [7] The variation of H_v with the applied load for the crystals are shown in fig.4. In this crystal, hardness increases, if we increase the load Thus, this crystal has good physical strength.



Figure 4. Load versus H_v

Second Harmonic Generation studies

Dynamic research has been engaged to find the NLO property of the crystal. The NLO conversion efficiency was tested using Kurtz and Perry setup [8]. A Q-switched Nd:YAG laser beam of wavelength 1064 nm was used. The output energy of the sample is 0.910 times of the KDP reference energy. Hence, the GPC compound crystal has nonlinearity nature.

Conclusion

Single crystals of GPC have been grown by slow evaporation method. The particle size is estimated using XRD. From UV-Vis-NIR spectral analysis, the crystal may be recommended for optoelectronic applications. In FT-IR spectrum analysis, the vibrational modes are identified. The physical strength of the crystal has been measured in the Vicker's hardness test. The GPC compound crystal has nonlinearity nature and it has been found out by Kurtz Perry method.

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providing instrumental facilities for characterization.

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