

# Piezoelectric and Mechanical Properties of Potassium Hydrogen Phthalate Single Crystal

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## Abstract

Potassium Hydrogen Phthalate is one of the most promising semi organic crystal with dielectric properties. A good quality crystal was harvested in a 30 days period using solution growth method. The grown crystal was subjected to various characterization techniques like Single crystal X-ray diffraction analysis, ferroelectric and micro hardness analysis. Unit cell dimensions of the grown crystal have been identified from XRD studies. Piezoelectric properties and Vickers's hardness test was done to study its mechanical property.

**Keywords:** KHP, Crystal growth, mechanical and piezo electric properties

## 1. INTRODUCTION

Semi-organic NLO crystals have attracted attention because they have been proposed as a new approach for materials with fascinating NLO properties which have the combined properties of both inorganic and organic crystals like high damage threshold, wide transparency range, less deliquescence and high non-linear coefficients which make them suitable for device fabrication. Potassium Hydrogen Phthalate (KHP) with the chemical unit formulae  $K(C_6H_4COOH-COO)$  is a semi-organic salt that belongs to the alkali acid phthalate series. KHP crystal presents long term stability and is used in devices due to its electro optical properties. KHP is chosen as model compound because of its well developed surface pattern on the (010) face consisting of very high and low growth steps which can be relatively easily observed by means of optical microscopy [1-5]. For any device application, various mechanical properties are very important. The mechanical behavior of a crystal is of paramount importance in technological applications. The hardness of the material is identified as an important mechanical property. The variation of Vickers micro hardness with applied load is studied. The grown sample is subjected to the

piezoelectric meter system, which is a special instrument for directly measuring the piezoelectric constants values of the given materials.

## 2. CRYSTAL GROWTH

The title compound was prepared by the slow evaporation method. KHP crystals were grown from high purity salt. The solution of KHP salt was prepared in a slightly under saturation condition at 30 °C. The solution was stirred well for six hours constantly using magnetic stirrer, then the solution was filtered using a filter paper. The solutions were kept undisturbed by covering with a thick sheet of paper for controlled slow evaporation. Transparent, good quality crystals of KHP were collected after 20 days. The photograph of grown crystals is shown in fig 1.



**Figure 1:** Grown crystal of KHP

## 3. CHARACTERIZATION:

Single crystal XRD analysis was carried out with APEX2v 2.0 diffractometer with Mo K $\alpha$  rays to identify the lattice parameters. Vickers's hardness was calculated to analyze the mechanical properties of the grown crystal. The piezoelectric constants value of the grown crystal also analysed.

## 4. RESULTS AND DISCUSSIONS:

### 4.1 Single Crystal X-Ray Diffraction Analysis

Single crystal X-ray diffraction is an analytical technique in which X-rays are employed to determine the actual arrangement of atoms within a crystalline specimen. With the set of X-ray diffraction data collected, it is possible to get unit cell

parameter, space groups, molecular structure of the crystalline solids and Miller indexing. The single crystal of pure KHP was subjected to single crystal XRD using a computer controlled Enraf Nonius – CAD4 X-ray diffractometer with Mo K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) to determine the unit cell dimension and morphology, and the unit cell dimensions determined by single crystal X-ray diffraction analysis are tabulated in table 4.1.

**Table 4.1:** Crystallographic data of pure KHP crystals

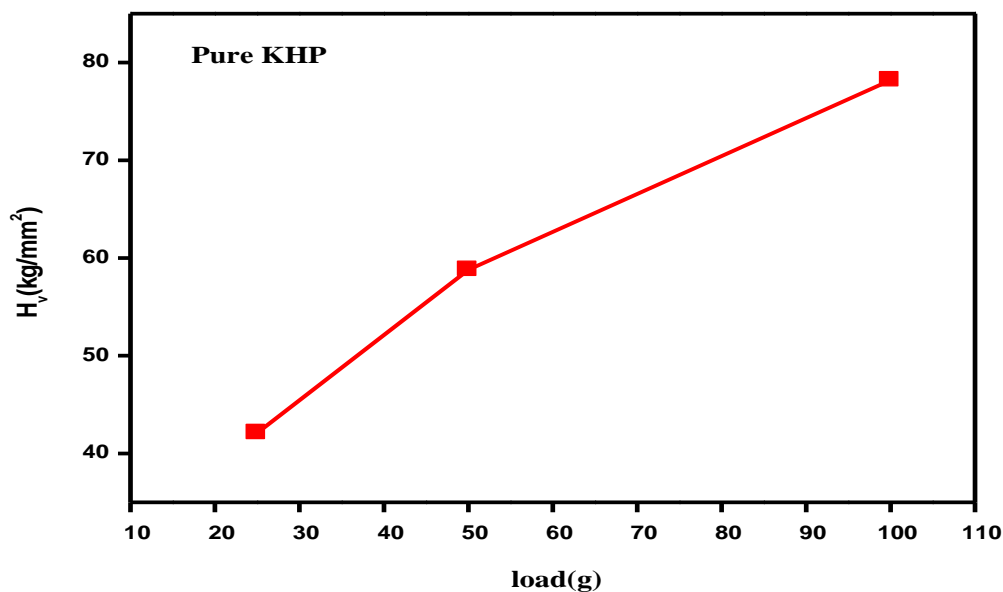
Chemical formula	K(C <sub>6</sub> H <sub>4</sub> COOH-COO)
Molecular Weight	204.22
Crystal system	Orthorhombic
Space group	Pca2 <sub>1</sub>
Density	1.64 g/cm <sup>3</sup>
a	9.638 $\text{\AA}$
b	13.353 $\text{\AA}$
c	6.494 $\text{\AA}$
$\alpha$	90°
$\beta$	90°
$\gamma$	90°
cell volume V	835.753 $\text{\AA}^3$

From the study, it was observed that the grown crystal belongs to the orthorhombic system with space group **Pca2<sub>1</sub>**. It was found that the lattice parameters and cell volumes are in good agreement with the literature values [6].

#### **4.2 Mechanical Study**

The mechanical properties of the grown crystal were studied by Vickers hardness test. Vickers hardness method is the reliable and the most common among the various methods of hardness measurement [7]. The applied loads were 25, 50 and 100 g. For each load P, several indentations are made and the average diagonal length (d) is used to calculate the microhardness number (H<sub>v</sub>) using the relation, **H<sub>v</sub> = 1.8544 P / d<sup>2</sup> kg-mm<sup>-2</sup>**

For KHP crystal, hardness increases with increasing load. The plot of hardness against the load is shown in figure 2. The work hardening coefficient is 3.77. As the value of n is greater than 2, it is inferred that KHP crystal is a soft type material [8].



**Figure 2:** Variation of hardness number with applied load for crystal.

### 4.3 Piezoelectric Study

The piezoelectric substance is one that produces an electric charge when a mechanical stress is applied. These materials are a class of low-symmetry materials that can be polarized. A special instrument for directly measuring the piezoelectric constants values of given materials is the piezoelectric meter system. The obtained piezoelectric coefficient ( $d_{33}$ ) value results indicate the presence of piezoelectric nature of the crystal. The obtained piezoelectric coefficient ( $d_{33}$ ) value for grown KHP crystal is 0.92 pC/N. The results indicate the piezoelectric nature of the crystal indicating its advantage in broadband transducer applications [9].

### CONCLUSION

Single crystals of KHP was grown and harvested in 20 days. Lattice parameters were confirmed by Single crystal X- ray studies. The work hardening coefficient ( $n$ ) was calculated which inferred that the grown KHP crystal is a soft type material. The piezoelectric nature of the crystal indicating its advantage in broadband transducer applications.

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