

Growth and Characterization of KI-Doped KDP Single Crystals

¹Md. Kamrul Hasan, ²Mohammad Khairul Islam Juman,
³Abdulla Noor

¹Lecturer (Physics), Faculty of Science, CCN University of Science & Technology, ²Assistant Professor & Chairman, Department of Business Administration, CCN University of Science & Technology, ³Department of Physics, Comilla University

DOI Link: <http://dx.doi.org/10.6007/IJARBSS/v16-i10/29146>

Published Date: 28 October 2026

Abstract

Crystalline materials are solids in which atoms, molecules, or ions are arranged in a regular and repeating three-dimensional structure. Potassium dihydrogen phosphate (KDP) is an important crystalline material because of its optical, ferroelectric, and piezoelectric characteristics. In the present study, the influence of potassium iodide (KI) incorporation on the properties of potassium dihydrogen phosphate (KDP) single crystals was investigated. Both undoped KDP and KI-doped KDP crystals containing 0.10 mole%, 0.15 mole%, and 0.20 mole% KI were prepared by the slow evaporation solution-growth method. The optical behavior was examined by UV-Visible spectroscopy over the wavelength interval of 200-1100 nm, while Fourier transform infrared (FTIR) spectroscopy was used to examine the characteristic functional groups and bonding environment. Thermogravimetric analysis (TGA) was also conducted to investigate the thermal behavior of the crystals. The obtained crystals were transparent and stable. The UV-Visible measurements showed a clear change in the transmission and absorption characteristics after KI incorporation, while the lower wavelength cut-off remained close to 400 nm for the investigated samples. The TGA profiles showed multi-stage thermal decomposition. The first major decomposition region was observed at 195.59°C for pure KDP, 221.09°C for 0.10 mole% KI-doped KDP, and 202.48°C for 0.20 mole% KI-doped KDP. These observations indicate that KI incorporation modifies the optical and thermal behavior of KDP single crystals.

Keywords: Slow Evaporation, Crystallization, Uv-Visible Spectroscopy, Ftir Spectroscopy, Tga

Introduction

Potassium dihydrogen phosphate (KDP), chemically represented as KH_2PO_4 and also referred to as monopotassium phosphate (MKP), is a widely investigated inorganic nonlinear optical (NLO) crystal. Its broad spectral response, efficient frequency conversion, high optical quality, and comparatively high resistance to laser-induced damage make it useful in nonlinear optical applications. KDP crystals are commonly employed for harmonic generation, including frequency doubling, tripling, and quadrupling of Nd:YAG laser radiation at room temperature.

Because KDP can be produced in large dimensions while maintaining a high laser-damage threshold, it has also been considered suitable for high-energy laser and fusion-related systems [16]. The choice of crystal-growth method depends on the physical and chemical characteristics of the material as well as the required crystal dimensions. The continuing development of coherent ultraviolet sources and nonlinear optical devices has increased the demand for crystals with improved optical and structural characteristics.

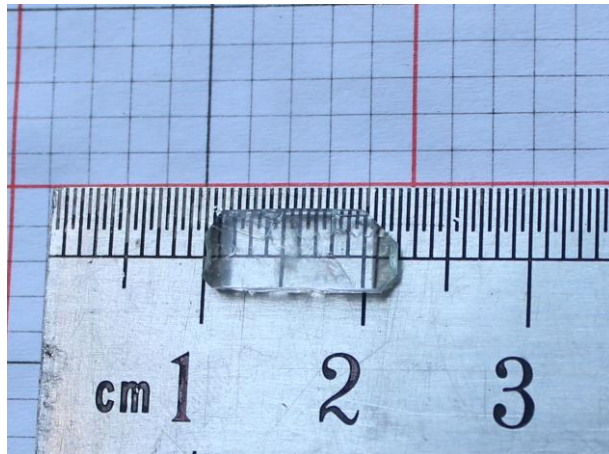
For a material to be useful in practical NLO devices, it should be obtainable as a high-quality bulk single crystal. Consequently, the development of crystal-growth techniques and the systematic evaluation of crystal properties remain important areas of materials science and engineering. NLO crystals are widely used for frequency conversion, signal processing, frequency doubling, and optical information-storage applications. KDP is particularly attractive because it combines a large nonlinear optical coefficient, good structural quality, broad transparency extending from the ultraviolet to the near-infrared region, and high laser-damage resistance. The present work focuses on the preparation and characterization of pure and KI-doped KDP single crystals using the slow evaporation solution-growth technique (SEST). KI concentrations of 0.10 mole%, 0.15 mole%, and 0.20 mole% were introduced to examine how the dopant affects crystal growth and the resulting optical, structural, and thermal characteristics. The synthesized samples were characterized by UV-Visible spectroscopy, FTIR spectroscopy, and thermogravimetric analysis, and their observed properties were compared with those of pure KDP.

Materials and Methods

High-purity KDP single crystals were prepared from aqueous solution using the slow evaporation technique at ambient temperature. Analytical Reagent (AR) grade KDP was dissolved in deionized water and continuously stirred for 240 minutes with a magnetic stirrer to obtain a homogeneous solution. The solution was then filtered through Whatman filter paper and transferred to a borosilicate beaker. The growth solution was kept in a vibration-isolated constant-temperature bath to provide stable growth conditions. The same procedure was followed for the preparation of KI-doped KDP solutions containing 0.10 mole%, 0.15 mole%, and 0.20 mole% KI. After approximately 25 days of controlled evaporation, transparent and stable single crystals with good visual quality were obtained.

Results and Discussion

High-quality single crystals of pure KDP and KI-doped KDP were successfully obtained from the prepared solutions. The crystals were transparent and displayed a tetrahedral morphology. Photographs of the grown samples, placed over graph paper for visual size comparison, are presented in the figure below.



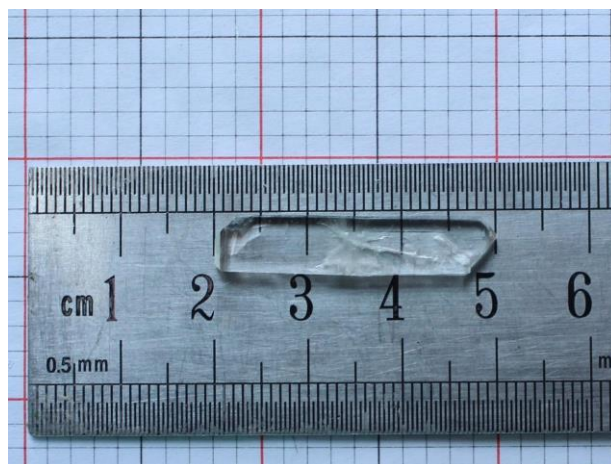
(a)



(b)



(c)



(d)

Figure Photographs of (a) pure KDP, (b) 0.10 mole% KI-doped KDP, (c) 0.15 mole% KI-doped KDP, and (d) 0.20 mole% KI-doped KDP single crystals

UV-Vis Spectra of Sample Crystals

The optical transmission characteristics of the pure and KI-doped KDP crystals were measured using a Shimadzu UV-1601 spectrophotometer. Measurements were performed in single-scan mode at medium scan speed with a sampling interval of 20 over the wavelength range of 200-1100 nm. Crystal specimens having a thickness of approximately 1.5 mm were used for the optical measurements.



Figure Shimadzu UV-1601 spectrophotometer used for UV-Visible measurements

The transmission spectra of the pure and KI-doped KDP samples at the investigated concentrations are presented in Figure-1. The measurements cover the ultraviolet and visible regions from 200 to 1100 nm and allow the effect of KI incorporation on optical transmission to be compared.

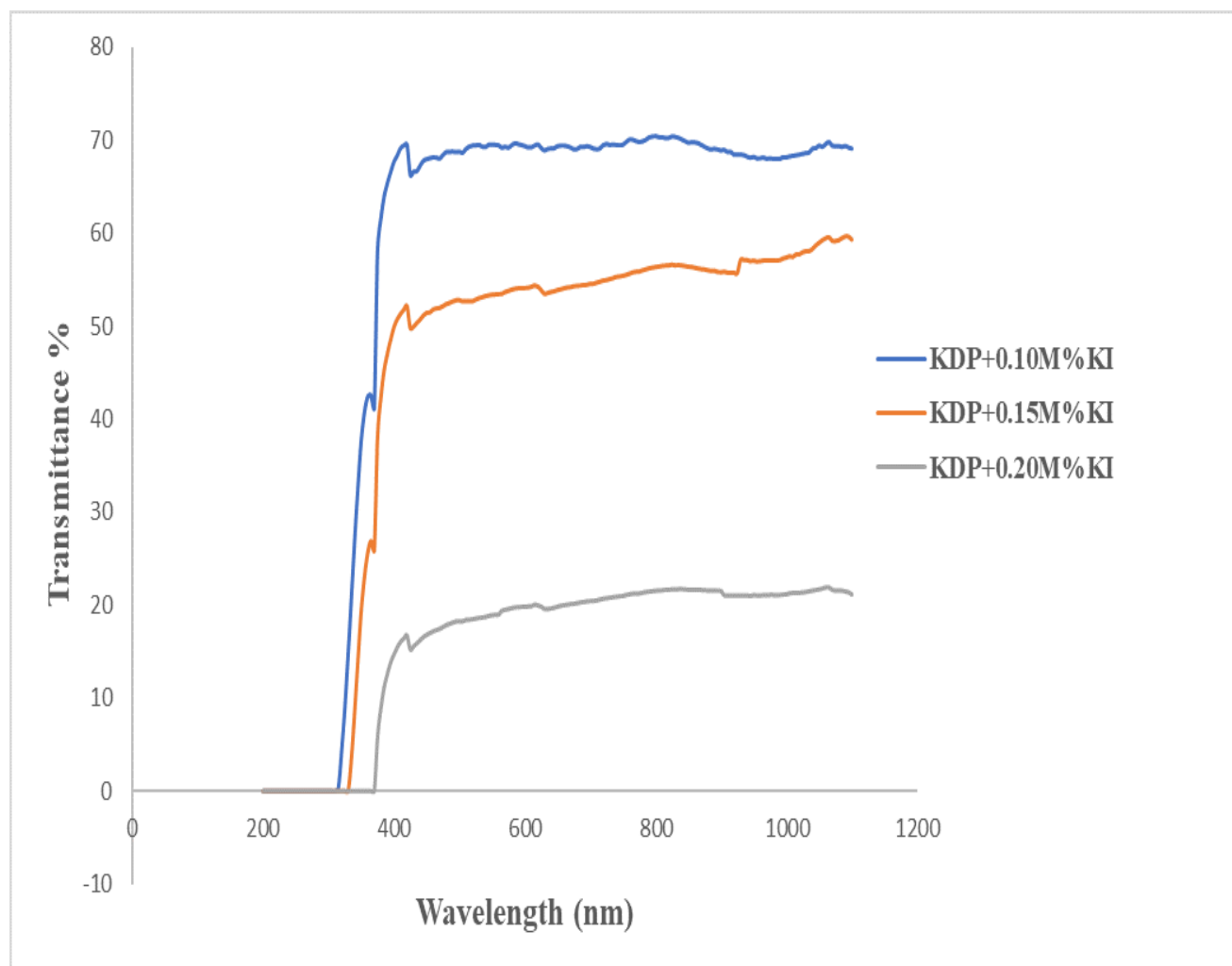


Figure-1 UV-Visible transmission spectra of KI-doped KDP single crystals.

The UV-Visible spectra show appreciable transmission in the visible region for the investigated crystals. The addition of KI changes the transmission level compared with the corresponding undoped material. A pronounced increase in transmission begins near 360 nm, after which the samples show comparatively higher transmission toward the visible and near-infrared regions.

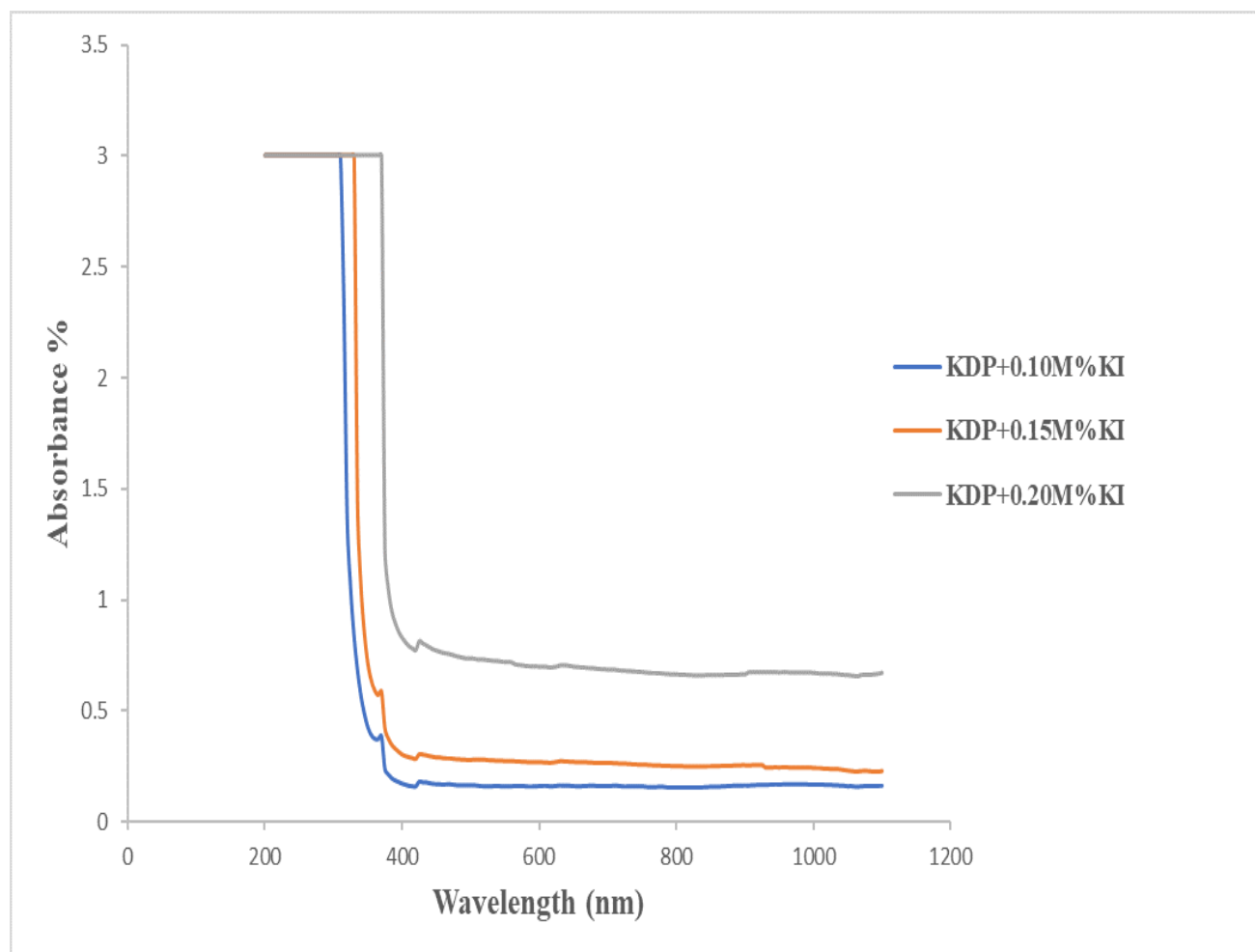


Figure-2 UV-Visible absorption spectra of KI-doped KDP single crystals.

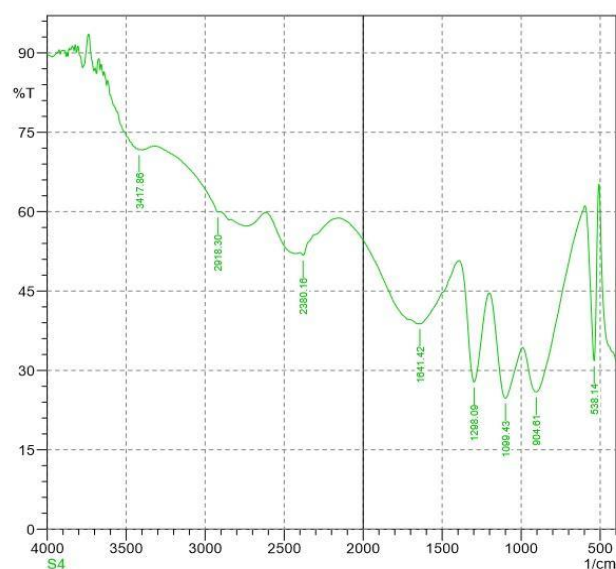
The absorption spectra indicate relatively low absorption throughout most of the visible region. KI incorporation modifies the absorption intensity, with the doped samples showing higher absorbance than the corresponding lower-absorption region of the spectra. A sharp decrease in absorbance is observed around 400 nm, after which the absorption remains comparatively low over the longer-wavelength region.

FTIR Spectroscopy

FTIR spectroscopy was employed to qualitatively examine the characteristic constituents and bonding environment of the grown crystals. The spectra were obtained using the KBr pellet method over the wavenumber range of 400-4000 cm^{-1} . The FTIR responses of the pure and KI-doped KDP samples are presented in the following figures.

SHIMADZU

CARS, DU



Peak	Intensit	Corr. In	Base (H	Base (L	Area	Corr. Ar
1	538.14	31.778	31.994	596	507.28	29.054
2	904.61	25.923	14.254	991.41	596	163.438
3	1099.43	24.742	14.851	1201.65	991.41	106.011
4	1298.09	27.802	19.906	1392.61	1201.65	80.905
5	1641.42	38.806	0.036	1647.21	1635.64	4.755
6	2380.16	51.761	1.057	2401.38	2154.49	62.236
7	2918.3	59.932	0.538	3307.92	2902.87	69.685
8	3417.86	71.687	0.152	3427.51	3406.29	3.059

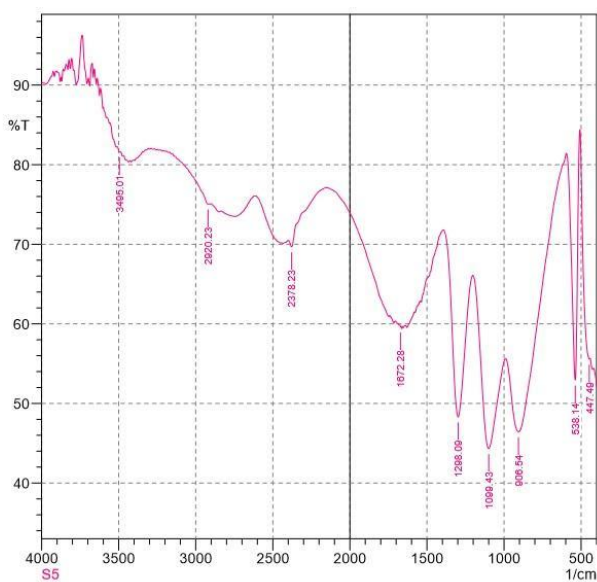
Comment;
S4

Date/Time; 10/23/2017 4:11:42 PM
No. of Scans;
Resolution;
Apodization;

(a)

SHIMADZU

CARS, DU

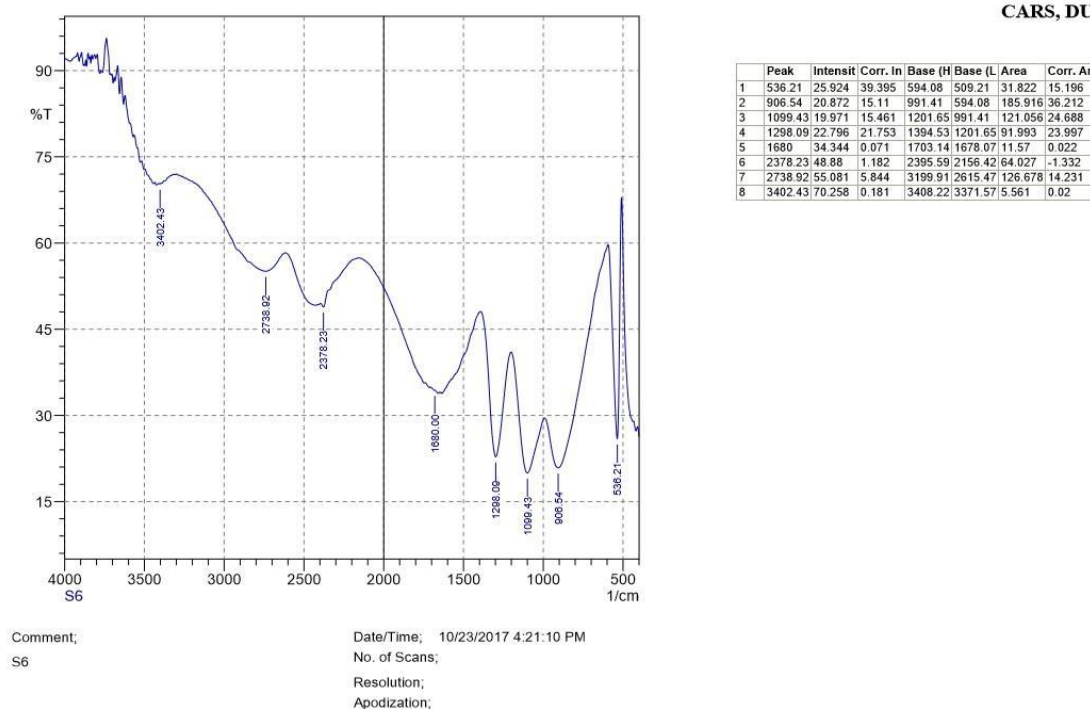


Peak	Intensit	Corr. In	Base (H	Base (L	Area	Corr. Ar
1	447.49	55.56	2.648	507.28	441.7	13.095
2	538.14	52.935	30.469	596	509.21	14.506
3	906.54	46.452	14.624	989.48	597.93	85.909
4	1099.43	44.319	16.685	1201.65	991.41	59.677
5	1298.09	48.297	20.683	1390.68	1203.58	43.072
6	1672.28	59.593	0.18	1678.07	1668.43	2.159
7	2378.23	69.688	1.399	2401.38	2150.63	32.436
8	2920.23	75.05	0.495	3170.97	2900.94	28.229
9	3495.01	81.587	0.232	3508.52	3489.23	1.682

Comment;
S5

Date/Time; 10/23/2017 4:18:00 PM
No. of Scans;
Resolution;
Apodization;

(b)



(c)

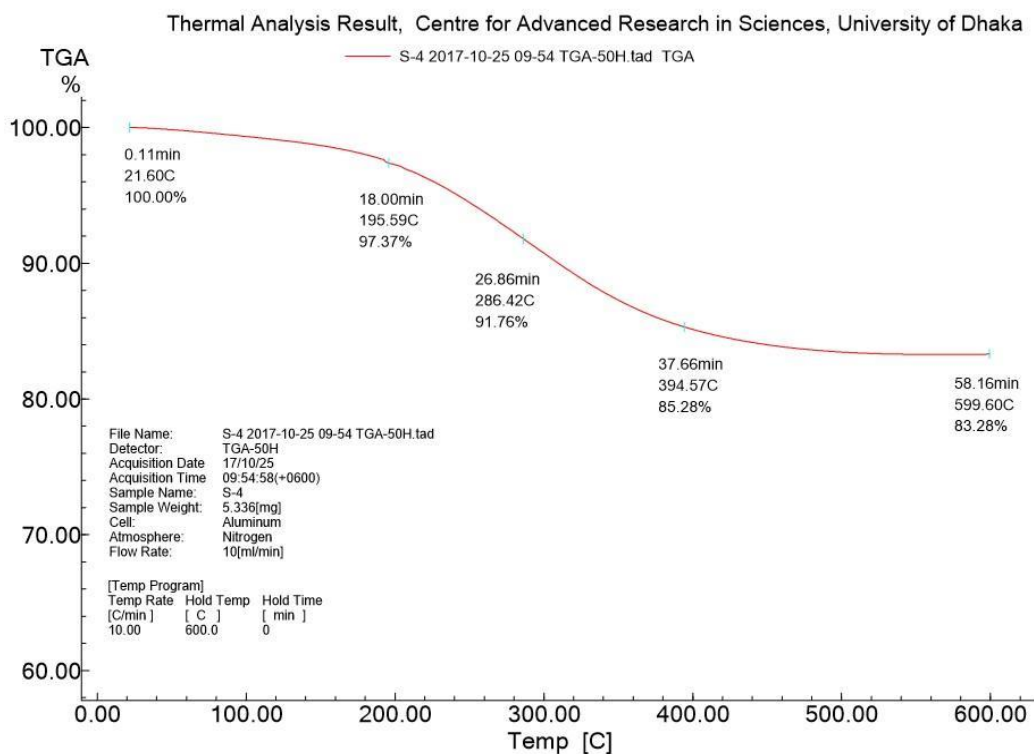
Figure-3 FTIR spectra of (a) pure KDP, (b) 0.10 mole% KI-doped KDP, and (c) 0.20 mole% KI-doped KDP

The FTIR spectrum of pure KDP contains an absorption band near 3448.8 cm^{-1} , while the corresponding band in the KI-doped samples shows a slight shift. These bands are associated with free O-H stretching vibrations, suggesting that the local O-H environment is affected by KI incorporation. A broader absorption region between approximately 2750 and 3200 cm^{-1} can be attributed to intermolecular hydrogen-bonded O-H stretching. The position of this hydrogen-bond-related feature changes as the dopant concentration is increased, indicating a modification of the hydrogen-bonding environment within the crystal.

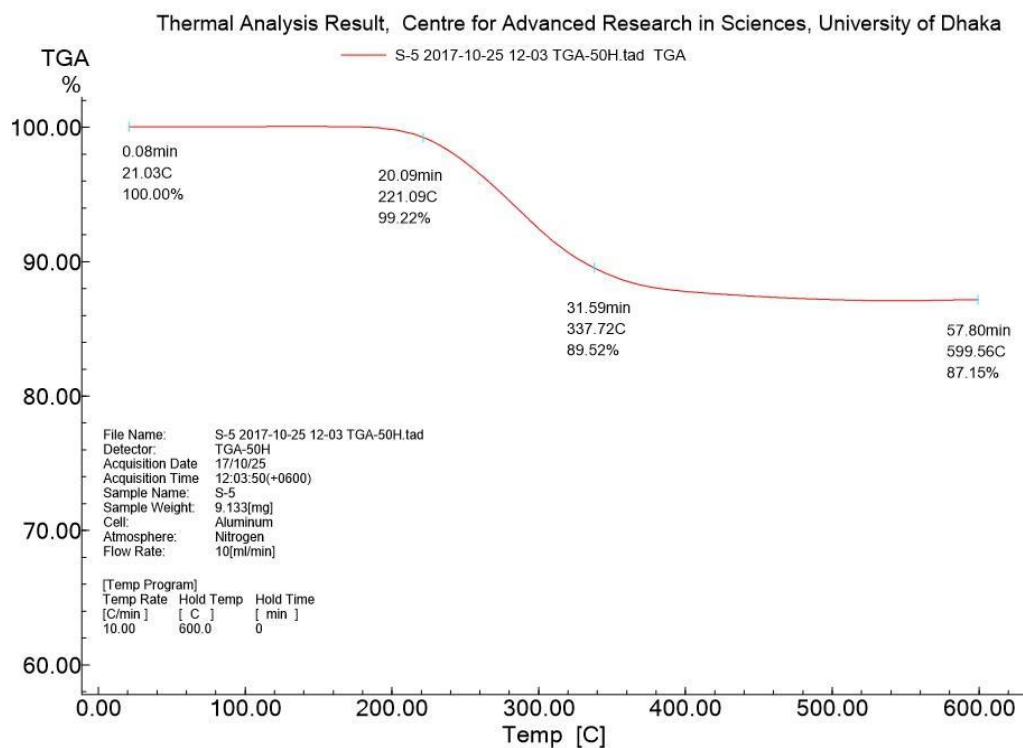
TGA/DTA Measurement of Sample Crystals

Thermogravimetric analysis (TGA) and differential thermal analysis (DTA) were carried out to evaluate the thermal behavior of pure and KI-doped KDP crystals. The measurements were performed with a TG/DTA-6300 thermal analyzer under a nitrogen atmosphere over a heating range of 30 – 500°C . A ceramic crucible was used during heating, and the heating rate was maintained at 20°C per minute. For the pure KDP measurement, the initial sample mass was 1.544 mg , while alumina with a mass of 2.830 mg was used as the reference material.

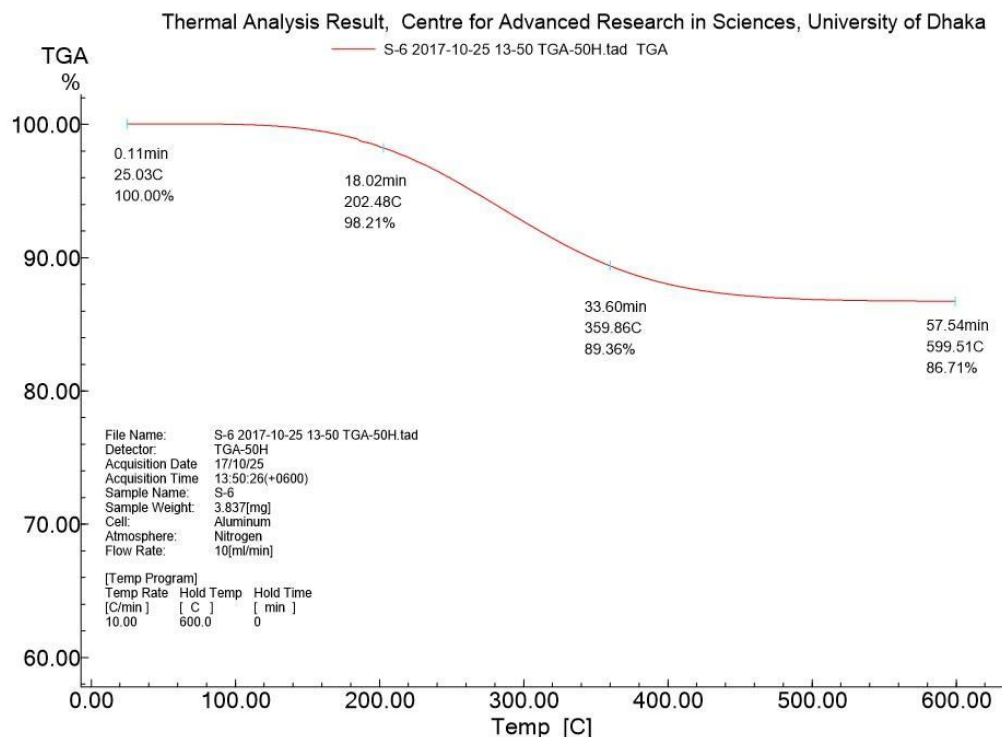
The recorded TG/DTA curves for pure KDP and the KI-doped KDP samples at the investigated concentrations are shown below.



(a)



(b)



(c)

Figure-4 TGA/DTA curves of (A) pure KDP, (B) KDP + 0.10% KI, and (C) KDP + 0.20% KI.

The TGA profiles demonstrate that both pure and KI-doped KDP undergo thermal changes in more than one stage. For pure KDP, the observed transition extends from approximately 195.59°C to 394.57°C. For the 0.10 mole% KI-doped sample, the corresponding transition occurs from about 221.09°C to 337.72°C, whereas the 0.20 mole% KI-doped sample shows a transition from approximately 202.48°C to 359.86°C. The observed mass-loss regions are associated with the thermal decomposition processes occurring in the KDP-based crystals.

Conclusion

The present study investigated the influence of potassium iodide (KI) doping on the optical, vibrational, and thermal properties of potassium dihydrogen phosphate (KDP) single crystals prepared using the slow evaporation technique. Pure KDP crystals and KI-doped samples containing 0.10, 0.15, and 0.20 mole% KI were examined to evaluate the effects of dopant concentration on their material properties. The findings reveal that the concentration of KI plays an important role in determining the optical transparency and thermal behavior of the resulting crystals.

Among the investigated compositions, the sample containing 0.10 mole% KI exhibited the most favorable overall performance. It showed the highest optical transmittance, reaching approximately 70% in the visible region, whereas the transmittance decreased to around 50–60% and 20% for the 0.15 and 0.20 mole% KI-doped samples, respectively. A similar improvement was observed in thermal behavior. The major thermal decomposition onset temperature increased from 195.59°C for pure KDP to 221.09°C for the 0.10 mole% KI-doped crystal. In comparison, the sample containing 0.20 mole% KI exhibited a major decomposition region beginning at approximately 202.48°C. These results suggest that a relatively low KI

concentration provides a more favorable balance between optical transparency and thermal resistance within the composition range investigated.

The FTIR analysis indicated that the characteristic bonding features of the KDP crystal remained identifiable following KI incorporation. The observed changes in the free O–H and intermolecular hydrogen-bonding regions further suggest modifications to the local hydrogen-bonding environment. In addition, the optical band gap was estimated to be 3.4531 eV, based on the absorption cut-off region around 360–400 nm. Collectively, these observations provide insight into the relationship between KI concentration and the optical, vibrational, and thermal characteristics of KDP crystals.

Despite these promising results, the study has certain limitations. The investigation was restricted to three KI concentrations within a relatively narrow range, and X-ray diffraction (XRD) analysis was not performed to establish possible structural changes associated with doping. Further research should therefore examine a broader range of dopant concentrations and incorporate XRD analysis to clarify the structural characteristics of the crystals. Additional quantitative optical and thermal measurements would also help establish the reproducibility of the observed trends. Overall, the present findings identify 0.10 mole% KI as the most promising composition among those examined, although further structural and experimental validation is required before drawing broader conclusions about its potential applications.

References

- Akhtar, F., & Podder, J. (2011). A study on structural, optical, electrical and etching characteristics of pure and L-alanine doped potassium dihydrogen phosphate crystals. *Journal of Crystallization Process and Technology*, 1(3), 55–62.
- Alexandru, H. V., Berbecaru, C., Grancea, A., & Iov, V. (1996). KDP prismatic faces: Kinetics and the mechanism of their growth from solutions. *Journal of Crystal Growth*, 166(1–4), 162–168.
- Islam Juman, M. K., Jalil, A., Yeasmin, K. F., Tamanna, N., Roy, T. C., & Jahan, I. (2025). AI-driven EdTech innovations for workforce reskilling: Bridging education and business needs. *International Journal of Academic Research in Business and Social Sciences*, 15(11), 808–829.
- Juman, M. K. I., Hasan, M. K., & Yeasmin, K. F. (2026). Financial Market Dynamics in the FinTech Era: A Statistical Physics-Inspired Business Analysis of Risk, Volatility, and Stability. *International Journal of Academic Research in Progressive Education and Development*, 15(2), 1619–1643.
- Begum, S. A., & Podder, J. (2009). Influence of co-doped bimetallic impurities on the metastable zone width and induction period for nucleation of KDP from aqueous solutions. *Trends in Applied Sciences Research*, 4(4), 241–247.
- Hirotaa, S., Miki, H., Fukui, K., & Maedaa, K. (2002). Coloring and habit modification of dyed KDP crystals as functions of supersaturation and dye concentration. *Journal of Crystal Growth*, 235, 541–546.
- Kanagathara, N., & Anbalagan, G. (2012). Growth, optical and dielectric studies on pure and L-lysine doped KDP crystals. *International Journal of Optics*, 2012, Article 826763.
- Yeasmin, K. F., Juman, M. K. I., Chowdhury, M. T. I., Synthia, T. I. C., Hossain, M., & Jalil, A. (2025). Towards sustainable AI: Green accounting-based model for measuring the environmental cost of intelligent systems. *International Journal of Academic Research*

- in Accounting, Finance & Management Sciences, 15*(4), 156–181. Human Resource Management Academic Research Society. <https://doi.org/10.6007/IJARAFMS/v15-i4/26812>
- Kumaresan, P., Moorthy Babu, S., & Anbarasan, P. M. (2005). Influence of dopants (L-glutamic acid, L-histidine and L-valine) on the performance of KDP crystals. *4th DAE-BRNS Laser Symposium*, 4, 521–522.
- Kumaresan, P., Moorthy Babu, B. S., & Anbarasan, P. M. (2007). Effect of metal ion and amino acid doping on the optical performance of KDP single crystals. *Journal of Optoelectronics and Advanced Materials*, 1(2), 65–69.
- Li, G., Xue, L., Su, G., Li, Z., Zhuang, X., & He, Y. (2005). Rapid growth of KDP crystal from aqueous solutions with additives and its optical studies. *Crystal Research and Technology*, 40(9), 867–870.
- Juman, M. K. I., Hasan, M. K., Rahaman, H., & Yeasmin, K. F. (2026). Nanotechnology Adoption, Green Innovation and ESG Performance: The Mediating Role of Environmental Accounting in Sustainable Business. *International Journal of Academic Research in Accounting, Finance and Management Sciences*, 16(4), 101–124.
- Loretta, F., Rani, T. J., Selvarajan, P., Perumal, S., & Ramalingom, S. (2011). Growth, structural and optical studies of pure and bithiourea zinc chloride doped potassium dihydrogen phosphate single crystals. *World Journal of Science and Technology*, 1(3), 1–6.
- Muley, G. G. (2012). Study on growth habit, SHG and thermal properties of urea phosphate doped KDP crystals. *Science and Technology*, 2(5), 109–113.
- Muley, G. G., Rode, M. N., & Pawar, B. H. (2009). FT-IR, thermal and NLO studies on amino acid (L-arginine and L-alanine) doped KDP crystals. *Acta Physica Polonica A*, 116, 1033–1038.
- Parikh, K. D., Dave, D. J., Parekh, B. B., & Joshi, M. J. (2007). Thermal, FT-IR and SHG efficiency studies of L-arginine doped KDP crystals. *Bulletin of Materials Science*, 30(2), 105–112.
- Roy, T. C., Tahera, K. T., Juman, M. K. I., Alin, A. I. J., & Jahan, I. (2026). FinTech Integration and Digital Accounting Systems in Enhancing Financial Performance of Startups. *International Journal of Academic Research in Accounting, Finance and Management Sciences*, 16(2), 97–114.
- Parikh, K. D., Dave, D. J., Parekh, B. B., & Joshi, M. J. (2010). Growth and characterization of L-alanine doped KDP crystals. *Crystal Research and Technology*, 45(6), 603–610.
- Juman, M. K. I., FarhanaYeasmin, K., Mazumder, N. H., Jalal, M. S., & Bhuiyan, M. M. (2026). Corporate Law Challenges of FinTech Adoption in Developing Countries Implications for Corporate Governance and Regulatory Compliance. *International Journal of Academic Research in Accounting, Finance and Management Sciences*, 16(1), 263–287.
- Podder, J. (2002). The study of impurities effect on the growth and nucleation kinetics of potassium dihydrogen phosphate. *Journal of Crystal Growth*, 237–239, 70–75.
- Pritula, I. M., Velikhov, Y. N., Levchenko, A. N., Kolybayeva, M. I., Puzikov, V. M., Tyutyunnik, V. B., & Doroshenko, A. O. (2004). Effect of organic dye on the growth and optical properties of KDP. *Functional Materials*, 11(4).
- Pritula, I., Gayvoronsky, V., Gromov, Y., Kopylovski, M., Kolybayeva, M., Puzikov, V., & Kosinova, A. (2008). The effect of thermal annealing on linear and nonlinear optical response of dyed KDP crystals. *Functional Materials*, 15(4).
- Chowdhury, M. T. I., Juman, M. K. I., & Yeasmin, K. F. (2026). Harnessing artificial intelligence for sustainable edupreneurship and next-generation knowledge business models.

- International Journal of Academic Research in Progressive Education and Development, 15(1), 331–361.
- Rahman, A., & Podder, J. (2010). Effect of EDTA on the growth kinetics and structural and optical properties of KDP crystal. *International Journal of Optics*, 2010, Article 978763.
- Shnidshtein, I. V., Strukov, B. A., Grabovsky, S. V., Pavlovskaya, T. V., & Carman, L. (2001). Effect of an organic dye on the ferroelectric phase transition in KH_2PO_4 (KDP). *Physics of the Solid State*, 43(12), 2276–2279.
- Singh, P., Hasmuddin, M., Rajveersingh, Wahab, M. A., & Shkir, M. (2012). Structural investigation on R6G dye and PbI_2 doped KDP single crystals by using powder X-ray diffraction. *Advanced Science, Engineering and Medicine*, 4, 415–420.
- Strukov, B., Shnidshtein, I., & Grabovsky, S. (2007). Phase transitions in KDP crystals with the complex organic and inorganic impurities. *Condensed Matter Physics*, 10(1), 111–118.
- Juman, M. K. I., Hyder, M. N. A., Rahaman, M., & Yeasmin, K. F. (2025). Artificial intelligence in business decision making: Legal, ethical, & strategic implications. *International Journal of Academic Research in Economics and Management Sciences*, 14(4), 301–322.
- Sun, X., Xu, X., Gao, Z., Fu, Y., Wang, S., Zeng, H., & Li, Y. (2000). Effect of EDTA on the light scatter in KDP crystals. *Journal of Crystal Growth*, 217, 404–409.
- Suresh Kumar, B., & Rajendra Babu, K. (2008). Effect of L-arginine, L-histidine and glycine on the growth of KDP single crystals and their characterization. *Indian Journal of Pure and Applied Physics*, 46(2), 123–126.
- Ugine Prince, M., & Perumal, S. (2012). Electrical properties of allylthiourea doped KDP single crystals. *Archives of Applied Science Research*, 4(1), 508–512.
- Velikhov, Y., Pritula, I., Ganina, I., Kolybayeva, M., Puzikov, V., & Levchenko, A. N. (2007). Growth and properties of dyed KDP crystals. *Crystal Research and Technology*, 42(1), 27–33.