J. Mountain Res. P-ISSN: 0974-3030, E-ISSN: 2582-5011
Vol. 21(S2), (2026) 94-103
DOI: https://doi.org/10.51220/jmr.v21-S2.12

# Effect of Electric Field on Phase Transition and Dielectric Properties of Deuterated $KD_2PO_4$(DKDP) Crystal

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**Received: 24.08.2025; Revised: 21.10.2025; Accepted: 19.11.2025**


**Abstract:** This study theoretically investigates the phase transition and ferroelectric characteristics of deuterated $KD_2PO_4$ (DKDP) crystals when subjected to an external electric field, denoted by E. To build upon previous research, we expanded the pseudo-spin model Hamiltonian. This modification takes into account extra spin-lattice interactions, cubic and quadratic phonon anharmonic interactions, spin-spin couplings, and the presence of an external electric field. Our approach involves employing Zuberav's double-time thermal-dependent Green's function method. This method enables us to explore a range of properties including acoustic attenuation, the behavior of smooth functions, relaxation time, electric conductivity, and Cochran's permittivity, and quality factor etc. By applying this theoretical framework, we have derived theoretical formulae for quality factor, tangent loss, permittivity, soft mode frequency and established a strong correspondence between our theoretical predictions and the experimental data outlined in prior studies conducted by Kaminow. This alignment validates our theoretical model's capability to capture the fundamental behaviors exhibited by the DKDP crystal under examination.

**Keywords:** Cochran's permittivity • Green's function • Phase Transition • Quality factor.

## Introduction

The 96% deuterated $KD_2PO_4$ (DKDP) crystal undergoes phase transition at about 173K. The study of $KD_2PO_4$ aroused an interest from several years due to non-linear, and laser technological applications such as second harmonic generation, oscillators, and high-power laser systems etc. Chabin and Gilleta, (1974) studied KDP crystals of the arsenate type, analyzing the pseudospin parameter $< S^z >$, which represents spontaneous polarization. They observed that pseudo-spin parameters $<S^x>$ and $<S^y>$exhibit a first-order phase transition under four-spin coupling $< S_i^z S_j^z S_k^z S_l^z >$ but this does not provide sufficient insight into the transition from ferroelectric to paraelectric states. The analysis of the arsenate-type KDP family's crystal structure revealed that higher-order phonon anharmonic interactions and four-spin coupling are significant at Curie temperature and above. Matysina and Eremenko (2003) examined quadrupole interactions in four $AsO_4$ or $PO_4$ groups and linked them to phonon-anharmonic effects influencing soft mode properties, aligning with Cochran's frequency theory (1960). Blinc et al. (1974) studied the dynamical susceptibility of an Ising model Hamiltonian under a transverse tunneling field. Their findings indicated that the soft mode spectra within the ordered phase can be underdamped but become overdamped above Tc. Deuteration reduces tunneling integral, eliminating the underdamped nature. Levitskii (2001) applied cluster theory to tunneling, observing that increasing the univalent ion size (K+→Rb+→Cs+) reduces first-order transition behavior, shifting it towards second-order transitions. Garland and Novotny (1969) investigated the ultrasonic properties of $KH_2PO_4$, measuring ultrasonic shear wave speed and attenuation above Tc = 122.82 K. They confirmed an elastic Curie-Weiss law and a cooperative relaxation time at constant stress. Pollina and Garland (1975) conducted ultrasonic and dielectric measurements on single-crystal cesium dihydrogen arsenate, examining dielectric constants along the free and clamped c-axis. They observed discrepancies of 20K between the free and clamped Curie temperatures, and the a-axis dielectric constant exhibited a first-order discontinuity with antiferroelectric properties between 90K to 300 K. Tuval and Nettleton (1976) analyzed ultrasonic attenuation in KDP from a microscopic perspective, focusing on longitudinal acoustic phonons modulating dipole-dipole separation. They applied Zubarev's (1960) double-time Green's function method within the random phase approximation. Chabin and Gilletta (1977) studied ferroelectric mode coupling, polarization, and dielectric properties of various KDP-type crystals, comparing spontaneous polarization with a four-cluster approximation model. Their results aligned with experimental data on dielectric constant values, excess specific heat, and latent heat of transition. Garland and Litov (1987) provided a comprehensive review of ultrasonic investigations on KDP-type crystals, covering microscopic and phenomenological theories. Their analysis linked experimental ultrasonic velocity and attenuation data with Silsbee, Uehling, and Schmidt's order-disorder model and the Landau relaxation theory. They examined proton tunneling's role in isomorphs, suggesting it alone cannot explain isotope effects on temperature and relaxation rates. Hu et al. (1990) explored ferroelectric phase transitions in $RbD_2PO_4$, measuring shear elastic wave attenuation and velocity. The softening of $C_{66}$ followed the Curie-Weiss law, and polarization relaxation time $\tau$ exhibited critical behavior, with Tc and $\tau 0$ highly sensitive to deuteration. Mizaras et al. (1994) investigated $PbHPO_4$'s dielectric properties near its phase transition using ultrasonic and microwave methods. Ultrasonic waves along the b-axis showed significant velocity and attenuation deviations, consistent with Landau-Khalatnikov theory. They proposed a temperature-dependent formula for polarization relaxation time and found that internal bias fields from imperfections influence ultrasonic velocity and relaxation times. Upadhyay et al. (2006) studied external electric field effects on KDP-style ferroelectrics, developing a pseudospin-lattice coupled model (PLCM). Their calculations, using the double-time Green's function method, indicated that both dielectric constant and loss tangent deccrease with the applied field. Starkov et al. (2012) examined the pyroelectric effect's influence on ferroelectric transition points. They linked polarization behavior to a transition from the Landau-Ginzburg-Devonshire model to the Landau-Khalatnikov equation, accounting for the pyroelectric effect. Their model accurately described temperature hysteresis. Upadhyay and Nautiyal (2013) investigated TGS crystals under external electric fields using a modified two sub-lattice pseudospin-lattice coupled model. Numerical simulations matched experimental findings from Bye et al. (1972) and Sreekumar (1994). Bist and Panwar (2016) studied dielectric properties and ultrasonic absorption in KDP-style ferroelectrics using a gentle dynamical model. They expanded Blinc model to include lattice inharmonicity up to the fourth order. Their results highlighted the relaxation mode of $H_2PO_4$ crystal and their random motion as a key factor influencing dielectric properties and ultrasonic absorption, with computed data closely aligning with experimental results. Sivakumar et al. (2019) investigated dielectric peculiarities of KDP crystals exposed to shock waves for microelectronic and optoelectronic applications. They found that shock-wave-loaded crystals exhibited reduced dielectric constants due to domain orientation shifts and lattice polarization changes. Their results suggested potential applications in microelectronics and optoelectronics. Khan and Upadhyay (2021) used a modified model Hamiltonian with a two-sublattice pseudospin lattice coupling approach and Green's function technique to study phase shifts in PbHPO4-

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like crystals. Their findings, aligning with Arend et al. (1976), confirmed the model's effectiveness.

Yukana et al. (2022) analyzed non-dehydrated triglycine sulfate using neutron diffraction, confirming its ferroelectric behavior at 20 K due to O-H-O hydrogen bonds. They refined double-minimum and single-minimum models at 298 K, finding comparable results with no significant structural differences across temperatures. Bhuva et al. (2023) studied glutamic acid-doped KDP crystals, noting enhanced second harmonic generation efficiency, reduced transmittance, and a slight decrease in the energy band gap. Impedance analysis showed non-Debye relaxation, while AC conductivity supported a limit hopping mechanism per Jonscher's power law. Singh et al. (2024) examined KDP's elastic properties via resonant ultrasonic spectroscopy, observing deviations in resonant modes and mechanical quality factors during the paraelectric-ferroelectric transition. Elastic constants $C_{ij}$ exhibited anomalous behavior, suggesting higher-order interactions in lattice polarization. Bist and Panwar (2015) extended Ganguli et al. (1980) pseudospin model with supplementary terms. Singh and Upadhyay (2006) refined this model further. Our research employs an advanced model incorporating spin-lattice terms, fourth-order phonon anharmonic interactions, and four-spin coupling terms in the modified Hamiltonian. Using Zuberav's statistical methods and retarded Green's function, we investigate Cochran's mode frequency near Curie temperature. Kaminow (1965) studied dielectric constants in deuterated KDP-type crystals, observing a monotonic rise in transition temperature and loss tangent. Proton tunneling was briefly considered. Kumar and Upadhyay (2022) modeled first-order phase transitions in $CsH_2AsO_4$, aligning their soft mode frequency and permittivity predictions with experimental results. Kandpal et al. (2023) applied a two-sublattice pseudospin model to colemanite crystals, achieving agreement with experimental mode frequency and permittivity data. Kumar and Upadhyay (2024) studied KDP-type crystals using a modified pseudospin model, producing theoretical results consistent with experiments on $CsH_2AsO_4$, $RbH_2AsO_4$, and $KH_2AsO_4$. Using a modified model and Green's function approach, Kumar and Upadhyay (2022) theoretically investigates spontaneous polarization and phase change in $KH_2PO_4$-type crystals, with findings that are consistent with experimental data.

Our approach diverges from previous studies by incorporating additional interaction terms rather than relying solely on strict decoupling techniques. This results in better theoretical insights into Cochran's frequency, energy shift, and width, achieving good agreement with experimental data on ferroelectric $KD_2PO_4$ (DKDP).

## Methods

### Theoretical Calculation

We have modified Ganguli's (1980) model as follows

$$
\begin{aligned}
H =& -2\Omega \sum_{i} (S_{1i}^{x} + S_{2i}^{x}) - \sum_{ij} J_{ij} [(S_{1i}^{z} + S_{2i}^{z}) + (S_{1i}^{z} + S_{2i}^{z})] - \sum_{ij} K_{ij} (S_{1j}^{z} S_{2i}^{z}) \\
& - \Delta \sum_{i} (S_{1i}^{z} + S_{2i}^{z}) - \sum_{ij} V_{ik} S_{1i}^{z} A_k - \sum_{ik} V_{ik} S_{2i}^{z} A_k^{+} \\
& + \frac{1}{4} \sum_{k} \omega_k (A_k A_k^{+} + B_k B_k^{+}) + \sum_{k_1 k_2 k_3} V^{(3)} (k_1, k_2, k_3) A_{k_1} A_{k_2} A_{k_3} \\
& + \textstyle\sum_{k_1 k_2 k_3 k_4} V^{(4)} (k_1, k_2, k_3, k_4) A_{k_1} A_{k_2} A_{k_3} A_{k4} - 2\mu E \sum_i S_i^{z} . \qquad \ldots\ldots \quad (1)
\end{aligned}
$$

Where Ω represents the tunneling frequency, $S^i$ denotes the pseudospin variable with components $S^x$ and $S^z$, and $V_{ik}$ corresponds to the spin-lattice interaction. $A_k$ and $B_k$ are the positional and momentum operators, $\omega_k$ indicates the harmonic phonon frequency, and $V^3$ and $V^4$ signify the cubic and quartic atomic force constants by Tuval (1976). $J_{ij}$ describes intra-sublattice dipole interactions, while $K_{ij}$ represents inter-sublattice dipole interactions.

Consider the analysis of Green's function (GF) based on Zubarev (1960)

$$G_{ij}(t-t') = \langle\langle S_{1i}^z(t); S_{1j}^z(t')\rangle\rangle$$
$$= -i\theta(t-t')\langle[S_{1i}^z(t); S_{1j}^z(t')]\rangle.$$

By applying Dyson's equation, performing a Fourier transformation, and differentiating Eq. (2) twice with respect to t and t' using the Hamiltonian from Eq. (1), the result is obtained.

$$G_{ij}(\omega) = G^0(\omega) + G^0(\omega)\tilde{p}(\omega)G^0(\omega),$$
....... (3)

Where $$G^0(\omega) = \frac{\Omega\langle S_{1i}^x\rangle\delta_{ij}}{\pi(\omega^2-4\Omega^2)}$$

and $$G_{ij}(\omega) = \frac{G^0(\omega)}{[1-G^0(\omega)\tilde{\tilde{P}}(\omega)]}$$

$$\tilde{P}(\omega) = \frac{\pi i\langle[F(t)S_{1j}^y]\rangle}{\Omega\langle S_{1i}^x\rangle^2} + \frac{\pi^2}{\Omega^2\langle S_{1i}^x\rangle^2}\langle\langle F_i(t); F_j'(t')\rangle\rangle$$

....... (6) where

$$F(t') = 2\Omega J_{ij}(S_{1j}^x S_{1i}^z + S_{1j}^z S_{1i}^x) - 2\Omega K_{ij}(S_{1i}^x S_{2i}^z)$$

$$+2\Omega V_{ik} S_{1i}^x A_k + 2\Omega\Delta(S_{1i}^x + S_{2i}^z) + 2\Omega V_{ik} A_k^{\dagger} S_{2i}^x.$$
..... (7)

The expression for Green's Function (GF) in Eq. (5) is given as follows:

$$G(\omega) = \frac{\Omega\langle S_{1i}^x\rangle\delta_{ij}}{\pi[\omega^2-\Omega^2-\tilde{\tilde{P}}(\omega)]},$$ ........... (8)

The lowest-order approximation for the renormalized frequency $\hat{\Omega}$ is given by:

$$\hat{\Omega}^2 = 4\Omega^2 + \frac{i}{\langle S_{1i}^x\rangle}\langle[F, S_{1i}^y]\rangle$$ ,......... (9)

The polarization operator $\tilde{\tilde{P}}(\omega)$ is also expressed as:

$$\tilde{\tilde{P}}(\omega) = \frac{\pi}{\Omega\langle S^x\rangle}\langle\langle[F_i(t);]F_j'(t')\rangle\rangle$$
............ (10)

so that

$$\hat{\Omega}^2 = a^2 + b^2 - bc$$
............. (11)

with

$$a = 2J_0\langle S_1^x\rangle + K_0\langle S_2^x\rangle + \Delta$$
$+2\mu E$........... (12)

$$b = 2\Omega$$
............... (13)

and

$$c = 2J\langle S_1^x\rangle + K\langle S_2^x\rangle$$
................ (14)

Green's function is finally obtained by substituting the values of $\tilde{\tilde{P}}(\omega)$ into Eq. (8).

$$G(\omega) = \frac{\Omega\langle S_{1i}^x\rangle\delta_{ij}}{\pi[\omega^2-\Omega^2-2i\Omega\Gamma(\omega)]}.$$ ....... (2)(15)

The equation $n_{ks} = \coth\frac{\tilde{\omega}_{ks}}{k_BT}$ where $k_B$ is Boltzmann constant and s is a numerical index (s = 1,2,3,4), is given as follows: The frequency $\hat{\Omega}$ is determined by:

$$\hat{\Omega}^2 = \tilde{\Omega}^2 + 2\Omega\Delta_{s-p}(\omega)$$ ................ (16)

and

$$\tilde{\tilde{\Omega}}^2 = \tilde{\Omega}^2 + 2\Omega\Delta_s(\omega)$$ ............(4)(17)

**Soft Mode Frequency and Transition Temperatures, Dielectric constant (5) and Loss Tangent**

The renormalized frequency is determined by repeatedly solving Eq. (10) as follows:

$$\hat{\Omega}_{\pm}^2 = \frac{1}{2}\left[\left(\tilde{\omega}_k^2 + \tilde{\tilde{\Omega}}^2\right) \pm \{\left(\tilde{\omega}_k^2 + \tilde{\tilde{\Omega}}^2\right)^2 + 8V_{ik}^2\langle S^x\rangle\}^{\frac{1}{2}}\Omega\right]$$
......... (18)

Phase transitions occur due to the soft mode frequency $\hat{\Omega}_{-}^2$, which exhibits strong temperature dependence.

A ferroelectric crystal with cubic symmetry exhibits scalar susceptibility in the paraelectric phase, represented as: $\chi(\omega) = -\chi_{\mu\nu}$ can be expressed as

$$\chi = \lim_{\epsilon\to 0}\{-2\pi N\mu^2 G_{ij}(\omega + i\epsilon)\},$$
......... (19)

where N is the highest number of unit cells in the sample, and $\mu$ represents the maximum dipole moment per unit cell.

The Green's function $G_{ij}(\omega + i\chi)$ is defined as:

$$G_{ij}(\omega + i\chi) = \langle\langle S_{1i}^{z}(t); S_{1j}^{z}(t')\rangle\rangle_{(\omega+i\chi)}. \quad ........... (20)$$

The real and imaginary parts $G_{ij}{}'(\omega)$ and $G_{ij}{}''(\omega)$ of the Green's function determine the phonon excitation frequency $\tilde{\tilde{\omega}}_k$ as:

$$\tilde{\tilde{\omega}}_k{}^2 = \tilde{\omega}_k{}^2 + 2\,\omega_k \Delta_k(\omega) \quad ........... (21)$$

The dielectric constant $\epsilon(\omega)$ is related to susceptibility as:

$$\epsilon(\omega) = 1 + 4\pi\chi = \epsilon'(\omega) - i\epsilon''(\omega) \quad ........... (22)$$

where $\epsilon'(\omega)$ and $\epsilon''(\omega)$ are the real and imaginary parts of dielectric constant, respectively. For ferroelectric crystals, $\epsilon(\omega) \gg 1$.

The following equation represents the real component of the dielectric constant

$$\epsilon'(\omega) = -8\pi N\mu^2 G_{ij}(\omega), \quad ...... (23)$$

Using the Green's function in Eq. (23), we obtain:

$$G_{ij}(\omega) = \frac{\Omega\langle S_i^x\rangle\delta_{ij}}{\pi[\omega^2 - \hat{\Omega}^2 - 2i\Omega\Gamma(\omega)]}, \quad ........... (24)$$

The real part of the dielectric constant $(\epsilon')$ is given by:

$$\epsilon'(\omega) = \frac{-8\pi N\mu^2\Omega\langle S_i^x\rangle\left(\omega^2 - \hat{\Omega}_{\pm}{}^2\right)}{\left[\left(\omega^2 - \hat{\Omega}_{\pm}{}^2\right)^2 + 4\Omega^2\Gamma^2(\omega)\right]}, \quad .. (25)$$

and the imaginary part $\epsilon''$ as

$$\epsilon''(\omega) = \mu^2 \frac{-8\pi N\mu^2\Omega\langle S_i^x\rangle\left(\omega^2 - \hat{\Omega}_{\pm}{}^2\right)}{\left[\left(\omega^2 - \hat{\Omega}_{\pm}{}^2\right)^2 + 4\Omega^2\Gamma^2(\omega)\right]}. \quad ........... (26)$$

Expanding Eq. (25) near the phase transition gives:

$$\epsilon(\omega) = \frac{C}{(T - T_c)}, \quad ........... (27)$$

where

$$C = \frac{8N\mu^2 \tanh\left(\frac{\Omega}{k_BT_c}\right) k_B T_c{}^2}{\Omega \tilde{J}_q\left(1 - \tanh^2\frac{\Omega}{2k_BT_c}\right)} \quad ........... (28)$$

the Curie-Weiss constant is represented by C. The well-known Curie-Weiss law is given in equation (27). The loss current of the total current I is represented by sin δ. Sin δ is sometimes referred to as the loss factor. However, when **δ** is small, sin δ ≈ δ ≈ tan δ**.** The two components, ϵ' and ϵ''**,** of the complex dielectric constant ϵ(ω) vary with frequency and are expressed as:

$$\epsilon'(\omega) = D_0 \operatorname{Cos}\delta/E_0. \quad ........... (29)$$

$$\epsilon''(\omega) = D_0 \operatorname{Sin}\delta/E_0. \quad ............. (30)$$

The displacement vector in a time-varying field will not be in phase with E, which is why there will be a phase difference δ between them. According to Equations (29) and (30),

$$\tan\delta = \frac{\epsilon''(\omega)}{\epsilon'(\omega)} \quad ........... (31)$$

When Eqs. (25) and (26) are substituted into Eq. (31), the expression for the dielectric loss (tangent loss) is as follows:

$$\tan\delta = -\frac{2\Omega\Gamma(\omega)}{\left(\omega^2 - \hat{\Omega}_{-}{}^2\right)}. \quad ........... (32)$$

When $\hat{\Omega} \gg \omega$ occurs at microwave frequencies, Eq. (32) is reduced to

$$\tan\delta = -\frac{2\Omega\Gamma(\omega)}{\left(\hat{\Omega}_{-}{}^2\right)}. \quad ........... (33)$$

By considering the temperature dependence of the square of the soft mode frequency $\hat{\Omega}^2 = K(T - T_c)$ and the breadth Γ(ω), the temperature dependence of the loss tangent in the paraelectric phase is computed as a polynomial.

$$(T - T_c)\tan\delta = (A + BT + CT^2), \quad ...... (34)$$

where A, B, and C are constants that are influenced by crystal defects and third- and fourth-order phonon-anharmonic interactions, respectively. While the second and third factors are particular to a single crystal, the first term on the right side vanishes for pure single crystals. The quality factor is defined by

$$Q = \frac{1}{\tan\delta} \quad ........... (35)$$

## Results and Discussion

Making use of the model parameters listed in table (1) from earlier literature Ganguli et al. (1980) in the obtained theoretical formulae given in the above equations of $\hat{\Omega}^2$, tangent loss, dielectric constant and quality factor. Throughout the calculation the value of $\Delta = 0,$ for $KD_2PO_4$ crystal and $E = 0\ Kv/cm,\ and\ E = 5\ Kv/cm$ is used.

**Table 1: Model values for $KD_2PO_4$ and their units by Ganguli et al (1980).**

| Parameters / Crystals | $\Omega$ $cm^{-1}$ | $J_{ij}$ $cm^{-1}$ | $J^*_{ij}$ $cm^{-1}$ | $K_{ij}$ $cm^{-1}$ | $V_{ik}$ $cm^{-1}$ | C (K) | $T_c$(K) | N $cm^{-1}$ | μ (esu) |
|---|---|---|---|---|---|---|---|---|---|
| $KD_2PO_4$ | 0.486 | 626 | 156.5 | 163 | 0.226 | 266 | 173K | $0.8\text{x}10^{21}$ | 1.8 |

The thermal behavior of $KD_2PO_4$ crystal is shown in Fig. 1, 2, 3, and 4. Fig. 1 exhibits that soft mode frequency $\widehat{\Omega}^2 \longrightarrow 0$ at $T_c$ and then slightly increases. It will increase because of the $(S^z)$ pseudospin parameter contribution given in Eqn. (18) for $KD_2PO_4$ crystal. The thermal variations $\widehat{\Omega}^2,$ shows good agreement with experimental correlated data of Kaminow (1965) at $E = 0Kv/cm$ by applied the formula $\varepsilon = \frac{8\pi N\mu^2\Omega}{\widehat{\Omega}^2}$ from Kumar and Upadhyay (2022). By increasing the electric field to $E = 5Kv/cm$ there is increases the dipole moment so that $\widehat{\Omega}^2,$ is also increases with temperature. From theoretical formulae of $\epsilon(\omega) \propto \left(\omega^2 - \widehat{\Omega}^2_-\right)^{-1}$ given in Eqn. (25) and loss tangent or $\tan(\delta) \propto \left(\omega^2 - \widehat{\Omega}^2_-\right)^{-1}$ given in Eqn. (33) we observed that the dielectric constant and loss tangent increases to maxima at Curie temperature because of the contribution of $\widehat{\Omega}^2$ term included within the formulae. Their thermal variations are shown in figs.2 and 3. They follows the same behavior by increasing the electric field from $E = 0\ Kv/cm\ to\ \ E = 5\ Kv/cm$ . Our theoretical results show better agreement with Kaminow (1965). The effect of all the contained pseudospins within the obtained shift and width, and this energy shift width contained in Eqn. (18). So, the total effect of these terms also shows in quality factor obtained in Eqn. (35) which is inversely proportional to $\tan(\delta)$ and their thermal variation with the action of electric field shows in Fig. 4 which decreases to minimum value at Curie temperature and then increases.

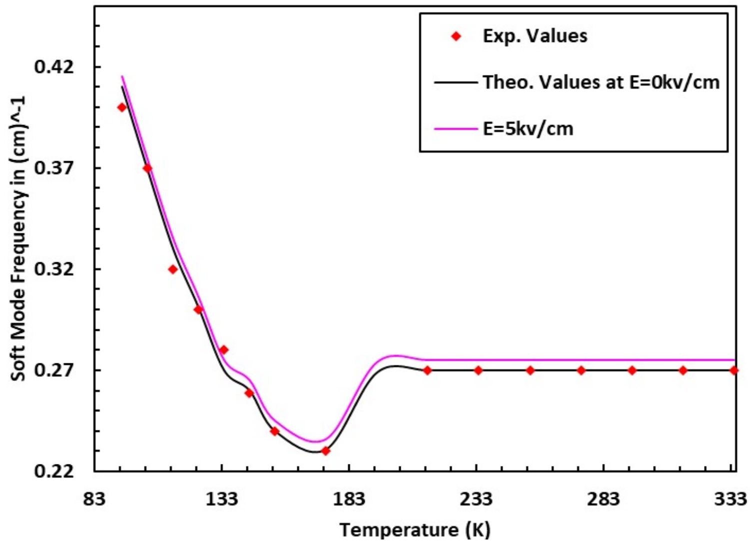


**Fig-1:** Thermal variation of soft mode frequency for $KD_2PO_4$ crystal (Thero. — Exp. ♦ and Elec. Field —)

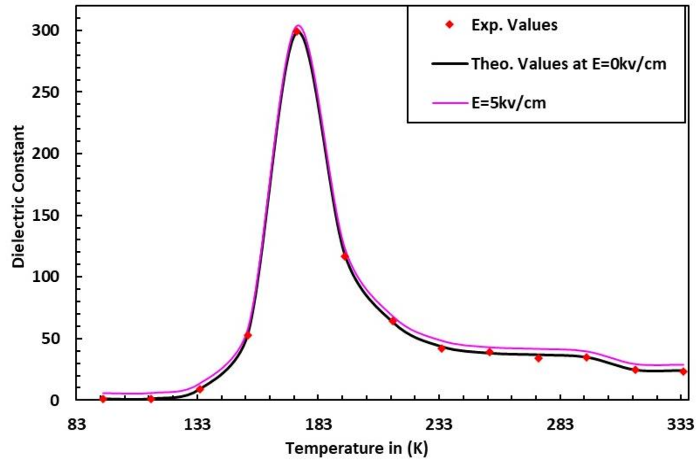


**Fig-2:** Thermal variation of dielectric constant for of $KD_2PO_4$crystal (Thero. —; Exp. ♦, Electric Field —)

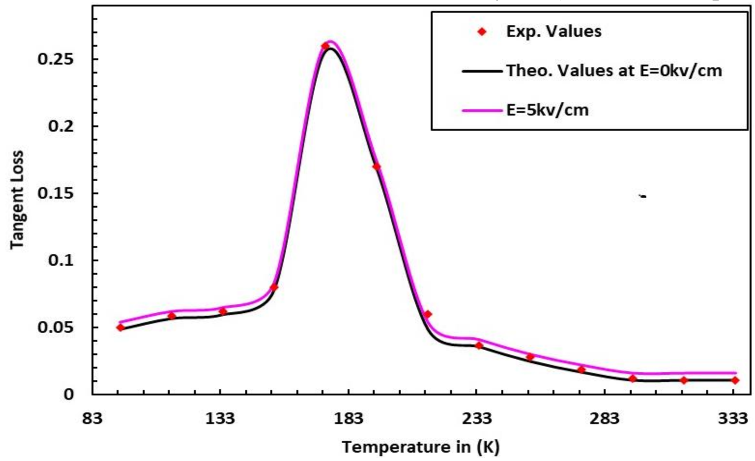


**Fig-3:** Thermal variation of tangent loss for of $KD_2PO_4$crystal (Thero. —; Exp.♦, Electric Field —)

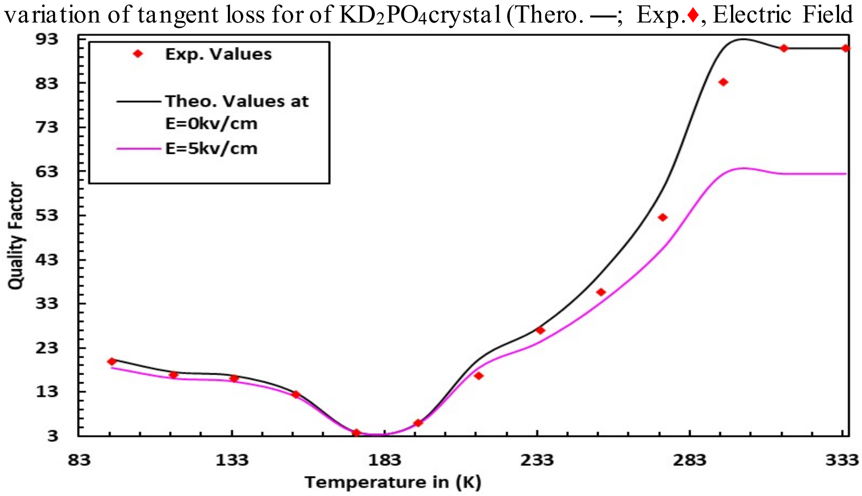


**Fig-4:** Thermal variation of quality factor for of $KD_2PO_4$ crystal (Thero. —; Exp. ♦, Electric Field —)

## Conclusion

In the study, we included phonons of third- and fourth-order anharmonic interaction terms together with a two-sublattice PLCM (Pseudo Lattice Coupled Model) model. These extra interaction factors are crucial for accurately characterizing the KD2PO4 crystal's thermally dependent soft mode frequency, dielectric constant, dielectric loss as well as quality factor.

## Acknowledgement

The authors are thankful Prof. T.C. Upadhyay, Prof. S.C. Bhatt, and the Department of Physics Ramjas College, University of Delhi for their kind encouragement. Kandpal is thankful to Sh. Satyawan Malik, Principal, Sh. Kamaljeet Singh, HOD Physics, and Dr. Vishal Redhu, Registrar, Govt. College, Jind, for help.

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