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Comparative Studies of Phonon Frequency Spectrum of HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ Through Normal Co-Ordinate Analysis.

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ABSTRACT

The prime application of Nano technology is High temperature superconductor**.** The Raman spectroscopy of HTSC explains that the role played by the phonons in the mechanism of superconductivity in the perovskite family of superconductors is not fully understood although a large series of experimental results has shown considerable coupling of some phonons to electronic excitation in these systems. Optical spectroscopy and especially Raman and Infrared spectroscopy revealed strong direct influences of the changes in the electronic states to the phonon at the center of the Brillouin. However, it is indispensable to have a precise knowledge of the zone –boundary phonons to investigate the contribution of electron-phonon coupling to T_c which can be achieved by neutron scattering techniques. The most commonly employed model is the valence force field model for computing phonon frequencies based on stretching bond and bending bond coordinates. Such models have the advantage of being well adopted to describe a covalent bonding but ignored the long–range Coulomb forces and wave vector dependence of the phonon spectrum. Even though a fairly good amount of literature is available on the vibrational spectra of high temperature superconductors, still some specific feature in the experimental vibration spectra could not be assigned reliable to a definite type of vibration. Hence a normal coordinate analysis (NCA) which is applicable to zero wave-vector normal-mode vibrations have been carried out for the high temperature superconductors and the assignment of specific features like phonon softening and hardening were looked in for the clear understanding of the superconducting mechanism in these new class materials. In the normal coordinate analysis, PED play an important role for characterization of the relative contributions from each internal coordinate to the total potential energy associated with particular normal coordinate of the molecule. The contribution to the potential energy from the individual diagonal elements give rise to a conceptual link between the empirical analysis of infrared spectra of complex molecules dealing with characteristic group frequencies and the theoretical approach from the computation of the normal modes. NCA gives complete assessment of all normal vibration modes of the system.

Keywords: High Temperature Superconductor Conductor (HTSC), NCA, Raman and IR-spectroscopy, Brillouin zone, Potential Energy Distribution (PED), etc.,

1. Introduction:

The study of normal coordinate analysis and the free carriers is important for the understanding of the physical nature of high temperature superconductors. Raman and far-infrared studies of these superconductors have contributed significantly to the understanding of new class of superconductors. The introduction of superconductivity above 30 K in CuO-pervoskites by Bednorz Muller[1] initiated tremendous efforts in solid state physics and material sciences with the aim to isolate the phases which are responsible for the superconductivity and to search for other substances beside the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ family which exhibit this phenomenon. These activities succeeded in the discovery of superconductivity in $YB_2Cu_3O_7$ at 92 K by Wu et al.[2] and the observation of a transition temperature above 100 K by Sheng et al.[3].

In this method the frequency of the normal vibration is determined by the kinetic and potential energies of the system. Wilson's GF matrix method [4] is applied for the calculation of optically active vibration frequencies. The kinetic energy is determined by the masses of their individual atoms and their geometrical arrangement in the molecules but the potential energy (PE) arises from interaction between the individual atoms described in terms of the force constants. Assuming reliable potential constants for various bonds, the vibration frequencies have been evaluated. Fine- tuning is done until the available observed frequency and the present evaluated frequency matches perfectly. Internal coordinates like bond length and bond angles are used in the kinetic energy expression. Since the potential and kinetic energies are described in terms of internal coordinates, they have clear physical meaning since these force constants are characteristics of bond- stretching and angle deformation involved[5]..

Besides non-central forces such as involved in angle bending can be included in the normal coordinate analysis, which was not possible in the lattice dynamics. Also in NCA, Potential Energy Distribution (PED) indicates the contribution of individual force constants to the vibration energy of normal mode for the clear understanding of the specific vibration the species involved. The normal coordinate calculations were performed to support the assignment of the vibration frequencies and to obtain PED for various mode.

2. Normal Co-Ordinate Analysis Of Superconductor HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$:

The stoichiometric compound HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ crystallize at high temperatures in the space group (D^{14}_{4h}-I4/mmm) with one chemical formula unit per unit cell (Jorgensen et al.[6]). At lower temperatures the crystals undergo a structural phase transition into an orthorhombic phase (D^{18}_{2h}-Cmca) by doubling the unit cell in a $\sqrt{2}a \times \sqrt{2}a$ fashion. The exact transition temperature depends on the oxygen stoichiometry of the sample and occurs between 430 K and 530 K (Johnsoton et al.[7]). Sometimes the structure is also denoted as (D^{18}_{2h}-Bmab). Both assignments may be transferred into each other changing the labels from the orthorhombic axes from *abc* to *acb*, respectively [8]. Table I. give the results of an analysis of the phonon symmetries at the Γ-point of the reciprocal lattice. In the high temperature phase four Raman-active and seven infrared active modes should be observable. Below the structural phase transition the number of Raman and IR-modes increases because the number of atoms in the unit cell is doubled.

The interest in the high-T_c superconducting cuprate-crystal is stimulated, on the one hand, by the possibility of phonons taking part in carrier pairing processes and, on the other hand, by peculiar dynamic properties of these complex compounds with a layered structure. It is not surprising; therefore, that many papers report studies of thermal excitations of the crystal lattice of high T_c superconducting cuprates and related compounds. In the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ crystal lattice oscillations are experimentally studied by means of neutron [9-11] and optical [12-13] spectroscopy. The results of inelastic neutron-scattering experiments giving information about phonon dispersion relation [5] or phonon spectral density [7-9] are usually interpreted in terms of collective oscillating excitations in each of which all the atoms take part. The information about the oscillations of individual atoms of the compound is thus lost.

Analysis of the literature shows that two approaches are used to get information about oscillating properties of single atoms of a complex compound. The first is based on model calculations of crystal-lattice dynamics, and the second on the analysis of indirect information about thermal atomic motions, obtained by neutron recoil spectroscopy for neutrons of energy ≈1 eV[10] by resonance neutron absorption and by neutron diffraction. All these methods suffer from an important short coming, namely the characteristics of thermal atomic motion are determined as fitting procedure parameters, together with a lot of other parameters, which, in some cases, can substantially affect the final result. Moreover, neutron diffraction data do not allow distinguishing between static and dynamic atomic displacements from equilibrium in the crystal lattice, the partial spectrum is determined by superposition of all normal modes with weight allowing for the *i*th atom displacement in lattice oscillations with energy E. As shown in Parshin *et.al* [12] and Soldatov *et.al* [13], the method of isotopic contrast in inelastic neutron scattering makes it possible to experimentally restore the partial oscillating spectra of single atoms.

3. Normal Coordinate Analysis of Zero Wave Vector Vibration of HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$

Cardona and coworkers [14] studied the infrared and Raman spectra of the super conducting cuparate perovskites $MBaCu_2O_2$ (M = Nd, Er, Dy, Tm and Eu) and reported the possible origins of phonon softening and the systematic variation of phonon frequencies with the ionic radius. Here an attempt has been made to perform the normal coordinate analysis for the phonon frequencies and the form of the zero wave vector vibrations for the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$.

The HTSC $GdBa_2Cu_3O_7$ systems crystallizes in the body-centered tetragonal (bct) systems, which belongs to the space group 14/mmm (D^{17}_{4h}). The body-centered tetragonal (bct) unit cell of HTSC $GdBa_2Cu_3O_7$ and the numbering of the atoms are shown in Fig.1. The 13 atoms of the unit cell yield a total of 35 optical vibrational modes. All the above calculations are made at q=0. One of B_{2u} and E_u modes corresponds to acoustic vibrations with frequency $\omega = O$. These normal modes are distributed as follows.

$B_{1u} + B_{2u} + E_u + B_{3u}$ from the motion of Gd atoms

$A_{1g} + B_{2g} + B_{3g} + B_{1u} + B_{2u} + E_u + B_{3u}\ _{3u}$ from the motion of Ba atoms

$A_{1g} + B_{2g} + B_{3g} + B_{1u} + B_{2u} + E_u + B_{3u}$ from the motion of Cu atom sandwitched between Gd and Ba atoms

$B_{1u} + B_{2u} + E_u + B_{3u}$ from the motion of Cu atom surrounded by Ba atom

$2A_{1g} + 2B_{2g} + 2B_{3g} + 2B_{1u} + 2B_{2u} + 2E_u + 2B_{3u}$ from the motion of 4 O atoms between Gd and Ba along c-axis

$A_{1g} + B_{2g} + B_{3g} + B_{1u} + B_{2u} + E_u + B_{3u}$ from the motion of O (1) atom along b-axis

$B_{1u} + B_{2u} + E_u + B_{3u}$ from the motion of O (1) atom along c-axis

Subtracting the translation modes $B_{2u} + B_{3u} + E_u$ at q = 0 optical modes involved in an irreducible representation are as follows.

$\Gamma_{opt} = 5A_{1g} + 5B_{2g} + 5\,B_{3g} + 7B_{1u} + 2B_{2u} + 5E_u + 6B_{3u}$

The species belonging to A_{1g} , B_{2g} and B_{3g} are Raman active modes whereas B_{2u} ,E_u and B_{2u} are infrared active modes. The A_{2u} and A_{1g} modes involve displacement along crystallographic c-axis, the B_{2u} and E_g modes along the b-axis and E_u modes along the a-axis.

Similarly, in **HTSC** $SmBa_2Cu_3O_7$ systems crystallizes in the simple tetragonal (st) systems, which belongs to the space group P4/mmm (D^{17}_{4h}). The simple tetragonal (st) unit cell of HTSC $SmBa_2Cu_3O_7$ and the numbering of the atoms are shown in Fig.2. The 13 atoms of the unit cell yield a total of 35 optical vibrational modes. All the above calculations are made at q=0. One of B_{2u} and E_u modes corresponds to acoustic vibrations with frequency $\omega = O$. These normal modes are distributed as follows.

$B_{1u} + B_{2u} + E_u + B_{3u}$ from the motion of Sm atoms

$A_{1g} + B_{2g} + B_{3g} + B_{1u} + B_{2u} + E_u + B_{3u\ 3u}$ from the motion of Ba atoms

$A_{1g} + B_{2g} + B_{3g} + B_{1u} + B_{2u} + E_u + B_3$ from the motion of Cu atom sandwitched between Sm and Ba atoms

$B_{1u} + B_{2u} + E_u + B_{3u}$ from the motion of Cu atom surrounded by Ba atom

$2A_{1g} + 2B_{2g} + 2\,B_{3g} + 2B_{1u} + 2B_{2u} + 2E_u + 2B_{3u}$ from the motion of 4 O atoms between Sm and Ba along a-axis

$A_{1g} + B_{2g} + B_{3g} + B_{1u} + B_{2u} + E_u + B_{3u}$ from the motion of O (1) atom along b-axis

$B_{1u} + B_{2u} + E_u + B_{3u}$ from the motion of O atom along c-axis

Subtracting the translation modes $B_{2u} + B_{3u} + E_u$ at q = 0 optical modes involved in an irreducible representation are as follows.

$\Gamma_{opt} = 5A_{1g} + 5B_{2g} + 5\,B_{3g} + 7B_{1u} + 2B_{2u} + 5E_u + 6B_{3u}$

The species belonging to A_{1g} , B_{2g} and B_{3g} are Raman active modes whereas B_{2u} ,E_u and B_{2u} are infrared active modes. The A_{2u} and A_{1g} modes involve displacement along crystallographic c-axis, the B_{2u} and E_g modes along the b-axis and E_u modes along the a-axis.

The normal coordinate calculation was performed using the programs GMAT and FPERT given by Fuhrer et al [15]. The general agreement between the evaluated and observed normal frequencies of $GdBa_2Cu_3O_7$ is good. The calculated force constants using the above programs are given in Table 1. It is interesting to note that the evaluated frequencies given in Table.2, agree favorably with the experiment values.

To check whether the chosen set of vibrational frequencies makes the maximum contribution to the potential energy associated with the normal coordinate frequencies of the super conducting material, the potential energy distributions was calculated using the equation.

PED = $(F_{ij} L^2_{ik})/ \lambda_k$

Where PED is the combination of the i-th symmetry coordinate to the potential energy of the vibration whose frequency is $V_k F_{ij}$ are potential constants, L_{ik} are L matrix elements and $\lambda_k = 4\pi^2 C^2 \upsilon^2_k$.

4. Result and Discussion :

The Normal Co-Ordinate analysis of high temperature superconductors $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ have been performed using rigid ion model. The modified three body shell model is adopted in the Normal Coordinate Analysis gives favourable phonon frequencies ,which are given as shown below:

5. Comparative studies of Normal Coordinate Analysis of HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$:

The Normal Coordinate Analysis calculations based on modified TSM reproduce the observed frequencies of Raman and infrared active modes reasonable which are given in table 2. The calculated frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ are in good agreement with the available experimental values are proved at various symmetries. The lowest calculated phonon frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ in A_{1g} symmetry are at 160 cm^{-1} and 202cm^{-1} are due to the vibration of Gd and Sm atoms respectively and these calculated frequencies agrees very well with the experimental frequencies at 162 cm^{-1} and 115 cm^{-1}respectively.. Similarly the calculated phonon Raman frequencies of HTSC $GdBa_2Cu_3O_7$ in A_{1g} symmetry are at 322 cm^{-1} , 421$cm^{-1}$and 435 cm^{-1} are due to the vibrations of Ba, Cu and O(2) atoms respectively and the calculated Raman frequencies of HTSC $SmBa_2Cu_3O_7$ in A_{1g} symmetry are at 328 cm^{-1} , 436 $cm^{-1}$and 457 cm^{-1} are due to the vibrations of Ba, Cu and O(2) atoms respectively. Similarly, the observed Raman frequencies of HTSC $GdBa_2Cu_3O_7$ in A_{1g} symmetry are at 320, 425 and 435 cm^{-1} and the observed Raman frequencies of frequencies of HTSC $SmBa_2Cu_3O_7$ in A_{1g} symmetry are at 215 cm^{-1} , 420 $cm^{-1}$and 445cm^{-1} agrees very well with the calculated frequencies respectively. The highest calculated Raman frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ in A_{1g} symmetry are at 560 cm^{-1} each are due to the vibration of O(2) atom respectively . Here, the observed frequencies of both of the HTSCs are at 550 cm^{-1} each agrees very well with the calculated frequency at 560 cm^{-1} each , which is confirmed by the PED calculation

The lowest calculated phonon frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ in B_{2g} symmetry are at 150 cm^{-1} and 155 cm^{-1} are due to the vibration of Gd and Sm atoms respectively and these calculated frequencies agrees very well with the experimental frequencies at 145 cm^{-1} and 80 cm^{-1}respectively.. Similarly, the calculated phonon Raman frequencies of HTSC $GdBa_2Cu_3O_7$ in B_{2g} symmetry are at 310 cm^{-1} , 450 $cm^{-1}$and 530 cm^{-1} are due to the vibrations of Ba,Cu and O(2) atoms respectively and the calculated Raman frequencies of HTSC $SmBa_2Cu_3O_7$ in B_{2g} symmetry are at 235 cm^{-1} , 450 $cm^{-1}$and 482 cm^{-1} are due to the vibrations of Ba,Cu and O(2) atoms respectively. Similarly, the observed Raman frequencies of HTSC $GdBa_2Cu_3O_7$ in B_{2g} symmetry are at 320, 480 and 550 cm^{-1} and the observed Raman frequencies of frequencies of HTSC $SmBa_2Cu_3O_7$ in B_{2g} symmetry are at 150 cm^{-1} , 480 $cm^{-1}$and 584cm^{-1} agrees very well with the calculated frequencies respectively. The highest calculated Raman frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ in B_{2g} symmetry are at 560 cm^{-1} and 594 cm^{-1} are due to the vibration of O(2) atom each. Here, the highest observed phonon frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ in B_{2g} symmetry are at 580 cm^{-1} and 630 cm^{-1} are due to the vibration of O(3) atoms each and these observed frequencies agree very well with the calculated frequencies at 560 cm^{-1} and 594 cm^{-1} respectively, which is confirmed by the PED calculation.

The lowest calculated phonon frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ in B_{3g} symmetry are at 115cm^{-1} and 135 cm^{-1} are due to the vibration of Gd and Sm atoms respectively and these calculated frequencies agrees very well with the experimental frequencies at 110 cm^{-1} and 78 cm^{-1}respectively.. Similarly the calculated phonon Raman frequencies of HTSC $GdBa_2Cu_3O_7$ in B_{3g} symmetry are at 290 cm^{-1} , 572 $cm^{-1}$and 580 cm^{-1} are due to the vibrations of Ba,Cu and O(2) atoms respectively and the calculated Raman frequencies of HTSC $SmBa_2Cu_3O_7$ in B_{2g} symmetry are at 230cm^{-1} , 464 $cm^{-1}$and 485 cm^{-1} are due to the vibrations of Ba, Cu and O(2) atoms respectively.

Similarly, the observed Raman frequencies of HTSC $GdBa_2Cu_3O_7$ in B_{3g} symmetry are at 270, 565 and 580 cm^{-1} and the observed Raman frequencies of frequencies of HTSC $SmBa_2Cu_3O_7$ in B_{3g} symmetry are at 127 cm^{-1} , 560 $cm^{-1}$and 570 cm^{-1} agrees very well with the calculated frequencies respectively. The calculated Raman frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ in B_{3g} symmetry are at 640 cm^{-1} and 600 cm^{-1} are due to the vibration of O(3) atom each. Here, the observed phonon frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ in B_{3g} symmetry agrees very well with the calculated frequencies at 640 cm^{-1} and 600 cm^{-1} respectively, which is confirmed by the PED calculation..

The evaluated Infrared (IR) phonon frequencies of HTSC $GdBa_2Cu_3O_7$ in B_{1u} symmetry are at 120 cm^{-1} and 180 cm^{-1} are due to the vibration of Gd and Ba atoms respectively, whereas the evaluated Infrared (IR) phonon frequencies of HTSC $SmBa_2Cu_3O_7$ in B_{1u} symmetry are at 248 cm^{-1} and 250 cm^{-1} are due to the vibration of Sm and Ba atoms respectively. The observed Infrared (IR) phonon frequencies in B_{1u} symmetry of HTSC $GdBa_2Cu_3O_7$ are at 120 cm^{-1} and 180 cm^{-1} and in HTSC $SmBa_2Cu_3O_7$ the experimental frequencies are at 80 cm^{-1} and 180 cm^{-1} which agrees very well with the calculated frequencies of both of the superconductors. The Calculated infrared phonon frequency of HTSC $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ are at 270 cm^{-1} and 325 cm^{-1}in B_{1u} symmetry are due to the vibration of Cu(1) atoms each. The observed frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ are at 270 cm^{-1} and 325 cm^{-1} respectively agrees very well with the calculated frequencies respectively. The IR frequencies' at 415 cm^{-1},482 cm^{-1} and 543 cm^{-1} of HTSC $GdBa_2Cu_3O_7$ are due to the vibration of Cu(2), O(1) and O(2) atoms respectively, whereas the IR frequencies at 435 cm^{-1},470 cm^{-1}, and 490 cm^{-1} of HTSC $SmBa_2Cu_3O_7$ are due to the vibration of Cu(2), O(1) and O(2) atoms respectively. The observed IR frequency of HTSC $GdBa_2Cu_3O_7$ are at 420 cm^{-1},480 cm^{-1} and 510 cm^{-1} and the observed IR frequency of HTSC $SmBa_2Cu_3O_7$ at 419 cm^{-1},480 cm^{-1} and 575 cm^{-1} agrees very well with the calculated frequencies. The highest calculated IR phonon frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ in B_{1u} symmetry are at 645 cm^{-1} and 560 cm^{-1} respectively are due to the vibration of O(3) atoms each and the observed frequencies of HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ are at 650 cm^{-1} and 630 cm^{-1} respectively agrees very well with the calculated frequencies ,which is confirmed by the PED calculation.

The calculated Infrared phonon frequencies of HTSC $GdBa_2Cu_3O_7$ in B_{2u} symmetry are at 625 cm^{-1} , and 638 cm^{-1} are due to the vibrations of O(2) and O(3) atoms respectively and the calculated Infrared frequencies of HTSC $SmBa_2Cu_3O_7$ in B_{2u} symmetry are at 590 cm^{-1} and 597 cm^{-1} are due to the vibrations of O(2) and O(3) atoms respectively. Similarly, the observed IR frequencies of HTSC $GdBa_2Cu_3O_7$ in B_{2u} symmetry are at 620 cm^{-1} and 630 cm^{-1} and the observed IR frequencies of HTSC $SmBa_2Cu_3O_7$ in B_{2u} symmetry are at 610 cm^{-1} and 630 cm^{-1} agrees very well with the calculated frequencies respectively, which is confirmed by the PED calculation.

The calculated IR frequency of HTSC $GdBa_2Cu_3O_7$ in E_u symmetry at 118 cm^{-1} is due to the vibration of Gd atom and its observed phonon frequency is at 118 cm^{-1} and this observed frequency agrees very well with the calculated frequency. The calculated IR frequencies at 180 cm^{-1} , 220 cm^{-1} and 570 cm^{-1} are due to the bending bond vibration of Ba, Ca, and O(1) atoms respectively and it corresponding observed phonon frequencies are at 180 cm^{-1} 212 cm^{-1} and 560 cm^{-1} agrees very well with the calculated frequencies. The highest calculated IR phonon frequency at 580 cm^{-1} in this symmetry is due to the vibration of O(3) atom which performs starched bending bond vibration and its observed frequency is at 575 cm^{-1} and it agrees very well with the calculated frequency. Similarly, The calculated IR frequencies of HTSCs $SmBa_2Cu_3O_7$in E_u symmetry at 150 cm^{-1} is due to the vibration of Sm atom and its observed phonon frequency is at 86 cm^{-1} and these observed frequency agrees very well with the calculated frequency. The calculated IR frequencies at 220 cm^{-1} , 280 cm^{-1} and 478 cm^{-1} are due to the bending bond vibration of Ba, Ca, and O(1) atoms respectively and its corresponding observed phonon frequencies are at 180 cm^{-1} ,189 cm^{-1} and 556 cm^{-1} respectively agrees very well with the calculated frequencies. The highest calculated IR phonon frequency of HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ at 580 cm^{-1} are at 530 cm^{-1} respectively are due to the vibration of O(3) atom each which performs starched bending bond vibrations and the observed frequencies of HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ are at 575 cm^{-1} and 587 cm^{-1} respectively agrees very well with the calculated frequencies. Therefore, the calculated and observed frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ agrees very well with each other which is confirmed by the PED calculation.

The calculated IR frequency of HTSC $GdBa_2Cu_3O_7$ in B_{3u} symmetry at 180 cm^{-1} is due to the vibration of Gd atom and its observed phonon frequency is at 175 cm^{-1} and this observed frequency agrees very well with the calculated frequency. The calculated IR frequencies at 190 cm^{-1} , 455 cm^{-1} , 530 cm^{-1} and 575 cm^{-1} are due to the bending bond vibration of Ba, Cu, and O(1) and O(2) atoms respectively and it corresponding observed phonon frequencies at 180 cm^{-1} 420 cm^{-1} 540 cm^{-1} and 580 cm^{-1} which agrees very well with the calculated frequencies. The highest calculated IR phonon frequency in this symmetry at 640 cm^{-1} is due to the vibration of O(3) atom which performs starched bending bond vibration and its observed frequency is at 635 cm^{-1} and it agrees very well with the calculated frequency. Similarly, The calculated IR frequencies of HTSCs $SmBa_2Cu_3O_7$ in B_{3u} symmetry at 233 cm^{-1} is due to the vibration of Sm atom and its observed phonon frequency is at 145 cm^{-1} and these observed frequency agrees very well with the calculated frequency. The calculated IR frequencies in this symmetry are at 280 cm^{-1} , 400 cm^{-1} ,460 cm^{-1} and 511cm^{-1} are due to the bending bond vibration of Ba, Ca, O(1) and O(2) atoms respectively and its corresponding observed phonon frequencies are at 196 cm^{-1} ,465 cm^{-1} 520 cm^{-1} and 570 cm^{-1} respectively agrees very well with the calculated frequencies. The highest calculated IR phonon frequency in this symmetry is at 580 cm^{-1} is due to the vibration of O(3) atom which performs starched bending bond vibration and its observed frequency is at 665 cm^{-1} which agrees very well with the calculated frequency. Therefore, the calculated and observed frequencies of both of the HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ agrees very well with each other which is confirmed by the PED calculation.

6. Conclusion:

In this present investigation , the Comparative Studies of Phonon Frequency Spectrum of HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$ Through Normal Coordinate Analysis calculations yielded the same phonon frequencies behaves as the bridge between Solid State Physics and Spectroscopy to understand the mechanism of superconductivity. The Raman and infrared studies of these HTSC have contributed significantly to their understanding. The assignment of the spectral features to specific lattice vibrations would be an important step in understanding their role in super conductivity In this work the Normal Coordinate Analysis technique have been adopted to give the evidence for electron, phonon interaction in HTSCs $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$**.** It is observed from the tables that the agreement between the calculated and observed frequencies were in good agreement with the systems that are considered here. This fact supports that the present vibrational assignments made for the infra red and Raman spectra are adequate. Therefore, it is concluded that the Normal Coordinate Analysis is the optically active vibrations of the vibrational spectra in cupurate oxides.

Therefore, the Normal Coordinate Analysis calculations yielded not only by the zone center phonon modes but also by the stable dispersions. Hence, it also supports the strong electron phonon interaction in high temperature super conductor (HTSC). The vibrational frequencies calculated by the method of Normal Coordinate Analysis are compared theoretically and experimentally, and they appears to be in good agreement that are further confirmed by the potential energy distribution calculation.

Therefore, it is concluded that metal – oxide (Cu-O) plays an important role for the occurrence of superconductivity. The Raman scattering has provided direct evidence for strong electron –phonon interaction in the high T_c superconducting oxides. The vibrational frequencies calculated by the methods of Normal Coordinate Analysis are compared and they appears to be in good agreement, which is confirmed by the Potential Energy Distribution calculation..

Finaly, these calculations yielded not only the zone center phonon modes but also the stable dispersions. Hence, it also supports the strong electron phonon interaction in high temperature super conductor (HTSC). The vibrational frequencies calculated by the method of normal coordinate analysis are compared theoretically and experimentally, and they appears to be in good agreement that are further confirmed by the potential energy distribution calculation.

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	Force Constants for $GdBa_2Cu_3O_7$			Force Constants for $SmBa_2Cu_3O_7$		
Force Constants	Bond Type	Distance (A^o)	Initial Value Constants	Bond Type	Distance (A^o)	Initial Value Constants
f_a	Cu(1)-O(1)	1.94	1.4	Cu(1)-O(1)	1.9	1.4
f_b	Cu(1)-O(2)	1.82	1.6	Cu(1)-O(2)	1.82	1.6
f_c	Cu(2)-O(3)	1.93	1.4	Cu(2)-O(3)	1.93	1.4
f_d	Cu(2)-O(4)	1.96	1.4	Cu(2)-O(4)	1.96	1.4
f_e	Cu(2)-O(2)	2.33	1.1	Cu(2)-O(2)	2.33	1.1
f_g	Ba-O(1)	2.91	0.8	Ba-O(1)	2.91	0.8
f_h	Ba-O(2)	2.75	1.0	Ba-O(2)	2.75	1.0
f_k	Ba-O(3)	2.94	0.8	Ba-O(3)	2.94	0.8
f_l	Ba-O(4)	2.94	1.0	Ba-O(4)	2.94	1.0
f_m	Gd-O(3)	2.40	1.0	Sm-O(3)	2.30	0.7
f_n	Gd-O(4)	2.30	0.5	Sm-O(4)	2.20	0.7
f_p	Cu(2)-Cu(2)	3.37	1.3	Cu(2)-Cu(2)	3.37	1.3
f_α	O(1)-Cu(1)-Cu(2)	---	1.3	O(1)-Cu(1)-Cu(2)	---	1.3
f_β	O(3)-Cu(2)-Cu(4)	---	0.5	O(3)-Cu(2)-Cu(4)	---	0.5
f_r	O(3)-Cu(3)-Cu(4)	---	0.5	O(3)-Cu(3)-Cu(4)	---	0.5

Table:1

Force Constants for $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$

(in units of 10^2 Nm^{-1})

(Stretching) and 10^{-18}Nm rad^{-2} (bending).

Symmetry species	Frequency(cm^{-1}) Normal Co-Ordinate Analysis of ***$GdBa_2Cu_3O_7$***	Frequency(cm^{-1}) Normal Co-Ordinate Analysis of ***$SmBa_2Cu_3O_7$***	Potential Energy Distribution(%) ***$GdBa_2Cu_3O_7$***	Potential Energy Distribution(%) ***$SmBa_2Cu_3O_7$***
A_{1g} (Raman)	560(550)	560(550)	f_b (70)f_e(10)	f_b (76)f_e(12)
	435(435)	457(445)	f_l (50)f_k(20)	f_l (55)f_k(26)
	421(425)	436(420)	f_k(50)f_n(21)	f_k(54)f_n(21)
	322(320)	328(215)	f_p(60)f_a (18)f_e(15)	f_p(65)f_a (28)f_e(11)
	160(162)	202(115)	f_g(64)fi(20)	f_g(68)fi(21)

B_{2g}	560(580)	594(630)	f_c (52)f_m (35)f_β(18)	f_c (57)f_m (30)f_β(17)
	530(550)	482(584)	f_c (70)	f_c (72)
	450(480)	450(480)	f_h (58)	f_h (59)
	310(320)	235(150)	f_β(70)fg(25)	f_β(67)f_g(24)
	150(145)	155(80)	f_g (60)fn(20)	f_g (65)f_n(28)
B_{3g}	640(640)	600(625)	f_c (59)f_α(20)	f_c (58)f_α(20)
	580(580)	485(570)	f_c (84)	f_c (74)
	572(565)	464(560)	f_h (90)	f_h (89)
	290(270)	230(127)	f_β(50)f_i(19)	f_β(55)f_i(20)
	115(110)	135(78)	f_g(54)f_m(30)f_i(15)	f_g(54)f_m(28)f_i(11)
B_{1u} (IR)	645(650)	560(630)	f_b(50) f_β(20)f_m(20)	f_b(56) f_β(20)f_m(12)
	543(510)	490(575)	f_b (71)f_β(17)	f_b (67)f_β(18)
	482(480)	470(480)	f_k (50)f_α(11)	f_k (55)f_α(11)
	415(420)	435(419)	f_n (51)f_k(20)f_m(15)	f_n (58)f_k(24)f_m(14)
	270(270)	325(250)	f_c (64)f_b(20)	f_c (65)f_b(23)
	180(180)	250(180)	f_l (53)f_k(20)	f_l (60)f_k(21)
	120(120)	248(80)	f_α (64)f_β(32)f_g(10)	f_α (68)f_β(30)f_g(14)
B_{2u}	638(630)	597(630)	f_β (48)f_c(30)f_m(20)	f_β (58)f_c(20)f_m(12)
	625(620)	590(610)	f_a (78)f_g(15)	f_a (70)f_g(17)
E_u	580(575)	530(587)	f_α (85)	f_α (75)
	570(560)	478(556)	f_h (42)f_e(20) f_α (12)	f_h (52)f_e(28) f_α (15)
	200(212)	280(189)	f_α (68) f_h (30)	f_α (69) f_h (23)
	180(180)	220(180)	f_m (70)f_β(20)	f_m (67)f_β(25)
	118(118)	150(86)	f_k (68) f_α (15)	f_k (65) f_α (25)
B_{3u}	640(635)	580(665)	f_β (41)f_n(28)f_c(20)	f_β (51)f_n(30)f_c(11)
	575(580)	511(570)	f_c (70) f_m (20)	f_c (69) f_m (24)
	530(540)	460(520)	f_h (78)	f_h (72)
	455(420)	400(465)	f_g (78) f_r (21)	f_g (75) f_r (22)
	190(180)	280(196)	f_γ (82)	f_γ (72)
	180(175)	233(145)	f_n (58)f_β(30)	f_n (68)f_β(23)

Table: 2.

Calculated Phonon frequencies of $GdBa_2Cu_3O_7$ and $SmBa_2Cu_3O_7$

(Values in the Parentheses are experiment frequencies.

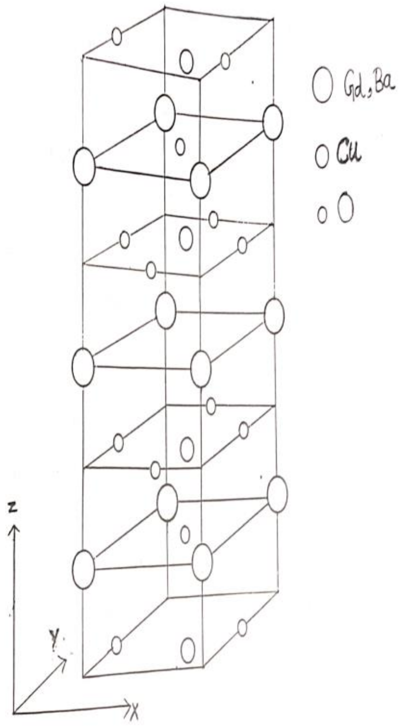

Fig:1 Crystal structure of GdBa2Cu3O7

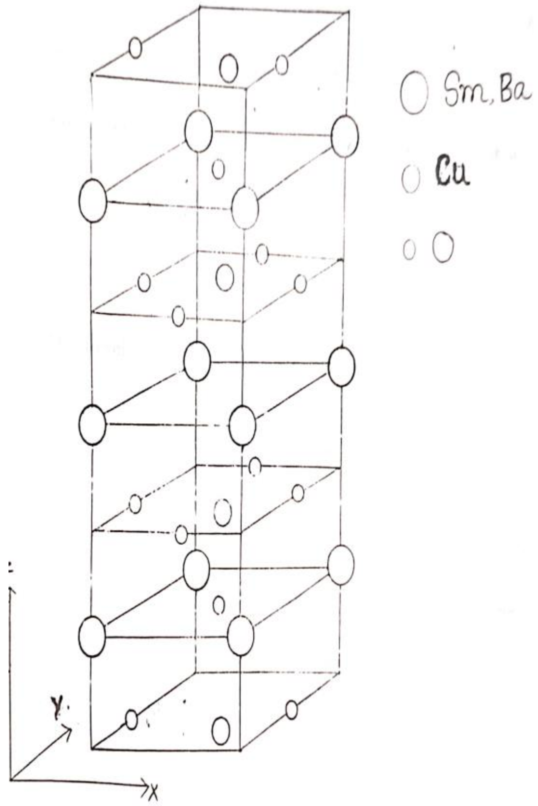

Fig:2 Crystal structure of SmBa2Cu3O7