

# Comparative Studies Between Lattice Dynamical Study And Normal Coordinate Analysis of HTSC $\text{EuBa}_2\text{Cu}_3\text{O}_6$

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## ABSTRACT

It is generally believed, that is needed to sign post the way to the development of materials with high critical temperature, even to room temperature and above, is the formulation of a proper theoretical understanding of superconductivity in these materials. Many experimental studies suggest an intimate relationship between phonons, and the superconducting transition in the high  $T_c$  oxides. For example, Raman frequencies and line widths, elastic constants and thermal conductivity all show changes around  $T_c$ . Nevertheless, there is not a well-developed theory to explain how the phonons are related to  $T_c$ . In conventional superconductors, the role of phonons is well established. However, in high  $T_c$  superconductors, the role played by phonons is controversial. Even if they do not mediate the pairing mechanism, they are likely to play an important subsidiary role. Hence there is much interest in the phonon structure of these materials.

The normal state and superconducting properties are believed to arise from the strongly correlated motion of the electronic charge carriers (electrons or holes) in the  $\text{CuO}_2$  planes that essentially define the layered cuprate HTSC. The other cations and oxygen atom in the structure provides structural stability and control the number of charge carriers in the  $\text{CuO}_2$  planes.

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.

**Keywords:** Superconducting, Raman spectroscopy, Brillouin, Three Body Force Shell Model, Normal Co-Ordinate Analysis, Lattice Dynamical Calculation, PED, etc.,

## 1. Introduction

The discovery of the high super conducting transition of the La-Ba-Cu-O system by Bednorz and Muller has caused unprecedented world wide activities in the search and characterization of high  $T_c$  superconductor is of importance, not only for the overall physical characterization of the role played by the phonons in the superconducting phenomenon.

Born-Killermann theory of ionic crystals explains the temperature variation of specific heats of many alkali halides reasonable well, but falls to describe the details of vibrational spectra. The three body

force shell model (TSM) developed from Verma and Singh [1] was reviewed by Cochran on the simple consideration that the electron shell is deformation. This deformation give rise to the three body interactions and accounts for the observed Cauchy discrepancy. The displacement on the other hand introduces the electronic polarization and accounts for the dielectric properties. Veram and Agarwal [2] redefined the shell and core charges suitably and hence the basic equation of the model have been modified. Woods et al. [3] has shown that TSM is equivalent to the breathing shell model (BSM).

## 2. Lattice Dynamics of HTSC $\text{EuBa}_2\text{Cu}_3\text{O}_6$ based on Three Body Force Shell Model

The new high  $T_c$  materials contain numerous particles in the unit cell. Thus, in a classical approach to lattice dynamics, a large number of unknown force constants has to be specified. Much attention has been paid, from several points of view, to copper-oxide-based high  $T_c$  Superconductors with the formula  $\text{EuBa}_2\text{Cu}_3\text{O}_6$  discovered by Cava et al. [4-12].

The study of the lattice dynamics of the high  $T_c$  Superconductors is of importance , not only for the overall physical characterization of these compounds, but also for an assessment of the role played by the phonons in the superconducting phenomenon. Our approach is based on the use of long -range Coulomb potentials and short-range repulsive Born Mayer potentials, as well as ionic polarizabilities, in the framework of the shell model.

The calculation of lattice dynamical vibration frequencies of  $\text{Tl}_2\text{Ba}_2\text{Cu}_1\text{O}_6$  system is performed by three-body force shell model (TSM) calculations. In the shell model calculation the equations of the motion for the core coordinate  $U$  and the shell coordinate  $W$  are expressed as [13] follows:

$$-M \omega^2 U = (R + ZC'Z) U + (T + ZC'Z) W$$

$$0 = (T - YC'Z) U + (S + K + YC'Y) W$$

with  $ZC'Z = Z [ Z + 12 f(a) ] C + V$  where  $M$ ,  $Z$  and  $Y$  are diagonal matrices representing the mass ionic charge on the shell,  $R$ ,  $S$ ,  $T$  are matrices specifying short-range core-core, shell-shell and core-shell interactions respectively,  $V$  is the matrix describing the three-body overlap interactions and  $f(a)$  is related to overlap integrals of electron wave function.  $U$  and  $W$  are the vectors describing the ionic displacements and deformations respectively.

In the earlier approaches the  $R$ ,  $S$  and  $T$  elements were considered to be equal to one another. In the present investigation, we have started with n approach such that  $R \neq S \neq T$  [10]. That is the various interactions between the ions are treated in a more general way without making them numerically equal. The dynamical matrix of the model consists of long-range Coulomb and three-body interactions and the short range overlap repulsions. The off-diagonal elements of this matrix along the symmetry directions chain a completely new term having a significant contribution for unequal  $R$ ,  $S$  and  $T$ .

The lattice dynamical calculation of high-temperature superconductors is explained using an inter ionic potential consisting of long-range Coulomb part and a short range Potential of Born-Mayer form [14-15].

$$V_{ij} = a_{ij} \exp. (-b_{ij}. r)$$

Where  $i, j$  label the ions and  $r$  is their separation. The parameters  $a_{ij}$  and  $b_{ij}$  are the pair potentials and the parameters  $Y$  and  $K$  determine the electronic polarizabilities. The parameters used in the present calculations are given in Table 1. Phonon frequencies are calculated using the force constants derived from the inter ionic potential. Following Leaner et al [14] inter-ionic pair potentials for short-rang interactions can be transferred from one structure to another in similar environments. The force constants evaluated by this method are in good agreement with the evaluated values [15-18]

### 3. Normal Co-Ordinate Analysis Of Superconductor $\text{EuBa}_2\text{Cu}_3\text{O}_6$ .

A molecule possesses three types of internal energy. These are electronic, vibrational, and rotational energies. Every molecule, at all temperatures, is continually executing vibrational motions. The complex, random, and seemingly a periodic internal motions of a vibrating molecule are the result of the superposition of a number of relatively simple vibratory motions known as the normal vibrations or normal modes of vibration of the molecule. Each of these has its own fixed frequency. Naturally, when many of them are superposed, the resulting motion must also be periodic, but it may have a period so long as to be difficult to discern the generalized co-ordinates, each one of them executing oscillations of one single frequency, are called normal co-ordinates.

### 4. Normal Co-ordinate Analysis of The Zero Wave-Vector Vibration of $\text{EuBa}_2\text{Cu}_3\text{O}_6$

The study of lattice vibrations 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. Cardona and coworkers [19] studied the infrared and Raman spectra of the super conducting cuprate perovskites  $\text{MBaCu}_2\text{O}_2$  ( $M = \text{Nd, Er, Dy, Tm and Eu}$ ) 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  $\text{EuBa}_2\text{Cu}_3\text{O}_6$  superconductors.

The high  $T_c$  superconductor  $\text{EuBa}_2\text{Cu}_3\text{O}_6$  System crystallizes in the body-centered tetragonal (bct) system, which belongs to the space group  $14/mmm (D_{4h}^{17})$ . The body-centered tetragonal (bct) unit cell of  $\text{EuBa}_2\text{Cu}_3\text{O}_6$  and the numbering of the atoms are shown in Fig.1. The 12 atoms of the unit cell yield a total of 24 optical vibrational modes. All the above calculations are made at  $q=0$ . Once of  $A_{2u}$  and  $E_u$  modes corresponds to acoustic vibrations with frequency  $\omega = 0$ . These normal modes are distributed as follows.

- $A_{1g} + E_g + A_{2u} + E_u$  □ from the motion of Eu atoms
- $A_{1g} + E_g + A_{2u} + E_u$  □ from the motion of 2 Ba atoms
- $A_{2u} + E_u$  □ from the motion Cu (1) atoms
- $E_g + A_{2u} + B_{2u} + 2E_u$  □ from the motion O (1) atoms alone c-axis
- $A_{1g} + E_g + A_{2u} + E_u$  □ from the motion O (2) atoms alone b-axis
- $A_{1g} + E_g + A_{2u} + E_u$  □ from the motion O (3) atoms alone a-axis

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

$$\Gamma_{\text{opt}} = 4A_{1g} + B_{1g} + 5E_g + 5A_{2u} + B_{2u} + 6E_u$$

The species belonging to  $A_{1g}$  and  $E_g$  Raman active modes whereas  $A_{2u}B_u$  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 [20]. The general agreement between the evaluated and observed normal frequencies of  $\text{EuBa}_2\text{Cu}_3\text{O}_6$  is good. The calculated force constants using the above programs are given in Table 2. It is interesting to note that the evaluated frequencies given in Table 3, agree favourably 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  $\lambda_k = 4\pi^2 C^2 v^2_k$ .

## 5. Result and Discussion

### 5.1 Lattice Dynamical Calculation HTSC $\text{EuBa}_2\text{Cu}_3\text{O}_6$ using Three Body Force Shell Model

The Lattice Dynamical calculations based on modified TSM reproduce the observed frequencies of Raman and infrared active modes reasonable which are given in table 3. The calculated frequencies are in good agreement with the available experimental values. The lowest calculated Raman active  $A_{1g}$  mode frequency at  $118 \text{ cm}^{-1}$  is due to the vibration of Eu atoms and this agrees very well with the experimental frequency at  $120 \text{ cm}^{-1}$ . Similarly the calculated Raman frequency is  $A_{1g}$  symmetry at  $184 \text{ cm}^{-1}$  and  $431 \text{ cm}^{-1}$  are due to the vibration of Ba and O(2) atoms respectively and the observed frequencies at  $185$  and  $435 \text{ cm}^{-1}$  agrees very well with the calculated frequency. The highest calculated Raman frequency  $462 \text{ cm}^{-1}$  in  $A_{1g}$  symmetry is due to the vibration of O(3) atoms which also agrees very well with the observed frequency at  $463 \text{ cm}^{-1}$ .

Further we have investigated the following Zone centre frequencies in the Raman active mode in the symmetry at  $80$ ,  $160$  and  $416 \text{ cm}^{-1}$  are due to the vibration of Ba, Cu and O(1) atoms respectively. The maximum vibrational frequency in  $E_g$  symmetry is  $515 \text{ cm}^{-1}$  which is due to the vibration of O(2) atoms. The calculated infrared frequency is  $A_{2u}$  symmetry at  $136 \text{ cm}^{-1}$  is due to the vibration of Cu(1), Ba and Tl atom whereas the atom Tl vibrates at  $180^\circ$  out of phase to Ba and Cu(1) atom and the observed frequency  $138 \text{ cm}^{-1}$  agrees very well with the experimental values. The infrared photon frequency at  $162 \text{ cm}^{-1}$  is due to the vibration of Ba and Cu (1) atoms and its experimental value is  $163 \text{ cm}^{-1}$ . The evaluated photon frequency at  $173 \text{ cm}^{-1}$  is due to the vibration of Cu (1) and O(1) atoms and its experimental values is  $173 \text{ cm}^{-1}$ . The evaluated infrared frequency at  $339 \text{ cm}^{-1}$  is due to the vibration of O(2), O(1) and Cu atoms in which O(1) atom vibrates at  $180^\circ$  out of phase to O(2) and Cu atoms. The highest evaluated phonon frequency in  $A_{2u}$  symmetry is  $497 \text{ cm}^{-1}$  which is due to the vibration of O(3) atom and its observed frequency at  $496 \text{ cm}^{-1}$  in  $A_{2u}$  symmetry modes agrees very well with each other.

The evaluated phonon frequency in  $B_{2u}$  symmetry mode at  $126 \text{ cm}^{-1}$  is due to the vibration of O(1) atoms. The Calculated infrared phonon frequency at  $103 \text{ cm}^{-1}$  in  $E_u$  symmetry is due to the vibration of Ba and Cu(1) atoms and its experimental frequency at  $104 \text{ cm}^{-1}$  agrees very well with the evaluated values. The infrared phonon frequency at  $134 \text{ cm}^{-1}$  is due to the vibration of Cu(1) and Ba atoms and its observed frequency  $133 \text{ cm}^{-1}$  agrees very well with the calculated frequency. The infrared phonon frequency at  $213 \text{ cm}^{-1}$  is due to the vibration of O(1) atom which performs bending bond vibrations and its observed frequency  $213 \text{ cm}^{-1}$  agrees very well with the calculated frequency. The highest infrared frequency  $514 \text{ cm}^{-1}$  is due to stretching of O(1) atoms and its experimental values  $513 \text{ cm}^{-1}$  agrees very well with observed frequency.

### 5.2 Normal coordinate analysis of HTSC $\text{EuBa}_2\text{Cu}_3\text{O}_6$

The G-matrix elements have been calculated from the equilibrium geometry. The initial force constants were taken from the related molecules. The final sets of potential constants provide the stability of the

crystal in relation to all vibrational modes. The vibrational frequencies and potential energy distribution values are presented in this work. The potential energy distribution indicates the contribution of an individual force constant to the vibrational energy of normal modes. It clearly indicates that there is mixing of the internal displacement coordinates.

The evaluated frequencies using the normal coordinate analysis method listed in table 3. agrees favourably with the calculated lattice dynamical frequencies and observed experimental frequencies. The calculated Raman phonon frequency at  $120\text{cm}^{-1}$  in  $A_{1g}$  symmetry agrees very well with the observed frequency at  $120\text{cm}^{-1}$ . This is the lowest phonon frequency due to the vibration of Eu atom, and is due to the bending vibration of O(2)-Cu-O(3), which is confirmed by the potential energy distribution calculation. The calculated Raman phonon frequencies at  $185\text{cm}^{-1}$ ,  $437\text{cm}^{-1}$  are due to the vibration of Cu and O(2) atoms, both the oscillation are due to the bending vibrations. The highest frequency in this mode is  $453\text{cm}^{-1}$  is due to the vibration of O(2). Both the frequencies agrees very well with the observed frequencies at  $463\text{cm}^{-1}$ .

The calculated Raman phonon frequencies in  $E_g$  symmetry at  $86\text{cm}^{-1}$ ,  $420\text{cm}^{-1}$  and  $437\text{cm}^{-1}$  are due the vibration of Eu, Cu and O(2) atoms respectively. All these vibrations are bending vibration which is confirmed by the potential energy distribution calculation. The highest calculated phonon frequency at  $5516\text{cm}^{-1}$  is due to the vibration of (O2)atom and it is due to stretched vibration.

The calculated infra red phonon frequencies in  $A_{2u}$  symmetry at  $136\text{cm}^{-1}$ ,  $169\text{cm}^{-1}$  are due to the vibration of Cu(1) and O(1) atoms and due to the stretched vibration. The calculated phonon frequencies and observed frequencies agrees very well with each other. The infrared phonon frequencies at  $173\text{cm}^{-1}$ ,  $339\text{cm}^{-1}$  and  $498\text{cm}^{-1}$  are due to the vibration of Cu(1), O(2) and O(3) atoms which is due to bending vibration. The frequency at  $498\text{cm}^{-1}$  in this symmetry is due to the bending vibration of O(2)-Ca-O(1).

The calculated infra red phonon frequencies in  $E_u$  mode at  $103\text{cm}^{-1}$  is due to the vibration of stretched vibration of Ba-O(1). The calculated highest infrared phonon frequency at  $551\text{cm}^{-1}$  is due to the vibration of O(3) atom, which agrees very well with the observed phonon frequency at  $513\text{cm}^{-1}$  is confirmed by the Potential Energy Distribution calculation.

## 6. Comparative Studies Between Lattice Dynamical Study And Normal Coordinate Analysis Of HTSC $\text{EuBa}_2\text{Cu}_3\text{O}_6$

The comparative study between Lattice dynamics and normal coordinate analysis of high temperature superconductors  $\text{EuBa}_2\text{Cu}_3\text{O}_6$ . In the present investigation the lattice dynamical calculations and normal coordinate analysis yield same phonon frequency a bridge between Solid State Physics and Spectroscopy to understand the mechanism of superconductivity. 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 superconductivity.

The lattice dynamics method is suited to determine the phonon frequencies in the proximity of the Brillouin zone centre only. But, the force constants obtained from that analysis do not provide a stable dynamics throughout the Brillouin zone. 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. This work



considered only the  $q=0$  modes and the number of model parameters exceeded the number of experimental data. The rigid ion model on the other hand, considers both the short-range repulsive interactions and the long range Coulomb interaction among various rigid ions in the crystal. The lattice dynamics of high temperature of high temperature superconductor have been performed using rigid ion model. The modified three body shell model adopted in the lattice dynamical study gives favourable phonon frequencies.

The lattice dynamical calculation based on modified TSM reproduce the observed frequencies of Raman and infrared active modes reasonably which are given in table 3. along with calculated normal coordinate analysis frequencies and the observed frequencies.

The calculated Raman phonon frequency at  $118\text{cm}^{-1}$  in  $A_{1g}$  symmetry is due to the vibration of Eu atom which agrees very well with the normal coordinate analysis's frequency at  $120\text{cm}^{-1}$  and it is due to the bending vibration of O(2)–Cu–O(3) which is confirmed by the potential energy distribution calculation. The highest frequency in this symmetry in lattice dynamical is  $462\text{cm}^{-1}$ , which is equal to  $463\text{cm}^{-1}$  in normal coordinate analysis which is due to the vibration of O(2) and this phonon frequency is due to the stretched vibration of O(2).

The phonon frequency at  $363\text{cm}^{-1}$  in lattice dynamics is more or less equal to the phonon frequency obtained by the normal coordinate analysis. This phonon frequency is due to the bending vibration. The phonon frequency  $416\text{cm}^{-1}$  and  $4371\text{cm}^{-1}$   $E_g$  symmetry in lattice dynamical calculation agrees very well with the frequencies obtained by the normal coordinate analysis at  $416\text{cm}^{-1}$  and  $437\text{cm}^{-1}$  respectively. Both these frequency are obtained in the bending vibration mode.

The minimum infrared phonon frequency in  $A_{2u}$  at  $136\text{cm}^{-1}$  in lattice dynamical calculation is due to the vibration of Ba atom which agrees very well with the frequency obtained by the normal coordinate analysis at  $138\text{cm}^{-1}$  which is performed by stretching vibration and it is confirmed by the potential energy distribution calculation. The maximum frequency in this symmetry is  $497\text{cm}^{-1}$  in lattice dynamics which agrees very well with the frequency obtained by the normal coordinate analysis at  $4961\text{cm}^{-1}$  is due to the stretched vibration of O(3), which is confirmed by PED calculation.

The phonon frequency in lattice dynamics at  $372\text{cm}^{-1}$  in  $E_u$  symmetry is due to the vibration of O(1) atom agrees very well with the frequency obtained by the normal coordinate analysis at  $373\text{cm}^{-1}$  which is due to bending vibration. Finally, the phonon frequency in this symmetry at  $514\text{cm}^{-1}$  in lattice dynamics agrees with the frequencies obtained by normal coordinate analysis at  $513\text{cm}^{-1}$  is due to the stretched vibration of O(3) atoms which is confirmed by the PED calculation.

## 7. Conclusion

In this work, two different methods viz, lattice dynamical study and normal coordinate analysis yielded the same phonon frequency for high temperature superconductor **EuBa<sub>2</sub>Cu<sub>3</sub>O<sub>6</sub>**. It is also seen from the tables, that the agreement between the calculated and observed frequencies wherever available are very good for the systems under consideration.

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 Lattice Dynamics and Normal Coordinate Analysis are compared and they appear to be in good agreement, which is confirmed by the Potential Energy Distribution calculation..

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**Table: 1 Force constants for EuBa<sub>2</sub>Cu<sub>3</sub>O<sub>6</sub>**

Parameters of the model: a, b are Born-Mayer constants: Z,Y,K, ionic charge, shell charge and on-site core-shell force constant of the ion, V<sub>a</sub> is the volume of the unit cell.

Interaction	a (eV)	b (Å <sup>-1</sup> )
Eu-O (Same plane)	3000	2.80
Eu-O (adj plane)	3000	3.55
Ba-O	2.90	3220
Cu-O	1260	3.35
O-O	1000	3.00

Ion	Z( e )	( e )	k(e <sup>2</sup>  V <sub>a</sub> )
Eu	2.70	2.00	1000
Ba	2.00	2.32	207
Cu	2.00	3.22	1248
O (Cu-O) Plane	-1.90	-2.70	310
O (Cu-O) Plane	-1.93	-2.70	210
O(Ba-O) Plane	-1.93	-2.70	310 (K <sub>1</sub> ) 2100 (K <sub>2</sub> )

**Table: 2**

Force constants for **EuBa<sub>2</sub>Cu<sub>3</sub>O<sub>6</sub>** (in units of 10<sup>2</sup> Nm<sup>-1</sup> (stretching) and 10<sup>-18</sup> Nm rad<sup>-2</sup> (bending))

Potential constant	bond type	distance (Å)	initial value
f <sub>b</sub>	Ba-O(1)	2.798	0.75
f <sub>c</sub>	Ba-O(2)	2.819	1.10
f <sub>d</sub>	Ba-O(3)	2.851	0.81
f <sub>e</sub>	Eu-O(1)	2.003	0.30
f <sub>g</sub>	Eu-O(2)	2.097	0.30
f <sub>h</sub>	Eu-O(3)	3.108	0.61
f <sub>k</sub>	Eu-O(3)	2.402	0.48
f <sub>l</sub>	Cu-O(1)	1.932	0.145
f <sub>m</sub>	Cu-O(2)	2.648	1.65
f <sub>n</sub>	Eu-O(3)-Eu	--	0.31
f <sub>p</sub>	O(1)-Cu-O(1)	--	0.25
f <sub>a</sub>	Eu-O(2)-Ba	--	0.46
f <sub>β</sub>	O(2)-Eu-O(3)	--	0.80

**Table.3 Calculated Phonon frequencies of EuBa<sub>2</sub>Cu<sub>3</sub>O<sub>6</sub>**  
(Values in the Parentheses are experiment frequencies)

Symmetry species	Frequency(cm <sup>-1</sup> ) Using Dynamics	Lattice	Using Normal Coordinate analysis	Potential Distribution(%)	Energy
A <sub>1g</sub> (Raman)	118(120)		120	f <sub>b</sub> (60)f <sub>d</sub> (20)f <sub>k</sub> (10)	
	184(185)		185	f <sub>i</sub> (70)f <sub>d</sub> (11)f <sub>p</sub> (10)	
	431(435)		437	f <sub>e</sub> (55)f <sub>a</sub> (31)	
	462(463)		463	f <sub>a</sub> (58)f <sub>e</sub> (30)f <sub>m</sub> (11)	
B <sub>1g</sub>	363		362	F <sub>1</sub> (68)fd(14)f <sub>m</sub> (10)	



E <sub>g</sub>	80(85)	86	f <sub>c</sub> (61)f <sub>e</sub> (11)f <sub>b</sub> (15)
	160(165)	164	f <sub>m</sub> (70) f <sub>i</sub> (21)
	416(416)	420	f <sub>a</sub> (45)f <sub>g</sub> (31)f <sub>n</sub> (20)
	437(437)	437	f <sub>n</sub> (64)f <sub>h</sub> (21)f <sub>m</sub> (15)
	515(513)	516	F <sub>k</sub> (66)fl(20)f <sub>m</sub> (15)
A <sub>2u</sub> (IR)	136(138)	136	f <sub>n</sub> (70)f <sub>a</sub> (12)
	162(163)	169	f <sub>m</sub> (65)f <sub>a</sub> (19)f <sub>d</sub> (15)
	173(173)	173	f <sub>p</sub> (59)f <sub>n</sub> (30)
	339(340)	339	f <sub>p</sub> (62)F <sub>b</sub> (19)f <sub>n</sub> (15)
	497(496)	498	f <sub>a</sub> (60)f <sub>e</sub> (21)f <sub>m</sub> (16)
B <sub>2u</sub>	126(120)	126	f <sub>p</sub> (51)f <sub>n</sub> (24)f <sub>e</sub> (16)
E <sub>u</sub>	103(104)	103	f <sub>b</sub> (70)f <sub>c</sub> (14)
	134(133)	132	f <sub>a</sub> (65)f <sub>e</sub> (22)
	213(213)	214	f <sub>a</sub> (49) f <sub>d</sub> (17) f <sub>e</sub> (21)
	372(372)	373	f <sub>a</sub> (60)f <sub>b</sub> (22)f <sub>k</sub> (11)
	415(411)	418	f <sub>b</sub> (66) f <sub>p</sub> (21)
	514(513)	515	f <sub>n</sub> (62)f <sub>a</sub> (20)

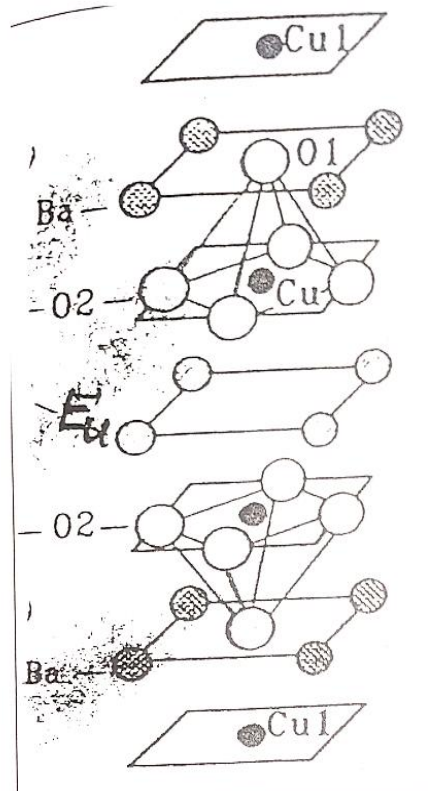


Fig 1: Unit Structure of HTSC EuBa<sub>2</sub>Cu<sub>3</sub>O<sub>6</sub>