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### RESEARCH ARTICLE

#### LATTICE DYNAMICAL STUDY OF EUROPIUM SULFIDE (EuS) USING TRI & TRSMODEL

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#### Abstract

In the present communication author's are reporting lattice dynamical study of Europium sulfide (EuS). Which is based on the two phenomenological models, by including the effect of three-body interactions (TBI) in the frame work of rigid ion model (TRIM) & rigid shell model (TRSM) with the satisfactory description of all phonon properties. The model parameters of both have used to the phonon spectra for the allowed 48-nonequivalent wave vectors in the first Brillouin zone. The frequencies along the symmetry directions have plotted against the wavevector to obtain the phonon dispersion curves (PDC) from both the models. With the help of available experimental data. We have also reported the Specific heat variation & Combined density of states (CDS) for complete description of the frequencies for the Brillouin zone included theoretical Debye temperature and elastic property of (second-third order) of EuS. So by using the present model the complete lattice property of EuS is reported successfully.

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#### Introduction:-

The electronic structure of Europium sulfide (EuS) which is a family of Europium Chalcogenides crystallize in f.c.c. NaCl structure and are also called rare earth europium chalcogenides. Complete experimental data on phonon dispersion is available for EuS, which has been reported. by Silberstein *et al.* [1]. Zeyher and Kress [2] discuss the complete phonon dispersion curves (PDC), combined density of states (CDS)[3] and Debye temperature variations curve given by [4]. The elastic constants [5], dielectric constants [6], the physical and natural properties of the (EuS) have attracted and their interpretations by means of different theoretical models [7-12], which has been described their interesting properties. It has been also found that three body interactions explain well the optical branches and Cauchy discrepancy both simultaneously and successfully to almost all the ionic and semiconducting crystals [13]. The remarkable success is achieved from rigid ion model (RIM) [14] and rigid shell model (RSM) [15] to describe the lattice dynamics of alkali halides and worthwhile to explore the adequacies of these model for EuS. The third-order elastic constants (TOEC), which is related to the energy products of three strain components, and the lowest order constants to enter the description of non-linear effects like the equation of state and the interaction of phonons. These TOEC is determined from velocity measurements on small amplitude sound waves in statically stressed media. The aim of present report is to test the applicability and utility of second-neighbor three-body rigid shell model (TBRSM) and second neighbor three-body rigid ion model (TBRIM) with the satisfactory description of phonon dispersion relations and other phonon properties of the EuS.

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## Materials and Methods: -

### Materials:

The lattice dynamics study of EuS compounds has important object of considerable and continuing interest in the solid state physics. It Having a lots of specific potential in modern technologies, europium chalcogenides are being used in magneto-optic memories and various electronic equipment's. The present model thus consists of the long-range Coulomb, TBI & the short-range overlap repulsion operative up to the second-neighbor for EuS. The relevant expression for the crystal potential per unit cell can be derived with TBFSM, is given as

$$\Phi = \Phi^C + \Phi^R + \Phi^{TBI} \quad (1)$$

where  $\Phi^C$  is long-range Coulomb interaction potential. The analytical expressions by the inverse and exponential power laws for the repulsive energy are given as

$$\Phi^R(r_{ij}) = ar_{ij}^{-n} \text{ (Born Potential) , } \Phi^R(r_{ij}) = b \exp(-r_{ij}/\rho) \text{ (B-M Potential)}$$

where, a (or b) and  $n$  (or  $\rho$ ) are the Born exponents called the strength and hardness parameters, respectively.  $\Phi^R$  is a short-range overlap repulsion potential. Third term  $\Phi^{TBI}$  long-range TBI interaction potential expressed as

$$\Phi^{TBI} = \alpha_m \frac{Z^2 e^2}{r_0} \left[ \frac{2n}{Z} f(r)_0 \right]$$

where, the term  $f(r)_0$  is the equilibrium electron wave-functions. Since we consider only one ion to be polarizable and deformable, the basic equations of Singh and verma's [16] model are modified. The secular determinant equation is given by

$$|D(\vec{q}) - \omega^2 MI| = 0 \quad (2)$$

Here  $D(\vec{q})$  is the (6 x 6) dynamical matrix for Rigid Shell model. The dipole-dipole (VWI) energy up to second neighbour is expressed as:

$$\Phi_{dd}^{VWI}(r) = -S_V \left| \frac{C_{++} + C_{--}}{6r^6} \right| = \Phi^V(r) \quad (3)$$

where,  $S_V$  is lattice sum and the constants  $C_{++}$  and  $C_{--}$  are the positive-positive and negative-negative ion pairs, respectively. By use of the secular equation (2) the expressions for elastic constants can derived and given as:

$$C_{11} = \frac{e^2}{4r_0^4} \left[ -5.112Z_m^2 + A_{12} + \frac{1}{2}(A_{11} + A_{22}) + \frac{1}{2}(B_{11} + B_{22}) + 9.3204 \xi'^2 \right] \quad (4)$$

$$C_{12} = \frac{e^2}{4r_0^4} \left[ 0.226Z_m^2 - B_{12} + \frac{1}{4}(A_{11} + A_{22}) - \frac{5}{4}(B_{11} + B_{22}) + 9.3204 \xi'^2 \right] \quad (5)$$

$$C_{44} = \frac{e^2}{4r_0^4} \left[ 2.556Z_m^2 + B_{12} + \frac{1}{4}(A_{11} + A_{22}) + \frac{3}{4}(B_{11} + B_{22}) \right] \quad (6)$$

at equilibrium condition  $[(d\Phi/dr)_0 = 0]$  we obtain

$$B_{11} + B_{22} + 2B_{12} = -0.6786 Z_m^2 \quad (7)$$

$$\text{where } Z_m^2 = Z^2 \left( 1 + \frac{16}{Z} f_0 \right) \quad \text{and} \quad \xi'^2 = Zr_0 f_0' \quad (8)$$

### Vibrational Properties of EuS:

The term  $f_0$  is function dependent on overlap integrals of electron wave functions. Similarly, expressions for two distinct optical vibration frequencies ( $\omega_L$  and  $\omega_T$ ) are obtained as:

$$(\mu\omega_L^2)_{q=0} = R'_0 + \frac{(Z'e)^2}{\nu f_L} \cdot \frac{8\pi}{3} (Z_m^2 + 6\xi'^2) \quad (9)$$

$$(\mu\omega_T^2)_{q=0} = R'_0 - \frac{(Z'e)^2}{\nu f_T} \cdot \frac{4\pi}{3} Z_m^2 \quad (10)$$

The frequency distribution function by use of Debye's model is given by

$$\Theta_D = hv_m/K \quad (11)$$

To determine the phonon density of states for each polarization is given by

$$g(\omega)=dN/d\omega= N \int \sum_{BZ} \delta[\omega - \omega_j(q)]dq = (VK^2/2\pi^2).dK/d\omega \quad (12)$$

and  $N = (L/2\pi)^3 (4\pi K^3/3)$  where N as a normalization, K is wave vector and  $L^3=V$ .

**Methods: -**

The input data along with their relevant references and calculated model parameters from SNTRSM and SNTRIM for EuS are given in Table- 1.

**Table-1:-** Input data, model parameters and Cauchy-Discrepancy (in units  $10^{12}$  dyne/cm<sup>2</sup>) for EuS-C<sub>ij</sub> (in  $10^{12}$  dyn/cm<sup>2</sup>),  $r_0$ (in  $10^{-8}$  cm)v(THz)  $\alpha_i$ (in  $10^{-24}$  cm<sup>3</sup>).

Input data for EuS		Model parameters for EuS			Cauchy-Discrepancy	
Properties	Values for EuS	Properties	Values for EuS		Property	Values for EuS
			(TRSM)	(TRIM)		
C <sub>11</sub>	13.1	r <sub>0</sub> f <sub>0</sub> '	-0.3005	-0.3005	C <sub>112</sub> - C <sub>166</sub>	-0.1536202
C <sub>12</sub>	1.10	Z <sub>m</sub> <sup>2</sup>	0.6745	0.6522	C <sub>123</sub> - C <sub>456</sub>	3.383992
C <sub>44</sub>	2.73	A	8.5110	8.396	C <sub>144</sub> - C <sub>456</sub>	1.1279974
r <sub>0</sub>	2.984	B	-0.7858	-0.7598	C <sub>123</sub> -C <sub>144</sub>	2.255995
α <sub>1</sub>	1.5	d <sub>1</sub>	0.01634	-----	C <sub>1112</sub> - C <sub>1166</sub>	56.266209
α <sub>2</sub>	5.5	d <sub>2</sub>	1.4081	-----	C <sub>1122</sub> - C <sub>1266</sub>	49.842597
		Y <sub>1</sub>	-0.7943	-----	C <sub>1122</sub> - C <sub>4444</sub>	32.475691
		Y <sub>2</sub>	-2.1497	-----	C <sub>1123</sub> - C <sub>1144</sub>	-7.98236
					C <sub>1123</sub> - C <sub>1456</sub>	-0.4595586
					C <sub>1123</sub> - C <sub>1244</sub>	-5.7288801
					C <sub>1123</sub> - C <sub>4466</sub>	-7.7757569

**Table-2:-** Combined Density States, TOEC and FOEC (in units  $10^{12}$  dyne / Cm<sup>2</sup>), Pressure derivatives of SOEC and TOEC (dimensionless) for EuS.

Raman Active -(Present study)			TOEC and FOEC (in units $10^{12}$ dyn / Cm <sup>2</sup> )		Pressure derivatives of SOEC and TOEC (dimensionless)	
Frequency In v (cm <sup>-1</sup> )	Branch	Values (cm <sup>-1</sup> )	Property	EuS (Present)	Property	EuS (Present)
53	LA(X)-TA(X)	54	C <sub>111</sub>	874.78016	dK'/dP	17.248192
90	LA-TA(L)	92	C <sub>112</sub>	-0.6960135	dS'/dP	8.8718618
128	TO-TA(X)	129	C <sub>123</sub>	4.620290	dC' <sub>44</sub> /dP	-0.4047117
155	LA+TA(Δ)	154	C <sub>144</sub>	2.3642958	dC' <sub>111</sub> /dP	-1296.827
184	2TA(L)	183	C <sub>166</sub>	-0.5423933	dC' <sub>112</sub> /dP	-1.0318125
208	2LA(Δ)	208	C <sub>456</sub>	1.2362984	dC' <sub>166</sub> /dP	8.863633
225	LA+TA(L)	225	C <sub>1111</sub>	877.65552	dC' <sub>123</sub> /dP	6.8493989
262	TO+TA(X)	262	C <sub>1112</sub>	61.749871	dC' <sub>144</sub> /dP	-3.5049752
290	TO+LA (Δ) LO+TA (Δ) LO+TA(X)	292	C <sub>1166</sub>	5.4836629	dC' <sub>456</sub> /dP	1.8327636
317	TO+LA(X)	316	C <sub>1122</sub>	52.219791		
357	2TO(Γ)	357	C <sub>1266</sub>	2.3771944		
412	LO+TO(L)	412	C <sub>4444</sub>	19.7441		
450	2LO(X)	450	C <sub>1123</sub>	-1.1414354		
483	2LO(Δ)	483	C <sub>1144</sub>	-6.8409246		
492	2LO(L)	491	C <sub>1244</sub>	-4.587447		
			C <sub>1456</sub>	-0.6818786		
			C <sub>4466</sub>	-6.6343215		

**Table-3:-** Comparison of frequencies from various sources at X and L point for EuS.

Crystal	Source	Frequency in (THz)
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		LO	TO	LA	TA
EuS X-Point	Experimental	-----	-----	-----	-----
	TRIM	6.4	5.8	3.3	1.8
	TRSM	6.75	5.87	3.62	2.0
EuS L-Point	Experimental	-----	-----	-----	-----
	TRIM	7.02	4.6	3.51	2.52
	TRSM	7.37	5.0	4.0	2.75

**Results and Discussion: -**

**Results:**

From figure- 1, it is clear that the results reported from SNTRSM for EuS are comparatively more close to the measured data on PDCs. These result are similar to the TMC but there are certain features in PDC of EuS which deserve special mention. The three body interactions have influenced both LO and TO branches much more than acoustic branches (LA and TA). Another striking feature of the present study is noteworthy from the excellent reproduction of optical and acoustic branches.

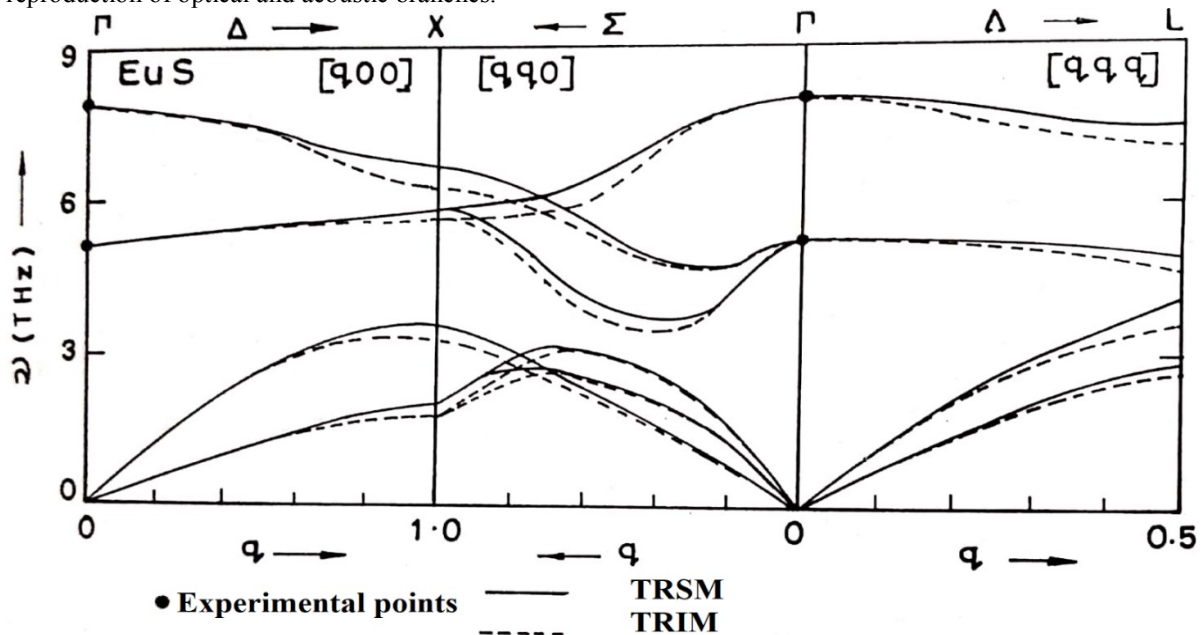


Fig.1:- Phonon dispersion curves of EuS.

The frequency along with symmetry directions have plotted against the wave vectors to obtain the phonon dispersion curves (PDCs) from both the models. For this purpose, the specific heat has been computed at different temperature using Blackmann's technique [17] and corresponding Debye temperature, plotted against absolute temperature (T). It may be concluded that TRSM provides agreement is certainly better than those fitted by experimental researchers and TRIM result closely to the experimental values. Although, qualitatively the agreement is achieved from our present model TRSM better than some of the used model values. In addition, some other researchers [18-22] in the same field has been also tried to explain PDCs and other properties of europium chalcogenides but only with moderate success.

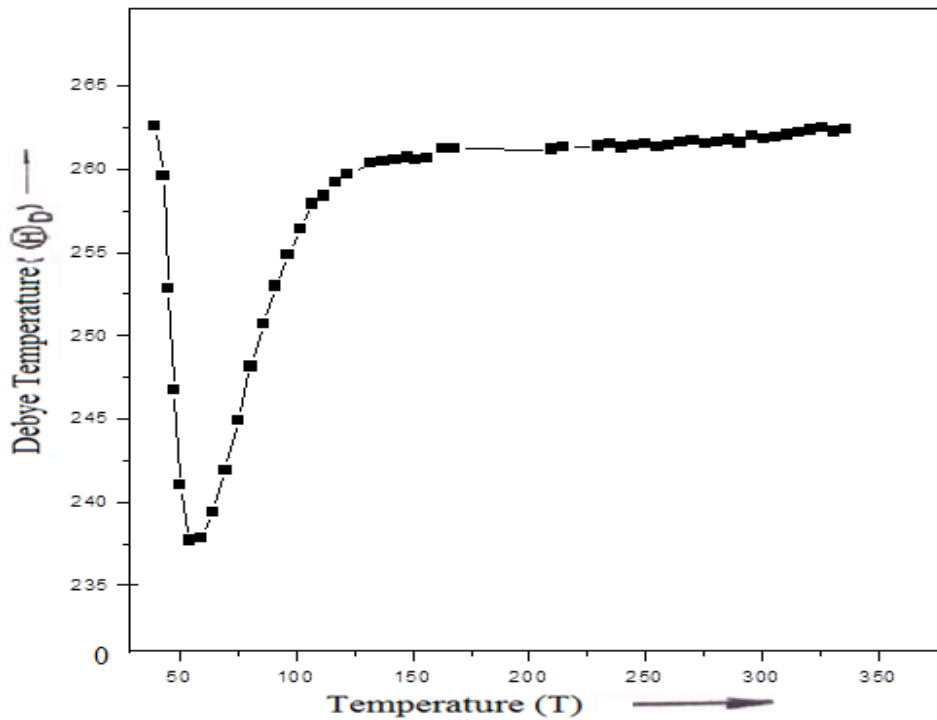


Fig.2:- Debye Temperature Curve for EuS.

Furthermore, in order to increase the merit of this work, we have tested the adequacy of our model by calculating 33 two phonon Raman/IR spectra and variation of Debye temperatures shown in figure-2. Since no observed data on two phonon IR/Raman spectra are available, these Combined density of states peaks has been compared with the assignments calculated by using our present theoretical data shown in figure-3. In order to interpret them the critical point analysis have been used following the method prescribed by Burstein *et al.* [23]. So the inclusion of the effect of short range overlap repulsive interaction upto second neighbours in the framework of TRIM and TRSM is important in EuS. The present approach has revealed much better description of the crystal dynamics of the such solid under consideration than those reported [1] by other models. It is expected that slight discrepancies still occurring between theory and experiment may be further improved by including the effect of free carrier screening (FCS), Van der Waals interactions (on data availability) and by including anharmonic vibrations in the present model (TRSM).

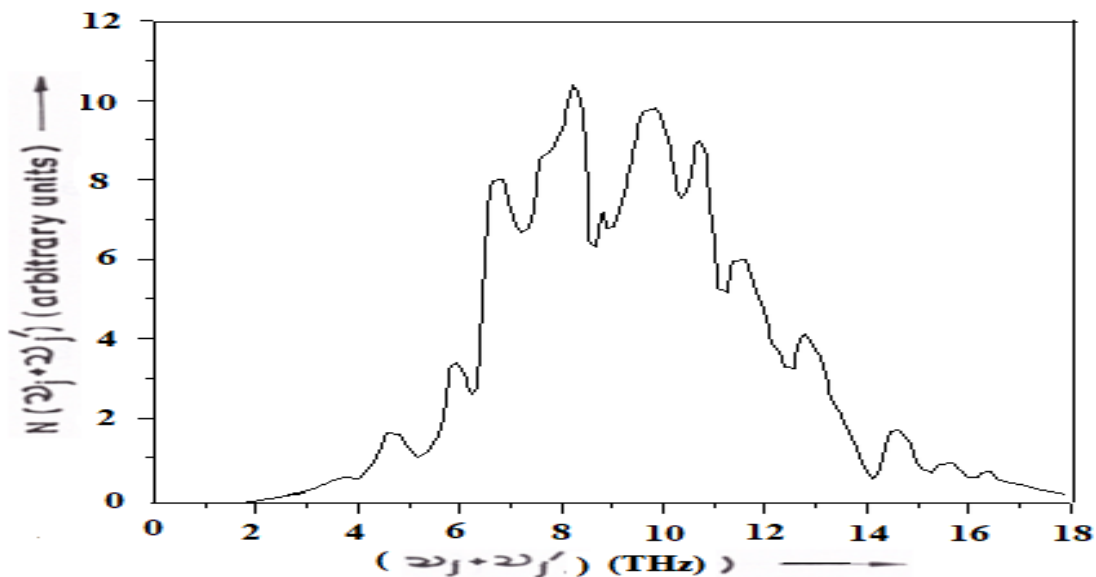


Fig. 3:- Combined density of States curve of EuS.

### Discussion:-

The present model is successfully provided complete description about EuS. The knowledge of the model parameters in Table-1 has been used to solve the secular equation for specified values of wave vectors in the first Brillouin zone, which is divided in an evenly spaced sample of 1000 wave vectors (Kellermann)[1]. Debye temperature variations at different temperatures by Blackman's [17] and (CDC) curves for (EuS) crystals have been computed by using VTBFMS model. By using the sampling technique and the corresponding values of  $\Theta_D$  have been compared with the available experimental data [20-22] and curve for  $\Theta_D$  Vs absolute temperature (T) plotted, are shown in Fig.-2 for EuS. The calculated ( $\Theta_D$ -T) curve for EuS has given excellent agreement with the experimental value [5]. The observed Raman spectra and critical point analysis have been interpreted with the help of PDS approach, using the above spectrum given in Fig-1. The third order and fourth order elastic constant and their pressure derivatives for EuS (Table-2) are probably the first reports and in the absence of experimental data, their reliability test is not possible.

### Conclusion: -

In the present communication eight parameters including elastic constants ( $C_{11}$ ,  $C_{12}$  and  $C_{44}$ ), six short range force constants a parameters  $r_0$ ,  $f_0$  arising from the deformation forces, the ionic charge  $z$ , the shell charge  $Y$ , polarizabilities ( $\alpha_1$ ,  $\alpha_2$ ), and mechanical polarizability 'd' developed by [16] have theoretically calculated for EuS and given in Table.1. By solving Eq.1 & 2 we can obtain the phonon spectra in the first Brillouin zone for the non-equivalent 48- allowed wave vectors. The frequency along with symmetry directions have been plotted against the wave vectors to obtain the phonon dispersion curves (PDCs) from both the models. These curves are compared with each other and with inelastic neutron scattering technique in Fig-1. The theoretical results obtained by three-body shell model. we have used the computed vibration spectra to study the dynamical properties like specific heat and IR/Raman spectra in the present paper. The specific heat and Debye temperature  $\Theta_D$  have been calculated as function of temperature T from the lattice frequency spectra is shown in Fig.2. The (CDSc) have been obtained by computing the density of states  $N(v_j + v'_j)$  of the combined frequencies ( $v_j + v'_j$ ) from the knowledge of lattice vibration frequency spectra in Fig.-3. The values of frequencies corresponding to theoretical and experimental peaks and Cauchy-Discrepancy for lattice dynamics of EuS have reported in Table.2. It is obvious that from table.3 the frequencies at X- and L-point reported by using present model TRSM which is very close to the experimental values. By using the present model many of the researchers have been successfully reported theoretical results for different alkali halides and semiconducting materials [24-33].

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