Indian J Phys (August 2017) 91(8):875–881
DOI 10.1007/s12648-017-0983-5

ORIGINAL PAPER

Electronic, elastic and optical properties of divalent ($R^{+2}X$) and trivalent ($R^{+3}X$) rare earth monochalcogenides

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Received: 01 August 2016 / Accepted: 17 January 2017

Abstract: Based on plasma oscillations theory of solids, simple relations have been proposed for the calculation of bond length, specific gravity, homopolar energy gap, heteropolar energy gap, average energy gap, crystal ionicity, bulk modulus, electronic polarizability and dielectric constant of rare earth divalent $R^{+2}X$ and trivalent $R^{+3}X$ monochalcogenides. The specific gravity of nine $R^{+2}X$, twenty $R^{+3}X$, and bulk modulus of twenty $R^{+3}X$ monochalcogenides have been calculated for the first time. The calculated values of all parameters are compared with the available experimental and the reported values. A fairly good agreement has been obtained between them. The average percentage deviation of two parameters: bulk modulus and electronic polarizability for which experimental data are known, have also been calculated and found to be better than the earlier correlations.

Keywords: Rare earth monochalcogenides; Electronic properties; Elastic properties; Optical properties; Electronic polarizability

PACS Nos.: 77.84.Bw; 84.30.Ng; 87.19.rd; 78.66.Qn; 32.10.Dk

1. Introduction

During the last few decades, an extensive research work has been done to understand the electronic, elastic and optical properties of rare earth materials because of their high electrical and thermal conductivities. Rare earth ions doped glasses crystallize in rare earth monochalcogenides (REX, RE = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er Tm, Yb, Lu; X = S, Se, Te) with rocksalt structure having 4f electrons. The presence of these 4f electrons in compounds are mainly responsible for their potential applications in the areas of glass-making, grinding alloys, composite lasers, electro-optic, electronic, opto-electronic and non-linear optical devices. The magnetic properties of these materials also help scientists to use rare earths in the form of fast light beam in addressing memory system of computers, in magneto-optic modulators, magnetic field activated electronic switches, spintronics and spin filtering devices [1–7]. The natural and free rare earth atoms have the electronic configuration: (Xe) $4f^{n}5d^{0,1}6\ s^{2}$. The divalent rare earths have the outer electronic structure $4f^{14}5d^{0}6\ s^{2}$ in which outer two 's' electrons contribute as valence electrons. In rare earth monochalcogenides, these two electrons fill the valence band derived from the 'p' state of the anion. However the trivalent state, the outer electronic structure of rare earth changes from $4f^{14}5d^{0}6\ s^{2}$ to $4f^{(14--X)}5d^{X}6\ s^{2}$. In a crystal, rare earths are in ionic form and the removal of 4f electrons let the ion shrink. Hence, the ionic radii of rare earths vary noticeably with their valence: for example Sm^{2+}: 1.16 Å, Sm^{3+}: 0.98 Å, and Tm^{2+}: 1.04 Å, Tm^{3+}: 0.87 Å. As a result, there is a variation of the lattice constant of the REX as one moves from one rare earth to the other in rare earth series. The divalent rare earth ($R^{+2}X$) compounds are semiconductors, which have a significantly larger lattice constant than the trivalent ($R^{+3}X$) compounds, which are metals. Most of the rare earth atoms are divalent but generally become trivalent in the metallic state. Butcher et al. [8] have shown that trivalent lanthanum monochalcogenides (LaS, LaSe and LaTe) are superconductors near 1 K. The superconducting

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*Corresponding author, E-mail: vkumar52@hotmail.com transition temperature and electronic specific heat coefficient increase as we move from mono sulfide (LaS) to mono telluride (LaTe), whereas the Debye temperature decreases from LaS to LaTe.

Crystal ionicity of materials is one of key parameters in describing the problems related to elastic constants, heats of formation, bulk modulus, cohesive energy and crystal structure. Various theoretical explanations have been given to calculate the ionicity of semiconducting materials. Phillips and Van Vechten (PV) [9, 10] have proposed dielectric theory for the calculation of ionic and covalent energy gaps, and hence the average energy gap, ionicity and covalency of binary semiconductors. Levine [11] has extended the dielectric theory of PV to ternary and multiband crystals and proposed bond charge model for the calculation of these parameters also considering the effect of d electrons. Verma [12] and Yadav [13] have recently proposed the modified form of PV model for the calculation of ionic energy gap of $R^{+2}X$ and $R^{+3}X$ monochalcogenides. Charifi et al. [14] have evaluated the elastic parameters C_{11}, C_{12}, C_{44}, B and G of B1(NaCl) and B2(CsCl) structures of REX using full-potential linearized-augmented plane wave (FP-LAPW) scheme in the frame of the generalized gradient approximation (GGA) and effect of pressure on these parameters. Binary rare earths ($R^{+2}X$) crystallize in the face centered cubic NaCl-type structure and show phase transition from B1(NaCl) to B2(CsCl) under high pressure. The theoretical and experimental investigations of high pressure structural behavior of lanthanum monochalcogenides have also been studied by Vaitheeswaran et al. [15]. Jayaraman et al. [16] have calculated bulk modulus of rocksalt type divalent and trivalent REX using effective valence product of the cation and the anion. The luminance and decay analysis of Eu^{3+} and Pr^{3+} ions doped lead telluride glasses for different concentrations in laser applications have been studied by other workers [17, 18]. The author [19, 20] have recently proposed simple relations, based on plasma oscillations theory of solids, for the calculation of bond length, covalent and ionic energy gaps of binary ionic rocksalt crystals. In this paper, we extend our earlier co-relations for the calculation of bond length (d), specific gravity (ρ), homopolar energy gap (E_h), heteropolar energy gap (E_c), average energy gap (E_g), crystal ionicity (f_i), bulk modulus (B), electronic polarizability (α_e) and dielectric constant (ε_∞) of $R^{+2}X$ and $R^{+3}X$ rare earths. The calculated values of all parameters are compared with the available experimental values of B and α_e in few compounds where the experiments are performed and the reported values of other parameters. Reasonably good agreement has been obtained between them.

2. Calculations

According to Phillips and Van Vechten [9, 10], the average energy gap (E_g) of A_mB_n binary crystals can be separated into covalent (E_h) and ionic (E_c) parts as $E_g^2 = E_h^2 + E_c^2$. The fraction of ionic (f_i) and covalent (f_c) characteristics of the individual bonds can be defined as $f_i = E_c^2/E_g^2$ and $f_c = E_h^2/E_g^2$. The generalized expression for E_h and E_c for an A_mB_n compound can be written as [9, 10]:

$$E_h = 39.74/d^{2.48} \tag{1}$$

and

$$E_c = 14.4b\left[\frac{Z_A}{r_o} - \frac{n}{m}\frac{Z_B}{r_o}\right]e^{-K_s r_o} \tag{2}$$

where d is the bond length, $r_0 = d/2$, b is the prescreening constant and $e^{-K_s r_0}$ the Thomas–Fermi screening factor. The above Eq. (1) shows the inverse relation between E_h and $d^{2.48}$. However, Eq. (2), signifies the difference between the screening Coulomb potential of atoms A and B having core charges Z_A and Z_B. These potentials are to be evaluated at the covalent radii r_0. Only a small part of the electrons are in the bond, the rest screen the ion cores, reducing their charges by Thomas–Fermi screening factor, which affects the chemical trends in a compound. The screening factor, as well as the bond length (d), both are related to the effective number of valence electrons in a compound. The plasmon energy also depends on the effective number of valence electrons in a compound. This shows that there must be a correlation between the physical process which involves the ionic and covalent contributions to the average energy gap (E_g) and the plasmon energy ($\hbar\omega_p$) of a compound. Based on this, the authors [19, 20] have proposed simple relations for the calculation of E_h and E_c of binary and ternary semiconductors. Recently, Verma [12] and Yadav [13] have modified PV theory and proposed the following relation for the calculation of covalent energy gap of $R^{+2}X$ and $R^{+3}X$ rare earth chalcogenides:

$$E_h = 40.468/d^{2.50} \tag{3}$$

where the numerator of PV Eq. (2), i.e., 39.74 has been modified by 40.468 and the denominator $d^{2.48}$ by $d^{2.50}$. Further Verma [12] and Yadav [13] have proposed empirical relations for the calculation of E_c, E_g, f_i, B, α_e and ε_∞ for rare earth chalcogenides, based on ionic charges, nearest neighbor distance and plasmon energy ($\hbar\omega_p$), and the values of $\hbar\omega_p$ have been calculated using the well-known relation:

$$\hbar\omega_p = 28.8\sqrt{\frac{Z\rho}{W}} \tag{4}$$

Table 1 Numerical values of the constants used in Eqs. (8) to (12)

Constants	K_1	K_2	K_3	K_4	K_5	K_6	K_7	K_8	K_9	K_{10}	K_{11}	K_{12}
Divalent ($R^{+2}X$)	2.5270	0.0537	0.4253	0.3939	1.0880	0.0190	71.350	8.1880	0.0629	73.520	7.826	0.2278
Trivalent ($R^{+3}X$)	2.5120	0.0335	1.1780	0.2505	1.1890	0.0308	686.50	86.020	−2.335	53.730	4.441	0.1014

where Z is the effective number of valence electrons taking part in plasma oscillations, ρ is the specific gravity and W the molecular weight. The experimental values of ρ are still not known for many $R^{+2}X$ and $R^{+3}X$ rare earths for which Verma [12] and Yadav [13] have calculated the values of $\hbar\omega_p$. Their calculations show that they have used our earlier relations [19] and back fitted the data of the bond length'd' in Eq. (5) for the calculation of $\hbar\omega_p$. In this paper, we extend our earlier correlations developed for 3-parameters d, E_h and E_c of NaCl crystals to 8-parameters d, E_h, E_c, ρ, E_g, f_i, B *and* α_e for $R^{+2}X$ and $R^{+3}X$ rare earths. The relation proposed for the calculations of nearest neighbor distance (bond length d) for $R^{+2}X$ and $R^{+3}X$ can be written as:

$$d = C(\hbar\omega_p)^{-2/3} \tag{5}$$

where C is the constant equals to17.669 and 18.369, respectively, for $R^{+2}X$ and $R^{+3}X$ rare earths.

Using Eqs. (4) and (5), we get the following relation for the calculation of specific gravity (ρ) of rare earth compounds:

$$\rho = \kappa\left(\frac{W}{d^3}\right) \tag{6}$$

where κ is the constant and equals to 0.83130 and 0.83029, respectively, for $R^{+2}X$ and $R^{+3}X$ rare earths. The calculated values of ρ are listed in column 2 of Tables 2 and 3, respectively, for $R^{+2}X$ and $R^{+3}X$ rare earths along with a few available experimental data for which experiments are performed and presented in parenthesis.

Using Eqs. (1) and (5), the covalent energy gap (E_h) of $R^{+2}X$ and $R^{+3}X$ rare earths can be expressed as:

$$E_h = K(\hbar\omega_p)^{1.6533} \tag{7}$$

where K is the constant and equals to 0.03207 and 0.02913, respectively, for $R^{+2}X$ and $R^{+3}X$ rare earths.

Further, we propose the following simple relations based on best fit of the data for the calculation of E_c, E_g, f_i, B and α_e for $R^{+2}X$ and $R^{+3}X$ rare earth monochalcogenides:

$$E_c = K_1 \exp[K_2(\hbar\omega_p)] \tag{8}$$

$$E_g = K_3 + K_4(\hbar\omega_p) \tag{9}$$

$$f_i = K_5 - K_6(\hbar\omega_p) \tag{10}$$

$$B = -K_7 + K_8(\hbar\omega_p) + K_9(\hbar\omega_p)^2 \tag{11}$$

$$\alpha_e = K_{10} - K_{11}(\hbar\omega_p) + K_{12}(\hbar\omega_p)^2 \tag{12}$$

where K_1 to K_{12} are the constants and their numerical values are listed in Table 1 for $R^{+2}X$ and $R^{+3}X$ rare earths. The values of these constants are obtained by simulating the known values of E_c, E_g, f_i, B and α_e and the calculated values of plasmon energy ($\hbar\omega_p$) using MATLAB software. We have also calculated the values of dielectric constant of $R^{+2}X$ and $R^{+3}X$ compounds using the relation proposed by Penn et al. [21]:

$$\varepsilon_\infty = 1 + \left[(\hbar\omega_p)^2 \big/ E_g^2\right] \tag{13}$$

3. Results and discussion

Based on plasma oscillations theory of solids, eight simple relations have been proposed for the calculation of various electronic, elastic and optical properties of $R^{+2}X$ and $R^{+3}X$ rare earth monochalcogenides. Using proposed Eqs. (5) to (12), the values of 8-parameters d, ρ, E_h, E_c, E_g, f_i, B and α_e have been calculated and listed in Tables 2 and 3, respectively, for $R^{+2}X$ and $R^{+3}X$ rare earths. The values of ε_∞ have also been calculated using Eq. (13) and listed in Tables 2 and 3. The calculated values of d from Eq. (6) and ionic radii data [22] are also listed in column 6 of Tables 2 and 3. The specific gravity (ρ) of 9 divalent and 20 trivalent rare earths have been calculated for the first time using Eq. (5) and listed in column 3 of Tables 2 and 3 along with the available experimental values. Our calculated values are in good agreement with the available experimental values. The average percentage deviations for B and α_e for which the experimental values are known have also been estimated using the relation, Percentage deviation = [(|Experimental values-Calculated values|)/Experimental values] × 100 and presented in the bottom row of Tables 2 and 3. In the case of B, the average percentage deviation of Eq. (11) has been estimated to be 2.318% against the earlier estimation of 5.989% for $R^{+2}X$, and 8.345% for $R^{+3}X$ against the earlier estimations of 7.302%. However, in the case of α_e, the average percentage deviation of Eq. (12) has been found to be 3.876% against the earlier estimation of 5.056% for

Table 2 Density (ρ), plasmon energy ($\hbar\omega_p$), bond length (d), energy gaps (E_h, E_c, E_g), ionicity (f_i), bulk modulus (B), electronic polarizability (α_e) and dielectric constant (ε_∞) of divalent($R^{+2}X$) rare earth monochalcogenides

Comp. (Z = 8)	Mol. Wt. (W) [22]	ρ[a] (g/cc) This work Eq. (6)	$\hbar\omega_p$ (eV) This work Eq. (4)	d (Å)		E_h (eV)		E_c (eV)			E_g (eV)		
				This work Eq. (5)	Known[b] [21, 22]	This work Eq. (7)	PVV [9]	This work Eq. (8)	PVV [9]	Yadav [13]	This work Eq. (9)	PVV [9]	Yadav [13]
1	2	3	4	5	6	7	8	9	10	11	12	13	14
SmS	182.42	5.702 (6.01 [24])	14.401	2.985	2.985	2.638	2.629	5.476	5.470	5.523	6.097	6.070	6.144
SmSe	229.32	6.399	13.607	3.100	3.100	2.401	2.373	5.247	5.209	5.118	5.785	5.724	5.667
SmTe	277.96	5.278	12.395	3.299	3.299	2.058	2.047	4.917	4.993	4.520	5.308	5.396	4.968
EuS	184.03	5.758 (5.75 [24])	14.408	2.984	2.984	2.640	2.631	5.478	5.420	5.523	6.101	6.025	6.144
EuSe	230.92	6.456	13.620	3.098	3.098	2.406	2.396	5.251	5.164	5.133	5.790	5.693	5.685
EuTe	279.56	6.473	12.395	3.299	3.299	2.058	2.047	4.917	4.952	4.535	5.308	5.358	4.985
TmS	201.00	8.395	16.648	2.710	2.710	3.352	3.347	6.178	6.353	6.145	6.983	7.181	6.879
TmSe	247.89	8.277	14.885	2.920	2.920	2.786	2.778	5.620	5.587	5.693	6.288	6.239	6.343
TmTe	296.53	8.195	13.542	3.110	3.110	2.383	2.373	5.229	5.415	4.868	5.759	5.912	5.375
YbS	205.10	7.530 (6.74 [24])	15.609	2.829	2.829	3.014	3.010	5.843	5.721	6.697	6.573	6.465	7.536
YbSe	252.00	8.328	14.809	2.930	2.930	2.763	2.754	5.597	5.498	5.775	6.258	6.149	6.441
YbTe	300.64	7.846	13.159	3.170	3.170	2.273	2.262	5.123	5.110	5.088	5.609	5.588	5.632
Average percentage deviation													

Comp. (Z = 8)	f_i			B (GPa)			α_e (Å^3)			ε_∞
	This work Eq. (10)	PVV [9]	Yadav [13]	This work Eq. (11)	Expt. [16, 23]	Yadav [13]	This work Eq. (12)	Known[c] [22]	Yadav [13]	This work Eq. (13)
1	15	16	17	18	19	20	21	22	23	24
SmS	0.814	0.812	0.809	59.613	60	58.47	8.061	8.18	8.165	6.577
SmSe	0.829	0.828	0.815	51.714	52	52.16	9.208	9.32	9.598	6.532
SmTe	0.852	0.856	0.827	39.803	40	43.29	11.515	11.49	12.489	6.453
EuS	0.814	0.809	0.808	59.685	61 ± 5	58.47	8.051	8.17	8.165	6.578
EuSe	0.829	0.823	0.815	51.844	52 ± 5	52.38	9.187	9.27	9.537	6.533
EuTe	0.852	0.854	0.827	39.803	40 ± 5	43.50	11.515	11.46	12.404	6.453
TmS	0.772	0.783	0.797	82.397	–	68.63	6.369	6.80	5.427	6.683
TmSe	0.805	0.802	0.805	64.462	–	61.18	7.502	7.78	7.430	6.603
TmTe	0.830	0.839	0.820	51.065	46 ± 5	48.39	9.316	10.09	9.718	6.528
YbS	0.791	0.783	0.789	71.779	72 ± 5	78.08	6.865	5.86	6.514	6.638
YbSe	0.807	0.800	0.803	63.697	61 ± 5	62.53	7.583	7.59	7.661	6.598
YbTe	0.838	0.836	0.815	47.289	46 ± 5	51.69	9.983	9.42	10.669	6.505
Average percentage deviation				2.318		5.989	3.876		5.056	

[a] The values of ρ have been calculated from Eq. (6) taking the known values of d given in column 6. The values given in parenthesis () are the experimental values

[b] Known values of d have been calculated from ionic radii data [21, 22]

[c] Calculated using Clasious–Mossoti relation [22]

Table 3 Density (ρ), plasmon energy ($\hbar\omega_p$), bond length (d), energy gaps (E_h, E_c, E_g), iconicity (f_i), bulk modulus (B), electronic polarizability (α_e) and dielectric constant (ε_∞) of trivalent ($R^{+3}X$) rare earth monochalcogenides

Comp (Z = 9)	Mol. Wt. (W) [22]	ρ^+ (g/cc) This work Eq. (6)	$\hbar\omega_p$(eV) This work Eq. (4)	d (Å)		E_h (eV)		E_c (eV)			E_g (eV)		
				This work Eq. (5)	Known* [21, 22]	This work Eq. (7)	PVV [9]	This work Eq. (8)	PVV [9]	Yadav [13]	This work Eq. (9)	PVV [9]	Yadav [13]
1	2	3	4	5	6	7	8	9	10	11	12	13	14
LaS	170.97	5.814 (5.86 [24])	15.933	2.901	2.901	2.832	2.761	4.284	4.303	4.673	5.169	5.113	5.699
LaSe	217.86	6.898	15.373	2.971	2.971	2.669	2.532	4.204	4.125	4.367	5.029	4.840	5.280
LaTe	266.50	6.940	13.942	3.171	3.171	2.271	2.142	4.007	3.902	3.887	4.670	4.451	4.667
CeS	172.18	6.022 (5.98 [24])	16.158	2.874	2.874	2.898	2.858	4.316	4.386	4.805	5.226	5.236	5.843
CeSe	219.07	7.128	15.585	2.944	2.944	2.731	2.609	4.234	4.200	4.472	5.082	4.936	5.416
CeTe	267.71	7.152	14.122	3.144	3.144	2.320	2.609	4.032	4.589	3.955	4.716	5.279	4.754
PrS	172.97	6.184 (6.08 [24], 6.01 [25])	16.337	2.853	2.853	2.952	2.895	4.342	4.394	4.857	5.270	5.262	5.910
PrSe	219.87	7.310 (6.87 [25])	15.754	2.923	2.923	2.779	2.651	4.258	4.204	4.527	5.124	4.970	5.486
PrTe	268.51	7.319 (7.00 [25])	14.265	3.123	3.123	2.359	2.278	4.051	4.036	4.012	4.751	4.635	4.827
NdS	176.31	6.425 (6.36 [24], 6.70 [26])	16.493	2.835	2.835	2.998	2.962	4.365	4.187	4.949	5.309	5.129	6.029
NdSe	223.20	7.559 (7.23 [26])	15.900	2.905	2.905	2.822	2.707	4.279	4.247	4.602	5.161	5.037	5.582
NdTe	271.84	7.540 (7.26 [26])	14.389	3.105	3.105	2.393	2.333	4.068	4.324	4.081	4.782	4.701	4.827
GdS	189.32	7.332 (7.26 [24])	17.003	2.778	2.778	3.153	3.121	4.440	4.460	5.155	5.437	5.440	6.295
GdSe	236.21	8.490	16.380	2.848	2.848	2.965	2.860	4.348	4.282	4.825	5.281	5.150	5.869
GdTe	284.85	8.352	14.795	3.048	3.048	2.505	2.450	4.123	4.116	4.247	4.884	4.790	5.126
TbS	190.99	7.518	17.142	2.763	2.763	3.196	3.201	4.461	4.520	5.261	5.472	5.538	6.433
TbSe	237.88	8.686	16.510	2.833	2.833	3.004	2.918	4.367	4.324	4.881	5.314	5.217	5.941
TbTe	286.52	8.526	14.904	3.033	3.033	2.536	2.489	4.139	4.146	4.301	4.911	4.836	5.195
DyS	194.57	7.785	17.282	2.748	2.748	3.239	3.242	4.482	4.530	5.314	5.507	5.570	6.502
DySe	241.46	8.959	16.642	2.818	2.818	3.043	2.936	4.387	4.307	4.913	5.347	5.213	5.582
1	2	3	4	5	6	7	8	9	10	11	12	13	14
DyTe	290.10	8.762	15.016	3.018	3.018	2.568	2.516	4.154	4.150	4.344	4.939	4.854	5.250
HoS	197.00	8.004	17.415	2.734	2.734	3.281	3.277	4.502	4.543	5.359	5.540	5.602	6.560
HoSe	243.89	9.185	16.767	2.804	2.804	3.081	2.977	4.405	4.323	4.961	5.378	5.249	6.045
HoTe	292.53	8.960	15.121	3.004	3.004	2.597	2.540	4.169	4.160	4.379	4.966	4.877	5.295
ErS	199.33	8.215 (7.10 [24])	17.540	2.721	2.721	3.320	3.332	4.521	4.558	5.433	5.572	5.646	6.565
ErSe	246.22	9.403	16.884	2.791	2.791	3.117	3.001	4.422	4.309	4.993	5.407	5.259	6.086
ErTe	294.86	9.149	15.220	2.991	2.991	2.625	2.570	4.183	4.163	4.422	4.990	4.893	5.350
LuS	207.03	8.831	17.844	2.690	2.690	3.415	3.513	4.567	4.464	5.553	5.648	5.681	6.812
LuSe	253.93	10.026	17.170	2.760	2.760	3.205	3.286	4.465	4.569	5.372	5.479	5.628	6.576
LuTe	302.57	9.687	15.459	2.960	2.960	2.694	2.780	4.216	4.354	4.693	5.050	5.166	5.699
Average percentage deviation													

Table 3 continued

Comp (Z = 9)	f_i			B (GPa)			α_e (Å^3)			ε_∞
	This work Eq. (10)	PVV [9]	Yadav [13]	This work Eq. (11)	Expt.	Reported	This work Eq. (12)	Known[#] [22]	Yadav [13]	This work Eq. (13)
1	15	16	17	18	19	20	21	22	23	24
LaS	0.698	0.708	0.677	91.296	89[a]	86[b], 87.8[a$]	8.712	8.96	8.813	10.500
LaSe	0.715	0.726	0.683	84.065	74[a]	74.8[a]	9.421	10.05	10.260	10.345
LaTe	0.759	0.767	0.693	58.921	55[c]	55[d], 59.4[a$]	11.523	12.27	13.140	9.911
CeS	0.691	0.702	0.676	93.791	82[e]	78.6[f], 96 [g$]	8.445	8.55	8.384	10.561
CeSe	0.709	0.724	0.681	86.975	76[e]	72.8[f], 83.4[g$]	9.145	9.66	9.758	10.405
CeTe	0.754	0.756	0.692	62.609	58[e]	60.8[f$], 68.3[g]	11.236	11.02	12.660	9.969
PrS	0.686	0.697	0.675	95.604	105.8[h]		8.241	8.41	8.194	10.608
PrSe	0.704	0.716	0.680	89.136	91.5[h]		8.933	9.46	9.510	10.451
PrTe	0.750	0.758	0.690	65.425	59.5[h]		11.013	11.55	12.280	10.014
NdS	0.681	0.666	0.673	97.063			8.067	8.15	7.874	10.649
NdSe	0.699	0.711	0.679	90.912			8.752	9.20	9.186	10.492
NdTe	0.746	0.753	0.689	67.799			10.822	11.19	11.840	10.052
GdS	0.665	0.671	0.669	101.046			7.534	7.61	7.223	10.779
GdSe	0.684	0.691	0.675	96.018			8.192	8.56	8.309	10.620
GdTe	0.733	0.738	0.685	75.048			10.221	10.48	10.890	10.176
TbS	0.661	0.666	0.668	101.918			7.399	7.36	6.916	10.813
TbSe	0.680	0.687	0.674	97.220			8.048	8.32	8.109	10.654
TbTe	0.730	0.735	0.684	76.880			10.064	10.27	10.600	10.209
DyS	0.657	0.661	0.667	102.711			7.265	7.24	6.770	10.848
DySe	0.676	0.683	0.673	98.356			7.906	8.26	9.186	10.688
1	15	16	17	18	19	20	21	22	23	24
DyTe	0.726	0.731	0.683	78.677			9.908	10.13	10.380	10.241
HoS	0.653	0.658	0.666	103.376			7.142	7.13	6.651	10.880
HoSe	0.672	0.678	0.672	99.355			7.774	8.10	7.833	10.720
HoTe	0.723	0.729	0.683	80.322			9.762	9.99	10.200	10.272
ErS	0.649	0.652	0.665	103.925	102 ± 1[a]		7.030	6.98	6.641	10.910
ErSe	0.669	0.673	0.672	100.228			7.654	8.02	7.727	10.749
ErTe	0.720	0.724	0.682	81.820			9.628	9.84	10.000	10.301
LuS	0.639	0.618	0.663	104.958		108[i]	6.771	6.73	6.168	10.982
LuSe	0.660	0.659	0.666	102.083		89.29[i]	7.372	7.11	6.619	10.820
LuTe	0.713	0.710	0.677	85.268		69.07[i]	9.309	8.89	8.813	10.369
Average percentage deviation				8.345		7.302	0.375	–	5.759	

[a] Ref. [15]; [b]Ref. [27]; [c]Ref. [28]; [d] Ref. [29]; [e]Ref. [30]; [f]Ref. [31]; [g] Ref. [32]; [h]Ref.[33]; [i] Ref. [34]

[+] The values of ρ have been calculated from Eq. (6) taking the known values of d given in column 6. The values given in parenthesis () are the experimental values

*Known value of d have been calculated from ionic radii data [21, 22]

[#] Calculated using Clasious–Mossoti relation [22]

[$] These values have been taken for the evaluation of average percentage deviation

$R^{+2}X$, and 0.375% for $R^{+3}X$ against the earlier values of 5.760%. In almost all cases except one, our percentage deviation of B and α_e is less than the earlier estimations. The percentage deviation of other parameters is not calculated due to unavailability of experimental data. However, our calculated values are in good agreement with the reported and known values. The main advantage of the present models is the simplicity of the formulas, which do not require any experimental data except the plasmon energy of the compound while the earlier models require the experimental values of Thomas–Fermi screening factor, ionic charges and bond length in their calculation, which are not known for many compounds. The proposed Eq. (7) for the calculation of E_h is based on PV Eq. (1), which further shows that dielectric theory of PV still holds good for binary crystals and gives better results than the modified models proposed by Verma [12] and Yadav [13].

4. Conclusions

Thus, one can calculate the values of d, ρ, E_h, E_c, E_g, f_i, B, α_e and ε_∞ of $R^{+2}X$ and $R^{+3}X$ groups of rare earth monochalcogenides from their plasmon energy data. The predictive nature of proposed equations is of great importance in predicting the values of these parameters for new compounds of these families. The lower percentage deviation shows the significant improvement over the earlier models, which further demonstrate the soundness of the proposed models.

Acknowledgements The authors are thankful to Prof. D C Panigrahi, Director, Indian Institute of Technology (Indian School of Mines), Dhanbad, Dr. P K Singh, Director, CSIR- Central Institute of Mining and Fuel Research, Dhanbad for their continuous support and Mr. Pradeep Khuntia for helping in the preparation of manuscript and calculations.

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