

Study of Cohesive and Harmonic Properties Of $\text{Nd}_4\text{Cl}-\text{Nd}_4\text{Br}$ Mixed Crystal

Alvin Daud

Department of Physics, Lucknow Christian College, Lucknow, INDIA

Abstract:

We have proposed a three-body Interaction potential for the study of cohesive, harmonic and anharmonic elastic properties of $\text{Nd}_4\text{Cl}-\text{Nd}_4\text{Br}$ mixed crystal. Present interaction potential shall consist of the long-range coulombs vdW dipole-dipole and dipole-quadrupole interactions and overlap repulsive potential of Born Mayer. This model potential has succeeded in predicting the Cohesive energy, and the Second order elastic constants of the mixed deuterated ammonium halides.

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I. Introduction

The materials with large concentration of substitutional impurity are called mixed crystals. They are an important example of randomly disordered matter, whose investigations have received much less attention by the physicist than did pure crystalline materials as is evident from the vast amount of work devoted in the study of static, dynamic, elastic and dielectric properties [1-20] of ionic crystals. This is so because the interaction mechanism in pure crystals is quite well known and also a wealth of experimental data exist on them. Their interaction system [21] mostly consists of the long-range Coulomb, three-body interaction (TBI), van-der Waal's (vdW) and short range overlap repulsion. Such interionic potential has been successfully used to describe the lattice, static, harmonic and anharmonic properties of perfect diatomic ionic crystals [22-25]. Such a potential has also been used to study the various properties of mixed crystals [26-28]. However the role played by these interactions has not been investigated in describing the properties of the mixed deuterated ammonium halides.

The first study of their static properties was carried out by Reitz et. al. using the Born Mayer potential [29] extended to incorporate the van-derwall (vdW) dipole-dipole (d-d) interactions. Later on, this potential was further modified to include the vdW dipole-quadrupole (d-q) interaction effect and used to describe the lattice static properties of several fluoride compounds by M.P. Tosi [30]. In these studies, the use has been made of the vdW coefficients, evaluated from the perturbation method which is not so accurate as the Slater and Kirkwood (SKV) method [31]. Also these potentials are essentially two body interactions, which failed to predict the Cauchy violation, exhibited by the second and higher order elastic constants of various crystal.

The Cauchy violation arise from the three body interaction (TBI), which have significant influence on lattice, static, dynamic and dielectric properties of Ionic crystals and semiconductors of rock salt [32] caesium chloride [33] and Fluorite [34] structure. These third body interaction (TBI) arise from the electron shell deformation caused due to the overlap integrals [32-34]. Such formation also occur in halides compounds and give rise to long [35] and short [range [36], three body interaction (TBI) in them. The influence of long range three body interaction (TBI) has been investigated on their cohesive [27] and harmonic and a harmonic elastic constant [37], while the same the short-range three-body interaction (TBI) has been done only for elastic properties [27-28]. However the influence of these third body interaction has not been investigated, so far in mixed halide crystals ($\text{NH}_4\text{Cl}_x-\text{Br}_{1-x}$, $\text{Nd}_4\text{Cl}_x-\text{Br}_{1-x}$ etc.), which are important subject as they provide a useful testing ground for theories to represent the interaction mechanism and describes various properties (elastic, dielectric and anharmonic) of their host crystals.

The mixed crystal according to virtual crystal approximation (VCA) are regarded as an array of "average ions" whose masses, force constants and effective charges are assumed to scale linearly with the concentration.

The interaction potential employed for the present investigation consists of the long-range coulomb forces and three body interaction (TBI), the short range vdW attraction and overlap repulsion. The required vdW coefficients for the host and mixed halides crystals have been obtained by us using the SKV approach [31] and considering the polarizability of the mixed crystals to vary linearly [27-28] with the concentration. The range parameters are different for different types of overlap repulsions. This interaction potential has only three model parameters and has been used to predict the cohesive energy, Second order elastic (SOE) constants of the host

and mixed $\text{Nd}_4\text{Cl}-\text{Br}_{1-x}$ crystals. The details of the present inter ionic potential are given in **Section 2** and discussed in **Section 3**.

II. Theory

In order to describe interactions between ammonium, deuterated ammonium and halides ion in the mixed crystals, we have assumed that

- (a) The symmetry of the mixed system remains the same as that of the host crystals.
- (b) The change in the force constants is limited to only short-range interactions ions.
- (c) Atoms are held together with harmonic elastic forces and there is no internal strain within the crystals.
- (d) The three –body interactions (TBI) have only localised effects.

III. A. Interionic Potential

In the view of these assumptions, the potential energy of the host and mixed crystals with halides structure and interionic separation (r) is written as.

$$\Phi(r)_{\text{Total}} = \Phi_c(r) + \Phi_v(r) + \Phi_T(r) + \Phi_R(r) \quad (1)$$

the first term represent the Coulomb energy, expressed as

$$\Phi_c(r) = - \sum_{lm} \frac{z_l z_m e^2}{r_{lm}} = - \frac{z^2 e^2 \alpha_m}{r} \quad (2)$$

with $\alpha_m (= 1.7629)$ as the Madelung constant and r_{lm} is the separation between l and m ions. and

$$\Phi_v(r) = \sum_{lm} - \frac{c_{lm}}{r_{lm}^6} + \sum_{lm} - \frac{d_{lm}}{r_{lm}^8} \quad (3)$$

With C_{lm} and d_{lm} as the vdW coefficients due to dipole–dipole and dipole–quadrupole interactions. These coefficients are calculated from the Slater Kirkwood variational approach [31]. However, the expression for C_{lm} and d_{lm} obtained by Slater and Kirkwood [31] and London et al. [43] have been slightly modified by us to take account of the doping effect. These expressions are written as

$$c_{lm} = \frac{3e\hbar}{2\sqrt{m}} \frac{\alpha_l \alpha_m}{[(\alpha_l/N_l)^{1/2} + (\alpha_m/N_m)^{1/2}]} \quad (4)$$

$$d_{lm} = \frac{27\hbar^2}{8m} \frac{[(\alpha_l/N_l)^{1/2} + (\alpha_m/N_m)^{1/2}]^2}{\left(\frac{\alpha_m}{N_m}\right) + \frac{20}{3} + (\alpha_l d_m / N_l N_m)^{1/2} + \left(\frac{\alpha_m}{N_m}\right)} \quad (5)$$

Where α_l and N_l are the polarizability and number of outermost electron of the cation, while α_m is given by

$$\alpha_m = \beta \alpha_1 + (1 - \beta) \alpha_2 \quad (6)$$

with α_1 and α_2 as the polarizability of the two type of anions (i.e. Cl^- and Br^- respectively). Also

$$N_m = \beta N_1 + (1 - \beta) N_2 \quad (7)$$

is the sum of outermost electrons in the two type of anions mentioned above. β is the concentration dependent parameters which assume value from zero to unity.

The third term of equation (1) represent three body interaction (TBI) energy, expressed as

$$\Phi_T(r) = \sum_{lm} \frac{z_l z_m e^2}{r_{lm}} f(r_{lm}) \quad (8)$$

is contributed by three–body interactions (TBI), which arise from the charge transfer effect between the adjacent ions. The function $f(r)$ is a TBI parameter dependent of the overlap integrals.

The last term of equation (1) represent the short –range overlap repulsive energy expressed as.

$$\Phi_R(r) = 8 \beta_{lm} b e^{(-r_{lm}/\rho)} \quad (9)$$

Here β_{lm} are defined as Pauling coefficients defined as

$$\beta_{lm} = 1 + \frac{z_l}{n_l} + \frac{z_m}{n_m} \quad (10)$$

With Z_l and Z_m are the valency and N_l and N_m are the numbers of the outermost electrons of l and m ions.

It is seen that there are only three unknown parameters in the above–mentioned interaction potential, viz. the repulsive strength parameter (b , ρ) and third body interaction (TBI) parameter $f(r)$. The two repulsive strength parameters (b , ρ) can be calculated from the equilibrium conditions.

$$\left(\frac{d\Phi_{\text{total}}(r)}{dr} \right)_{r=r_0} = 0 \quad (11)$$

And bulk modulus expression

$$\left(\frac{d^2\Phi_{\text{total}}(r)}{dr^2}\right)_{r=r_0} = \frac{18r_0}{\beta r} \tag{12}$$

The three body interaction (TBI) parameter can be evaluated by the expression of the second order elastic constant expression [44] .

$$C_{11} = \frac{e^2}{4a^4} \left[0.7010 Z_m^2 + \frac{A_{lm} + 2 B_{lm}}{6} + 5.4283 Z r_0 f_0' \right] \tag{13}$$

$$C_{12} = \frac{e^2}{4a^4} \left[-0.6898 Z_m^2 + \frac{A_{lm} - 4 B_{lm}}{6} + 5.4283 Z r_0 f_0' \right] \tag{14}$$

$$C_{44} = \frac{e^2}{4a^4} \left[-0.3505 Z_m^2 + \frac{A_{lm} + 2 B_{lm}}{6} \right] \tag{15}$$

COMPUTATIONS

The vdW coefficient (C_{lm} and d_{lm}) required for the present study have been calculated by using the expression (4) and (5) for the mixed $\text{ND}_4\text{Cl}-\text{ND}_4\text{Br}$ crystals. Their value listed in Table 4 for the host and mixed $\text{ND}_4\text{Cl}-\text{ND}_4\text{Br}$ crystals and used to obtain repulsive strength parameters (b, ρ) whose values are listed in table 2. The required three body interaction (TBI) parameters $f(r)$ have been calculated by using the expression (13) to (15). The equilibrium in inter ionic separation r_0 are used as input data are listed in Table 1. A linear variation of r_0 with concentration, as depicted in Fig. 1, is a feature identical to that exhibited by other mixed crystals ($\text{AgCl}-\text{AgBr}$) [42], $\text{KCl}-\text{KBr}$ [27] and $\text{KBr}-\text{KI}$ & $\text{KI}-\text{KCl}$ [28] mixed crystals.

The values of these models parameter together with vdW coefficient listed in table 4 and 2 have been used to compute the cohesive energy and the second order elastic constant (SOE) using the equation given from (13) to (15). Their value have been listed in Table 1-5 and plotted respectively in figure 1 and figure 2 against the percentage concentration of $\text{ND}_4\text{Cl}-\text{ND}_4\text{Br}$ mixed crystals.

Our results on the cohesive energy and harmonic and elastic constant of $\text{ND}_4\text{Cl}-\text{ND}_4\text{Br}$ have been compared with the available experimental and other theoretical results. Such comparison for the mixed crystals could not be possible in the absence of measured data on them.

TABLE – 1

Input data of the mixed crystal $\text{ND}_4\text{Cl}-\text{ND}_4\text{Br}$.

Input ND_4Cl

$r_0 = 3.307 \times 10^{-8} \text{ cm}$
 $C_{11} = 4.79 \times 10^{11} \text{ dyn./cm}^2$
 $C_{12} = 1.64 \times 10^{11} \text{ dyn./cm}^2$
 $C_{44} = 1.43 \times 10^{11} \text{ dyn./cm}^2$
 $\alpha_+ = 1.154 \times 10^{-24} \text{ Ref 5}$
 $\alpha_- = 3.355 \times 10^{-24}$
 $N_+ = 17.0$
 $N_- = 17.0$

Input ND_4Br

$r_0 = 3.51 \times 10^{-8} \text{ cm}$
 $C_{11} = 3.4293 \times 10^{11} \text{ dyn./cm}^2$
 $C_{12} = 0.7716 \times 10^{11} \text{ dyn./cm}^2$
 $C_{44} = 0.7605 \times 10^{11} \text{ dyn./cm}^2$
 $\alpha_+ = 1.154 \times 10^{-24} \text{ Ref 5}$
 $\alpha_- = 4.157 \times 10^{-24}$
 $N_+ = 17.0$
 $N_- = 22.0$

Table- 1: Input data of the Mixed Crystal $\text{ND}_4\text{Cl}-\text{ND}_4\text{Br}$

% Crystal	$r_0 = (1-\beta)r_{0,\text{Cl}} + \beta r_{0,\text{Br}}$	$C_{11} = (1-\beta)C_{11,\text{Cl}} + \beta C_{11,\text{Br}}$	$C_{12} = (1-\beta)C_{12,\text{Cl}} + \beta C_{12,\text{Br}}$	$C_{44} = (1-\beta)C_{44,\text{Cl}} + \beta C_{44,\text{Br}}$	$\alpha = (1-\beta)\alpha_{\text{Cl}} + \beta\alpha_{\text{Br}}$	$N = [(1-\beta)N_{\text{Cl}} + \beta N_{\text{Br}}]$
$\text{ND}_4\text{Cl}_{100}\text{Br}_0$	3.3070 [37]	4.79000 [39]	1.64000 [39]	1.43000 [39]	3.3550 [41]	17.00
$\text{ND}_4\text{Cl}_{90}\text{Br}_{10}$	3.3273	4.65393	1.55316	1.36305	3.4352	17.5
$\text{ND}_4\text{Cl}_{80}\text{Br}_{20}$	3.3476	4.51786	1.46632	1.29600	3.5154	18
$\text{ND}_4\text{Cl}_{70}\text{Br}_{30}$	3.3679	4.38179	1.37948	1.29915	3.5956	18.5
$\text{ND}_4\text{Cl}_{60}\text{Br}_{40}$	3.3882	4.24572	1.29264	1.16220	3.6758	19.0
$\text{ND}_4\text{Cl}_{50}\text{Br}_{50}$	3.4085	4.10965	1.2058	1.09525	3.7560	19.5
$\text{ND}_4\text{Cl}_{40}\text{Br}_{60}$	3.4288	3.97358	1.11896	1.0283	3.8362	20.0
$\text{ND}_4\text{Cl}_{30}\text{Br}_{70}$	3.4491	3.83751	1.03212	0.96135	3.9164	20.5
$\text{ND}_4\text{Cl}_{20}\text{Br}_{80}$	3.4694	3.70144	0.94528	0.8944	3.9966	21.0
$\text{ND}_4\text{Cl}_{10}\text{Br}_{90}$	3.4897	3.56537	0.85844	0.82745	4.0768	21.5
$\text{ND}_4\text{Cl}_0\text{Br}_{100}$	3.5100 [38]	3.4293 [40]	0.77160[40]	0.7605 [40]	4.1570 [41]	22.0

Where β is the concentration of mixed crystal.

**Table -2 : Model Parameter of mixed crystal
 b and ρ are in unit of 10^{-8} cm**

% Crystal	$f(r)$	$r_0 f_0'$	b	ρ	Zm^2
$\text{ND}_4\text{Cl}_{100}\text{Br}_0$	-0.0193552	0.0089146	1.3009872	0.2975072	0.6903168
$\text{ND}_4\text{Cl}_{90}\text{Br}_{10}$	-0.0189825	0.0082702	1.1787965	0.3021544	0.696279
$\text{ND}_4\text{Cl}_{80}\text{Br}_{20}$	-0.0186131	0.0075873	1.0575996	0.3072031	0.70219
$\text{ND}_4\text{Cl}_{70}\text{Br}_{30}$	-0.0182642	0.0068643	0.9391605	0.3126968	0.7077721
$\text{ND}_4\text{Cl}_{60}\text{Br}_{40}$	-0.017931	0.0061014	0.8251143	0.3186851	0.7131036
$\text{ND}_4\text{Cl}_{50}\text{Br}_{50}$	-0.0176142	0.0052961	0.7169051	0.3252252	0.7181721
$\text{ND}_4\text{Cl}_{40}\text{Br}_{60}$	-0.0173145	0.0044476	0.6157548	0.3323826	0.7229665
$\text{ND}_4\text{Cl}_{30}\text{Br}_{70}$	-0.0170328	0.0035548	0.5225989	0.3402343	0.7274742
$\text{ND}_4\text{Cl}_{20}\text{Br}_{80}$	-0.0167697	0.0026164	0.4380948	0.3488702	0.7316833
$\text{ND}_4\text{Cl}_{10}\text{Br}_{90}$	-0.0165261	0.0016312	0.3626045	0.3583957	0.7355813
$\text{ND}_4\text{Cl}_0\text{Br}_{100}$	-0.0163027	0.0005979	0.296205	0.3689367	0.7391555

Table - 3: Model parameters of $\text{ND}_4\text{Cl}-\text{ND}_4\text{Br}$ Mixed Crystals

% Crystal	A_1	B_1	$C_1 = A_1^2/B_1$
$\text{ND}_4\text{Cl}_{100}\text{Br}_0$	4.2138736	-0.3254832	-54.554984
$\text{ND}_4\text{Cl}_{90}\text{Br}_{10}$	4.1812719	-0.3273004	-53.415867
$\text{ND}_4\text{Cl}_{80}\text{Br}_{20}$	4.1441856	-0.3292266	-52.165512
$\text{ND}_4\text{Cl}_{70}\text{Br}_{30}$	4.1023594	-0.33127	-50.802526
$\text{ND}_4\text{Cl}_{60}\text{Br}_{40}$	4.055537	-0.3334319	-49.327555
$\text{ND}_4\text{Cl}_{50}\text{Br}_{50}$	4.00344	-0.3357167	-47.741241
$\text{ND}_4\text{Cl}_{40}\text{Br}_{60}$	3.9458633	-0.3381293	-46.046992
$\text{ND}_4\text{Cl}_{30}\text{Br}_{70}$	3.8824728	-0.3406781	-44.245859

$ND_4 Cl_{20} Br_{80}$	3.8129571	-0.3433694	-42.341111
$ND_4 Cl_{10} Br_{90}$	3.7389666	-0.3462042	-40.337233
$ND_4 Cl_0 Br_{100}$	3.6541123	-0.3491897	-38.238633

Table 4: Calculation of Van-der Waal's Coefficients

Crystal %	C_{ij}	C_{ii}	C_{jj}	d_{ij}	d_{ii}	d_{jj}	C*	D**
$ND_4 Cl_{100} Br_0$	138.22069	64.30364	318.76133	76.3555	25.3027	213.866	1882.6424	885.68052
$ND_4 Cl_{90} Br_{10}$	-141.76414	64.30364	335.08072	78.1523	25.3027	224.213	1942.4244	911.70771
$ND_4 Cl_{80} Br_{20}$	-145.30654	64.30364	351.80399	79.9494	25.3027	234.804	2002.9131	938.00548
$ND_4 Cl_{70} Br_{30}$	-148.84795	64.30364	368.93113	81.7468	25.3027	245.64	2064.109	964.57491
$ND_4 Cl_{60} Br_{40}$	-152.38845	64.30364	386.46217	83.5444	25.3027	256.72	2126.0128	991.41409
$ND_4 Cl_{50} Br_{50}$	-155.92811	64.30364	404.39713	85.3422	25.3027	268.045	2188.6251	1018.5241
$ND_4 Cl_{40} Br_{60}$	-159.46698	64.30364	422.73601	87.1403	25.3027	279.614	2251.9464	1045.9047
$ND_4 Cl_{30} Br_{70}$	-163.00513	64.30364	441.47882	88.9385	25.3027	291.427	2315.9773	1073.5542
$ND_4 Cl_{20} Br_{80}$	-166.54258	64.30364	460.62558	90.7369	25.3027	303.485	2380.7181	1101.4746
$ND_4 Cl_{10} Br_{90}$	-170.0794	64.30364	480.1763	92.5354	25.3027	315.788	2446.1693	1129.665
$ND_4 Cl_0 Br_{100}$	-173.61563	64.30364	500.13095	94.3341	25.3027	328.334	2512.3313	1158.1241

* C has unit of $10^{-60} \text{ erg-cm}^6$

** D has unit of $10^{-76} \text{ erg-cm}^8$

Table 5: Calculation of the Cohesive Energy in K. Cal/mole of ND_4Cl-ND_4Br

Crystal %	Φ_c	Φ_v	Φ_I	Φ_R	Φ_{total}	$\Phi_{exp} \cdot \Phi_{other}$
$ND_4 Cl_{100} Br_0$	-177.15973	-13.885705	1.1366323	22.3069	-167.6019	-150.2 Φ_{exp} -145.51 Φ_{other}
$ND_4 Cl_{90} Br_{10}$	-176.07889	-13.719433	1.0579127	22.422153	-166.31826	
$ND_4 Cl_{80} Br_{20}$	-175.01113	-13.549836	0.9748422	22.566076	-165.02005	
$ND_4 Cl_{70} Br_{30}$	-173.95625	-13.377457	0.8869959	22.741838	-163.70487	
$ND_4 Cl_{60} Br_{40}$	-172.91401	-13.202793	0.7938566	22.952464	-162.37048	
$ND_4 Cl_{50} Br_{50}$	-171.88419	-13.026298	0.6948682	23.201844	-161.01378	
$ND_4 Cl_{40} Br_{60}$	-170.86656	-12.848388	0.5893434	23.494012	-159.63159	
$ND_4 Cl_{30} Br_{70}$	-169.86091	-12.669441	0.4765087	23.833866	-158.21998	
$ND_4 Cl_{20} Br_{80}$	-168.86702	-12.489801	0.3554247	24.227313	-156.77408	
$ND_4 Cl_{10} Br_{90}$	-167.8847	-12.309783	0.2249995	24.680836	-155.28865	
$ND_4 Cl_0 Br_{100}$	-166.91375	-12.129678	0.0839175	25.202502	-153.75701	-143.0 Φ_{exp} -130.65 Φ_{other}

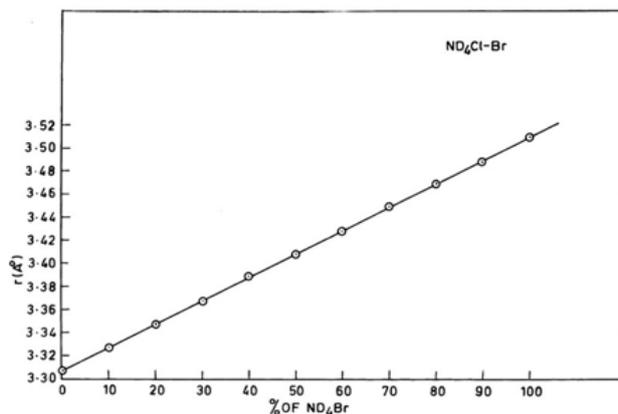


Figure -1

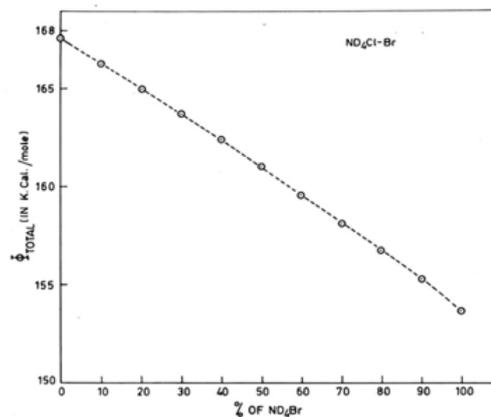


Figure-2

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