

## Thermal properties [compressibility and Moelwyn-Hughes Parameter] of NaCl crystals under high pressure

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### Abstract

Many inter ionic potential functions have been proposed since the Born and Lande's inverse function. An exponential function for the repulsive component of the potential has been proposed by Born and Lande', none of the potential function proposed is successful. A new interionic function proposed by Jha and Thakur to study the properties of ionic crystal under high pressure. Its repulsive component includes both an inverse power function due to Born and Lande' and an exponential function due to Born and Mayer. Jha has used it to study the thermal properties of NaCl and CsCl crystal under high pressure up to 100 Kilo bar.

**Keywords:** NaCl crystals; Moelwyn-Hughes parameter, Isothermal compressibility

### 1. Introduction

In the early part of 20<sup>th</sup> century there was a revolution in solid state physics. To study the theory of solid the Born model of ionic solids [1] provides a method for calculating elastic and thermal properties of ionic crystal under high pressure. The calculations are based on an inter ionic potential function. An important component of the potential function is the repulsive term. Born and Lande''s describe this term by inverse power function while Born and Mayer used an exponential function to describe this term. In accounting for the compression for the sodium halide crystals Roberts and Smith [2] have shown that neither of these functions is successful.

### 2. Theory

An inter ionic potential function has been proposed by Jha and Thakur [3]. Its repulsive components includes both an inverse power function due to Born and Lande' and an exponential function due to Born and Mayer. Jha [4] has used it the thermal properties of NaCl and CsCl crystal under high pressure. In the present work I shall report the success of this potential in describing the elastic properties of NaCl crystals under high pressure up to 100 Kilo bar. The new inter ionic potential for the crystal under study using reduced units of equilibrium inter ionic distance  $R_0$  for distance and  $e^2/R_0$  can be written as [3] .

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$$\varphi(r) = \frac{A}{r^m} \exp[-B(r^n - 1)] - \frac{M}{r} - \frac{C}{r^6} - \frac{D}{r^8} \quad (1)$$

Where  $r$  is the inter ionic distance,  $A$ ,  $B$ ,  $m$  &  $n$  are the potential parameters which are constants for a given crystal,  $M$  is the Madeline constant,  $C$  &  $D$  are Van dar Walls constants for dipole-dipole and dipole-quadruple interactions, respectively and  $e$  is the electronic charge. Crystal properties have also been calculated using Born-Lande'' and Born Mayer potential for the sake of comparison. These can be written as

$$\varphi(r) = \frac{A_1}{r^{m1}} - \frac{M}{r} - \frac{C}{r^6} - \frac{D}{r^8} \quad (2)$$

And

$$\varphi(r) = A_2 \exp(-r/\rho) - \frac{M}{r} - \frac{C}{r^6} - \frac{D}{r^8} \quad (3)$$

### 3. Results and Discussion

Potential parameters of the Born – Lande' and Born - Mayer potentials have been calculated in the usual manner. The parameters of the new potential have been calculated using a procedure described by Jha & Thakur [3].  $m$  has been given integer values and  $n$  has been varied and  $n$  has been varied in steps of 0.1. Input crystal data are taken from Tosi [1] and Ashcroft and Mermin [5]. Values of potential parameters for the crystal under study have been listed in table 1.

At a given compression, the pressure have been calculate with the help of Debye's equation of state [6]

$$P = - (\partial E_0 / \partial V) + \gamma E_D / V \quad (4)$$

where  $E_0$  is the internal energy of the volume,  $p$  pressure at 0 Kelvin,  $E_D$  the Debye energy of the crystal at the temperature at which the crystal properties are being studied, and  $\gamma$  the Gruneisen parameter.

**Table 1:** Potential parameters of NaCl crystals in reduced (dimensionless) units

Parameter	Value	Parameter	Value
C	0.0446	Born - Lande' potential	
D	0.0056	m1	7.81
New potential		A1	0.264
M	4	Born - Mayer potential	
N	3.1	1/ $\rho$	9.049
A	0.2142	A2	1978.83
B	1.8122		

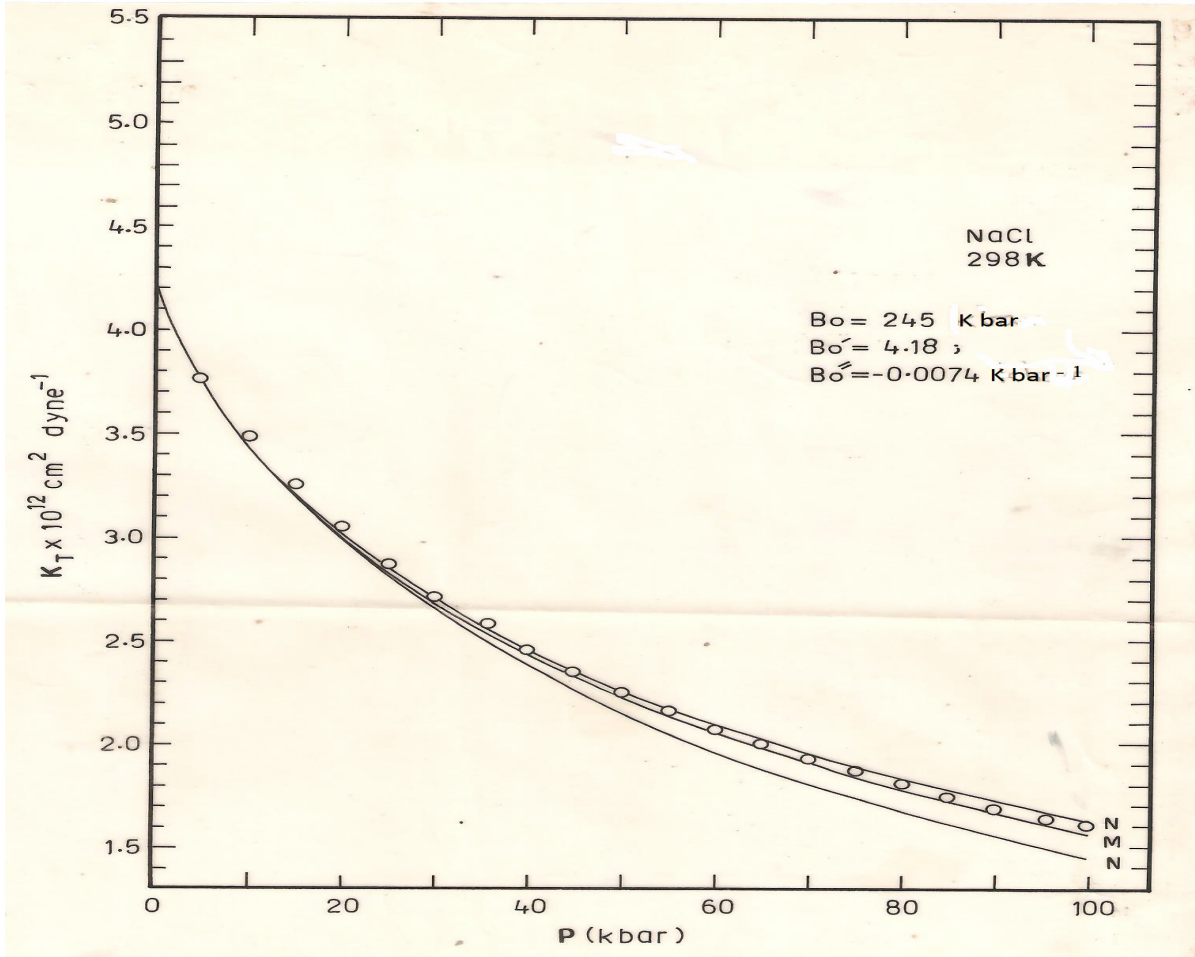


Figure 1: Variation of isothermal compressibility with pressure

Here we have taken in to account the variation of  $E_D$  and  $\gamma$  with pressure, but their temperature has been ignored.  $E_D$  has been calculated by calculating the Debye temperature. Jha and Thakur[3] explained the calculation of Gruneisen parameter and Debye temperature.

The isothermal compressibility has been calculated with the relation

$$K_T = - 1/V (\partial V/\partial p)_T \tag{5}$$

The Moelwyn-Hughes parameters[7,8] is the pressure derivative of the isothermal Bulk modulus  $B_T$ . It is defined by

$$C_1 = (\partial B_T/\partial P)_T \tag{6}$$

The computed results have been displayed in fig. 1 and 2. Fig. 1 shows the variation of  $K_T$  with pressure at room temperature (298 K). Fig. 2 shows the variation of  $C_1$  with pressure at room temperature. Curves marked L have been drawn using the Born-Landé' potential, curves marked M using the Born-Mayer Potential and curves marked N using the new potential. The open circles are estimates of  $K_T$  and  $C_1$  obtained from the compression data of Bridgman [9] using a modified Murnaghan equation [10,11]. This equation helps us to express  $B_T$  as a parabolic function of P,

$$B_T = B_0 + B_1P + 1/2B_2P^2 \quad (7)$$

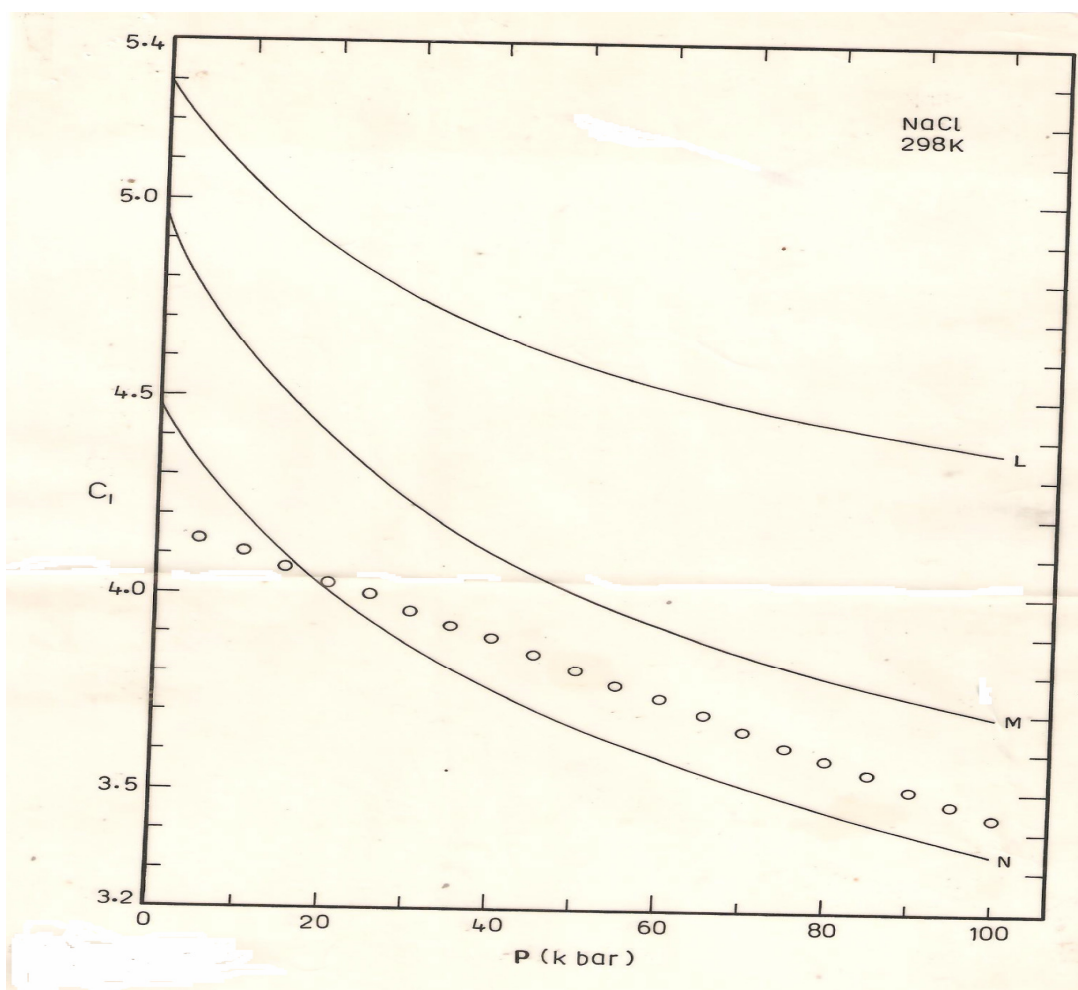


Figure 2: Variation of Moelwyn-Hughes parameter with pressure

It follows from the definition of the Moelwyn-Hughes parameter that

$$C_1 = B_1 + B_2P \quad (8)$$

Values of  $B_0, B_1$  &  $B_2$  have been mentioned in figure 1.

#### 4. Conclusion

It is seen that the inverse power law of Born Lande' is not suitable for predicting the elastic properties of NaCl crystal under high pressure, whereas the exponential laws is better for studying the elastic properties of crystal under high pressure. The new potential is most successful in explaining mechanical and thermal properties of NaCl crystal under high pressure i.e, from 100 kilo bar study.

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## Further reading

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