

## COHESIVE ENERGIES IN MAGNESIUM CHLORIDE

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### ABSTRACT

The cohesive energies or interaction potential energies of magnesium chloride are calculated using a three-body interaction potential. The experimental and theoretical results are in good agreement.

### INTRODUCTION

Magnesium chloride is the name for the chemical compound with the formula  $MgCl_2$  and its various hydrates  $MgCl_2 \cdot (H_2O)_x$ . These salts are typical ionic halides, being highly soluble in water. The hydrated magnesium chloride can be extracted from brine or sea water.

In North America, magnesium chloride is produced primarily from Green salt Lake brine. It is extracted in a similar process from the dead sea in the Jordan valley. Magnesium chloride, as the natural mineral bischofite, is also extracted (by solution mining) out of ancient seabeds, for example the zechstein seabed in northwest Europe. Some magnesium chloride is made from solar evaporation of seawater. Anhydrous magnesium chloride is the principal precursor to magnesium metal which is produced on a large scale. Hydrated magnesium chloride is the form most readily available.

Its molar mass is 95.211 g/ mol, melting point is 714 degree centigrade and boiling point is 1,412 degree centigrade.

Several investigators <sup>(1-25)</sup> have studied the cohesive energies using both two-body <sup>(1-3)</sup> and three-body <sup>(4-7)</sup> potentials. The latter potentials have given their prediction better than those revealed by other potential <sup>(1-3)</sup>. Elastic constants are measured by Lundqvist Potential <sup>(8)</sup> Singh and Verma <sup>(9)</sup> Karlsson <sup>(10)</sup>.

In the present paper, we have used three-body potential to explain the cohesive energies of magnesium chloride.

Calculations have been performed using the expression for the model parameters.

Given by Verma and co-workers <sup>(4)</sup> and those for the pressure derivatives of SOE constants are given by Garg et al <sup>(5)</sup> respectively. The essential theory and calculations are given in section 2. The results are presented and discussed in section 3.

### 2. THEORY AND METHOD OF CALCULATIONS:

Interaction potential energy of rock salt structure solid with contribution from the long-range coulomb and three-body interactions and the short-range repulsive and van der Waals dipole-dipole and dipole –quadrupole attractions is given by

$$W(r) = \alpha_m Z (Z+6) f(r)/r + [W_1(r)+W_2(r)] e^2 \quad (1)$$

First term is the Coulomb interaction with a  $\alpha_m$  as the Madelung constant,  $Ze$  is the ionic charge and  $e$  is the electronic charge. Here  $r (=r_0)$  and  $r_1 (=2r_0)$  are the first and second neighbor distances.  $f(r)$  is the three-body force parameter dependent on  $r$ .  $W_1$  and  $W_2$  are the short-range interactions defined as

$$W_1(r) = b\beta/e^2\beta_+ \exp(r_+ + r_- - r)/\rho_+ - C_+/r^6 - d_+/r^8 \quad (2)$$

$$W_2(r) = b\beta/e^2\beta_+ \exp(2r_+ + r')/\rho_{++} + b\beta_-/e^2 \exp(2r_- - r')/\rho_- - (c_{++} + c_-)/r^6 - (d_{++} + d_-)/r^8 \quad (3)$$

$$\text{Where } \beta_{ij} = 1 + (z_i/n_i) + (z_j/n_j) \quad (4)$$

With  $n_i$  as the number of electrons in outermost orbit. Here,  $b$  and  $\rho$  are the repulsive strength and hardness parameters, respectively. In our calculations value of ionic radii ( $r_i$ ) and van der Waals coefficients ( $c_{ij}$  and  $d_{ij}$ ) have been taken from Singh <sup>(9)</sup> and co-workers <sup>(11-19)</sup>. The values of  $\rho_{ij}$  for the cesium bromide have been

taken from Hafemeister and Flygare<sup>(20)</sup>. The values of  $b$  for them have been evaluated from the equilibrium condition

$$dW(r) / dr = 0 \quad \text{at } r=r_0 \quad (5)$$

Using the values of  $f(r)$  obtained from the knowledge of overlap integral and its derivatives from the knowledge of overlap integral (5).

$$f(r_0) = f_0 \exp(-r_0 \rho_{+-}) = \epsilon_{+-} S_{+-}^2 \quad (6)$$

$$\text{With } f_0 = A_{+-} (1 - 2r_+/r_0) \quad (7)$$

Values of overlap integral ( $S_{+-}$ ) and constants ( $A_{+-}$ ) are directly taken from<sup>(14)</sup>. Values of parameters ( $\rho_{ij}$ ,  $b$  and  $f_0$ ) have been given in Table 1 together with the equilibrium nearest neighbour distance  $r_0$ , which is the only input data used for the calculation of the parameter  $b$ .

### 3. RESULT AND DISCUSSIONS:

**TABLE: 3.1 Values of input for ionic crystal.**

CRYSTAL	$r_0$	$r_+$	$r_-$	$C_{11}$	$C_{12}$	$C_{44}$
	$10^{-8}$ cm (a)	$10^{-8}$ cm (b)	$10^{-8}$ cm (b)	$10^{11}$ dyne / $\text{cm}^2$ (a)	$10^{11}$ dyne / $\text{cm}^2$ (a)	$10^{11}$ dyne / $\text{cm}^2$ (a)
MgCl <sub>2</sub>	3.51	2.57	4.07	3.13	1.00	0.76

**Table 3.2 Model Parameters for ionic solids**

CRYSTAL	$\rho$	$b$ (in $10^{-12}$ erg)	$f(r)$
MgCl <sub>2</sub>	0.23	0.16	-000015

**Table 3.3 Values of Cohesive Energies In Magnesium Chloride.**

CRYSTAL	Experimental Value	Theoretical Value
MgCl <sub>2</sub>	326.52	310.41

The model parameters listed in Table 3.1 have been used to evaluate the various –order derivatives of the short-range interactions.  $B_i, C_i, D_i$  ( $i=1, 2$ ). Those parameters are the same as those defined by Verma and co-workers<sup>4</sup> except for the difference that we have included the effect of short range Vander Waals attraction and represented the overlap repulsion by the HF potential. With the knowledge of parameters and input data we have calculated the cohesive energies of Magnesium Chloride using their relevant expressions reported (4, 5).

Results obtained in the table are in good agreement with the experimental results which shows that the agreement between experimental and our theoretical results are better.

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