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COHESIVE ENERGIES IN MAGNESIUM FLUORIDE

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

INTRODUCTION

Magnesium fluoride is an inorganic compound with the formula MgF_2. The compound is a white crystalline salt and is transparent over a wide range of wavelengths, with commercial uses in optics that are also used in space telescopes. It occurs naturally as the rare mineral sellaite.It is prepared from magnesium oxide with sources of hydrogen fluoride such as ammonium bifluoride.

$$MgO + (NH_4)\,HF2 \rightarrow MgF_2 + NH3 + H2O$$

The compound crystallizes as tetragonal birefringent crystals. The structure of compound is similar to that in rutile, featuring octahedral Mg^{2+} centres and 3-coordinate fluoride centres.

Magnesium fluoride is transparent over an extremely wide range of wavelengths windows, lenses and prisms made of this material can be used over the wide range of wavelength from 0.120micrometer (vacuum ultraviolet) to 8.0micrometer (infrared).His quality synthetic VUV grade MgF_2 is quite expansive, in the region of $3/Kg (2007) but the real cost of optics in this material is due to relatively low volume manufacture. However, with lithium fluoride it is one of the two materials that will transmit in the vacuum ultraviolet range at 121nm (Lyman alpha) and this is where it find its application. Lower grade MgF_2 is sometimes used in the infrared but here it is inferior to calcium fluoride.MgF_2 is tough and works and polishes well, but it is slightly birefringent and should be cut with the optic axis perpendicular to the plane of the window or lens.

Due to its suitable refractive index of 1.37, thin layers of MgF_2 are very commonly used on the surfaces of optical elements as inexpensive anti-reflective coatings. The Verdet constant of MgF_2 AT 632.8nm is 0.00810 arcmin/G.cm. Its molar mass is 3.148 g/cm^3, melting point is 1263^{0}C, boiling point is 2,260^{0}C, solubility in water 0.013g/100mL but is insoluble in ethanol. Magnetic susceptibility(X) is -22.7× 10^{-6}cm^3/mol. Its crystal structure is Rutile (tetragonal) tP6, space group is $P4_2$/mnm No.136, Heat capacity(C) is 61.6 Jmol^{-1}K^{-1} Standard molar entropy is 57.2 Jmol^{-1}K^{-1} Standard enthalpy of formation is -1124.2 KJmol^{-1}, Gibbs free energy is -1071KJ/mol.

Co-workers [1-27] have studied the interaction potential energies using both two-body [1-3] and three-body [4-7]) potentials. The latter potentials have given their prediction better than those revealed by other potential [1-3].Elastic constants are measured by Lindquist Potential [8] Singh and Verma [9] Karlsson [10]. In the present paper, we have used three-body potential to explain the cohesive energies or interaction potential energies of magnesium fluoride.

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Calculations have been performed using the expression for the model parameters given by Verma and co-workers [4] and those for the pressure derivatives of Second order elastic SOE constants are given by Garg et al [5] 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

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

First term is the Coulomb interaction with a α_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

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

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

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

With n_i as the number of electrons in outermost orbit. Here, b and ρ 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[9] and co-workers[11-19].The values of ρ_{ij} for the rubidium iodide have been taken from Hafemeister and Flygare[20].The values of b for them have been evaluated from the equilibrium condition

$dW(r) / dr = 0$ at $r=r_o$ (5)

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

$f(r_0) = f_0 \exp(-r_0\backslash\rho_{+-}) = €_{+-}S_{+-}^2$ (6)

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

Values of overlap integral (S_{+-}) and constants (A_{+-}) are directly taken from [14]. Values of parameters (ρ_{ij}, b and f_0) have been given in Table 1 together with the equilibrium nearest neighbor 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 10^{-8} cm (a)	r_+ 10^{-8} cm (b)	r_- 10^{-8} cm (b)	C_{11} 10^{11} dyne/ cm^2 (a)	C_{12} 10^{11} dyne/ cm^2 (a)	C_{44} 10^{11} dyne/ cm^2 (a)
MgF_2	2.01	1.33	3.00	3.10	1.00	0.11

Table 3.2 Model Parameters for ionic solids

CRYSTAL	**ρ**	**b (in 10^{-12} erg)**	**f (r)**
MgF_2	0.111	0.10	-0.00002

Table 3.3 Values of Cohesive Energies of Magnesium Fluoride in (KJ/Mol)

CRYSTAL	**Experimental Value**	**Theoretical Value**
MgF_2	**2908**	2901

The model parameters listed in Table 3.1 have been used to evaluate the various –order derivatives of the short-range interactions. $_I$, Bi, Ci, Di (i=1, 2).Those parameters are the same as those defined by Verma and co-workers[4] 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 or interaction potential energies of magnesium fluoride using their relevant expressions reported (4, 5).

Results obtained in the table are in good agreement with the experimental results which shows that the

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agreement between experimental and our theoretical results are better.

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