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PHASE TRANSITION IN SILVER CHLORIDES

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ABSTRACT
The phase transition in silver chlorides, interaction potential energies are calculated using a three-body interaction potential. The experimental and theoretical results are in good agreement.

INTRODUCTION

Silver Chloride is a chemical compound with the chemical formula AgCl. This is white crystalline solid well known for its low solubility in water (this behaveiour being reminiscent of the chlorides of Tl plus and Pb two plus). Upon illumination or heating, silver chloride converts to silver, which is signaled by grey to black or purplish coloration to some samples. Its molar mass is 143.32 gm /mol, IUPAC ID is silver (I) chloride, solubility in water is 520micro gram/100gram at 50 degree centigrade, other anions are silver fluoride, silver bromide, silver iodide. Refractive index nd is 2.071, crystals structure is halite, boiling point is 1547degree centigrade(2,817degree Farehenite, 1820 Kelvin),CAS number is 7783-90-6.Appearence is white solid, density 5.56 gm centimeter cube minus 3,magnetic susceptibility(X)is -49.0*10 power minus 6,standard molar entropy is 96 J Mol inverse K inverse, standard enthalpy of formation -127 KJ mol inverse.

AgCl occurs naturally as a mineral chlorargyrite.It is easily synthesized by combining aqueous solution of silver nitrate and sodium chloride.The solid adopts the fcc NaCl structure, in which each Ag plus ion is sourrounded by an octahedron of six chloride ligands.AgF and AgBr crystallize similarly. However, the crystallography depends on the condition of crystallization, primarily free silver ion concentration.

AgCl dissolves in solution containing ligands such as chlorides, cyanide, triphenylphosphine, thiosulphate, thiocyanate and ammonia. Silver chloride does not react with nitric acid most complexes derived from AgCl are two, three and in rare cases, four coordinate, adopting linear trigonal planar and tetrahedral coordination geometries respectively. Silver chloride electrodes are used in electrochemistry, for production of inglaze lusture, used as an antidote for mercury poisoning assisting in the elimination mercury,also used to make photographic paper,in photographic lenses, in bandages, as an infrared transmissive optical component,as an antimicrobialagent.

Co-workers [1-26] 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 phase transition, interaction potential energies of silver chloride.

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 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

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

Phase transition pt can be calculated by difference of interaction potential energies (U1 – U2) divided to the difference in volumes (V2-V1) in two phases.

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)
AgCl	2.01	1.40	3.00	3.10	1.00	0.16

Table 3.2 Model Parameters for ionic solids

CRYSTAL	**ρ**	**b (in 10^{-12} erg)**	**f (r)**
AgCl	0.113	0.10	-0.00009

Table 3.3 Values of Cohesive Energies In Silver Chloride and phase transition value (Pt)

CRYSTAL	**Experimental Value**	**Theoretical Value**
AgCl(U1-U2)	**190.11**	183.09
AgCl (Pt)	**2.3**	2.0
AgCl(V2-V1)	**3**	2.4

The model parameters listed in Table 3.1 have been used to evaluate the various –order derivatives of the

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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 phase transition, interaction potential energies of silver 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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