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333

ON THE ELECTROSTATIC THEORY OF IONIC CRYSTALS

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It is impossible to define a sharp boundary between typical ionic crystals and typical molecular crystals.

1. It is well known, that ionic compounds evaporate in the form of molecules, which are quite stable. Their energy of dissociation (into ions) is in the range of 160 to 40 kcal/mole and exceeds the sublimation heat of the same crystals. Considering the formation of liquid and solid state as the result of condensation of molecular vapor, it is possible to expect the molecules to be conserved, to some degree, also in the crystalline state.

2. A considerable part of the molecules of ionic compounds have large dipole moments, and the interaction between them can supply binding energies on the order of the sublimation heat of these substances. For example, for the molecules of CsI, $\mu = 10 \times 10^{-18}$ CGS electrostatic units. Supposing that the intermolecular distances are equal to 5×10^{-8} cm, we find the work of the attraction forces between two molecules to be 11 kcal/mole. Hence the contribution of the dipole interaction to the energy in the molecular lattice of CsI is approximately equal to $11(l/2) = 66$ kcal/mole (assuming that the coordination number is $l = 12$ for a hypothetical lattice comprising two atomic molecules). In those cases, when the molecules of the ionic compounds have no dipole moments, as for example $HgCl_2$, the Van-der-Waals interaction between them can provide a binding energy on the order of their sublimation heat. Example:

The energy of the dispersion interaction between two $HgCl_2$ molecules is 3 kcal/mole (taking the ionization potential as 12 ev, the coefficient of polarization as $9 \times 10^{-24}\,\mathrm{cm}^{-3}$, and the distances between molecules as 4.3×10^{-8} cm) and the lattice energy is approximately equal to $3(l/2) = 18$ kcal/mole (if $l = 12$). In practice the sublimation heat of $HgCl_2$ is 20 kcal/mole.

3. The principal feature of the molecular structure of crystals is the existence of differences in the interatomic distances between a given atom (ion) and its nearest neighbor. In these cases it is possible to distinguish the "molecules" in the structure. At the same time, the structure is characterized by the distances (radii) between the molecules and inside the molecules. The majority of studied heteropolar compounds exhibit this feature, although, with some exceptions, no attempt has yet been made to describe the structures of the ionic compounds as molecular ones. Things are different for a comparatively small number of heteropolar compounds with structures of the NaCl, CsCl, ZnS type. It is therefore possible to consider these structures not as the rule, but as an exception in the group of heteropolar substances.

4. In many compounds such as NaCl, $HgCl_2$ or HCl properties such as the temperature and the heat of melting and evaporation, as well as compressibility, change gradually from typical ionic to typical molecular structures, which indicates a gradual change in the degree of molecularity of the crystals, and the presence, to a certain degree, of bonds of molecular character in typical ion substances.

5. Based on the above, one might think that many properties of ionic crystals are determined by the energy U^s of "small" intermolecular interaction, which is less than the Born lattice energy E^B. In particular cases, $U^e = S$, the sublimation heat. The question of the dimensions and forms of the molecules in crystals of different substances should be resolved separately. In some cases one must consider the "molecules" that make

up the crystals as infinitely long unidimensional or two-dimensional atom complexes, bound together by "small" forces of one nature, whereas in the complex itself the atoms are bound by "big" forces of another nature.

6. The difference between the typical molecular crystals (e.g., the CH_4 or C_6H_6 crystals) and the heteropolar molecular crystals (such as the NaCl, $HgCl_2$ or PbS crystals) lies: (1) in the degree of molecularity β; (2) in the nature of the forces in the molecules; (3) in the nature of intermolecular forces. The quantity β is defined as the ratio of the intramolecular energy $U^a \cong D$ (D is the energy of dissociation of the diatomic molecule into ions) to the intermolecular energy U^e per bond. For the substances for which β is given below, it is possible to take $U^e \approx 2S/l$. Example:

$\beta = 300\,(CH_4),\ 200\,(HCl),\ 22\,(HgCl_2),\ 10\,(NaCl)$ taking $l = 12$ in all four cases.

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334

ERRATA

Page	Line	Reads	Should Read
Volume 5			
1043	Eq. (4)		$W = y^2 a_{14}^2 \sin 2\phi/2\rho\,(a_{11} a_{44} - \alpha_{14}^2 \sin^2 3\phi)$ The coefficient k_2 equals $0.185 \times 10^{-3}\,cm^{-1}$.
1044	3 from bottom (l.h.)	$\Delta y = 2.87 \times 10^{-3}$ cm	$\Delta y = 3.18 \times 10^{-3}$ cm
	4 from top (r.h.)	$\Delta\vartheta_\Sigma = 7.2 \times 10^{-5}$ radians	$\Delta\vartheta_\Sigma = 5.9 \times 10^{-5}$ radians
Volume 6			
1090	4 and 5 from top	2—(d, 3n); and of the I_{53}^{127} cross section, 3—(d, 2n); 4—(d, 3n)	2—(d, 3n) on I_{53}^{127} and 3—(d, 3n); 4—(d, 3n) on Bi_{83}^{209}
1091	6 from bottom expression for determinant C(y)	ρ, γp, h, $1/\rho$	ρy_2, $\gamma p y_2$, $h y_2$, y_2/ρ
1094	7 from bottom	For $\gamma = 5/3$, μ has . . .	Here μ has . . .
Volume 7			
55	16 from bottom	Correct submittal date is April 5, 1957	
169	17 from bottom	Delete "Joint Institute for Nuclear Research"	
215	Table	Add: Note. Columns 2—9 give the number of counts per 10^6 monitor counts	
215	Table, column headings	1, 2, 3, 4-7, 8	1, 2, 3, 4, 8-7
312	Eq. (8)	$\ldots (1 \pm \mu/2M)^2$	$\ldots (1 \mp \mu/2M)^2$
313	2, r.h. col.	$\alpha_{33} = 0.235$	$a_{33} = 0.235$
692	Eq. (5)	$m_B/M_B = \ldots \mp [1 + \ldots]$	$m_B/M_B = \mp [1 + \ldots]$
461	Title	. . . Elastically Conducting	. . . Electrically Conducting