where E_K is the kinetic energy and E_L is of eq. (1). And the equation of state is

$$P - T \cdot \frac{\beta}{K} - \frac{dE_L}{dV} - \left(\frac{\partial E_K}{\partial V}\right)_T \qquad (3)$$

where β, K are the coefficient of thermal expantion and the isothermal compressibility of the ionic crystal. As far as we are concerned with the problem near room temperature, we can neglect the entropy term and the kinetic energy term in eq. (3). We can say this by comparing our results with other authors'[1][2][3]. Hence E_L in eq. (2) may be considered as the internal energy of the ionic crystal at room temperature, and eq. (3) becomes

$$P = \frac{\alpha\, e^2\, a}{3V} \left\{ \frac{1}{a_0{}^2} \exp\left(\frac{a_0 - a}{\rho}\right) - \frac{1}{a^2} \right\}. \qquad (4)$$

The relation between volume and the nearest neighbor distance is of the form

$$V = c\, Na^3, \qquad (5)$$

where c is a constant value determined from the crystal structure and N is the number of positive or negative ions in the crystal. For the NaCl structure c is 2, and eq. (4) becomes

$$P = \frac{\alpha}{6} \cdot \frac{e^2}{K^{4/3} a_0{}^4} \left[K^{2/3} \exp\left\{ \frac{a_0}{\rho}(1 - K^{1/3}) \right\} - 1 \right] \qquad (6)$$

where K is defined as $K = (a/a_0)^3$.

The unknown parameter p is determined from the compressibility K_0 at room temperature and atmospheric pressure which has the relation between the lattice energy as

$$\frac{1}{K_0\, V_0} = \left(\frac{d^2\, E_L}{dV^2}\right)_{V_0}, \qquad (7)$$

substitution of eq. (2) into eq. (7) yields

$$\frac{a_0}{\rho} = \frac{18\, a_0{}^4}{K_0\, \alpha\, e^2} + 2. \qquad (8)$$

In Table 1. the compressibilities K_0's, the nearest neighbor distances a_0's[4], the calculated a_0/p's and p's are given. The P-K relations are shown in Fig. 1. Here we compare our results with the experimental values of Bridgman[5] (we extended the calculations to the slable regions of the CsCl structure for some alkali halides). NaI shows considerable discrepancy between the calculated values and the observed values, this may be due to the small effective number of two of the observed compressibility. Hence we shall exclude LiI, NaI, KF and RbCl (These have the effective number of two, others have three) in calculating the ionic radii at high pressure (we shall calculate the ionic radii last of all). Fig. 2 shows P-a relations which were calculated to examine additive character of ionic radii at high pressure.

At atmospheric pressure, to a fair approximation, ionic radii are additive quantities. We shall examine whether this approximation is also fair at high pressure or not. The examination is made as follows. We denote AX as a certain alkali halide. A is an alkali metal ion and X is a halide ion. The additive character of ionic radii is shown by the equations

$$AX - A'X = AX' - A'X' = \cdots\cdots$$

or

$$AX - AX' = A'X - A'X' - \cdots\cdots$$

Table 1.

| Compound	$K_0 \times 10^{12}\left(\dfrac{cm^2}{dyn}\right)$ $T=273°C,\ P=0$	a (A) $T=273°C,\ P=0$	a_0/ρ	ρ (A)
LiF	1.53	2.008	6.747	0.299
LiCl	3.48	2.563	7.540	0.350
LiBr	4.28	2.756	8.022	0.344
LiI	7.2	3.040	7.299	0.421
NaF		2.312		
NaCl	4.16	2.812	8.715	0.323
NaBr	5.09	2.978	8.903	0.335
NaI	7.1	3.225	8.807	0.367
KF	3.3	2.669	8.870	0.307
KCl	5.64	3.137	9.670	0.324
KBr	6.66	3.290	9.859	0.334
KI	8.54	3.522	10.05	0.350
RbF		2.815		
RbCl	7.4	3.262	8.835	0.369
RbBr	7.95	3.437	9.842	0.350
RbI	9.58	3.664	10.41	0.352
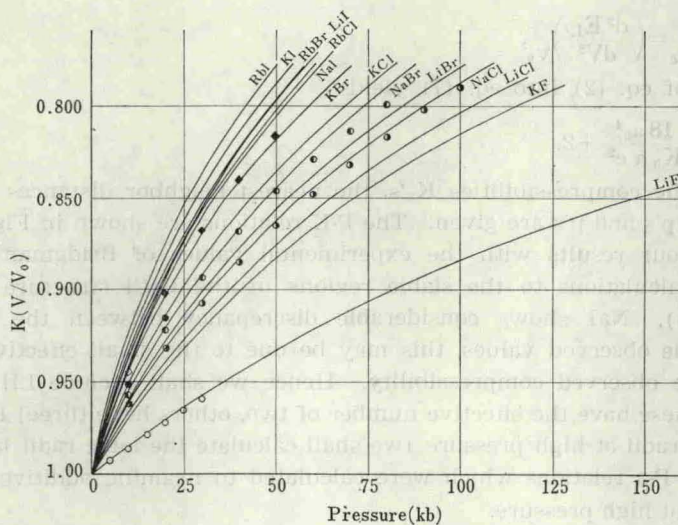
Fig. 1. The volume decreases of alkali halides in the NaCl structure as a
function of pressure. Solid curves, the calculated results (extended
to pressure range in which the CsCl structure is more stable for
some alkali halides). The observed values (5), ◯ LiF, ● KCl, ◑ NaCl,
◑ NaBr, ◇ KBr, ◆ NaI.

The equalities are fairly satisfied at atmospheric pressure. So, if we examine
these differences at high pressure, we can see whether the additive character