

ANHARMONIC PROPERTIES OF ALKALI HALIDES AND CYANIDES

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Anharmonic properties of 16 alkali halides and 4 alkali cyanides are investigated using long-range Coulomb and short-range Börn-Mayer potentials starting from the nearest-neighbour distance and repulsive parameter. This study includes the prediction of second, third and fourth order elastic constants, the pressure derivatives of second and third order elastic constants and partial contractions at elevated temperatures. The results obtained in present investigations are in reasonable agreement compared with experimental studies.

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1. Introduction

The elastic energy density for a deformed crystal can be expanded as a power series of strains and the coefficients of quadratic, cubic and quartic terms are known as second, third and fourth order elastic constants (SOEC, TOEC and FOEC), respectively. When the values of SOEC, TOEC and FOEC are known for a crystal, many of the anharmonic properties of the lattice can be treated within the limit of the continuum approximation in a quantitative manner. Crystal anharmonicities such as thermal expansion, high temperature specific heat, temperature variation of acoustic velocity and attenuation, first order pressure derivatives of SOEC, Grüneisen numbers and temperature derivatives of SOEC are directly related to SOEC and TOEC. While discussing higher order anharmonicities such as the first order pressure derivatives of TOEC, the second order pressure derivatives of SOEC, deformation of crystals under large forces and partial contractions, FOEC are to be considered extensively.

In recent years, some efforts have been made in studying the elastic properties of materials of different kinds [1-7]. Some fruitful work has been done by various investigators while studying the anharmonic properties of solids of several types. They have studied temperature dependence of SOEC of rare gas solids [8], of some alkali halides [9], of a few alkali cyanides using ultrasonic [10-12] and Brillouin scattering [13, 14] methods and of mixed alkali halide cyanide crystals

[15]. The theoretical evaluations of TOEC of a few alkali halides [16, 17], chalcogenides [18], rare gas solids [8, 19] and fluorite crystals [20] have been done by some workers. TOEC of NaCN and KCN are measured by Haussühl et al. [21] at 293 K. Few efforts have been made while investigating FOEC of crystals of various natures [7, 16, 17, 22]. No complete theoretical or experimental efforts have been so far made in obtaining the temperature variation of SOEC, TOEC and FOEC, pressure derivatives of SOEC and TOEC and partial contractions of alkali halides and cyanides.

The present theory deals with the formulation for evaluating SOEC, TOEC and FOEC at any temperature, the first order pressure derivatives of SOEC and TOEC, second order pressure derivatives of SOEC and partial contractions assuming long-range Coulomb and short-range Börn-Mayer potentials starting from the nearest-neighbour distance and repulsive parameter. The results are tabulated for all alkali halides and cyanides of the rock salt structure.

2. Formulation

The elastic strain energy density for a crystal of a cubic symmetry can be expanded up to quartic terms as follows [23]:

$$\begin{aligned}
 U_0 &= U_2 + U_3 + U_4 \\
 &= \frac{1}{2!} C_{ijkl} x_{ij} x_{kl} + \frac{1}{3!} C_{ijklmn} x_{ij} x_{kl} x_{mn} + \frac{1}{4!} C_{ijklmnpq} x_{ij} x_{kl} x_{mn} x_{pq} \\
 &= \frac{1}{2} C_{11}(x_{11}^2 + x_{22}^2 + x_{33}^2) + C_{12}(x_{11}x_{22} + x_{22}x_{33} + x_{33}x_{11}) \\
 &\quad + 2C_{44}(x_{12}^2 + x_{23}^2 + x_{31}^2) + \frac{1}{6} C_{111}(x_{11}^3 + x_{22}^3 + x_{33}^3) \\
 &\quad + \frac{1}{2} C_{112}[x_{11}^2(x_{22} + x_{33}) + x_{22}^2(x_{33} + x_{11}) + x_{33}^2(x_{11} + x_{22})] \\
 &\quad + C_{123}x_{11}x_{22}x_{33} + 2C_{144}(x_{11}x_{23}^2 + x_{22}x_{31}^2 + x_{33}x_{12}^2) \\
 &\quad + 2C_{166}[x_{12}^2(x_{11} + x_{22}) + x_{23}^2(x_{22} + x_{33}) + x_{31}^2(x_{33} + x_{11})] \\
 &\quad + 8C_{456}x_{12}x_{23}x_{31} + \frac{1}{24} C_{1111}(x_{11}^4 + x_{22}^4 + x_{33}^4) \\
 &\quad + \frac{1}{6} C_{1112}[x_{11}^3(x_{22} + x_{33}) + x_{22}^3(x_{33} + x_{11}) + x_{33}^3(x_{11} + x_{22})] \\
 &\quad + \frac{1}{4} C_{1122}(x_{11}^2x_{22}^2 + x_{22}^2x_{33}^2 + x_{33}^2x_{11}^2) \\
 &\quad + \frac{1}{2} C_{1123}x_{11}x_{22}x_{33}(x_{11} + x_{22} + x_{33}) \\
 &\quad + C_{1144}(x_{11}^2x_{23}^2 + x_{22}^2x_{31}^2 + x_{33}^2x_{12}^2) \\
 &\quad + C_{1155}[x_{11}^2(x_{31}^2 + x_{12}^2) + x_{22}^2(x_{12}^2 + x_{23}^2) + x_{33}^2(x_{23}^2 + x_{31}^2)] \\
 &\quad + 2C_{1255}[x_{11}x_{22}(x_{23}^2 + x_{31}^2) + x_{22}x_{33}(x_{31}^2 + x_{12}^2) + x_{33}x_{11}(x_{12}^2 + x_{23}^2)] \\
 &\quad + 2C_{1266}(x_{11}x_{22}x_{12}^2 + x_{22}x_{33}x_{23}^2 + x_{33}x_{11}x_{31}^2) \\
 &\quad + 8C_{1456}x_{12}x_{23}x_{31}(x_{11} + x_{22} + x_{33}) + \frac{2}{3} C_{4444}(x_{12}^4 + x_{23}^4 + x_{31}^4)
 \end{aligned}$$

$$+ 4C_{4455}(x_{12}^2x_{23}^2 + x_{23}^2x_{31}^2 + x_{31}^2x_{12}^2), \quad (1)$$

where C_{ijkl} , C_{ijklmn} and $C_{ijklmnpq}$ are SOEC, TOEC and FOEC in tensorial form, x_{ij} are the Lagrangian strain components, C_{IJ} , C_{IJK} and C_{IJKL} are SOEC, TOEC and FOEC in Brügger's definition [24] and Voigt notations.

The elastic constants of the second, third and fourth order are defined as [24]

$$C_{ijkl} = C_{IJ} = \left(\frac{\partial^2 U}{\partial x_{ij} \partial x_{kl}} \right)_{x=0},$$

$$C_{ijklmn} = C_{IJK} = \left(\frac{\partial^3 U}{\partial x_{ij} \partial x_{mn} \partial x_{kl}} \right)_{x=0}$$

and

$$C_{ijklmnpq} = \left(\frac{\partial^4 U}{\partial x_{ij} \partial x_{kl} \partial x_{mn} \partial x_{pq}} \right)_{x=0}. \quad (2)$$

The free energy density [25, 26] of a crystal at a finite temperature T is

$$U_{\text{Total}} = U_0 + U^{\text{vib}}, \quad U^{\text{vib}} = \frac{kT}{NV_c} \sum_{i=1}^{3sN} \ln 2 \sinh \left(\frac{\hbar \omega_i}{kT} \right), \quad (3)$$

where U_0 is the internal energy per unit volume of the crystal when all ions are at rest on their lattice points, U^{vib} is the vibrational free energy, V_c is the volume of the primitive cell, N is the number of the primitive cells in the crystal and s is the number of ions in the elementary cell. Other notations used in this equations have their usual meanings.

An elastic constant can be separated into two parts:

$$C_{IJ} = C_{IJ}^0 + C_{IJ}^{\text{vib}}, \quad C_{IJK} = C_{IJK}^0 + C_{IJK}^{\text{vib}}$$

and

$$C_{IJKL} = C_{IJKL}^0 + C_{IJKL}^{\text{vib}}. \quad (4)$$

The first part is the strain derivative of the internal energy U_0 and is known as "static" elastic constant and the second part is the strain derivative of the vibrational free energy U^{vib} and is called "vibrational" elastic constant. The superscript "0" has been introduced to emphasize that the static elastic constants correspond to absolute zero temperature.

The energy density of the nondeformed crystal is expressed as

$$U_0 = \frac{1}{2V_c} \sum_{v=1}^s \sum_{\binom{m}{v} \neq \binom{o}{v}} Q_{uv}(R_{uv}^{mo}) = \sum' \frac{Q_{uv}(R)}{2V_c}, \quad (5)$$

where R_{uv}^{mo} is the distance between the v -th ion in the o -th cell and the u -th ion in the m -th cell and Q_{uv} is the interaction potential between the ions. The indices (v, o) and (u, m) are sometimes dropped when no confusion occurs. One assumes that Q_{uv} is the sum of the electrostatic and the Börn-Mayer [27] short-range repulsive potentials

$$Q_{uv}(R) = \pm(e^2/R) + A \exp(-R/q), \quad (6)$$

where e is the electric charge, \pm signs apply to like and unlike ions, respectively and A and q are some parameters. One includes the short-range interactions up to the second nearest-neighbours. The general expressions for the short-range interactions up to the second nearest-neighbours will be of three types:

- (i) unlike ions: $A_{+-} \exp(-r_1/q_{+-})$,
- (ii) like positive ions: $A_{++} \exp(-r_2/q_{++})$,
- (iii) like negative ions: $A_{--} \exp(-r_2/q_{--})$.

Such a model would require six parameters. One further assumes that A and q are the same for all short-range interactions, where q is the repulsive parameter of the crystal and A is given by

$$A = -0.29126q(e^2/r_0^4)/[\exp(-r_0/q) + 2\sqrt{2} \exp(-r_0\sqrt{2}/q)]. \quad (7)$$

When the crystal is deformed homogeneously, the distance between (v, o) and (u, m) ion in the deformed and nondeformed states, R_{uv}^{mo} and r_{uv}^{mo} , are related to the Lagrangian strains x_{ij} as follows:

$$(R_{uv}^{mo})^2 - (r_{uv}^{mo})^2 = 2Y_{uvi}^{mo}Y_{uvj}^{mo}x_{ij} = 2Z_{uv}^{mo}, \quad (8)$$

where Y_{uvi}^{mo} is the i -th Cartesian component of the vector r_{uv}^{mo} . The definition of the quantity Z_{uv}^{mo} is also expressed in Eq. (8). The internal energy U_0 given by Eq. (5) can be expanded in terms of Z , which yields quadratic, cubic and quartic terms as shown below

$$\begin{aligned} U_2 &= \frac{1}{2V_c} \sum' \left[\frac{Z^2 D^2 Q(R)}{2!} \right]_{R=r} = \frac{1}{4V_c} \left[x_{ij} x_{kl} \sum' Y_i Y_j Y_k Y_l D^2 Q(R) \right]_{R=r}, \\ U_3 &= \frac{1}{2V_c} \sum' \left[\frac{Z^3 D^3 Q(R)}{3!} \right]_{R=r} \\ &= \frac{1}{12V_c} \left[x_{ij} x_{kl} x_{mnp} \sum' Y_i Y_j Y_k Y_l Y_m Y_n D^3 Q(R) \right]_{R=r}, \\ U_4 &= \frac{1}{2V_c} \sum' \left[\frac{Z^4 D^4 Q(R)}{4!} \right]_{R=r} \\ &= \frac{1}{48V_c} \left[x_{ij} x_{kl} x_{mnp} x_{pq} \sum' Y_i Y_j Y_k Y_l Y_m Y_n Y_p Y_q D^4 Q(R) \right]_{R=r} \end{aligned} \quad (9)$$

with the abbreviation $D = \frac{d}{(RdR)}$. With reference to Eqs. (3) and (4) and comparison of Eqs. (1) and (9), one obtains the static elastic constants which are shown in Table I (all tables are collected in Sec. 5).

For a central force model, there are only two independent SOEC, three independent TOEC and four independent FOEC at 0 K.

As in the case of the internal energy U_0 , the vibrational free energy is also expanded in terms of strains; the quadratic, cubic and quartic terms are as below

$$\begin{aligned} U_2 &= \frac{1}{V_c 2!} \sum' \sum' [ZZ'(D'D)U^{\text{vib}}]_{Z=0} = \frac{1}{2V_c} x_{ij} x_{kl} f_{ijkl}, \\ U_3 &= \frac{1}{V_c 3!} \sum' \sum' \sum' [ZZ'Z''(D''D'D)U^{\text{vib}}]_{Z=0} = \frac{1}{6V_c} x_{ij} x_{kl} x_{mnp} f_{ijklmnp}, \end{aligned}$$

$$\begin{aligned}
 U_4 &= \frac{1}{V_c 4!} \sum' \sum' \sum' \sum' [Z Z' Z'' Z''' (D''' D'' D' D) U^{\text{vib}}]_{Z=0} \\
 &= \frac{1}{24 V_c} x_{ij} x_{kl} x_{mn} x_{pq} f_{ijklmnpq},
 \end{aligned} \tag{10}$$

where

$$\begin{aligned}
 f_{ijkl} &= \sum' \sum' [Y_i Y_j Y_k Y_l (D' D) U^{\text{vib}}]_{R=r} \\
 f_{ijklmn} &= \sum' \sum' \sum' [Y_i Y_j Y_k Y_l Y_m Y_n (D'' D' D) U^{\text{vib}}]_{R=r}
 \end{aligned}$$

and

$$f_{ijklmnpq} = \sum' \sum' \sum' \sum' [Y_i Y_j Y_k Y_l Y_m Y_n Y_p Y_q (D''' D'' D') U^{\text{vib}}]_{R=r}.$$

Here the abbreviations $Z_{u'v'}^{m'o} \rightarrow Z'$, $\left(\frac{d}{R_{u'v'}^{m'o} dR_{u'v'}^{m'o}}\right) \rightarrow D'$, etc. are used and by comparing Eqs. (1) and (10), one can determine the vibrational elastic constants. These are given in Table II. These are shown as a combination of g_n and F_n which are evaluated conveniently by taking crystal's symmetry [28] into account and the expressions for g_n and F_n are shown in Table III. By adding the vibrational elastic constants to the static elastic constants, one may get SOEC, TOEC and FOEC at any temperature.

The first order pressure derivatives of SOEC are related to SOEC and TOEC, the first order pressure derivatives of TOEC and second order pressure derivatives of SOEC are concerned with SOEC, TOEC and FOEC and partial contractions are mere combinations of FOEC. The expressions for the pressure derivatives [29, 30] and partial contractions [31, 32] are given in Tables IV and V, respectively.

3. Evaluation

Using the concept of the nearest-neighbour distance [28, 33] and repulsive parameter [17, 34], the SOEC, TOEC and FOEC are computed at 0 K (Table I) and are given in Table VI for different alkali halides and cyanides. The temperature coefficients F_n (Table III) are also evaluated and are shown in Table VII. The calculated values of SOEC, TOEC and FOEC at 300 K adding the vibrational contributions are presented in Tables VIII and IX. The first order pressure derivatives of SOEC and TOEC, second order pressure derivatives of SOEC and partial contractions using room temperature data are investigated and are given in Tables X and XI.

4. Results and discussions

Tables VIII and IX show that there are three independent SOEC, six independent TOEC and eleven independent FOEC for halides and cyanides of alkali metals at room temperature. The experimental values of SOEC and TOEC are in good agreement for alkali halides and differ in a certain ratio for alkali cyanides. One may obtain better results to a certain extent by changing the repulsive parameter. Due to the lack of experimental studies of FOEC no comparison can be

made. The first order pressure derivatives of SOEC (Table X) are also in reasonable agreement with the experimental results. The values of the first order pressure derivatives of TOEC may be of help for other workers in further investigations. The experimental data of the second order pressure derivatives of SOEC for some alkali halides are available which are in good agreement for rubidium halides and are in reasonable agreement for sodium halides (Table XI). The overall good agreement between theoretical and experimental investigations supports the validity of the interaction model used in the present work.

5. Tables*

TABLE I

Expressions for the second, third and fourth order elastic constants at 0 K.

$$\begin{aligned}
 C_{11}^0 &= -1.56933P + P_1 + 2P_2, \quad C_{12}^0 = C_{44}^0 = 0.347775P + P_2, \\
 C_{111}^0 &= 10.2639P - P_3 - 2P_4, \quad C_{112}^0 = C_{166}^0 = 1.208625P - P_4, \\
 C_{123}^0 &= C_{144}^0 = C_{456}^0 = 0.678375P, \quad C_{1111}^0 = -80.71455P + P_5 + 2P_6, \\
 C_{1112}^0 &= C_{1155}^0 = 4.43205P + P_6, \quad C_{1122}^0 = C_{1266}^0 = C_{4444}^0 = 5.615925P + P_6, \\
 C_{1123}^0 &= C_{1144}^0 = C_{1255}^0 = C_{1456}^0 = C_{4455}^0 = -1.584975P, \\
 \text{where } P &= e^2/r_0^4, \quad P_1 = (1/r_0 + 1/q)Q(r_0)/qr_0, \\
 P_2 &= (\sqrt{2}/2r_0 + 1/q)Q(r_0\sqrt{2})/qr_0, \quad P_3 = (3/r_0^2 + 3/qr_0 + 1/q^2)Q(r_0)/q, \\
 P_4 &= (3\sqrt{2}/r_0^2 + 6/qr_0 + 2\sqrt{2}/q^2)Q(r_0\sqrt{2})/4q, \\
 P_5 &= (15/r_0^3 + 15/qr_0^2 + 6/q^2r_0 + 1/q^3)r_0Q(r_0)/q, \\
 P_6 &= (15\sqrt{2}/4r_0^3 + 15/2qr_0^2 + 3\sqrt{2}/q^2r_0 + 1/q^3)r_0Q(r_0\sqrt{2})/2q.
 \end{aligned}$$

TABLE II

Expressions for vibrational contribution to the second, third and fourth order elastic constants.

$$\begin{aligned}
 C_{11}^{\text{vib}} &= g_1F_1^2 + g_1F_2; \quad C_{12}^{\text{vib}} = g_2F_1^2 + g_1F_5; \quad C_{44}^{\text{vib}} = g_1F_5; \\
 C_{111}^{\text{vib}} &= g_3F_1^3 + g_2F_2F_1 + g_1F_3; \quad C_{112}^{\text{vib}} = g_1F_1^3 + g_2F_1(2F_5 + F_2) + g_1F_6; \\
 C_{123}^{\text{vib}} &= g_3F_1^3 + 3g_2F_1F_5; \quad C_{144}^{\text{vib}} = g_2F_1F_5; \quad C_{166}^{\text{vib}} = g_2F_1F_5 + g_1F_6; \quad C_{456}^{\text{vib}} = 0; \\
 C_{1111}^{\text{vib}} &= g_4F_1^4 + 6g_3F_1^2F_2 + 3g_2F_2^2 + 4g_2F_1F_3 + g_1F_4; \quad C_{1456}^{\text{vib}} = 0; \\
 C_{1112}^{\text{vib}} &= g_4F_1^4 + 3g_3F_1^2(F_5 + F_2) + 3g_2F_5F_2 + g_2F_1(3F_6 + F_3) + g_1F_7; \\
 C_{1122}^{\text{vib}} &= g_4F_1^4 + 2g_3F_1^2(2F_5 + F_2) + g_2(2F_5^2 + F_2^2) + 4g_2F_1F_2 + g_1F_7; \\
 C_{1123}^{\text{vib}} &= g_4F_1^4 + g_3F_1^2(5F_5 + F_2) + g_2F_1(2F_5 + F_2) + 2g_2F_1F_6; \\
 C_{1144}^{\text{vib}} &= g_3F_1^2F_5 + g_2F_5F_2; \quad C_{4444}^{\text{vib}} = 3g_2F_5^2 + g_2F_7; \\
 C_{1155}^{\text{vib}} &= g_3F_1^2F_5 + g_2F_5F_2 + 2g_2F_1F_6 + g_1F_7; \quad C_{4455}^{\text{vib}} = g_2F_5^2; \\
 C_{1255}^{\text{vib}} &= g_3F_1^2F_5 + g_2F_5^2 + g_2F_1F_6; \\
 C_{1266}^{\text{vib}} &= g_3F_1^2F_5 + g_2F_5^2 + 2g_2F_1F_6 + g_1F_7.
 \end{aligned}$$

*For technical reasons the tables are not given in their numerical order.

TABLE III

Expressions for g_n and F_n .

$$\begin{aligned}
g_1 &= g_0 S; & g_2 &= -g_0[(X/S_1) + S]/2; & g_0 &= \hbar\omega_0/8r_0^3; \\
g_3 &= g_0[(2X^2S/3S_1) + (X/S_1) + S]/48; & X &= \hbar\omega_0/2kT; \\
g_4 &= -g_0[(X^3S^2/3S_1) + (X^3/6S_1^2) + (X^2S/S_1) + (5X/4S_1) + (5S/4)]/144; \\
\omega_0 &= (1/M^+ + 1/M^-)/qr_0F_0; & S &= \coth X; & S_1 &= \sinh^2 X.
\end{aligned}$$

$$\begin{aligned}
F_0 &= 1/[(q_0 - 2)Q(r_0) + 2(q_0 - \sqrt{2})Q(r_0\sqrt{2})], & q &= r_0/q; \\
F_1 &= 2[(2 + 2q_0 - q_0^2)Q(r_0) + 2(\sqrt{2} + 2q_0 - \sqrt{2}q_0^2)Q(r_0\sqrt{2})]F_0; \\
F_2 &= 2(-6 - 6q_0 - q_0^2 + q_0^3)Q(r_0)F_0 + F_5; \\
F_3 &= 2(30 + 30q_0 + 9q_0^2 - q_0^3 - q_0^4)Q(r_0)F_0 + F_6; \\
F_4 &= 2(-210 - 210q_0 - 75q_0^2 - 5q_0^3 + 4q_0^4 + q_0^5)Q(r_0)F_0 + F_7; \\
F_5 &= (-3\sqrt{2} - 6q_0 - \sqrt{2}q_0^2 + 2q_0^3)Q(r_0\sqrt{2})F_0; \\
F_6 &= [(15/\sqrt{2}) + 15q_0 - (9/\sqrt{2})q_0^2 - q_0^3 - \sqrt{2}q_0^4]Q(r_0\sqrt{2})F_0; \\
F_7 &= [-(105/2\sqrt{2}) - (105/2)q_0 - (75/2\sqrt{2})q_0^2 - (5/2)q_0^3 + 2\sqrt{2}q_0^4 + q_0^5]Q(r_0\sqrt{2})F_0.
\end{aligned}$$

TABLE IV

Expressions for the first order pressure derivatives of the second and third order elastic constants and expressions for the second order pressure derivatives of the second order elastic constants.

$$\begin{aligned}
dC_{11}/dp &= (C_{11} + C_Q + C_{111} + C_{112})C_0; & C_Q &= C_{11} + 2C_{12}; \\
dC_{12}/dp &= -(-C_{11} + C_{12} + C_{123} + 2C_{112})C_0; & C_0 &= 1/C_Q; \\
dC_{44}/dp &= -(C_Q + C_{44} + C_{144} + 2C_{166})C_0; \\
dC_{111}/dp &= -(-3C_Q + 3C_{111} + C_{1111} + 2C_{1112})C_0; \\
dC_{112}/dp &= -(C_Q + 3C_{112} + C_{1112} + C_{1122} + C_{1123})C_0; \\
dC_{123}/dp &= -(-C_Q + 3C_{123} + 3C_{1123})C_0; \\
dC_{144}/dp &= -(C_Q + 3C_{144} + C_{1144} + 2C_{1244})C_0; \\
dC_{166}/dp &= -(-C_Q + 3C_{166} + C_{1166} + 2C_{1244})C_0; \\
dC_{456}/dp &= -(-C_Q + 3C_{456} + 3C_{1456})C_0; \\
d^2C_{11}/dp^2 &= [(1 + 3C_p)C_{11} + (4 + 3C_p)(C_{111} + 2C_{112}) + C_{1111} + \\
&\quad 4C_{1112} + 2C_{1122} + 2C_{1123}]C_0^2; \\
d^2C_{12}/dp^2 &= [(1 + 3C_p)C_{12} + (4 + 3C_p)(2C_{112} + C_{123}) + \\
&\quad 2C_{1122} + 5C_{1123}]C_0^2; \\
d^2C_{44}/dp^2 &= [(1 + 3C_p)C_{44} + (4 + 3C_p)(C_{144} + 2C_{166}) + \\
&\quad C_{1144} + 2C_{1166} + 4C_{1244} + 2C_{1266}]C_0^2; \\
C_p &= (4C_{11} + C_{111} + 6C_{112} + 2C_{123})C_0.
\end{aligned}$$

TABLE V
Expressions for partial contractions of the fourth order
elastic constants.

$$Y_{11} = C_{1111} + 4C_{1112} + 2C_{1122} + 2C_{1123};$$

$$Y_{12} = 2C_{1112} + 2C_{1122} + 5C_{1123};$$

$$Y_{44} = C_{1144} + 2C_{1166} + 4C_{1244} + 2C_{1266}.$$

TABLE XI

The second order pressure derivatives of the second order elastic constants in 10^{-10} dyn/cm² and partial contractions in 10^{13} dyn/cm².

Sub.	$\frac{d^2 C_{11}}{dp^2}$	$\frac{d^2 C_{12}}{dp^2}$	$\frac{d^2 C_{44}}{dp^2}$	Y_{11}	Y_{12}	Y_{44}	Ref.
LiF	-14.24	-12.14	-3.30	-1158	-1189	-259.9	this work
LiCl	-8.30	-9.45	-2.32	-144.7	-158.9	-33.77	this work
LiBr	-6.100	-8.67	-2.00	-80.65	-92.17	-19.30	this work
LiI	-5.57	-10.07	-2.28	-50.76	-59.96	-12.53	this work
NaF	-2.85	-4.33	-1.01	-157.9	-182.5	-38.32	this work
	-7.2	-0.8	0.2				[47]
NaCl	-1.22	-3.79	-0.64	-27.39	-40.32	-7.985	this work
	-9.4	-0.4	-0.6				[47]
NaBr	3.96	-3.01	-0.32	-10.86	-21.39	-4.006	this work
	-6.2	-3.4	-0.8				[47]
NaI	-6.78	-3.24	-0.24	-5.15	-13.43	-2.468	this work
	-10.4	-3.4	-1.0				[47]
KF	-0.49	-4.35	-0.89	-52.07	-68.48	-14.04	this work
KCl	-4.67	-4.46	-0.76	-14.02	-25.26	-5.105	this work
KBr	-8.63	-3.13	-0.31	-3.689	-13.42	-2.582	this work
KI	-12.89	-3.04	-0.16	-0.449	-8.292	-1.566	this work
	-12.7	-1.6	-1.08				[32]
RbF	-1.39	-3.88	-0.71	-29.95	-44.48	-8.970	this work
RbCl	-8.13	-3.67	-0.50	-5.839	-16.22	-3.228	this work
	-11.3	-0.3	-1.1	11.20	-0.20	0.16	[31]
RbBr	-13.39	-2.09	0.02	1.839	-7.243	-1.337	this work
	-15.6	-3.5	-1.2	9.10	-0.9	0.18	[31]
RbI	-18.26	-1.65	0.24	3.476	-4.204	-0.747	this work
	-18.4	-2.3	-1.3	7.7	-0.41	0.21	[31]
LiCN	-5.39	-4.58	-1.16	-945.3	-972.2	-207.5	this work
NaCN	-0.79	-1.79	-0.30	-106.9	-131.1	-25.39	this work
KCN	-0.11	-1.89	-0.29	-56.84	-78.67	-15.10	this work
RbCN	1.13	-1.67	-0.20	-32.11	-52.55	-9.817	this work

TABLE VI

Nearest-neighbour distances and repulsive parameters in 10^{-8} cm and the second, third and fourth order elastic constants at 0 K in 10^{11} dyn/cm² of alkali halides and cyanides.

Sub.	r_0	q	C_{11}^0	C_{12}^0	C_{111}^0	C_{112}^0	C_{123}^0	C_{1111}^0	C_{1112}^0	C_{1122}^0	C_{123}^0
LiF	2.0032	0.249	14.167	6.167	-217.04	-25.176	9.719	2943.0	122.09	117.18	139.05
LiCl	2.5467	0.297	6.327	2.301	-100.38	-9.379	3.721	1406.4	45.87	43.12	52.36
LiBr	2.7136	0.311	5.107	1.772	-81.81	-7.218	2.886	1156.8	35.36	33.01	40.39
LiI	2.9529	0.325	3.979	1.244	-65.23	-5.049	2.058	942.7	24.80	22.71	28.32
NaF	2.3032	0.256	10.528	3.373	-171.59	-13.709	5.562	2466.8	67.31	61.94	77.01
NaCl	2.7865	0.296	5.405	1.547	-90.40	-6.258	2.596	1332.6	30.77	27.62	35.30
NaBr	2.9567	0.310	4.378	1.214	-73.79	-4.904	2.048	1095.7	24.11	21.46	27.68
NaI	3.1967	0.326	3.385	0.879	-57.98	-3.538	1.498	874.7	17.38	15.19	20.00
KF	2.6568	0.278	6.743	1.861	-113.77	-7.514	3.141	1691.4	36.95	32.85	42.43
KCl	3.115	0.296	4.300	0.956	-76.75	-3.800	1.669	1206.2	18.57	15.33	21.48
KBr	3.2580	0.305	3.683	0.791	-66.37	-3.134	1.389	1053.1	15.29	12.43	17.71
KI	3.4840	0.319	2.929	0.600	-53.51	-2.368	1.062	860.6	11.51	9.15	13.37
RbF	2.7914	0.284	5.849	1.511	-100.33	-6.078	2.577	1515.6	29.87	26.05	34.36
RbCl	3.2564	0.298	3.842	0.786	-70.20	-3.103	1.392	1129.4	15.04	11.98	17.51
RbBr	3.4263	0.305	3.289	0.636	-61.13	-2.495	1.135	1000.3	12.06	9.29	14.05
RbI	3.6220	0.315	2.740	0.506	-51.66	-1.973	0.909	857.8	9.49	7.11	11.08
LiCN	1.7013	0.265	13.142	12.918	-179.68	-51.740	18.681	2206.0	238.22	232.34	270.83
NaCN	2.0721	0.266	11.376	5.458	-171.31	-22.267	8.489	2286.3	107.39	103.85	122.20
KCN	2.2892	0.267	9.689	3.524	-153.70	-14.367	5.699	2153.4	70.26	66.06	80.21
RbCN	2.4104	0.268	8.771	2.814	-142.92	-11.430	4.636	2054.2	56.12	51.65	64.12

TABLE X

The first order pressure derivatives of the second and third order elastic constants.

Sub.	$\frac{dC_{11}}{dp}$	$\frac{dC_{12}}{dp}$	$\frac{dC_{44}}{dp}$	$\frac{ds}{dp}$	$\frac{dk}{dp}$	$\frac{dC_{111}}{dp}$	$\frac{dC_{112}}{dp}$	$\frac{dC_{123}}{dp}$	$\frac{dC_{144}}{dp}$	$\frac{dC_{156}}{dp}$	$\frac{dC_{158}}{dp}$	Ref.
LiF	-8.48	1.83	0.28	3.11	4.33	1366	1441	1450	-1.23	482	2.42	this work [44]
LiCl	-9.25	1.76	0.15	3.60	5.30	382	468	477	-1.22	158	2.32	this work [44]
LiBr	-9.46	1.74	0.12	3.70	5.63	254	343	351	-1.21	116	2.30	this work [44]
LiI	-9.95	1.69	0.04	3.75	5.68	202	299	306	-1.20	101	2.24	this work [44]
NaF	-9.84	1.69	0.06	3.91	4.63	243	341	349	-1.20	115	2.26	this work [45]
NaCl	-10.40	1.65	-0.02	4.23	4.76	46.6	153	100	-1.19	52.8	2.20	this work [45]
NaBr	-10.56	1.63	-0.05	4.79	5.107	-7.64	101	108	-1.18	35.6	2.18	this work [45]
NaI	-10.91	1.61	-0.09	4.83	5.29	-30.0	83.4	90.4	-1.18	30.0	2.14	this work [45]
KF	-10.59	1.63	-0.05	4.80	5.40	10.1	211	218	-1.19	72.3	2.17	this work [45]
KCl	-11.81	1.52	-0.21	5.03	5.10	0.42	130	137	-1.16	46.1	2.05	this work [45]
KBr	-12.01	1.51	-0.23	5.61	5.34	-52.1	81.6	87.7	-1.16	29.8	2.03	this work [45]

TABLE IX

The fourth order elastic constants in 10^{11} dyn/cm² at room temperature.

Sub.	C_{1111}	C_{1112}	C_{1122}	C_{1123}	C_{1144}	C_{1155}	C_{1255}	C_{1266}	C_{1456}	C_{4444}	C_{4453}
LiF	-10477	-13134	-13128	-13274	-23.24	118.3	-22.99	141.5	-22.71	142.8	-22.76
LiCl	-478.9	-1736	-1738	-1789	-8.961	43.43	-8.822	53.37	-8.693	53.99	-8.715
LiBr	28.97	-1001	-1003	-1042	-6.967	33.22	-6.848	41.19	-6.744	41.72	-6.761
LiI	184.3	-649.7	-652.9	-678.2	-4.986	22.85	-4.888	29.00	-4.809	29.41	-4.821
NaF	245.5	-1985	-1988	-2062	-13.37	62.29	-13.16	78.34	-12.99	79.20	-1.302
NaCl	759.4	-427.3	-432.1	-46.27	-6.278	27.74	-6.156	35.97	-6.065	36.47	-6.077
NaBr	748.6	-221.1	-226.1	-249.1	-4.964	21.55	-4.859	28.24	-4.785	28.65	-4.794
NaI	630.2	-136.8	-141.9	-157.1	-3.644	15.24	-3.559	20.43	-3.502	20.75	-3.508
KF	777.3	-735.9	-741.9	-78.4	-7.586	33.00	-7.443	43.23	-7.339	43.79	-7.352
KCl	791.3	-266.3	-275.2	-288.6	-4.055	15.38	-3.959	-21.94	-3.901	22.29	-3.907
KBr	780.2	-136.8	-145.5	-155.5	-3.378	12.46	-3.295	18.09	-3.246	1.839	-3.249
KI	658.6	-82.20	-90.69	-96.68	-2.589	9.173	-2.521	13.67	-2.482	13.92	-2.485
RbF	875.6	-473.5	-480.4	-508.1	-6.237	26.15	-6.109	35.03	-6.023	35.52	-6.033
RbCl	814.1	-167.5	-177.6	-186.28	-3.384	12.01	-3.300	17.88	-3.252	18.19	-3.256
RbBr	791.3	-69.44	-79.83	-84.97	-2.765	9.313	-2.693	14.36	-2.653	14.61	-2.656
RbI	692.4	-37.36	-47.60	-50.09	-2.217	7.126	-2.157	11.34	-2.125	11.55	-2.127
LiCN	-6785	-10658	-10627	-10931	-44.25	234.1	-44.09	274.1	-43.65	275.6	-43.77
NaCN	662.5	-1390	-1384	-1513	-20.28	104.3	-20.08	123.9	-19.83	124.9	-19.88
KCN	1113	-829.5	-829.7	-909.8	-13.68	66.35	-13.49	81.46	-13.31	82.32	-13.34
RbCN	1304	-547.5	-550.6	-611.7	-11.16	51.85	-10.98	65.26	-10.83	66.01	-10.85

TABLE VII

Temperature coefficients (F_n) and natural frequency (ω_0) in 10^{13} s^{-1} .

Sub.	F_1	F_2	F_3	F_4	F_5	F_6	F_7	ω_0
LiF	-15.92	133.0	-1247	460.9	4.915	-32.33	230.4	7.680
LiCl	-16.97	152.1	-1519	473.1	4.520	-31.42	236.5	5.237
LiBr	-17.26	157.6	-1602	475.2	4.405	-31.16	237.6	4.593
LiI	-17.97	171.4	-1812	477.7	4.130	-30.29	238.8	4.096
NaF	-17.80	167.9	-1759	477.4	4.198	-30.52	238.7	4.698
NaCl	-18.62	184.3	-2019	477.3	3.880	-29.38	238.6	3.142
NaBr	-18.86	189.3	-2098	476.5	3.787	-29.01	238.3	2.562
NaI	-19.39	200.3	-2279	-473.7	3.587	-28.18	236.8	2.223
KF	-18.90	190.1	-2110	476.4	3.773	-28.95	238.2	3.559
KCl	-20.79	230.7	-2803	459.9	3.085	-25.80	229.9	2.476
KBr	-21.12	238.3	-2939	455.3	2.970	-25.20	227.6	1.965
KI	-21.60	249.2	-3138	448.2	2.812	-24.35	224.1	1.688
RbF	-19.44	201.1	-2295	473.4	3.571	-28.10	236.7	3.053
RbCl	-21.61	249.5	-3143	448.0	2.809	-24.32	224.0	2.041
RbBr	-22.22	263.8	-3409	437.9	2.615	-23.22	218.9	1.499
RbI	-22.74	276.4	-3650	428.3	2.455	-22.27	214.1	1.258
LiCN	-12.71	81.56	-597.4	371.3	5.852	-31.41	185.6	8.031
NaCN	-15.42	124.3	-1127	452.1	5.097	-32.57	226.0	4.606
KCN	-16.97	152.0	-1519	473.1	4.521	-31.48	236.5	3.746
RbCN	-17.79	167.8	-1757	477.4	4.200	-30.52	238.7	3.168

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