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Maria Carolina Monard
Alicia Batana
Jorge Bruno

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Maria Carolina Monard[*]
Universidade de São Paulo
Instituto de Ciências Matemáticas de São Carlos
Departamento de Ciências de Computação e Estatística
Caixa Postal 668, 13560-970 - São Carlos, SP, Brasil
e-mail: mcmonard@icmsc.sc.usp.br

Alicia Batana[†]
Jorge Bruno[†]
Universidad de Buenos Aires
Facultad de Ciencias Exactas y Naturales
Departamento de Química Inorgánica Analítica y Química Física
and
Universidad Nacional de La Patagonia San Juan Bosco
Facultad de Ciencias Naturales
e-mail: {batana,jbruno}@q1.fcen.uba.ar

Abstract

An empirical method based on two models, with parameters fitted to ab initio and experimental data, has been developed for the evaluation of the pressure dependence of ionic polarizabilities in ionic crystals. The importance of this method is its predictive nature, particularly useful in the study of more complex materials for which there are no experimental data at high pressures. Both models have been implemented as Maple procedures and experimental results using these procedures on different salts are shown.

Fevereiro 2003

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1 Introduction

High pressure studies of ionic materials are of geophysical interest; further importance is that one may also obtain a critical study of the theoretical models involved. The concept of ionic properties appears in these studies, such as polarizabilities of ions in the theories of dielectric constants, refractive index and optical properties of ionic solids.

In the study of more complex systems, in general, there are no high pressure data available, thus it is important to have theoretical methods to evaluate these magnitudes; these may be based either on data only at $P = 0$ or on high pressure data of other solids that have either a cation or an anion in common with the one of interest.

In this work we propose an alternative way, based on two different models [8], for evaluating high pressure ionics polarizabilities in more complex solids than the ones we used in previous work [1, 2, 9, 10, 11, 12, 13, 14]. Both models have been implemented as Maple procedures and experimental results obtained using different salts are shown and discussed.

This work is organized as follows: in Section 2 the method proposed is presented and in Section 3 the corresponding Maple implementation is described. Experimental results are shown in Section 4 and conclusions are presented in Section 5.

2 Method

Ab initio calculations for complex materials at high pressures are time consuming and expensive. We therefore propose to extend to these systems the behavior obtained in previous ab initio calculations of simple systems [4, 5, 6, 8]. In these studies it is shown that the anion polarizability curves α_- *vs* R, can be represented by different models — equations 1 and 2

$$\frac{\alpha_-}{\alpha_-^\infty} = e^{-\frac{a}{R^2}} \tag{1}$$

$$\frac{\alpha_-^\infty}{\alpha_-} = (1 + aR^{-s}) \; for \; s = 3 \; or \; s = 4 \tag{2}$$

where

- R is the equilibrium anion-cation distance (pressure $p = 0$);
- α_-^∞ is the value of α_- at $R \to \infty$
- a is a parameter for a given anion in a given salt.

For a given salt we propose to evaluate the parameter a that appears in both models by knowledge of α_- at the equilibrium R and α_-^∞ that should be evaluated independently. $\frac{\partial \alpha_-}{\partial R}$ is therefore obtained by diferentiating at the equilibrium R. If we know the value of the compressibility χ_T one may evaluate $\frac{\partial \alpha_-}{\partial p}$ as

$$\frac{\partial \alpha_-}{\partial p} = \frac{\partial \alpha_-}{\partial R}(-\frac{\chi_T R}{3}) \tag{3}$$

To evaluate the cation contribution $\frac{\partial \alpha_+}{\partial p}$ we propose to use the method we described previously [2]— equation 4

$$\frac{1}{\alpha_+}\frac{\partial \alpha_+}{\partial p} - \frac{1}{\alpha_-}\frac{\partial \alpha_-}{\partial p} = 3(\frac{1}{r_+}\frac{\partial r_+}{\partial p} - \frac{1}{r_-}\frac{\partial r_-}{\partial p}) \tag{4}$$

where

- r_+ and r_- are the cation and anion radii respectively;
- $\frac{\partial r_+}{\partial p}$ and $\frac{\partial r_-}{\partial p}$ are their pressure derivatives.

The method has been implemented in Maple 6 [3], a comprehensive computer system for advanced mathematics. Maple 6 includes facilities for interactive algebra, calculus, discrete mathematics, graphics, numerical computation and many other areas of mathematics. It also provides a unique environment for rapid development of mathematical programs using its vast library of built-in functions and operations.

3 Maple Implementation

Both models have been implemented as Maple procedures. In what follows we shall refer as Model 1 and Model 2 to the models described by equation 1 and equation 2 respectively.

For Model 1 only the data related to the salt needs to be informed. For Model 2 the data related to the salt and the aditional information related to the value of $s = 3$ or $s = 4$ are needed. Furthermore, for each model we want to calculate $\frac{\partial \alpha_-}{\partial p}$ using equation 3 as well as $\frac{\partial \alpha_+}{\partial p}$ using equation 4. Thus, as we would like the procedures to execute interactively as well as in batch, we decided to keep together all data needed for the calculations related to each individual salt, as described in next section.

3.1 Data Structure

Maple has a rich set of build-in data structures and we decided to use the *list* data structure to group each salt's data. A list is an ordered sequence of distinct expressions enclosed in square brackets. The elements of a list may be extracted via the selection operation. Thus, if `L` is a list then the ith element of `L` can be obtained by `L[i]`.

In our implementation, a salt is described by a list of 11 elements where each element in the list is indexed only through the following defined Maple constants

```
> alfaMinus:=1: Requil:=2: xi:=3: alfaMinusRinfinity:= 4: a:=5:
  SaltName:=6: alfaPlus:=7: rPlus:=8: rMinus:=9: DerRPlusDp:=10:
  DerRMinusDp:=11:
```

Table 1 shows the mapping between these Maple constants and the corresponding information held by these list's elements.

Constant	Data
`alfaMinus`	α_-
`Requil`	R
`xi`	χ_T
`alfaMinusRinfinity`	α_-^∞
`a`	a
`SaltName`	*Salt's name*
`alfaPlus`	α_+
`rPlus`	r_+
`rMinus`	r_-
`DerRPlusDp`	$\frac{\partial r_+}{\partial p}$
`DerRMinusDp`	$\frac{\partial r_-}{\partial p}$

Table 1: List's Elements Mapping

```
LiF_1:=[0.89, 1.996, 1.43, 2.4525, -100, "LiF_1", 0.03, 0.60,
1.36, -0.2784, -0.6709]:
```

Table 2: Data for LiF in *cgs* units

This data structure allows to identify any salts's data through its name. For example, the data related to salt LiF has been defined (*cgs* units) as shown in Table 2

thus, the value of α_- for this salt is given by `LiF_1[alfaMinus]`, the value of R at equilibrium by `LiF_1[Requil]`, the value of χ_T by `LiF_1[xi]` and so on — Table 1.

Observe that the 5th element of the list is negative (-100) corresponding to the value of a, this means that the value of a for this salt is unknown. Also, a 4th element negative value means that the value of α_-^∞ for that salt is unknown. The Maple implementation of both models is described next.

3.2 Model 1

The Model 1 algorithm is presented in Algorithm 1

Algorithm 1 for a given salt is implemented by `Model_1/1` Maple procedure, where:

- `<arg-1>` = Salt

```
> Model_1 := proc(Salt::list)
> local Calc_a, Calc_alfaMinusRinfinity,
> todraw, DerAlfMinusDR, DerAlfMinusDp,DerAlfPlusDp;
> print("Model 1 for salt ", Salt[SaltName],Salt);
```

Algorithm 1: **Model 1**

Require: *Salt*

procedure Model_1(*Salt*)
if α_-^∞ is known **then**
  $a := R^2(\ln \alpha_- - \ln \alpha_+)$
else
  $\alpha_-^\infty := \alpha_- e^{\frac{a}{R^2}}$
end if
$todraw(R) := \alpha_-^\infty e^{-\frac{a}{R^2}}$ Model 1 equation 1
$\frac{\partial \alpha_-}{\partial R} := \frac{\partial todraw(R)}{\partial R}$
$\frac{\partial \alpha_-}{\partial p} = \frac{\partial \alpha_-}{\partial R}(-\frac{\chi_T R}{3})$ {at the equilibrium R equation 3}
$\frac{\partial \alpha_+}{\partial p} := \alpha_+(\frac{1}{\alpha_-}\frac{\partial \alpha_-}{\partial p} + 3(\frac{1}{r_+}\frac{\partial r_+}{\partial p} - \frac{1}{r_-}\frac{\partial r_-}{\partial p}))$ {at the equilibrium R equation 4}
print all values
plot $todraw(R)$ and at the equilibrium R
end

```
> if Salt[alfaMinusRinfinity] > 0
> then Calc_alfaMinusRinfinity := Salt[alfaMinusRinfinity];
> Calc_a := calculate_aORRequilModel_1(Salt);
> print("DataalfaMinusRinfinity=", Calc_alfaMinusRinfinity,
> "Calculated a=" , Calc_a)
> else Calc_a := Salt[a];
> Calc_alfaMinusRinfinity := calculate_aORRequilModel_1(Salt);
> print("CalculatedalfaMinusRinfinity=",Calc_alfaMinusRinfinity,"Data
> a=", Calc_a) fi;
> todraw := alfMinusModel_1(Calc_alfaMinusRinfinity,Calc_a,R);
> print("todraw=" ,todraw);
> DerAlfMinusDR := eval(diff(todraw,R),R=Salt[Requil]);
> print("DerAlfMinusDR=", DerAlfMinusDR);
> DerAlfMinusDp := -DerAlfMinusDR*Salt[xi]*Salt[Requil]/3;
> print("DerAlfMinusDp=", DerAlfMinusDp);
> DerAlfPlusDp:=CationPressureDerivative(Salt,DerAlfMinusDp);
> print("DerAlfPlusDp",DerAlfPlusDp);
> plot({[[Salt[Requil],0],[Salt[Requil],eval(todraw,R=Salt[Requil])]],
> todraw },R=0.5..4*Salt[Requil],title=Salt[SaltName]);
> end:
```

`Model_1/1` calls the following three Maple procedures

1. `calculate_aORRequilModel_1/1`
2. `alfMinusModel_1/2`

3. `CationPressureDerivative/2` which is also called by `Model_2/2`

Procedure `calculate_aORRequilModel_1/1` calculates, for a given salt, the value of a if the value of α_{-}^{∞} is known else, the value of a is known and it calculates the value of α_{-}^{∞} using, in both cases, equation 1 for Model 1.

```
> calculate_aORRequilModel_1:=proc(Salt::list)
> if Salt[alfaMinusRinfinity] > 0
> then -(Salt[Requil]^2)*
> (ln(Salt[alfaMinus])-ln(Salt[alfaMinusRinfinity]))
> else Salt[alfaMinus]*exp(Salt[a]/(Salt[Requil]^2)) fi end:
```

Procedure `alfMinusModel_1/2` calculates the value of α_{-} related to equation 1 for Model 1, where:

- `<arg-1>` α_{-}^{∞}
- `<arg-2>` a
- `<arg-3>` free variable used for plotting

```
> alfMinusModel_1:=proc(AlfInf::float,a::float,R)
> AlfInf*exp(-a/(R^2)) end:
```

Procedure `CationPressureDerivative/2` calculates the cation pressure derivative $\frac{\partial \alpha_{+}}{\partial p}$ (equation 4) of a given salt, given the anion pressure derivative $\frac{\partial \alpha_{-}}{\partial p}$ (equation 3) previously computed. This procedure is used for Model 1 and 2 procedures.

- `<arg-1>` salt
- `<arg-2>` $\frac{\partial \alpha_{-}}{\partial p}$

```
> CationPressureDerivative := proc(Salt::list,DerAlfMinusDp::float)
> eval(Salt[alfaPlus]*(3*(Salt[DerRPlusDp]/Salt[rPlus]-
> Salt[DerRMinusDp]/Salt[rMinus]) + DerAlfMinusDp/Salt[alfaMinus]))
> end:
```

In order to illustrate it follows an execution example of `Model_1/1` Maple procedure for salt LiF — Table 2 pg.3. The call

```
> Model_1(LiF_1);
```

has the following output as well as the graph shown in Figure 1

"Model 1 for salt ", "LiF_1",
[.89, 1.996, 1.43, 2.4525, −100, "LiF_1", .03, .60, 1.36, −.2784, −.6709]
"Data alfaMinusRinfinity=", 2.4525, "Calculated a=", 4.03836

"todraw=", $2.4525\, e^{(-4.03836\, \frac{1}{R^2})}$

"DerAlfMinusDR=", .903953
"DerAlfMinusDp=", −.860043
"DerAlfPlusDp", −.0263523

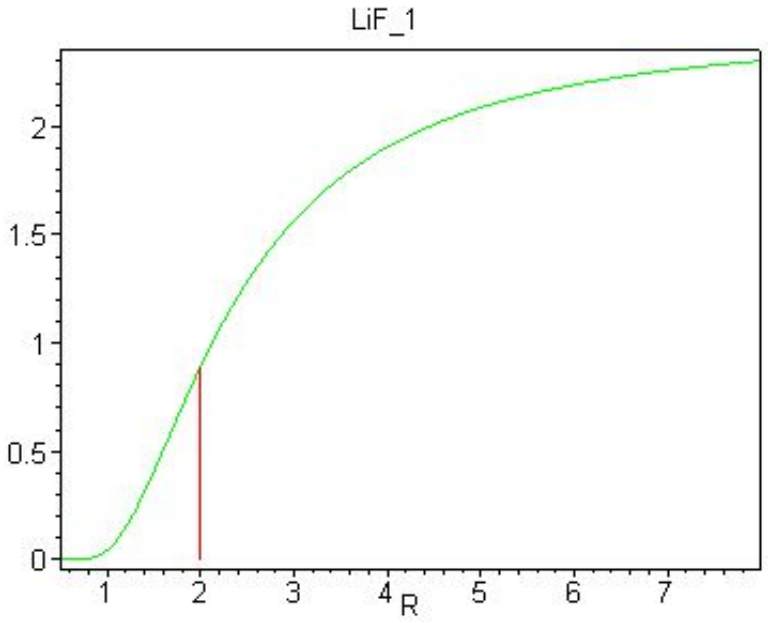

Figure 1: $\alpha_- = \alpha_-^{\infty} e^{-\frac{a}{R^2}}$ for salt LiF – Model 1

Furthermore, as Maple handles symbols, it is possible to execute Maple procedures although some data is not available. As an example, consider the case of salt $CaCl_2$ where the value of χ_T is unknown. The data related to this salt has been defined (*cgs* units) as shown in Table 3. In this case, it is possible to execute Model 1 procedure obtaining some partial results.

```
CaCl2_1:=[2.8740, 3.0307, xiunknown, 5.3643, -100, "CaCl2_1*",.4732, .99, 1.81,
-.2194, -1.9148];
```

Table 3: Data for $CaCl_2$ in *cgs* units

```
> Model_1(CaCl2_1);
```

"Model 1 for salt ", "CaCl2_1*", [2.8740, 3.0307, *xiunknown*, 5.3643, −100, "CaCl2_1*", .4732, .99, 1.81, −.2194, −1.9148]

"Data alfaMinusRinfinity=", 5.3643, "Calculated a=", 5.73217

"todraw=", $5.3643\, e^{(-5.73217\, \frac{1}{R^2})}$

"DerAlfMinusDR=", 1.18359

"DerAlfMinusDp=", $-1.19570\,xiunknown$

```
Error, (in Model_1) CationPressureDerivative expects its 2nd argument,
DerAlfMinusDp, to be of type float, but received -1.19570*xiunknown
```

3.3 Model 2

The Model 2 algorithm is presented in Algorithm 2

Algorithm 2: **Model 2**

Require: *Salt, s*

1: **procedure** Model_2(*Salt,s*)
2: **if** α_{-}^{∞} is known **then**
3: $a := \frac{\alpha_{-}^{\infty} - \alpha_{-}}{\alpha_{-} R^{s}}$
4: **else**
5: $\alpha_{-}^{\infty} := \alpha_{-}(1 + R^2)$
6: **end if**
7: $todraw(R) := \frac{\alpha_{-}^{\infty}}{1 + aR^{s}}$ {Model 2 equation 2}
8: $\frac{\partial \alpha_{-}}{\partial R} := \frac{\partial todraw(R)}{\partial R}$
9: $\frac{\partial \alpha_{-}}{\partial p} = \frac{\partial \alpha_{-}}{\partial R}(-\frac{\chi_T R}{3})$ {at the equilibrium R equation 3}
10: $\frac{\partial \alpha_{+}}{\partial p} := \alpha_{+}(\frac{1}{\alpha_{-}}\frac{\partial \alpha_{-}}{\partial p} + 3(\frac{1}{r_{+}}\frac{\partial r_{+}}{\partial p} - \frac{1}{r_{-}}\frac{\partial r_{-}}{\partial p}))$ {at the equilibrium R equation 4}
11: **print** all values
12: **plot** $todraw(R)$ and at the equilibrium R
13: **end**

Algorithm 2 for a given salt and $s = 3$ or $s = 4$ is implemented by `Model_2/1` Maple procedure, where:

- `<arg-1>` = Salt
- `<arg-2>` = s value for Model 2. Should be set as 3 or 4 otherwise the procedure informs the erro.

```
> Model_2 := proc(Salt::list, ModelSet::integer)
> local Calc_a, Calc_alfaMinusRinfinity,
> todraw, DerAlfMinusDR, DerAlfMinusDp,DerAlfPlusDp;
> if ModelSet=3 then print("Model 2 for salt ", Salt[SaltName],Salt)
> elif ModelSet=4 then print("Model 3 for salt ",
> Salt[SaltName],Salt); print("s=",ModelSet)
> else print("ERROR ModelSet should be 3 or 4!!!!") fi;
```

```
> if Salt[alfaMinusRinfinity] > 0
> then Calc_alfaMinusRinfinity := Salt[alfaMinusRinfinity];
> Calc_a := calculate_aORRequilModel_2(Salt,ModelSet);
> print("Data alfaMinusRinfinity=",
> Calc_alfaMinusRinfinity, "Calculated a=" ,Calc_a)
> else Calc_a :=Salt[a];
> Calc_alfaMinusRinfinity := calculate_aORRequilModel_2(Salt,ModelSet);
> print("Calculated alfaMinusRinfinity=",Calc_alfaMinusRinfinity,"Data
> a=", Calc_a) fi;
> todraw := alfMinusModel_2(Calc_alfaMinusRinfinity,
> Calc_a,R,ModelSet);
> print("todraw=" ,todraw);
> DerAlfMinusDR := eval(diff(todraw,R),R=Salt[Requil]);
> print("DerAlfMinusDR=", DerAlfMinusDR);
> DerAlfMinusDp := -DerAlfMinusDR*Salt[xi]*Salt[Requil]/3;
> print("DerAlfMinusDp=", DerAlfMinusDp);
> DerAlfPlusDp := CationPressureDerivative(Salt,DerAlfMinusDp);
> print("DerAlfPlusDp",DerAlfPlusDp);
> plot({[[Salt[Requil],0],[Salt[Requil],eval(todraw,
> R=Salt[Requil])]],todraw },R=0.5..4*Salt[Requil],title=Salt[SaltName]);
> end:
```

`Model_2/2` calls the following three Maple procedures

1. `calculate_aORRequilModel_2/2`
2. `alfMinusModel_2/2`
3. `CationPressureDerivative/2` which is also called by `Model_1/1` and has been described in Section 3.2 pg. 3

Procedure `calculate_aORRequilModel_2/2` calculates, for a given salt and s the value of a if the value of α_{-}^{∞} is known else it calculates the value of α_{-}^{∞} using Model 2 equation 2 for $s = 3$ or $s = 4$.

```
> calculate_aORRequilModel_2
> :=proc(Salt::list, ModelSet::integer)
> if Salt[alfaMinusRinfinity] > 0
> then (Salt[alfaMinusRinfinity]-Salt[alfaMinus])/
> ((Salt[Requil]^(-ModelSet))*Salt[alfaMinus])
> else Salt[alfaMinus]*(1+Salt[a]*Salt[Requil]^(-ModelSet)) fi end:
```

Procedure `alfMinusModel_2/2` calculates the value of α_- related to equation 2 for Model 2, where:

- `<arg-1>` α_-^∞
- `<arg-2>` a
- `<arg-3>` free variable used for plotting
- `<arg-4>` value of s for Model 2. Should be 3 or 4

```
> alfMinusModel_2:=proc(AlfInf::float,a::float,
> R, ModelSet::integer)
> AlfInf/(1+a*(R^(-ModelSet))) end:
```

In order to illustrate it follows an execution example of `Model_2/2` Maple procedure for salt LiF — Table 2 pg.3 — with $s = 3$ and $s = 4$. The call

```
> Model_2(LiF_1,3);
```

has the following output as well as the graph shown in Figure 2

"Model 2 for salt ", "LiF_1",
[.89, 1.996, 1.43, 2.4525, −100, "LiF_1", .03, .60, 1.36, −.2784, −.6709]
"s=", 3
"Data alfaMinusRinfinity=", 2.4525, "Calculated a=", 13.9609
$$\text{"todraw="}, 2.4525\,\frac{1}{1+\frac{13.9609}{R^3}}$$
"DerAlfMinusDR=", .852235
"DerAlfMinusDp=", −.810843
"DerAlfPlusDp", −.0246939

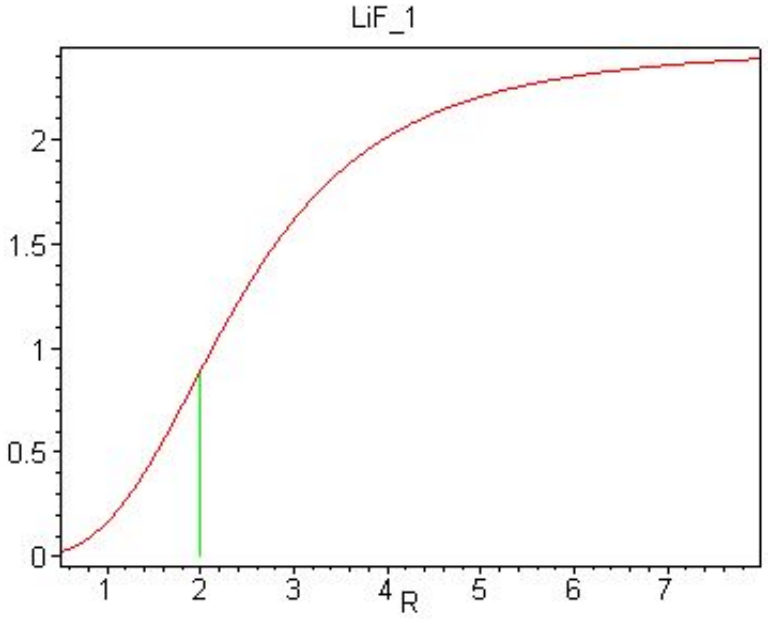

Figure 2: $\alpha_- = \alpha_-^\infty \frac{1}{1+aR^2}$ for salt LiF – Model 2 $s = 3$

The call

```
> Model_2(LiF_1,4);
```

has the following output as well as the graph shown in Figure 3

$$\text{“Model 3 for salt ”, “LiF\_1”,}$$
$$[.89,\ 1.996,\ 1.43,\ 2.4525,\ -100,\ \text{“LiF\_1”},\ .03,\ .60,\ 1.36,\ -.2784,\ -.6709]$$
$$\text{“s=”, 4}$$
$$\text{“Data alfaMinusRinfinity=”, 2.4525, “Calculated a=”, 27.8658}$$
$$\text{“todraw=”, } 2.4525\ \frac{1}{1+\frac{27.8658}{R^4}}$$
$$\text{“DerAlfMinusDR=”, 1.13632}$$
$$\text{“DerAlfMinusDp=”, } -1.08113$$
$$\text{“DerAlfPlusDp”, } -.0338046$$

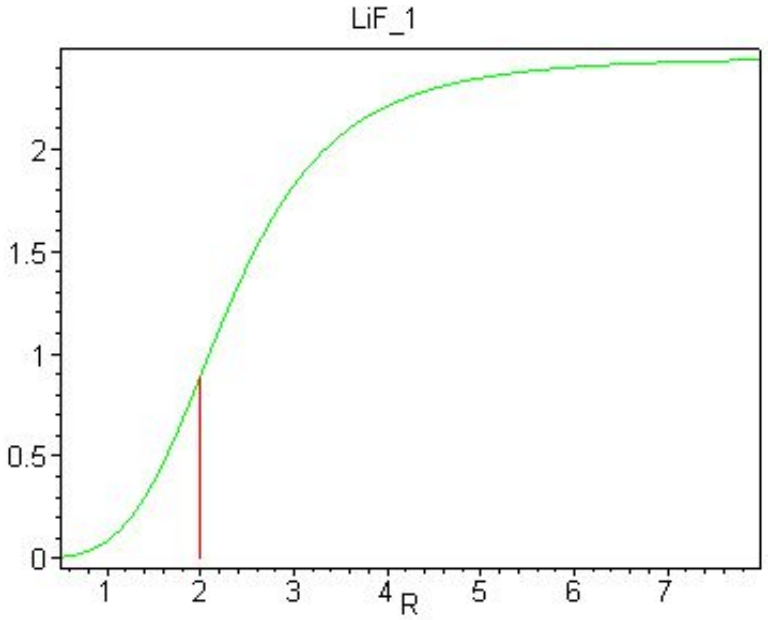

Figure 3: $\alpha_- = \alpha_-^\infty \frac{1}{1+aR^2}$ for salt LiF – Model 2 $s = 4$

4 Experimental Results

In this section the results obtained for different salts using data in *cgs* and *au* units are listed.

Salt	a	α_-^∞	$\frac{\partial \alpha_-}{\partial R}$	$\frac{\partial \alpha_-}{\partial p}$	$\frac{\partial \alpha_+}{\partial p}$
LiF	4.0384		0.9039	-0.8600	-0.0263
LiCl	3.8767		1.3927	-3.7717	0.0150
LiBr	2.8947		1.1974	-4.5479	0.0492
LiI	3.0	8.7358	1.4452	-8.2174	0.0860
	4.0	9.7988	1.9270	-10.9565	0.0727
NaF	4.6208		0.7798	-1.1872	-0.3465
NaCl	4.1657		1.2059	-4.4618	-0.1353
NaBr	3.1205		1.0363	-4.7958	0.0499
NaI	3.0	8.5209	1.1693	-8.0296	0.2424
	4.0	9.3985	1.5591	-10.7062	0.1805
KF	5.0120		0.6478	-1.7727	-3.7681
KCl	4.5423		1.0089	-5.5121	-2.5285
KBr	3.1777		0.8313	-5.5769	-1.4174
KI	3.0	8.5212	0.9408	-8.4801	-0.2759
	5.0	10.0428	1.5681	-14.1336	-0.9635
RbF	5.6907		0.6191	-2.1927	-8.3664
RbCl	4.6880		0.9345	-6.4973	-6.4212
RbBr	3.3705		0.7786	-6.8060	-4.2819
RbI	3.5	8.8714	0.9968	-11.4277	-2.5815
	5.5	10.3272	1.5664	-17.9578	-3.8778
CsF	5.8547		0.5604	-2.3680	-15.6616
CsCl	5.1005		0.8338	-4.4343	-10.2580
CsBr	3.6599		0.6932	-4.6125	-7.4059
CsI	3.5	8.5702	0.8025	-7.2432	-4.1760
	6.0	10.0997	1.3757	-12.4168	-5.9537
AgBr	3.1821		1.1110	-2.6204	
	1.0843		0.4875	-1.1410	
NaCN	3.5	4.5764	0.8599		
	4.0	4.8548	0.9827		
KCN	4.0	4.7475	0.7576	-5.7260	1.7579
	5.0	5.2190	0.9470	-7.1576	1.4013
$NaClO_3$	3.5	6.7949	0.9753	-4.1624	0.1298
	4.5	7.4579	1.2540	-5.3516	0.0941
$NaBrO_3$	3.5	8.1314	1.1068	-4.0152	0.0161
	4.5	8.8882	1.4230	-5.1624	-0.0122
NH_4F	5.3905		0.6667	-4.5298	-3.9389
NH_4Cl	5.2356		0.9336	-5.8277	-17.1863
NH_4Br	3.7272		0.7764	-5.8599	-15.3688
NH_4I	4.3827		1.0714	-8.9487	-24.1114
$CaCl_2$	5.7322		1.1836		
$SrCl_2$	4.3308		1.0413		
$SrBr_2$	5.7094		1.2479		
$BaCl_2$	4.1103		0.9918		
$BaBr_2$	3.7394		0.9529		
Results Using Interpolated α_- Values					
NaCN	3.0	5.6293	0.9618		
	4.0	6.3349	1.2824		
KCN	3.0	5.9781	0.7865	-5.9446	2.1146
	5.0	7.2243	1.3109	-9.9078	1.4013
$NaClO_3$	3.0	9.6518	1.2441	-5.3092	0.1476
	4.0	10.5935	1.6588	-7.0790	0.1120
$NaBrO_3$	3.0	10.7095	1.3063	-4.7390	0.0303
	4.0	11.7064	1.7418	-6.3187	0.0020

Table 4: Results from Model 1 with Data in *cgs* Units

Salt	a	α_-^∞	$\frac{\partial \alpha_-}{\partial R}$	$\frac{\partial \alpha_-}{\partial p}$	$\frac{\partial \alpha_+}{\partial p}$
LiF	13.9609		0.8522	-0.8108	-0.0247
LiCl	13.4967		1 .5699	-4.2518	0.0101
LiBr	9.6217		1.4850	-5.6403	0.0413
LiI	9.0	8.3579	1.6322	-9.2805	0.0809
	14.0	9.5622	2.2192	-12.6181	0.0647
NaF	16.9763		0.7788	-1.1856	-0.3463
NaCl	15.3677		1.4005	-5.1819	-0.1690
NaBr	11.0817		1.3068	-6.0479	0.0069
NaI	11.0	8.4937	1.5053	-10.3371	0.1890
	17.0	9.6630	2.0449	-14.0424	0.1033
KF	19.3798		0.6943	-1.8998	-3.8540
KCl	18.0474		1.2087	-6.6035	-2.7916
KBr	12.0796		1.0779	-7.2318	-1.7127
KI	12.0	8.5417	1.2615	-11.3706	-0.6275
	19.0	9.6393	1.7600	-15.9533	-1.1848
RbF	23.3949		0.6586	-2.3327	-8.5265
RbCl	19.2063		1.1333	-7.8795	-6.9620
RbBr	13.3327		1.0139	-8.8626	-4.8881
RbI	13.0	8.6512	1.2032	-13.7940	-3.0512
	23.0	10.0752	1.8279	-20.9558	-4.4730
CsF	24.7074		0.6159	-2.6025	-16.0936
CsCl	22.1951		1.0247	-5.4495	-10.9271
CsBr	15.4174		0.9101	-6.0561	-8.1308
CsI	15.4	8.5755	1.0780	-9.7296	-5.0303
	25.0	9.6761	1.5509	-13.9982	-6.4971
AgBr	11.1706		1.3840	-3.2645	
	3.3363		0.6855	-1.6169	
NaCN	11.0	4.3784	0.9631		
	17.0	5.1154	1.2740		
KCN	12.0	4.3873	0.7773	-5.8748	1.7209
	19.0	5.0502	1.0691	-8.0807	1.1712
$NaClO_3$	11.0	6.4382	1.0689	-4.5618	0.1178
	17.0	7.2742	1.4621	-6.2397	0.0675
$NaBrO_3$	11.0	7.6942	1.2047	-4.3705	0.0074
	17.0	8.6429	1.6575	-6.0130	-0.0332
NH_4F	21.4659		0.6946	-4.7123	-3.9779
NH_4Cl	22.3680		1.1100	-6.9911	-17.7548
NH_4Br	15.2951		1.0054	-7.5886	-16.0290
NH_4I	19.4057		1.3845	-11.5640	-25.4581
$CaCl_2$	24.1209		1.3207		
$SrCl_2$	16.7701		1.2455		
$SrBr_2$	24.3503		1.4264		
$BaCl_2$	15.7918		1.2042		
$BaBr_2$	14.5104		1.2006		
Results Using Interpolated α_- Values					
NaCN	11.0	5.7132	1.2568		
	17.0	6.6750	1.6624		
KCN	12.0	6.0731	1.0759	-8.1321	1.7209
	19.0	6.9907	1.4700	-11.1856	1.1712
$NaClO_3$	11.0	9.5808	1.5907	-6.7885	0.1178
	17.0	10.8249	2.1758	-9.2856	0.0675
$NaBrO_3$	11.0	10.5949	1.6589	-6.0182	0.0074
	17.0	11.9012	2.2824	-8.2799	-0.0332

Table 5: Results from Model 2 for $s = 3$ with Data in *cgs* Units

Salt	a	α_-^∞	$\frac{\partial \alpha_-}{\partial R}$	$\frac{\partial \alpha_-}{\partial p}$	$\frac{\partial \alpha_+}{\partial p}$
LiF	27.8658		1.1363	-1.0811	-0.0338
LiCl	34.2680		2.0932	-5.6690	-0.0044
LiBr	26.1036		1.9700	-7.5203	0.0276
LiI	26.1	8.3203	2.1483	-12.2150	0.0667
	34.3	8.9897	2.6130	-14.8574	0.0538
NaF	38.9606		1.0384	-1.5808	-0.4033
NaCl	42.8605		1.8673	-6.9092	-0.2499
NaBr	32.7353		1.7424	-8.0338	-0.0624
NaI	32.7	8.3452	1.9013	-13.0563	0.1261
	42.9	8.9675	2.3212	-15.9401	0.0593
KF	51.3179		0.9257	-2.5331	-4.2814
KCl	56.2360		1.6116	-8.8047	-3.3222
KBr	39.4037		1.4373	-9.6424	-2.1428
KI	34.4	8.2060	1.4386	-12.9661	-0.8215
	56.2	9.1859	2.0995	-18.9234	-1.5461
RbF	65.2482		0.8781	-3.1102	-9.4160
RbCl	62.5933		1.5111	-10.5060	-7.9898
RbBr	45.4646		1.3519	-11.8168	-5.7589
RbI	45.5	8.5859	1.5594	-17.8782	-3.8620
	65.2	9.3591	2.0500	-23.5023	-4.9786
CsF	73.6946		0.8212	-3.4600	-17.6920
CsCl	78.0158		1.3663	-7.2660	-12.1245
CsBr	56.4970		1.2135	-8.0649	-9.1445
CsI	56.5	8.4701	1.3683	-12.3501	-5.9307
	78.0	9.1018	1.7579	-15.8661	-7.1389
AgBr	32.1712		1.8454	-4.3528	
	9.6085		0.9140	-2.1559	
NaCN	32.0	4.3779	1.2839		
	43.0	4.8423	1.5598		
KCN	34.0	4.2416	0.9345	-7.0633	1.4247
	56.0	4.8827	1.3371	-10.1064	0.6665
$NaClO_3$	32.0	6.2659	1.2998	-5.5471	0.0883
	43.0	6.7335	1.6253	-6.9363	0.0467
$NaBrO_3$	32.0	7.4644	1.4370	-5.2131	-0.0134
	43.0	7.9833	1.8055	-6.5498	-0.0464
NH_4F	56.4553		0.9261	-6.2924	-4.3018
NH_4Cl	75.0668		1.4933	-9.3214	-18.8937
NH_4Br	53.7776		1.3405	-10.1180	-16.9950
NH_4I	73.4507		1.8461	-15.4188	-27.4431
$CaCl_2$	73.1033		1.7609		
$SrCl_2$	50.8321		1.6607		
$SrBr_2$	77.0248		1.9019		
$BaCl_2$	48.3322		1.6056		
$BaBr_2$	46.7821		1.6008		
Results Using Interpolated α_- Values					
NaCN	32.0	5.7127	1.6753		
	43.0	6.3186	2.0353		
KCN	34.0	5.8714	1.2936	-9.7773	1.4247
	56.0	6.7587	1.8509	-13.9896	0.6665
$NaClO_3$	32.0	9.3244	1.9343	-8.2548	0.0882
	43.0	10.0203	2.4187	-10.3220	0.0468
$NaBrO_3$	32.0	10.2785	1.9787	-7.1784	-0.0134
	43.0	10.9930	2.4861	-9.0190	-0.0464

Table 6: Results from Model 2 for $s = 4$ with Data in *cgs* Units

Salt	a	α_-^∞	$\frac{\partial \alpha_-}{\partial R}$	$\frac{\partial \alpha_-}{\partial p}$	$\frac{\partial \alpha_+}{\partial p}$
LiF	14.4213		3.2281	-5.8039	-0.1778
LiCl	13.8438		4.9733	-25.4529	0.1009
LiBr	10.3373		4.2760	-30.6912	0.3297
LiI	14.4	66.3717	6.9369	-74.5360	0.4880
	10.3	58.1739	4.9619	-53.3140	0.5908
NaF	16.5009		2.7848	-8.0114	-2.3386
NaCl	14.8760		4.3064	-30.1103	-0.9134
NaBr	11.1435		3.7006	-32.3635	0.3366
NaI	16.5	67.4012	6.4310	-83.4550	1.1716
	11.1	58.1156	4.3263	-56.1427	1.8039
KF	17.8981		2.3135	-11.9625	-25.4287
KCl	16.2212		3.6029	-37.1977	-17.0631
KBr	11.3479		2.9685	-37.6350	-9.5651
KI	17.8	67.6867	5.5826	-95.0843	-6.4668
	11.3	58.2858	3.5440	-60.3623	-2.2439
RbF	20.3214		2.2107	-14.7972	-56.4545
RbCl	16.7416		3.3373	-43.8467	-41.2525
RbBr	12.0365		2.7806	-45.9300	-28.8913
RbI	20.3	70.6758	5.7815	-125.254	-26.9728
	12.0	58.2353	3.4176	-74.0413	-16.8057
CsF	20.9076		2.0013	-15.9802	-105.691
CsCl	18.2147		2.9778	-29.9251	-69.2261
CsBr	13.0699		2.4754	-31.1272	-39.9779
CsI	20.9	67.4994	4.7922	-81.7350	-39.4719
	13.1	58.4778	3.0037	-51.2310	-28.9902
AgBr	11.3636		3.9674	-17.6840	
	3.8725		1.7411	-7.7605	
NaCN	16.5	35.2523	4.0538		
	11.1	28.4873	2.7271		
KCN	17.8	35.1679	3.3714	-48.1523	9.4939
	11.3	29.6009	2.1402	-30.5684	13.8752
$NaClO_3$	16.5	50.8956	4.5979	-37.0810	0.6065
	11.1	44.2126	3.0932	-24.9453	0.9701
$NaBrO_3$	16.5	60.6277	5.2179	-35.7707	-0.1051
	11.1	52.9935	3.5102	-24.0640	0.139
NH_4F	5.3905		0.6667	-4.5298	-3.9389
NH_4Cl	18.6969		3.3340	-39.3273	-115.979
NH_4Br	13.3107		2.7726	-39.5460	-103.730
NH_4I	15.6508		3.8261	-60.3883	-141.518
$CaCl_2$	20.4700		4.2267		
$SrCl_2$	15.4654		3.7188		
$SrBr_2$	20.3889		4.4563		
$BaCl_2$	14.6784		3.5419		
$BaBr_2$	13.3537		3.4031		
Results Using Interpolated α_- Values					
NaCN	16.5	46.0001	5.2897		
	11.1	38.4775	3.5585		
KCN	17.8	48.6805	4.6668	-66.6540	9.4940
	11.3	40.9744	2.9626	-42.3137	13.8552
$NaClO_3$	16.5	75.7389	6.8423	-55.1810	0.6065
	11.1	65.7938	4.6030	-37.1217	0.9701
$NaBrO_3$	16.5	83.4841	7.1850	-49.2560	-0.1051
	11.1	72.9718	4.8335	-33.1358	0.1839

Table 7: Results from Model 1 with Data in *au* Units

Salt	a	α_-^∞	$\frac{\partial \alpha_-}{\partial R}$	$\frac{\partial \alpha_-}{\partial p}$	$\frac{\partial \alpha_+}{\partial p}$
LiF	94.2133		3.0434	-5.4718	-0.1666
LiCl	91.0807		5.6064	-28.6928	0.0679
LiBr	64.9294		5.3030	-38.0623	0.2761
LiI	94.2	64.4619	7.9098	-84.9890	0.4373
	65.0	57.4283	6.1264	-65.8267	0.5302
NaF	114.560		2.7812	-8.0009	-2.3370
NaCl	103.706		5.0014	-34.9700	-1.1409
NaBr	74.7808		4.6668	-40.8130	0.0464
NaI	114.5	64.1656	7.2930	-94.6413	0.9127
	74.8	57.4287	5.4062	-70.1563	1.4795
KF	130.783		2.4794	-12.8206	-26.0079
KCl	121.793		4.3163	-44.5630	-18.8386
KBr	81.5174		3.8494	-48.8020	-11.5574
KI	130.8	65.4548	6.4083	-109.149	-8.1774
	81.5	57.7240	4.5277	-77.1173	-4.2816
RbF	157.874		2.3518	-15.7418	-57.5353
RbCl	129.613		4.0472	-53.1740	-44.9024
RbBr	89.9707		4.6208	-59.8080	-32.9819
RbI	157.8	68.3593	6.6006	-142.999	-30.4958
	89.9	58.6906	4.3799	-94.3890	-20.9445
CsF	166.734		2.1994	-17.5623	-108.606
CsCl	149.785		3.6596	-36.7760	-73.7421
CsBr	104.041		3.2501	-40.8683	-54.8693
CsI	166.7	65.0674	5.4920	-93.6720	-43.5735
	104.0	57.8794	3.8519	-65.6970	-33.9610
AgBr	75.3825		4.9425	-22.0303	
	22.5141		2.4480	-10.9115	
NaCN	114.5	34.4932	4.5443		
	74.8	28.6164	3.4575		
KCN	130.8	34.3250	3.8671	-55.2333	7.7295
	81.5	29.6561	2.7889	-39.8333	11.5668
$NaClO_3$	114.5	49.0573	5.2144	-42.0530	0.4575
	74.8	43.5260	3.8394	-30.9663	0.7898
$NaBrO_3$	114.5	58.2909	5.9113	-40.5247	-0.2225
	74.8	52.0134	4.3278	-29.6688	0.0455
NH_4F	144.860		2.4805	-31.8478	-26.8448
NH_4Cl	150.949		3.9995	-47.1783	-119.817
NH_4Br	103.218		3.5904	-51.2103	-108.168
NH_4I	130.955		4.9443	-78.0387	-149.423
$CaCl_2$	162.779		4.7164		
$SrCl_2$	113.169		4.4478		
$SrBr_2$	164.325		5.0937		
$BaCl_2$	106.572		4.3005		
$BaBr_2$	97.9193		4.2873		
Results Using Interpolated α_- Values					
NaCN	114.5	45.0096	5.9298		
	74.8	38.6460	4.5117		
KCN	130.8	47.5137	5.3530	-76.4557	7.7297
	81.5	41.0510	3.8605	-55.1390	11.5667
$NaClO_3$	114.5	73.0034	7.7598	-62.5800	0.4575
	74.8	64.7721	5.7135	-46.0773	0.7898
$NaBrO_3$	114.5	80.2663	8.1399	-55.8023	-0.2225
	74.8	71.6222	5.9594	-40.8540	0.0455

Table 8: Results from Model 2 for $s = 3$ with Data in *au* Units

Salt	a	α_-^∞	$\frac{\partial \alpha_-}{\partial R}$	$\frac{\partial \alpha_-}{\partial p}$	$\frac{\partial \alpha_+}{\partial p}$
LiF	355.363		4.0579	-7.2958	-0.2281
LiCl	437.005		7.4752	-38.2570	-0.0297
LiBr	332.878		7.0706	-50.7497	0.1840
LiI	355.4	57.1225	8.0518	-86.5157	0.4299
	332.8	56.1467	7.6709	-82.4223	0.4498
NaF	496.834		3.7082	-10.6678	-2.7214
NaCl	546.572		6.6685	-46.6267	-1.6866
NaBr	417.442		6.2224	-54.4177	-0.4209
NaI	496.8	58.8921	7.7348	-100.374	0.7700
	417.4	56.3287	6.7943	-88.1700	1.0625
KF	654.434		3.3059	-17.0942	-28.8925
KCl	717.166		5.7550	-59.4170	-22.4194
KBr	502.497		5.1325	-65.0697	-14.4597
KI	654.4	60.5078	7.0138	-119.461	-9.4315
	502.4	56.8930	5.7268	-97.5407	-6.7656
RbF	832.061		3.1358	-20.9890	-63.5385
RbCl	798.232		5.3963	-70.8987	-51.8380
RbBr	579.763		4.8277	-79.7440	-38.8583
RbI	832.1	63.1716	7.3248	-158.690	-33.6109
	579.7	57.9293	5.5648	-120.559	-26.0408
CsF	939.797		2.9325	-23.4165	-119.392
CsCl	994.928		4.8794	-49.0343	-81.8222
CsBr	720.474		4.3334	-54.4913	-61.7102
CsI	939.8	60.5688	6.0148	-102.589	-56.6376
	720.4	57.1574	4.8858	-83.3327	-40.0208
AgBr	410.263		6.5800	-29.3737	
	122.531		3.2640	-14.5487	
NaCN	496.8	31.5256	5.2307		
	417.4	29.7519	4.6567		
KCN	654.4	32.0287	4.5014	-64.2930	5.4724
	502.4	29.6949	3.7288	-53.2570	8.2221
$NaClO_3$	496.8	44.2798	5.3961	-43.5177	0.4136
	417.4	42.4938	4.7242	-38.0990	0.5760
$NaBrO_3$	496.8	52.5873	5.9844	-41.0253	-0.2348
	417.4	50.6053	5.2249	-35.8187	-0.1063
NH_4F	719.957		3.3073	-42.4637	-29.0302
NH_4Cl	957.303		5.3327	-62.9043	-127.501
NH_4Br	685.808		4.7872	-68.2803	-114.686
NH_4I	936.673		6.5924	-104.051	-161.073
$CaCl_2$	932.265		6.2884		
$SrCl_2$	648.222		5.9304		
$SrBr_2$	982.264		6.7917		
$BaCl_2$	616.376		5.7339		
$BaBr_2$	596.623		5.7164		
Results Using Interpolated α_- Values					
NaCN	496.8	41.1373	6.8255		
	417.4	38.8227	6.0765		
KCN	654.4	44.3352	6.2311	-88.9967	5.4724
	502.4	41.0907	5.1615	-73.7197	8.2221
$NaClO_3$	496.8	65.8938	8.0300	-64.7597	0.4136
	417.4	63.2361	7.0302	-56.6963	0.5759
$NaBrO_3$	496.8	72.4124	8.2905	-56.4920	-0.2348
	417.4	69.6832	7.1946	-49.3223	-0.1063

Table 9: Results from Model 2 for $s = 4$ with Data in *au* Units

5 Conclusions

Salts for which there are experimental data at high pressures were studied in order to establish the validity of the model. Results of $\frac{\partial \alpha}{\partial p}$ obtained with the method developed in this report and implemented as Maple procedures are, in absolute value, lower than those calculated via experimental data; on the other hand, the empirical method we proposed previously [13] gave values higher than the experimental ones.

We may therefore predict upper and lower bounds of the experimental data. Results for more complex materials are given in this report showing the same behaviour as described previously when compared to results obtained with other methods.

6 Appendix - Experimental Data

Experimental data used in this work has been taken from the experimental data at Low Temperature – LT – and Room Temperature – RT – described in [7]. It should be noted that some data was not available at LT, in those cases the missing data (data with an $*$ in Table 10) has been substituted by data at RT from the same source.

Struct.	Salt	α_+ $10^{-24}cm^3$	α_- $10^{-24}cm^3$	R $10^{-8}cm$	χ_T $10^{-12}cm^2dyn^{-1}$
fcc	Li	0.030			
C=2	LiF		0.89	1.996	1.43
	LiCl		2.94	2.539	3.20
	LiBr		4.13	2.713	*4.20
	LiI		6.19	2.951	*5.7803
	Na	0.147			
	NaF		1.02	2.295	1.99
	NaCl		3.14	2.789	3.98
	NaBr		4.28	2.954	4.70
	NaI		6.35	3.194	6.45
	K	0.81			
	KF		1.20	2.648	3.10
	KCl		3.36	3.116	5.26
	KBr		4.54	3.262	6.17
	KI		6.66	3.489	7.75
	Rb	1.35			
	RbF		1.18	2.789	*3.81
	RbCl		3.45	3.259	*6.40
	RbBr		4.58	3.410	*7.69
	RbI		6.80	3.628	*9.48
	Cs	2.34			
	CsF		1.27	2.9827	*4.25
bcc	Cs	2.34			
C= $\frac{8}{3\sqrt{3}}$	CsCl		3.55	3.5150	4.5387
	CsBr		4.66	3.6645	5.4476
	CsI		6.81	3.9018	6.9396
	AgBr		4.17	2.88	2.457
			5.37		
	NaCN		3.0271	2.91	
	KCN		3.2509	3.25	6.9767
	$NaClO_3$		4.9055	3.2775	3.90625
	$NaBrO_3$		5.9550	3.3445	3.24675
	NH_4F	0.2316	1.125	2.63	7.75
	NH_4Cl	1.647	3.37	3.356	5.58
	NH_4Br	1.729	4.527	3.516	6.44
	NH_4I	3.413	6.628	3.785	6.62
	Ca	0.47315			
	$CaCl_2$		2.8740	3.0307	
	Sr	0.7706			
	$SrCl_2$		3.3481	3.0311	
	$SrBr_2$		3.4589	3.1632	
	Ba	1.4967			
	$BaCl_2$		3.4590	3.0606	
	$BaBr_2$		4.2711	3.2243	

Table 10: Experimental Data at Low Temperatures

The following values of r_+, $-\frac{\partial r_+}{\partial p}$, r_- and $-\frac{\partial r_-}{\partial p}$ for different anions and cations at Low Temperature have been used.

Cation	r_+	$-\frac{\partial r_+}{\partial p}$	Anion	r_-	$-\frac{\partial r_-}{\partial p}$
Li	0.60	0.2780	F	1.36	0.6709
Na	0.95	0.8466	Cl	1.81	1.9148
K	1.33	2.0636	Br	1.95	2.6866
Rb	1.48	2.8707	I	2.16	4.0229
Cs	1.69	3.5537	CN	1.94	5.4953
Ag		0.0981	ClO_3	2.33	3.4175
Ca	0.99	0.2194	BrO_3	2.40	2.7684
Sr	1.13	0.5256			
Ba	1.35	0.8974			
NH_4F	1.27	6.1218			
NH_4Cl	1.55	6.1218			
NH_4Br	1.57	6.1218			
NH_4I	1.63	6.1218			

Table 11: Values of $\frac{1}{r_+}$, $-\frac{\partial r_+}{\partial p}$, $\frac{1}{r_-}$ and $-\frac{\partial r_-}{\partial p}$ at Low Temperatures in *cgs* Units

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