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Abstract

A new way of evaluating the pressure dependence of ionic radii was developed previously and used for alkali halides. It is now extended and applied to crystals with more complex ions and results are compared to those obtained with the first method we developed previously.

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1 Introduction

The importance of the evaluation of the pressure dependence of ionic radii is reflected not only by the magnitude itself, but also due to its use in the evaluation of ionic polarizabilities and dielectric constants at high pressures [1, 2, 15, 11, 12, 10, 13, 14]. As the ionic contributions cannot be compared to experimental values, it is important to have different ways of evaluating them as we described in the references mentioned above. In this work we apply the evaluation of $\frac{\partial r_i}{\partial p}$ to more complex ions using both the methods mentioned.

This work is organized as follows: in Section 2 the method implemented by the Maple V module PRad is described. In Section 3 two case study are presented showing the correspondence among the salts being studied and the $\frac{\partial R}{\partial p}$ notation used by the PRad module. For each case study several results obtained using different constraints to run the module are also shown. Similarly, the method implemented by the Maple V module PDac is described in Section 4. Results obtained considering the same two case study are shown in Section 5. Conclusions are presented in Section 6.

2 Module PRad Description

This module, implemented in Maple V [3]and described in detail in [13], is responsible for the calculation of the maximum values of the absolute value of the quantities $\frac{\partial r_+}{\partial p}$, $\frac{\partial r_-}{\partial p}$ and $\frac{\partial R}{\partial p}$ such that they verify

$$\frac{\partial r_+}{\partial p} + \frac{\partial r_-}{\partial p} \leq \frac{\partial R}{\partial p} \tag{1}$$

using data from Table 22.

The general notation used by this module is similar to the one used by the PDac module from the Polariz System — see Section 4 — but considering only the derivatives, i.e. the input to the system are the derivatives. The notation used by the system is shown in Table 1, assuming we have n_c different cations $\mathbf{c}$ and n_a different anions $\mathbf{a}$ with $md = n_c + n_a$

Cations	$\mathbf{c}_1$	$\mathbf{c}_2$	$\mathbf{c}_3$	$\ldots$	$\mathbf{c}_{n_c}$
	$\frac{\partial r_1}{\partial p}$	$\frac{\partial r_2}{\partial p}$	$\frac{\partial r_3}{\partial p}$	$\ldots$	$\frac{\partial r_{n_c}}{\partial p}$
Anions	$\mathbf{a}_{n_c+1}$	$\mathbf{a}_{n_c+2}$	$\mathbf{a}_{n_c+3}$	$\ldots$	$\mathbf{a}_{n_c+n_a}$
	$\frac{\partial r_{n_c+1}}{\partial p}$	$\frac{\partial r_{n_c+2}}{\partial p}$	$\frac{\partial r_{n_c+3}}{\partial p}$	$\ldots$	$\frac{\partial r_{n_c+n_a}}{\partial p}$

Table 1: General Notation

the system implements the linear programming problem of the form

$$maximize\ Z = \sum_{k=1}^{md} \frac{\partial r_k}{\partial p} \tag{2}$$

subject to the restrictions

$$\frac{\partial r_i}{\partial p} + \frac{\partial r_j}{\partial p} \leq \frac{\partial R_{ij}}{\partial p} \; for \begin{cases} i \; is \; any \; value \; in \; \{1..n_c\} \\ j \; is \; any \; value \; in \; \{n_c + 1..n_c + n_a\} \end{cases} \tag{3}$$

all nonnegative. All instances of i and j values are user defined through the corresponding companion matrix, such that they verify the restrictions defined by the system of inequalities (3) as ilustrated later on. To solve this problem the user is also allowed to fix one or more $\frac{\partial r_k}{\partial p}$.

Also, for each one of the equations of the system the linear error e_{ij} is calculated for user's defined i and j as

$$e_{ij} = \frac{\partial r_i}{\partial p} + \frac{\partial r_j}{\partial p} - \frac{\partial R_{ij}}{\partial p} \tag{4}$$

as well as

$$e = \sqrt{\sum_{i,j} (e_{ij})^2} \tag{5}$$

3 Examples and Results

In this section two case study are presented showing the correspondence among the salts being studied and the $\frac{\partial R_{ij}}{\partial p}$ notation used by this module. Furthermore, we show the results of using different constraints to run the module. It should be observed that the system has too many degree of freedom and some times a solution $\frac{\partial r_k}{\partial p} = 0$ is factible. Adding constraints allows the user to study the behavior of the system as well as testing specific $\frac{\partial r_k}{\partial p}$values.

In what follows the symbol $\oplus$ in front of a value means that this value has been fixed by the user for that run, while a $\bullet$ indicates that a zero value is a solution to the system.

3.1 Module PRad - Case Study 6

This sixth case study considers the same anions and cations than case 5 published in [13], incremented by just one anion CN^- and one salt KCN as shown in Table 2.

Cations	Li^+ $\frac{\partial r_1}{\partial p}$	Na^+ $\frac{\partial r_2}{\partial p}$	K^+ $\frac{\partial r_3}{\partial p}$	Rb^+ $\frac{\partial r_4}{\partial p}$	Cs^+ $\frac{\partial r_5}{\partial p}$	Ca^{2+} $\frac{\partial r_6}{\partial p}$	Sr^{2+} $\frac{\partial r_7}{\partial p}$	Ba^{2+} $\frac{\partial r_8}{\partial p}$	Mg^{2+} $\frac{\partial r_9}{\partial p}$	NH_4^+ $\frac{\partial r_{10}}{\partial p}$
Anions	F^- $\frac{\partial r_{11}}{\partial p}$	Cl^- $\frac{\partial r_{12}}{\partial p}$	Br^- $\frac{\partial r_{13}}{\partial p}$	I^- $\frac{\partial r_{14}}{\partial p}$	O^{2-} $\frac{\partial r_{15}}{\partial p}$	ClO_3^- $\frac{\partial r_{16}}{\partial p}$	BrO_3^- $\frac{\partial r_{17}}{\partial p}$	CN^- $\frac{\partial r_{18}}{\partial p}$		

Table 2: Case 6 – Cations and Anions Considered

Thus $n_c = 10$, $n_a = 8$ and $md = 18$ with

$$maximize \; Z = \sum_{k=1}^{18} \frac{\partial r_k}{\partial p} \tag{6}$$

subject to the restrictions

$$\frac{\partial r_i}{\partial p} + \frac{\partial r_j}{\partial p} \leq \frac{\partial R_{ij}}{\partial p} \; for \begin{cases} i \in \{1..10\} \\ j \in \{11..18\} \end{cases}$$

all nonnegative making 35 inequalities where the correspondence among the salts being studied and the $\frac{\partial R_{ij}}{\partial p}$ notation is shown in Table 3.

LiF $\frac{\partial R_{1,11}}{\partial p}$	LiCl $\frac{\partial R_{1,12}}{\partial p}$	LiBr $\frac{\partial R_{1,13}}{\partial p}$	LiI $\frac{\partial R_{1,14}}{\partial p}$	NaF $\frac{\partial R_{2,11}}{\partial p}$	NaCl $\frac{\partial R_{2,12}}{\partial p}$	NaBr $\frac{\partial R_{2,13}}{\partial p}$	NaI $\frac{\partial R_{2,14}}{\partial p}$	$NaClO_3$ $\frac{\partial R_{2,16}}{\partial p}$	$NaBrO_3$ $\frac{\partial R_{2,17}}{\partial p}$
KF $\frac{\partial R_{3,11}}{\partial p}$	KCl $\frac{\partial R_{3,12}}{\partial p}$	KBr $\frac{\partial R_{3,13}}{\partial p}$	KI $\frac{\partial R_{3,14}}{\partial p}$	KCN $\frac{\partial R_{3,18}}{\partial p}$	RbF $\frac{\partial R_{4,11}}{\partial p}$	RbCl $\frac{\partial R_{4,12}}{\partial p}$	RbBr $\frac{\partial R_{4,13}}{\partial p}$	RbI $\frac{\partial R_{4,14}}{\partial p}$	
CsF $\frac{\partial R_{5,11}}{\partial p}$	CsCl $\frac{\partial R_{5,12}}{\partial p}$	CsBr $\frac{\partial R_{5,13}}{\partial p}$	CsI $\frac{\partial R_{5,14}}{\partial p}$						
CaF $\frac{\partial R_{6,11}}{\partial p}$	CaO $\frac{\partial R_{6,15}}{\partial p}$	SrF $\frac{\partial R_{7,11}}{\partial p}$	SrCl $\frac{\partial R_{7,12}}{\partial p}$	SrO $\frac{\partial R_{7,15}}{\partial p}$	BaF $\frac{\partial R_{8,11}}{\partial p}$	BaO $\frac{\partial R_{8,15}}{\partial p}$	MgO $\frac{\partial R_{9,15}}{\partial p}$		
NH_4F $\frac{\partial R_{10,11}}{\partial p}$	NH_4Cl $\frac{\partial R_{10,12}}{\partial p}$	NH_4Br $\frac{\partial R_{10,13}}{\partial p}$	NH_4I $\frac{\partial R_{10,14}}{\partial p}$						

Table 3: Case 6 – Correspondence Among Salts

In matrix form $\mathbf{Ar} \leq \mathbf{R}$ where $\mathbf{A}$, $\mathbf{r}$, and $\mathbf{R}$ are defined as shown in (7).

$$\mathbf{A} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0
\end{pmatrix} \quad \mathbf{r} = \begin{pmatrix}
\frac{\partial r_1}{\partial p} \\ \frac{\partial r_2}{\partial p} \\ \frac{\partial r_3}{\partial p} \\ \frac{\partial r_4}{\partial p} \\ \frac{\partial r_5}{\partial p} \\ \frac{\partial r_6}{\partial p} \\ \frac{\partial r_7}{\partial p} \\ \frac{\partial r_8}{\partial p} \\ \frac{\partial r_9}{\partial p} \\ \frac{\partial r_{10}}{\partial p} \\ \frac{\partial r_{11}}{\partial p} \\ \frac{\partial r_{12}}{\partial p} \\ \frac{\partial r_{13}}{\partial p} \\ \frac{\partial r_{14}}{\partial p} \\ \frac{\partial r_{15}}{\partial p} \\ \frac{\partial r_{16}}{\partial p} \\ \frac{\partial r_{17}}{\partial p} \\ \frac{\partial r_{18}}{\partial p}
\end{pmatrix} \quad \mathbf{R} = \begin{pmatrix}
\frac{\partial R_{1,11}}{\partial p} \\ \frac{\partial R_{1,12}}{\partial p} \\ \frac{\partial R_{1,13}}{\partial p} \\ \frac{\partial R_{1,14}}{\partial p} \\ \frac{\partial R_{2,11}}{\partial p} \\ \frac{\partial R_{2,12}}{\partial p} \\ \frac{\partial R_{2,13}}{\partial p} \\ \frac{\partial R_{2,14}}{\partial p} \\ \frac{\partial R_{2,16}}{\partial p} \\ \frac{\partial R_{2,17}}{\partial p} \\ \frac{\partial R_{3,11}}{\partial p} \\ \frac{\partial R_{3,12}}{\partial p} \\ \frac{\partial R_{3,13}}{\partial p} \\ \frac{\partial R_{3,14}}{\partial p} \\ \frac{\partial R_{3,18}}{\partial p} \\ \frac{\partial R_{4,11}}{\partial p} \\ \frac{\partial R_{4,12}}{\partial p} \\ \frac{\partial R_{4,13}}{\partial p} \\ \frac{\partial R_{4,14}}{\partial p} \\ \frac{\partial R_{5,11}}{\partial p} \\ \frac{\partial R_{5,12}}{\partial p} \\ \frac{\partial R_{5,13}}{\partial p} \\ \frac{\partial R_{5,14}}{\partial p} \\ \frac{\partial R_{6,11}}{\partial p} \\ \frac{\partial R_{6,15}}{\partial p} \\ \frac{\partial R_{7,11}}{\partial p} \\ \frac{\partial R_{7,12}}{\partial p} \\ \frac{\partial R_{7,15}}{\partial p} \\ \frac{\partial R_{8,11}}{\partial p} \\ \frac{\partial R_{8,15}}{\partial p} \\ \frac{\partial R_{9,15}}{\partial p} \\ \frac{\partial R_{10,11}}{\partial p} \\ \frac{\partial R_{10,12}}{\partial p} \\ \frac{\partial R_{10,13}}{\partial p} \\ \frac{\partial R_{10,14}}{\partial p}
\end{pmatrix} \tag{7}$$

Table 4 shows the results obtained by different tests T under the restrictions given by equa-

tion (7) where

$$\begin{aligned}\mathbf{R}^t = (&.9514, 2.7083, 3.7982, 5.6859, 1.5224, 3.7000, 4.6279, 6.8671, 4.2676,\\ &3.6196, 2.7363, 5.4634, 6.7088, 9.0133, 7.5581, 3.5420, 6.9525,\\ &8.7410, 11.4645, 4.2308, 5.3178, 6.6542, 9.0256, .8915, .7206,\\ &1.1981, 3.3128, .9592, 1.5703, 1.2436, .4255, 6.79417, 6.24216,\\ &7.54768, 8.35223)\end{aligned}$$

The Z column correspond to the Z value defined by equation (6) and the e column is defined by equation (8).

$$e = \sqrt{\sum_{i,j}(e_{ij})^2} \; for \begin{cases} i \in \{1..10\} \\ j \in \{11..18\} \end{cases} \tag{8}$$

$\frac{\partial r_i}{\partial p}$	T0-1	T-2	T-3	T-4	T-5	T-6
$\frac{\partial r_1}{\partial p}$	.7805	.2805	$\oplus$.2780	.5798	$\oplus$.2780	.2805
$\frac{\partial r_2}{\partial p}$	•	$\oplus$.8466	$\oplus$.8466	$\oplus$.8466	$\oplus$.8466	$\oplus$.8466
$\frac{\partial r_3}{\partial p}$	2.5654	$\oplus$2.0636	$\oplus$2.0636	$\oplus$2.0636	$\oplus$2.0636	$\oplus$2.0636
$\frac{\partial r_4}{\partial p}$	3.3711	2.8711	2.8711	3.1704	3.0269	2.8711
$\frac{\partial r_5}{\partial p}$	3.6056	3.1056	2.8875	3.4358	3.1031	3.4358
$\frac{\partial r_6}{\partial p}$	.7206	.2206	2206	.3764	.3764	.2206
$\frac{\partial r_7}{\partial p}$	.95920	.5272	.5272	.6150	.6150	.5272
$\frac{\partial r_8}{\partial p}$	1.2436	.8994	.8994	.8994	.8994	.8994
$\frac{\partial r_9}{\partial p}$	.42550	.0813	.0813	.0813	.0813	.0813
$\frac{\partial r_{10}}{\partial p}$	4.5299	4.0300	2.9443	4.3293	4.0275	4.3293
$\frac{\partial r_{11}}{\partial p}$	.1709	$\oplus$.6709	$\oplus$.6709	.3715	.5151	$\oplus$.6709
$\frac{\partial r_{12}}{\partial p}$	1.7122	2.2122	2.4303	1.8819	2.2147	1.8819
$\frac{\partial r_{13}}{\partial p}$	3.0177	3.5177	3.5202	3.2183	3.5202	3.2183
$\frac{\partial r_{14}}{\partial p}$	3.8222	4.3222	5.4079	$\oplus$4.0229	$\oplus$4.0229	$\oplus$4.0229
$\frac{\partial r_{15}}{\partial p}$	•	$\oplus$.3442	$\oplus$.3442	$\oplus$.3442	$\oplus$.3442	$\oplus$.3442
$\frac{\partial r_{16}}{\partial p}$	4.2676	3.4210	3.4210	3.4210	3.4210	3.4210
$\frac{\partial r_{17}}{\partial p}$	3.6196	2.7730	2.7730	2.7730	2.7730	2.7730
$\frac{\partial r_{18}}{\partial p}$	4.9927	5.4945	5.4945	5.4945	5.4945	5.4945
Z	39.8045	37.6817	37.6816	37.9254	37.6234	37.3824
e	7.9549	6.9958	6.0692	7.4026	7.3744	7.7299

Table 4: Case Study 6 Tests using Absolute Values of $\frac{\partial r_i}{\partial p}$

Table 5 shows, for each one of the equations, the linear error as defined by equation (9).

$$e_{ij} = \frac{\partial r_i}{\partial p} + \frac{\partial r_j}{\partial p} - \frac{\partial R_{ij}}{\partial p} \; for \begin{cases} i \in \{1..10\} \\ j \in \{11..18\} \end{cases} \tag{9}$$

Several other tests have been carried out such as

$e_{i,j}$	T0-1	T-2	T-3	T-4	T-5	T-6
$e_{1,11}$	0	0	-.0025	0	-.1583	0
$e_{1,12}$	-.2156	-.2156	0	-.2465	-.2156	-.5458
$e_{1,13}$	0	0	0	0	0	-.2993
$e_{1,14}$	-1.0831	-1.0831	0	-1.0831	-1.3850	-1.3825
$e_{2,11}$	-1.3515	-.0049	-.0049	-.3042	-.1607	-.0049
$e_{2,12}$	-1.9878	-.6412	-.4231	-.9714	-.6387	-.9714
$e_{2,13}$	-1.6102	-.2636	-.2611	-.5629	-.2611	-.5629
$e_{2,14}$	-3.0448	-1.6982	-.6126	-1.9976	-1.9976	-1.9976
$e_{2,16}$	0	0	0	0	0	0
$e_{2,17}$	0	0	0	0	0	0
$e_{3,11}$	0	-.0018	-.0018	-.3011	-.1576	-.0018
$e_{3,12}$	-1.1858	-1.1876	-.9695	-1.5178	-1.1851	-1.5178
$e_{3,13}$	-1.1257	-1.1275	-1.1250	-1.4268	-1.1250	-1.4268
$e_{3,14}$	-2.6256	-2.6274	-1.5418	-2.9268	-2.9268	-2.9268
$e_{3,18}$	0	0	0	0	0	0
$e_{4,11}$	0	0	0	0	0	0
$e_{4,12}$	-1.8692	-1.8692	-1.6511	-1.9001	-1.7109	-2.1994
$e_{4,13}$	-2.3522	-2.3522	-2.3497	-2.3522	-2.1939	-2.6515
$e_{4,14}$	-4.2711	-4.2711	-3.1855	-4.2711	-4.4147	-4.5705
$e_{5,11}$	-.4543	-.4543	-.6724	-.4234	-.6126	-.1240
$e_{5,12}$	0	0	0	0	0	0
$e_{5,13}$	-.0309	-.0309	-.2465	0	-.0309	0
$e_{5,14}$	-1.5977	-1.5977	-.7302	-1.5668	-1.8996	-1.5668
$e_{6,11}$	0	0	0	-.1435	0	0
$e_{6,15}$	0	-.1558	-.1558	0	0	-.1558
$e_{7,11}$	-.0680	0	0	-.2115	-.0680	0
$e_{7,12}$	-.6414	-.5734	-.3553	-.8158	-.4831	-.9036
$e_{7,15}$	0	-.0878	-.0878	0	0	-.0878
$e_{8,11}$	-.1558	0	0	-.2993	-.1558	0
$e_{8,15}$	0	0	0	0	0	0
$e_{9,15}$	0	0	0	0	0	0
$e_{10,11}$	-2.0933	-2.0933	-3.1789	-2.0933	-2.2516	-1.7939
$e_{10,12}$	0	0	-.8675	-.03089	0	-.0309
$e_{10,13}$	0	0	-1.0831	0	0	0
$e_{10,14}$	0	0	0	0	-.3018	0

Table 5: Case Study 6: Linear Error using Absolute Values

- (T_0-1) With $\frac{\partial r_1}{\partial p} = 0.2780$, related to Li^+, as constraint then $\frac{\partial r_2}{\partial p}$, $\frac{\partial r_3}{\partial p}$ and $\frac{\partial r_{15}}{\partial p}$, related to Na^+, K^+ and O^{2-} respectively, are zero.
- (T_0-2) With $\frac{\partial r_{11}}{\partial p} = 0.6709$, related to F^-, as constraint then $\frac{\partial r_2}{\partial p}$, $\frac{\partial r_3}{\partial p}$ and $\frac{\partial r_{15}}{\partial p}$, related to Na^+, K^+ and O^{2-} respectively, are zero.
- (T_0-3) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, as constraint then $\frac{\partial r_3}{\partial p}$ and $\frac{\partial r_{15}}{\partial p}$, related to K^+ and O^{2-} respectively, are zero.
- (T_0-4) With $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, as constraint then $\frac{\partial r_2}{\partial p}$ and $\frac{\partial r_{15}}{\partial p}$, related to Na^+ and O^{2-} respectively, are zero.
- (T_0-5) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+ and $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, as constraints then $\frac{\partial r_{15}}{\partial p}$, related to O^{2-} is zero.
- (T_06) With $\frac{\partial r_1}{\partial p} = 0.2780$, related to Li^+, $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+ and $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, as constraints then $\frac{\partial r_{11}}{\partial p}$, related to F^- and $\frac{\partial r_{15}}{\partial p}$, related to O^{2-} are zero.

- (T_0-7) With $\frac{\partial r_{14}}{\partial p} = 4.0229$, related to I^- as constraint then $\frac{\partial r_2}{\partial p}$, $\frac{\partial r_3}{\partial p}$ and $\frac{\partial r_{15}}{\partial p}$, related to Na^+, K^+ and O^{2-} respectively, are zero.
- (T_0-8) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+ and $\frac{\partial r_{14}}{\partial p} = 4.0229$, related to I^- as constraint then $\frac{\partial r_{15}}{\partial p}$, related to O^{2-} is zero.
- (T_0-9) With $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} then $\frac{\partial r_2}{\partial p}$, $\frac{\partial r_3}{\partial p}$ related to Na^+ and K^+ respectively, are zero.
- (T_0-10) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+ and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_3}{\partial p}$ related to Na^+ and $\frac{\partial r_{11}}{\partial p}$, related to F^- are zero.
- (T_0-11) With $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+ and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_2}{\partial p}$, related to Na^+ is zero
- (T_0-12) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+ and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_{11}}{\partial p}$, related to F^- is zero.
- (T_0-13) With $\frac{\partial r_1}{\partial p} = 0.2780$, related to Li^+, $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_{11}}{\partial p} = 0.6709$, related to F^- and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_3}{\partial p}$, related to K^+ is zero.
- (T_0-14) With $\frac{\partial r_1}{\partial p} = 0.2780$, related to Li^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_{11}}{\partial p} = 0.6709$, related to F^- and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_2}{\partial p}$, related to Na^+ is zero
- (T_0-15) With $\frac{\partial r_{14}}{\partial p} = 4.0229$, related to I^- and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_2}{\partial p}$, related to Na^+ and $\frac{\partial r_3}{\partial p}$, related to K^+ are zero.
- (T_0-16) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_{14}}{\partial p} = 4.0229$, related to I^- and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_3}{\partial p}$, related to K^+ is zero.
- (T_0-17) With $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_{14}}{\partial p} = 4.0229$, related to I^- and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_2}{\partial p}$, related to Na^+ is zero.
- (T_0-18) With $\frac{\partial r_{11}}{\partial p} = 0.6709$, related to F^-, , $\frac{\partial r_{14}}{\partial p} = 4.0229$, related to I^- and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_2}{\partial p}$, related to Na^+ and $\frac{\partial r_3}{\partial p}$, related to K^+ are zero.
- (T_0-19) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_{11}}{\partial p} = 0.6709$, related to F^-, , $\frac{\partial r_{14}}{\partial p} = 4.0229$, related to I^- and $\frac{\partial r_{15}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_3}{\partial p}$, related to K^+ is zero.

These results are sumarized in Tables 6 and 7

$\frac{\partial r_i}{\partial p}$	T_0-1	T_0-2	T_0-3	T_0-4	T_0-5	T_0-6	T_0-7	T_0-8	T_0-9	T_0-10
$\frac{\partial r_1}{\partial p}$	$\oplus$					$\oplus$				
$\frac{\partial r_2}{\partial p}$	$\bullet$	$\bullet$	$\oplus$	$\bullet$	$\oplus$	$\oplus$	$\bullet$	$\oplus$	$\bullet$	$\oplus$
$\frac{\partial r_3}{\partial p}$	$\bullet$	$\bullet$	$\bullet$	$\oplus$	$\oplus$	$\oplus$	$\bullet$	$\oplus$	$\bullet$	$\bullet$
$\frac{\partial r_4}{\partial p}$										
$\frac{\partial r_5}{\partial p}$										
$\frac{\partial r_6}{\partial p}$										
$\frac{\partial r_7}{\partial p}$										
$\frac{\partial r_8}{\partial p}$										
$\frac{\partial r_9}{\partial p}$										
$\frac{\partial r_{10}}{\partial p}$										
$\frac{\partial r_{11}}{\partial p}$		$\oplus$				$\bullet$				$\bullet$
$\frac{\partial r_{12}}{\partial p}$										
$\frac{\partial r_{13}}{\partial p}$										
$\frac{\partial r_{14}}{\partial p}$							$\oplus$	$\oplus$		
$\frac{\partial r_{15}}{\partial p}$	$\bullet$	$\bullet$	$\bullet$	$\bullet$	$\bullet$	$\bullet$	$\bullet$	$\bullet$	$\oplus$	$\oplus$
$\frac{\partial r_{16}}{\partial p}$										
$\frac{\partial r_{17}}{\partial p}$										
$\frac{\partial r_{18}}{\partial p}$										
Z	39.8045	38.5283	38.9578	39.8044	38.9579	38.3896	39.8044	38.9578	38.7719	37.9252
e	9.6164	9.7224	8.2304	6.5243	6.4765	6.6618	10.2510	7.2265	9.9959	8.1890

Table 6: Case Study 6: Tests with Zero Solutions

$\frac{\partial r_i}{\partial p}$	T_0-11	T_0-12	T_0-13	T_0-14	T_0-15	T_0-16	T_0-17	T_0-18	T_0-19
$\frac{\partial r_1}{\partial p}$			$\oplus$	$\oplus$					
$\frac{\partial r_2}{\partial p}$	$\bullet$	$\oplus$	$\oplus$	$\bullet$	$\bullet$	$\oplus$	$\bullet$	$\bullet$	$\oplus$
$\frac{\partial r_3}{\partial p}$	$\oplus$	$\oplus$	$\bullet$	$\oplus$	$\bullet$	$\bullet$	$\oplus$	$\bullet$	$\bullet$
$\frac{\partial r_4}{\partial p}$									
$\frac{\partial r_5}{\partial p}$									
$\frac{\partial r_6}{\partial p}$									
$\frac{\partial r_7}{\partial p}$									
$\frac{\partial r_8}{\partial p}$									
$\frac{\partial r_9}{\partial p}$									
$\frac{\partial r_{10}}{\partial p}$									
$\frac{\partial r_{11}}{\partial p}$		$\bullet$	$\oplus$	$\oplus$				$\oplus$	$\oplus$
$\frac{\partial r_{12}}{\partial p}$									
$\frac{\partial r_{13}}{\partial p}$									
$\frac{\partial r_{14}}{\partial p}$					$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$
$\frac{\partial r_{15}}{\partial p}$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$
$\frac{\partial r_{16}}{\partial p}$									
$\frac{\partial r_{17}}{\partial p}$									
$\frac{\partial r_{18}}{\partial p}$									
Z	38.7719	37.9252	37.6817	38.5283	38.7719	37.9253	38.7719	38.2289	37.3823
e	7.7399	5.9979	9.2887	7.1928	10.3094	9.8475	7.9938	10.1340	10.0315

Table 7: Case Study 6: More Tests with Zero Solutions

3.2 Module PRad - Case Study 7

This seventh case study considers the same anions and cations than case 6 incremented by just one cation Ag^+ and two salts, AgCl and AgBr, as shown in Table 8.

Cations	Li^+ $\frac{\partial r_1}{\partial p}$	Na^+ $\frac{\partial r_2}{\partial p}$	K^+ $\frac{\partial r_3}{\partial p}$	Rb^+ $\frac{\partial r_4}{\partial p}$	Cs^+ $\frac{\partial r_5}{\partial p}$	Ca^{2+} $\frac{\partial r_6}{\partial p}$	Sr^{2+} $\frac{\partial r_7}{\partial p}$	Ba^{2+} $\frac{\partial r_8}{\partial p}$	Mg^{2+} $\frac{\partial r_9}{\partial p}$	NH_4^+ $\frac{\partial r_{10}}{\partial p}$	Ag^+ $\frac{\partial r_{11}}{\partial p}$
Anions	F^- $\frac{\partial r_{12}}{\partial p}$	Cl^- $\frac{\partial r_{13}}{\partial p}$	Br^- $\frac{\partial r_{14}}{\partial p}$	I^- $\frac{\partial r_{15}}{\partial p}$	O^{2-} $\frac{\partial r_{16}}{\partial p}$	ClO_3^- $\frac{\partial r_{17}}{\partial p}$	BrO_3^- $\frac{\partial r_{18}}{\partial p}$	CN^- $\frac{\partial r_{19}}{\partial p}$			

Table 8: Case 7 – Cations and Anions Considered

Thus $n_c = 11$, $n_a = 8$ and $md = 19$ with

$$maximize\ Z = \sum_{k=1}^{19} \frac{\partial r_k}{\partial p} \tag{10}$$

subject to the restrictions

$$\frac{\partial r_i}{\partial p} + \frac{\partial r_j}{\partial p} \leq \frac{\partial R_{ij}}{\partial p}\ for \begin{cases} i \in \{1..11\} \\ j \in \{12..19\} \end{cases}$$

all nonnegative making 37 inequalities where the correspondence among the salts being studied and the $\frac{\partial R_{ij}}{\partial p}$ notation is shown in Table 9.

LiF $\frac{\partial R_{1,12}}{\partial p}$	LiCl $\frac{\partial R_{1,13}}{\partial p}$	LiBr $\frac{\partial R_{1,14}}{\partial p}$	LiI $\frac{\partial R_{1,15}}{\partial p}$	NaF $\frac{\partial R_{2,12}}{\partial p}$	NaCl $\frac{\partial R_{2,13}}{\partial p}$	NaBr $\frac{\partial R_{2,14}}{\partial p}$	NaI $\frac{\partial R_{2,15}}{\partial p}$	$NaClO_3$ $\frac{\partial R_{2,17}}{\partial p}$	$NaBrO_3$ $\frac{\partial R_{2,18}}{\partial p}$
KF $\frac{\partial R_{3,12}}{\partial p}$	KCl $\frac{\partial R_{3,13}}{\partial p}$	KBr $\frac{\partial R_{3,14}}{\partial p}$	KI $\frac{\partial R_{3,15}}{\partial p}$	KCN $\frac{\partial R_{3,19}}{\partial p}$	RbF $\frac{\partial R_{4,12}}{\partial p}$	RbCl $\frac{\partial R_{4,13}}{\partial p}$	RbBr $\frac{\partial R_{4,14}}{\partial p}$	RbI $\frac{\partial R_{4,15}}{\partial p}$	
CsF $\frac{\partial R_{5,12}}{\partial p}$	CsCl $\frac{\partial R_{5,13}}{\partial p}$	CsBr $\frac{\partial R_{5,14}}{\partial p}$	CsI $\frac{\partial R_{5,15}}{\partial p}$						
CaF $\frac{\partial R_{6,12}}{\partial p}$	CaO $\frac{\partial R_{6,16}}{\partial p}$	SrF $\frac{\partial R_{7,12}}{\partial p}$	SrCl $\frac{\partial R_{7,13}}{\partial p}$	SrO $\frac{\partial R_{7,16}}{\partial p}$	BaF $\frac{\partial R_{8,12}}{\partial p}$	BaO $\frac{\partial R_{8,16}}{\partial p}$	MgO $\frac{\partial R_{9,16}}{\partial p}$		
NH_4F $\frac{\partial R_{10,12}}{\partial p}$	NH_4Cl $\frac{\partial R_{10,13}}{\partial p}$	NH_4Br $\frac{\partial R_{10,14}}{\partial p}$	NH_4I $\frac{\partial R_{10,15}}{\partial p}$	AgCl $\frac{\partial R_{11,13}}{\partial p}$	AgBr $\frac{\partial R_{11,14}}{\partial p}$				

Table 9: Case 7 – Correspondence Among Salts

In matrix form $\mathbf{Ar} \leq \mathbf{R}$ where $\mathbf{A}$, $\mathbf{r}$, and $\mathbf{R}$ are defined as shown in (11).

$$
\mathbf{A} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\quad
\mathbf{r} = \begin{pmatrix}
\frac{\partial r_1}{\partial p} \\
\frac{\partial r_2}{\partial p} \\
\frac{\partial r_3}{\partial p} \\
\frac{\partial r_4}{\partial p} \\
\frac{\partial r_5}{\partial p} \\
\frac{\partial r_6}{\partial p} \\
\frac{\partial r_7}{\partial p} \\
\frac{\partial r_8}{\partial p} \\
\frac{\partial r_9}{\partial p} \\
\frac{\partial r_{10}}{\partial p} \\
\frac{\partial r_{11}}{\partial p} \\
\frac{\partial r_{12}}{\partial p} \\
\frac{\partial r_{13}}{\partial p} \\
\frac{\partial r_{14}}{\partial p} \\
\frac{\partial r_{15}}{\partial p} \\
\frac{\partial r_{16}}{\partial p} \\
\frac{\partial r_{17}}{\partial p} \\
\frac{\partial r_{18}}{\partial p} \\
\frac{\partial r_{19}}{\partial p}
\end{pmatrix}
\quad
\mathbf{R} = \begin{pmatrix}
\frac{\partial R_{1,12}}{\partial p} \\
\frac{\partial R_{1,13}}{\partial p} \\
\frac{\partial R_{1,14}}{\partial p} \\
\frac{\partial R_{1,15}}{\partial p} \\
\frac{\partial R_{2,12}}{\partial p} \\
\frac{\partial R_{2,13}}{\partial p} \\
\frac{\partial R_{2,14}}{\partial p} \\
\frac{\partial R_{2,15}}{\partial p} \\
\frac{\partial R_{2,17}}{\partial p} \\
\frac{\partial R_{2,18}}{\partial p} \\
\frac{\partial R_{3,12}}{\partial p} \\
\frac{\partial R_{3,13}}{\partial p} \\
\frac{\partial R_{3,14}}{\partial p} \\
\frac{\partial R_{3,15}}{\partial p} \\
\frac{\partial R_{3,19}}{\partial p} \\
\frac{\partial R_{4,12}}{\partial p} \\
\frac{\partial R_{4,13}}{\partial p} \\
\frac{\partial R_{4,14}}{\partial p} \\
\frac{\partial R_{4,15}}{\partial p} \\
\frac{\partial R_{5,12}}{\partial p} \\
\frac{\partial R_{5,13}}{\partial p} \\
\frac{\partial R_{5,14}}{\partial p} \\
\frac{\partial R_{5,15}}{\partial p} \\
\frac{\partial R_{6,12}}{\partial p} \\
\frac{\partial R_{6,16}}{\partial p} \\
\frac{\partial R_{7,12}}{\partial p} \\
\frac{\partial R_{7,13}}{\partial p} \\
\frac{\partial R_{7,16}}{\partial p} \\
\frac{\partial R_{8,12}}{\partial p} \\
\frac{\partial R_{8,16}}{\partial p} \\
\frac{\partial R_{9,16}}{\partial p} \\
\frac{\partial R_{10,12}}{\partial p} \\
\frac{\partial R_{10,13}}{\partial p} \\
\frac{\partial R_{10,14}}{\partial p} \\
\frac{\partial R_{10,15}}{\partial p} \\
\frac{\partial R_{11,13}}{\partial p} \\
\frac{\partial R_{11,14}}{\partial p}
\end{pmatrix}
\tag{11}
$$

Table 10 shows the results obtained by different tests T under the restrictions given by equation (11) where

$$\begin{aligned}\mathbf{R}^t = (&.9514, 2.7083, 3.7982, 5.6859, 1.5224, 3.7000, 4.6279, 6.8671, 4.2676,\\ &3.6196, 2.7363, 5.4634, 6.7088, 9.0133, 7.5581, 3.5420, 6.9525,\\ &8.7410, 11.4645, 4.2308, 5.3178, 6.6542, 9.0256, .8915, .7206,\\ &1.1981, 3.3128, .9592, 1.5703, 1.2436, .4255, 6.79417, 6.24216,\\ &7.54768, 8.35223, 2.0938, 2.3587)\end{aligned}$$

The Z column correspond to the Z value defined by equation (10) and the e column is defined by equation (12).

$$e = \sqrt{\sum_{i,j}(e_{ij})^2} \; for \begin{cases} i \in \{1..11\} \\ j \in \{12..19\} \end{cases} \tag{12}$$

$\frac{\partial r_i}{\partial p}$	T0-1	T-2	T-3
$\frac{\partial r_1}{\partial p}$	.9514	.4363	$\oplus$.2780
$\frac{\partial r_2}{\partial p}$	•	$\oplus$.8466	$\oplus$.8466
$\frac{\partial r_3}{\partial p}$	•	$\oplus$2.0636	$\oplus$2.0636
$\frac{\partial r_4}{\partial p}$	3.5420	$\oplus$2.8707	$\oplus$2.8707
$\frac{\partial r_5}{\partial p}$	3.5609	3.4030	3.4030
$\frac{\partial r_6}{\partial p}$	.7206	.3764	.3764
$\frac{\partial r_7}{\partial p}$	.9592	.6150	.6150
$\frac{\partial r_8}{\partial p}$	1.2436	.8994	.8994
$\frac{\partial r_9}{\partial p}$	.4255	.0813	.0813
$\frac{\partial r_{10}}{\partial p}$	3.6177	3.1026	4.3274
$\frac{\partial r_{11}}{\partial p}$	.3369	.1790	.1790
$\frac{\partial r_{12}}{\partial p}$	•	.5151	.5151
$\frac{\partial r_{13}}{\partial p}$	1.7569	$\oplus$1.9148	$\oplus$1.9148
$\frac{\partial r_{14}}{\partial p}$	2.0218	2.1797	2.1797
$\frac{\partial r_{15}}{\partial p}$	4.7345	5.2496	4.0249
$\frac{\partial r_{16}}{\partial p}$	•	$\oplus$.3442	$\oplus$.3442
$\frac{\partial r_{17}}{\partial p}$	4.2676	3.4210	3.4210
$\frac{\partial r_{18}}{\partial p}$	3.6196	2.7730	2.7730
$\frac{\partial r_{19}}{\partial p}$	7.5581	5.4945	5.4945
Z	39.3163	36.7658	36.6076
e	10.9440	8.0662	8.7674

Table 10: Case Study 7: Tests using Absolute Values of $\frac{\partial r_i}{\partial p}$

Table 11 shows, for each one of the equations, the linear error as defined by equation (13).

$$e_{ij} = \frac{\partial r_i}{\partial p} + \frac{\partial r_j}{\partial p} - \frac{\partial R_{ij}}{\partial p} \; for \begin{cases} i \in \{1..11\} \\ j \in \{12..19\} \end{cases} \tag{13}$$

$e_{i,j}$	T0-1	T-2	T-3
$e_{1,12}$	0	0	-.1583
$e_{1,13}$	0	-.3572	-.5155
$e_{1,14}$	-.8250	-1.1822	-1.3405
$e_{1,15}$	0	0	-1.3830
$e_{2,12}$	-1.5224	-.1607	-.1607
$e_{2,13}$	-1.9431	-.9386	-.9386
$e_{2,14}$	-2.6061	-1.6016	-1.6016
$e_{2,15}$	-2.1326	-.7709	-1.9956
$e_{2,17}$	0	0	0
$e_{2,18}$	0	0	0
$e_{3,12}$	-2.7363	-.1576	-.1576
$e_{3,13}$	-3.7065	-1.4850	-1.4850
$e_{3,14}$	-4.6870	-2.4655	-2.4655
$e_{3,15}$	-4.2788	-1.7001	-2.9248
$e_{3,19}$	0	0	0
$e_{4,12}$	0	-.1562	-.1562
$e_{4,13}$	-1.6536	-2.1670	-2.1670
$e_{4,14}$	-3.1772	-3.6906	-3.6906
$e_{4,15}$	-3.1880	-3.3442	-4.5689
$e_{5,12}$	-.6699	-.3127	-.3127
$e_{5,13}$	0	0	0
$e_{5,14}$	-1.0715	-1.0715	-1.0715
$e_{5,15}$	-.7302	-.3730	-1.5977
$e_{6,12}$	-.1709	0	0
$e_{6,16}$	0	0	0
$e_{7,12}$	-.2389	-.0680	-.0680
$e_{7,13}$	-.5967	-.7830	-.7830
$e_{7,16}$	0	0	0
$e_{8,12}$	-.3267	-.1558	-.1558
$e_{8,16}$	0	0	0
$e_{9,16}$	0	0	0
$e_{10,12}$	-3.1764	-3.1764	-1.9517
$e_{10,13}$	-.8675	-1.2247	0
$e_{10,14}$	-1.9081	-2.2653	-1.0406
$e_{10,15}$	0	0	0
$e_{11,13}$	0	0	0
$e_{11,14}$	0	0	0

Table 11: Case Study 7: Linear Error using Absolute Values

Several other thests have been carried out such as

- (T_0-1) With $\frac{\partial r_1}{\partial p} = 0.2780$, related to Li^+, as constraint then $\frac{\partial r_2}{\partial p}$, $\frac{\partial r_3}{\partial p}$, $\frac{\partial r_{12}}{\partial p}$, and $\frac{\partial r_{16}}{\partial p}$, related to Na^+, K^+, F^- and O^{2-} respectively, are zero.
- (T_0-2) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, as constraint then $\frac{\partial r_3}{\partial p}$, $\frac{\partial r_{12}}{\partial p}$, and $\frac{\partial r_{16}}{\partial p}$, related to K^+, F^- and O^{2-} respectively, are zero.
- (T_0-3) With $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, as constraint then $\frac{\partial r_2}{\partial p}$, $\frac{\partial r_{12}}{\partial p}$, and $\frac{\partial r_{16}}{\partial p}$, related to Na^+, F^- and O^{2-} respectively, are zero.
- (T_0-4) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+ and$\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, then $\frac{\partial r_{12}}{\partial p}$, and $\frac{\partial r_{16}}{\partial p}$, related to F^- and O^{2-} respectively, are zero.
- (T_0-5) With $\frac{\partial r_{12}}{\partial p} = 0.6709$, related to F^-, as constraints then $\frac{\partial r_2}{\partial p}$, $\frac{\partial r_3}{\partial p}$, and $\frac{\partial r_{16}}{\partial p}$, related to Na^+, K^+ and O^{2-} respectively, are zero.

- ($T_0$6) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+ and $\frac{\partial r_{12}}{\partial p} = 0.6709$, related to F^- as constraints then $\frac{\partial r_{16}}{\partial p}$, related to O^{2-} respectively, is zero.

- (T_0-7) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_{12}}{\partial p} = 0.6709$, related to F^- and $\frac{\partial r_{16}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_{11}}{\partial p}$ related to Ag^+ is zero

- (T_0-8) With $\frac{\partial r_1}{\partial p} = 0.2780$, related to Li^+, $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_{12}}{\partial p} = 0.6709$, related to F^- and $\frac{\partial r_{16}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_{11}}{\partial p}$ related to Ag^+ is zero.

- (T_0-9) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_{10}}{\partial p} = 4.0274$, related to NH_4^+ and $\frac{\partial r_{12}}{\partial p} = 0.6709$, related to F^- as constraints then $\frac{\partial r_{11}}{\partial p}$ related to Ag^+ is zero.

- (T_0-10) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_{10}}{\partial p} = 4.0274$, related to NH_4^+ and $\frac{\partial r_{16}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_{11}}{\partial p}$ related to Ag^+ and $\frac{\partial r_{12}}{\partial p}$, related to F^- are zero.

- (T_0-11) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_{10}}{\partial p} = 4.0274$, related to NH_4^+, $\frac{\partial r_{12}}{\partial p} = 0.6709$, related to F^- and $\frac{\partial r_{16}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_{11}}{\partial p}$ related to Ag^+ is zero.

- (T_0-12) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+ and $\frac{\partial r_4}{\partial p} = 2.8707$, related to Rb^+ as constraints then $\frac{\partial r_{12}}{\partial p}$, related to F^- and $\frac{\partial r_{16}}{\partial p}$, related to O^{2-} are zero.

- (T_0-13) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_4}{\partial p} = 2.8707$, related to Rb^+ and $\frac{\partial r_{12}}{\partial p} = 0.6709$, related to F^- as constraints then $\frac{\partial r_{11}}{\partial p}$ related to Ag^+ is zero.

- (T_0-14) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_4}{\partial p} = 2.8707$, related to Rb^+, $\frac{\partial r_{12}}{\partial p} = 0.6709$, related to F^- and $\frac{\partial r_{16}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_{11}}{\partial p}$ related to Ag^+ is zero.

- (T_0-15) With $\frac{\partial r_2}{\partial p} = 0.8466$, related to Na^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_4}{\partial p} = 2.8707$, related to Rb^+ and $\frac{\partial r_{13}}{\partial p} = 1.9148$, related to Cl^- as constraints then $\frac{\partial r_{11}}{\partial p}$ related to Ag^+ is zero.

- (T_0-16) With $\frac{\partial r_1}{\partial p} = 0.2780$, related to Li^+, $\frac{\partial r_3}{\partial p} = 2.0636$, related to K^+, $\frac{\partial r_4}{\partial p} = 2.8707$, related to Rb^+, $\frac{\partial r_{13}}{\partial p} = 1.9148$, related to Cl^- and $\frac{\partial r_{16}}{\partial p} = 0.3442$, related to O^{2-} as constraints then $\frac{\partial r_2}{\partial p}$, related to Na^+ and $\frac{\partial r_{11}}{\partial p}$ related to Ag^+ are zero.

These results are sumarized in Tables 12 and 13

$\frac{\partial r_i}{\partial p}$	T_0-1	T_0-2	T_0-3	T_0-4	T_0-5	T_0-6	T_0-7	T_0-8	T_0-9	T_0-10
$\frac{\partial r_1}{\partial p}$	$\oplus$							$\oplus$		
$\frac{\partial r_2}{\partial p}$	$\bullet$	$\oplus$	$\bullet$	$\oplus$	$\bullet$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$
$\frac{\partial r_3}{\partial p}$	$\bullet$	$\bullet$	$\oplus$	$\oplus$	$\bullet$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$
$\frac{\partial r_4}{\partial p}$										
$\frac{\partial r_5}{\partial p}$										
$\frac{\partial r_6}{\partial p}$										
$\frac{\partial r_7}{\partial p}$										
$\frac{\partial r_8}{\partial p}$										
$\frac{\partial r_9}{\partial p}$										
$\frac{\partial r_{10}}{\partial p}$									$\oplus$	$\oplus$
$\frac{\partial r_{11}}{\partial p}$							$\bullet$	$\bullet$	$\bullet$	$\bullet$
$\frac{\partial r_{12}}{\partial p}$	$\bullet$	$\bullet$	$\bullet$	$\bullet$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\bullet$
$\frac{\partial r_{13}}{\partial p}$										
$\frac{\partial r_{14}}{\partial p}$										
$\frac{\partial r_{15}}{\partial p}$										
$\frac{\partial r_{16}}{\partial p}$	$\bullet$	$\bullet$	$\bullet$	$\bullet$	$\bullet$	$\bullet$	$\oplus$	$\oplus$		$\oplus$
$\frac{\partial r_{17}}{\partial p}$										
$\frac{\partial r_{18}}{\partial p}$										
$\frac{\partial r_{19}}{\partial p}$										
Z	38.6430	38.4698	39.3164	38.4697	37.3693	36.5227	36.5226	36.5201	36.5226	37.4371
e	10.8589	12.7851	10.9963	7.88575	11.9735	9.2007	7.9259	7.6613	8.1321	7.7159

Table 12: Case Study 7: Tests with Zero Solutions

$\frac{\partial r_i}{\partial p}$	T_0-11	T_0-12	T_0-13	T_0-14	T_0-15	T_0-16
$\frac{\partial r_1}{\partial p}$						$\oplus$
$\frac{\partial r_2}{\partial p}$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\bullet$
$\frac{\partial r_3}{\partial p}$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$
$\frac{\partial r_4}{\partial p}$		$\oplus$	$\oplus$	$\oplus$	$\oplus$	$\oplus$
$\frac{\partial r_5}{\partial p}$						
$\frac{\partial r_6}{\partial p}$						
$\frac{\partial r_7}{\partial p}$						
$\frac{\partial r_8}{\partial p}$						
$\frac{\partial r_9}{\partial p}$						
$\frac{\partial r_{10}}{\partial p}$	$\oplus$					
$\frac{\partial r_{11}}{\partial p}$	$\bullet$		$\bullet$	$\bullet$		$\bullet$
$\frac{\partial r_{12}}{\partial p}$	$\oplus$	$\bullet$	$\oplus$	$\oplus$		
$\frac{\partial r_{13}}{\partial p}$					$\oplus$	$\oplus$
$\frac{\partial r_{14}}{\partial p}$						
$\frac{\partial r_{15}}{\partial p}$						
$\frac{\partial r_{16}}{\partial p}$	$\oplus$	$\bullet$		$\oplus$	$\bullet$	$\oplus$
$\frac{\partial r_{17}}{\partial p}$						
$\frac{\partial r_{18}}{\partial p}$						
$\frac{\partial r_{19}}{\partial p}$						
Z	36.5226	37.7984	36.5223	36.5222	37.7985	37.4541
e	8.1321	10.1069	8.2544	7.6610	8.7408	8.3161

Table 13: Case Study 7: More Tests with Zero Solutions

4 Module PDac Description

This module, responsible for the evaluation of $\frac{dr_-}{dp}$ and $\frac{dr_+}{dp}$, is part of the Polariz system which is described in detail in [10] and [11]. It uses the experimental data related to the values of R^0_{ij} and χ_{ij}, from Table 21, for the salts treated.

The general notation used by this module is shown in Table 14, assuming we have n_c different cations $\mathbf{c}$ and n_a different anions $\mathbf{a}$ with $md = n_c + n_a$

Cations	$\mathbf{c}_1$	$\mathbf{c}_2$	$\mathbf{c}_3$	...	$\mathbf{c}_{n_c}$
	r_1	r_2	r_3	...	r_{n_c}
Anions	$\mathbf{a}_{n_c+1}$	$\mathbf{a}_{n_c+2}$	$\mathbf{a}_{n_c+3}$	...	$\mathbf{a}_{n_c+n_a}$
	r_{n_c+1}	r_{n_c+2}	r_{n_c+3}	...	$r_{n_c+n_a}$

Table 14: General Notation

the system implements the linear programming problem of the form

$$maximize\ Z = \sum_{k=1}^{md} r_k$$

subject to the restrictions

$$r_i + r_j \leq R_{ij}\ for \begin{cases} i\ is\ any\ value\ in\ \{1..n_c\} \\ j\ is\ any\ value\ in\ \{n_c+1..n_c+n_a\} \end{cases}$$

all nonnegative. All instances of i and j values are user defined through the corresponding companion matrix, as explained later on. To solve this problem the user can also fix one or more r_k at zero pressure (p_0) and iteratively solve

$$R'_{ij} = R^0_{ij} - \frac{\chi_{ij} R^0_{ij}}{3}(p' - p_0) \tag{14}$$

such that it must verify for $p'' > p' > p_0$

$$\begin{array}{llll} R''_{ij} & < R'_{ij} & < R_{ij} & all\ i\ and\ j\ defined\ by\ the\ user \\ r''_k & < r'_k & < r_k & k = 1..md \end{array}$$

From p_0 to $p' = 0.001$ GPa a step of 10^{-4} is used and from $p' = 0.001$ GPa to $p'' = 0.01$ GPa a step of 10^{-3} (10 times higher) is used, making a total of 20 iterations. This module allows for a wide range of experimental settings such as the inclusion of fixed values of one or more $r_k, k = 1..md$ at different pressures, where every r_k may be evaluated at each value of p and may then be fixed in each maximization procedure.

To obtain the restriction that for $p'' > p' > p_0$ then $r''_k < r'_k < r_k$, aditional constraints may be used in each iteration $(n+1)$ of the form

$$r_k^{(n+1)} \leq r_k^{(n)} - \Delta r_k \Delta p \tag{15}$$

where Δr_k can be fixed by the user. The value of the objective function Z being minimized

$$Z^{(n)} = \sum_{k=1}^{md} r_k^{(n)} \tag{16}$$

in each of the $n = 20$ iterations is calculated. Also, for each one of the total number of equations of the system the error $e_{ij}^{(n)}$ in every iteration n is calculated for user's defined i and j

$$e_{ij}^{(n)} = r_i^{(n)} + r_j^{(n)} - R_{ij}^{(n)}$$

as well as

$$e^{(n)} = \sqrt{\sum_{i,j} (e_{ij}^{(n)})^2} \tag{17}$$

Finally, $r_k = f(p)$ for $k = 1..md$ is calculated for the 20 calculated pressures and using leastsquares, a linear function is interpolated for the following two cases: all 20 pressures and only the first 10 pressures. From that the module calculates its output $\frac{\partial r}{\partial p}$ for both cases. All those results can also be plotted.

To obtain the restriction that for $p'' > p' > p_0$ then $r_k'' < r_k' < r_k$ in each iteration $(n+1)$ of the form

$$r_i^{(n+1)} \leq r_i^{(n)} - \Delta r_i \Delta p$$

we experimented with different values of Δr_i such as $\Delta r_i = constant$, Δr_i proportional to the ionic radii and others. Results presented in this work for both cases 6 and 7, correspond to the first option with $\Delta r_i = 1$.

5 Examples and Results

In what follows, the same two case study considered in Section 3 are presented showing the correspondence among the salts being studied and the R_{ij} notation used by this module. As before, we show the results of using different constraints to run the module since the system has too many degree of liberty and some times a solution $r_k = 0$ is factible. Adding constraints allows the user to study the behavior of the system as well as testing specific $r_k$values.

5.1 Module PDac - Case Study 6

This case study considers the same anions and cations than in Section 3.1 as shown in Table 15.

Cations	Li^+	Na^+	K^+	Rb^+	Cs^+	Ca^{2+}	Sr^{2+}	Ba^{2+}	Mg^{2+}	NH_4^+
	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8	r_9	r_{10}
Anions	F^-	Cl^-	Br^-	I^-	O^{2-}	ClO_3^-	BrO_3^-	CN^-		
	r_{11}	r_{12}	r_{13}	r_{14}	r_{15}	r_{16}	r_{17}	r_{18}		

Table 15: Case 6: Module PDac – Cations and Anions Considered

Thus $n_c = 10$, $n_a = 8$ and $md = 18$ with

$$maximize\ Z = \sum_{k=1}^{18} r_k \tag{18}$$

subject to the restrictions

$$r_i + r_j \leq R_{ij}\ for \begin{cases} i \in \{1..10\} \\ j \in \{11..18\} \end{cases}$$

all nonnegative making 35 inequalities where the correspondence among the salts being studied and the R_{ij} notation is shown in Table 16.

LiF	LiCl	LiBr	LiI	NaF	NaCl	NaBr	NaI	$NaClO_3$	$NaBrO_3$
$R_{1,11}$	$R_{1,12}$	$R_{1,13}$	$R_{1,14}$	$R_{2,11}$	$R_{2,12}$	$R_{2,13}$	$R_{2,14}$	$R_{2,16}$	$R_{2,17}$
KF	KCl	KBr	KI	KCN	RbF	RbCl	RbBr	RbI	
$R_{3,11}$	$R_{3,12}$	$R_{3,13}$	$R_{3,14}$	$R_{3,18}$	$R_{4,11}$	$R_{4,12}$	$R_{4,13}$	$R_{4,14}$	
CsF	CsCl	CsBr	CsI						
$R_{5,11}$	$R_{5,12}$	$R_{5,13}$	$R_{5,14}$						
CaF	CaO	SrF	SrCl	SrO	BaF	BaO	MgO		
$R_{6,11}$	$R_{6,15}$	$R_{7,11}$	$R_{7,12}$	$R_{7,15}$	$R_{8,11}$	$R_{8,15}$	$R_{9,15}$		
NH_4F	NH_4Cl	NH_4Br	NH_4I						
$R_{10,11}$	$R_{10,12}$	$R_{10,13}$	$R_{10,14}$						

Table 16: Case 6: Module PDac – Correspondence Among Salts

In matrix form $\mathbf{Ar} \leq \mathbf{R}$ where $\mathbf{A}$, $\mathbf{r}$, and $\mathbf{R}$ are defined as shown in (19).

$$\mathbf{A} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0
\end{pmatrix} \mathbf{r} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \\ r_6 \\ r_7 \\ r_8 \\ r_9 \\ r_{10} \\ r_{11} \\ r_{12} \\ r_{13} \\ r_{14} \\ r_{15} \\ r_{16} \\ r_{17} \\ r_{18} \end{pmatrix} \mathbf{R} = \begin{pmatrix} R_{1,11} \\ R_{1,12} \\ R_{1,13} \\ R_{1,14} \\ R_{2,11} \\ R_{2,12} \\ R_{2,13} \\ R_{2,14} \\ R_{2,16} \\ R_{2,17} \\ R_{3,11} \\ R_{3,12} \\ R_{3,13} \\ R_{3,14} \\ R_{3,18} \\ R_{4,11} \\ R_{4,12} \\ R_{4,13} \\ R_{4,14} \\ R_{5,11} \\ R_{5,12} \\ R_{5,13} \\ R_{5,14} \\ R_{6,11} \\ R_{6,15} \\ R_{7,11} \\ R_{7,12} \\ R_{7,15} \\ R_{8,11} \\ R_{8,15} \\ R_{9,15} \\ R_{10,11} \\ R_{10,12} \\ R_{10,13} \\ R_{10,14} \end{pmatrix} \tag{19}$$

where

$$\mathbf{R}^t = (1.996, 2.539, 2.713, 2.951, 2.295, 2.789, 2.954, 3.194, 3.2775, 3.3445, 2.648, 3.116, 3.262, 3.489, 3.25, 2.789, 3.259, 3.410, 3.628, 2.9827, 3.5150, 3.6645, 3.9018, 2.30, 2.3995, 2.51, 3.0311, 2.5698, 2.69, 2.8129, 2.1066, 2.63, 3.356, 3.516, 3.785)$$

Table 17 shows the results obtained for $\frac{\partial r}{\partial p}$ using the first 10 pressures as well as all the 20 pressures for different tests T. Z corresponds to the Z value defined by equation (16) and e is defined by equation (17) for $n = 20$

It follows a description of each test T. Whenever not explicitly stated, and in order to obtain $r''_k < r'_k < r_k$ for $p'' > p' > p_0$ in each iteration $(n + 1)$ aditional constraints given by equation 15 with $\Delta r_k = 1$ as well as $\Delta p = 0.00001$ for $n = 1$ to 10 and $\Delta p = 0.0001$ for $n = 11$ to 20 were used.

- T-1 fixing the following values at p_0

$$r_{11} = \frac{R^{(0)}_{1,11}}{\sqrt{2}} \qquad r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_2 = R^{(0)}_{2,11} - r_{11} \qquad r_3 = R^{(0)}_{3,11} - r_{11} \tag{20}$$

- T-2 fixing the following values at p_0

$$r_{11} = \frac{R^{(0)}_{1,11}}{\sqrt{2}} \qquad r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{14} = \frac{R^{(0)}_{1,14}}{\sqrt{2}} \qquad r_2 = R^{(0)}_{2,11} - r_{11} \qquad r_3 = R^{(0)}_{3,11} - r_{11} \tag{21}$$

- T-3 fixing the following values at p_0

$$\begin{aligned} &r_{11} = \frac{R^{(0)}_{1,11}}{\sqrt{2}} \qquad r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{13} = \frac{R^{(0)}_{1,13}}{\sqrt{2}} \qquad r_{14} = \frac{R^{(0)}_{1,14}}{\sqrt{2}} \\ &r_2 = R^{(0)}_{2,11} - r_{11} \qquad r_3 = R^{(0)}_{3,11} - r_{11} \qquad r_{15} \geq 1.2 \end{aligned} \tag{22}$$

  In each maximization procedure the following values were also fixed

$$\begin{aligned} r'_2 &= \frac{R^0_{2,11} - \frac{\chi_{2,11} R^0_{2,11}}{3}(p' - p_0)}{\sqrt{2}} - r'_{11} \qquad r'_3 = \frac{R^0_{2,11} - \frac{\chi_{3,11} R^0_{3,11}}{3}(p' - p_0)}{\sqrt{2}} - r'_{11} \\ r'_{11} &= \frac{R^0_{1,11} - \frac{\chi_{1,11} R^0_{1,11}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{12} = \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p' - p_0)}{\sqrt{2}} \\ r'_{13} &= \frac{R^0_{1,13} - \frac{\chi_{1,13} R^0_{1,13}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{14} = \frac{R^0_{1,14} - \frac{\chi_{1,14} R^0_{1,14}}{3}(p' - p_0)}{\sqrt{2}} \end{aligned} \tag{23}$$

- T-4 fixing the same values than in T-3, but only at p_0.

- T-5 fixing the same values at p_0 than in T-3, *i.e.*

$$\begin{aligned} &r_{11} = \frac{R^{(0)}_{1,11}}{\sqrt{2}} \qquad r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{13} = \frac{R^{(0)}_{1,13}}{\sqrt{2}} \qquad r_{14} = \frac{R^{(0)}_{1,14}}{\sqrt{2}} \\ &r_2 = R^{(0)}_{2,11} - r_{11} \qquad r_3 = R^{(0)}_{3,11} - r_{11} \qquad r_{15} \geq 1.2 \end{aligned} \tag{24}$$

  In each maximization procedure the same values than in T-3, except the values of r'_2 and r'_3, were also fixed, *i.e.*

$$\begin{aligned} r'_{11} &= \frac{R^0_{1,11} - \frac{\chi_{1,11} R^0_{1,11}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{12} = \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p' - p_0)}{\sqrt{2}} \\ r'_{13} &= \frac{R^0_{1,13} - \frac{\chi_{1,13} R^0_{1,13}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{14} = \frac{R^0_{1,14} - \frac{\chi_{1,14} R^0_{1,14}}{3}(p' - p_0)}{\sqrt{2}} \end{aligned} \tag{25}$$

- T-6 similar to T-5 including only the aditional constraint

$$r_2' = \frac{R^0_{2,11} - \frac{\chi_{2,11} R^0_{2,11}}{3}(p' - p_0)}{\sqrt{2}} - r'_{11}, \quad p > 0$$

- T-7 fixing the following values at p_0

$$r_{11} = \frac{R^{(0)}_{1,11}}{\sqrt{2}} \qquad r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_2 = R^{(0)}_{2,11} - r_{11} \qquad r_3 = R^{(0)}_{3,11} - r_{11} \qquad r_{15} \geq 1.2 \tag{26}$$

In each maximization procedure the following values were also fixed

$$\begin{aligned} r_2' &= \frac{R^0_{2,11} - \frac{\chi_{2,11} R^0_{2,11}}{3}(p' - p_0)}{\sqrt{2}} - r'_{11} \qquad & r_3' &= \frac{R^0_{2,11} - \frac{\chi_{3,11} R^0_{3,11}}{3}(p' - p_0)}{\sqrt{2}} - r'_{11} \\ r'_{11} &= \frac{R^0_{1,11} - \frac{\chi_{1,11} R^0_{1,11}}{3}(p' - p_0)}{\sqrt{2}} & r'_{12} &= \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p' - p_0)}{\sqrt{2}} \end{aligned} \tag{27}$$

- T-8 fixing the following values at p_0

$$\begin{aligned} &r_{11} = \frac{R^{(0)}_{1,11}}{\sqrt{2}} \qquad r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_2 = R^{(0)}_{2,11} - r_{11} \qquad r_3 = R^{(0)}_{3,11} - r_{11} \\ &r_{10} = R^{(0)}_{10,11} - r_{11} \qquad r_{15} \geq 1.2 \end{aligned} \tag{28}$$

In each maximization procedure the following values were also fixed

$$\begin{aligned} r_2' &= \frac{R^0_{2,11} - \frac{\chi_{2,11} R^0_{2,11}}{3}(p' - p_0)}{\sqrt{2}} - r'_{11} \qquad & r_3' &= \frac{R^0_{2,11} - \frac{\chi_{3,11} R^0_{3,11}}{3}(p' - p_0)}{\sqrt{2}} - r'_{11} \\ r'_{10} &= \frac{R^0_{10,11} - \frac{\chi_{10,11} R^0_{10,11}}{3}(p' - p_0)}{\sqrt{2}} - r'_{11} & & \\ r'_{11} &= \frac{R^0_{1,11} - \frac{\chi_{1,11} R^0_{1,11}}{3}(p' - p_0)}{\sqrt{2}} & r'_{12} &= \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p' - p_0)}{\sqrt{2}} \end{aligned} \tag{29}$$

Test T-3(20) in Table 17 shows good results.

$\frac{\partial r_i}{\partial p}$	T-1		T-2		T-3		T-4	
	T-1(20)	T-1(10)	T-2(20)	T-2(10)	T-3(20)	T-3(10)	T-4(20)	T-4(10)
$\frac{\partial r_1}{\partial p}$	.0974	.0909	.0974	.0909	**.2780**	.2636	.0972	.0954
$\frac{\partial r_2}{\partial p}$	4.1667	4.1591	3.5191	3.5227	**.8466**	.8500	3.5193	3.5182
$\frac{\partial r_3}{\partial p}$	7.4566	7.4545	3.3279	6.3182	**2.0636**	2.0909	.0972	.0909
$\frac{\partial r_4}{\partial p}$	9.9090	9.9091	4.9421	.7273	**2.8707**	2.8636	.0972	.1364
$\frac{\partial r_5}{\partial p}$	.0995	.0909	.0995	.0909	**3.5537**	3.6364	.0972	.0909
$\frac{\partial r_6}{\partial p}$	.0981	.0909	.0981	.0909	**.2194**	.2273	.0972	.0909
$\frac{\partial r_7}{\partial p}$	.6307	.6818	.6307	.6364	**.6307**	.6364	.6332	.6364
$\frac{\partial r_8}{\partial p}$	.0966	.0909	.0972	.1364	**.8974**	.9091	.0972	.1364
$\frac{\partial r_9}{\partial p}$	.0981	.1136	.0981	.1136	**.0981**	.1136	.0979	.1136
$\frac{\partial r_{10}}{\partial p}$	.0966	.1364	2.6668	2.6364	**6.1218**	6.0909	2.6679	2.6591
$\frac{\partial r_{11}}{\partial p}$	6.6954	6.6818	4.1259	4.1364	**.6709**	.6364	4.1264	4.1364
$\frac{\partial r_{12}}{\partial p}$	.0981	.0909	.0981	.0909	**1.9148**	1.8636	.0996	.1136
$\frac{\partial r_{13}}{\partial p}$	.0995	.0454	3.3808	.3636	**2.6866**	2.6364	.1020	.0682
$\frac{\partial r_{14}}{\partial p}$	1.5542	1.5454	.0974	.1364	**4.0229**	4.0000	.0996	.1591
$\frac{\partial r_{15}}{\partial p}$	.3259	.3182	.3259	.3182	**.3259**	.3182	.3272	.3409
$\frac{\partial r_{16}}{\partial p}$	.1023	.0909	.7478	.7273	**3.4173**	3.4545	.7478	.7500
$\frac{\partial r_{17}}{\partial p}$	.1023	.0909	.1023	.0909	**2.7675**	2.7273	.1023	.1136
$\frac{\partial r_{18}}{\partial p}$	.0995	.0454	4.2253	1.2273	**5.4953**	5.5227	7.4552	7.4318
Z	26.2770		26.1476		25.9359		26.1398	
e	.5746		.7522		.9588		.7965	

	T-5		T-6		T-7		T-8	
	T-5(20)	T-5(10)	T-6(20)	T-6(10)	T-7(20)	T-7(10)	T-8(20)	T-8(10)
$\frac{\partial r_1}{\partial p}$	.2780	.2500	.2780	.2636	.2784	.2500	.2780	.2636
$\frac{\partial r_2}{\partial p}$	3.5191	3.5227	.8466	.8500	.8466	.8409	.8466	.8500
$\frac{\partial r_3}{\partial p}$	2.0636	2.0909	2.0636	2.0909	2.0632	2.1136	2.0636	2.0909
$\frac{\partial r_4}{\partial p}$	2.8707	2.8636	2.8707	2.8636	3.2651	2.8864	3.2651	2.8636
$\frac{\partial r_5}{\partial p}$	3.5537	3.6364	3.5537	3.6364	3.5537	3.5909	3.5537	3.6364
$\frac{\partial r_6}{\partial p}$	.2194	.2273	.2194	.2273	.2194	.2273	.2194	.2273
$\frac{\partial r_7}{\partial p}$	.6307	.6364	.6307	.6364	.6307	.6364	.5256	.5000
$\frac{\partial r_8}{\partial p}$	.8974	.9090	.8974	.9090	.8974	.8864	.8974	.9090
$\frac{\partial r_9}{\partial p}$	.0981	.1136	.0981	.1136	.0981	.1136	.0981	.1136
$\frac{\partial r_{10}}{\partial p}$	6.1218	6.0909	6.1218	6.0909	6.1218	6.0909	6.1218	6.0909
$\frac{\partial r_{11}}{\partial p}$	.6709	.6364	.6709	.6364	.6709	.6364	.6709	.6364
$\frac{\partial r_{12}}{\partial p}$	1.9148	1.8636	1.9148	1.8636	1.9148	1.8636	1.9148	1.8636
$\frac{\partial r_{13}}{\partial p}$	2.6866	2.6364	2.6866	2.6364	4.6423	4.6364	4.6423	4.6364
$\frac{\partial r_{14}}{\partial p}$	4.0229	4.0000	4.0229	4.0000	8.2023	8.5454	8.2023	8.5454
$\frac{\partial r_{15}}{\partial p}$	.3259	.3182	.3259	.3182	.3259	.3182	.4346	.4545
$\frac{\partial r_{16}}{\partial p}$	.7478	.7273	3.4175	3.4545	3.4175	3.4545	3.4175	3.4545
$\frac{\partial r_{17}}{\partial p}$	.1023	.0909	2.7684	2.7273	2.7684	2.7273	2.7684	2.7273
$\frac{\partial r_{18}}{\partial p}$	5.4953	5.5000	5.4953	5.500	5.4953	5.5000	5.4953	5.5227
Z	25.9626		25.9359		26.1868		26.1413	
e	.9726		.9588		.7096		.7151	

Table 17: Case 6: Module PDac – Absolute Values of $\frac{\partial r_i}{\partial p}$

5.2 Module PDac - Case Study 7

This case study considers the same anions and cations than in Section 3.2 as shown in Table 18.

Cations	Li^+	Na^+	K^+	Rb^+	Cs^+	Ca^{2+}	Sr^{2+}	Ba^{2+}	Mg^{2+}	NH_4^+	Ag^+
	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8	r_9	r_{10}	r_{11}
Anions	F^-	Cl^-	Br^-	I^-	O^{2-}	ClO_3^-	BrO_3^-	CN^-			
	r_{12}	r_{13}	r_{14}	r_{15}	r_{16}	r_{17}	r_{18}	r_{19}			

Table 18: Case 7: Module PDac – Cations and Anions Considered

Thus $n_c = 11$, $n_a = 8$ and $md = 19$ with

$$maximize\ Z = \sum_{k=1}^{19} r_k \tag{30}$$

subject to the restrictions

$$r_i + r_j \leq R_{ij}\ for \begin{cases} i \in \{1..11\} \\ j \in \{12..19\} \end{cases}$$

all nonnegative making 37 inequalities where the correspondence among the salts being studied and the R_{ij} notation is shown in Table 19.

LiF	LiCl	LiBr	LiI	NaF	NaCl	NaBr	NaI	$NaClO_3$	$NaBrO_3$
$R_{1,12}$	$R_{1,13}$	$R_{1,14}$	$R_{1,15}$	$R_{2,12}$	$R_{2,13}$	$R_{2,14}$	$R_{2,15}$	$R_{2,17}$	$R_{2,18}$
KF	KCl	KBr	KI	KCN	RbF	RbCl	RbBr	RbI	
$R_{3,12}$	$R_{3,13}$	$R_{3,14}$	$R_{3,15}$	$R_{3,19}$	$R_{4,12}$	$R_{4,13}$	$R_{4,14}$	$R_{4,15}$	
CsF	CsCl	CsBr	CsI						
$R_{5,12}$	$R_{5,13}$	$R_{5,14}$	$R_{5,15}$						
CaF	CaO	SrF	SrCl	SrO	BaF	BaO	MgO		
$R_{6,12}$	$R_{6,16}$	$R_{7,12}$	$R_{7,13}$	$R_{7,16}$	$R_{8,12}$	$R_{8,16}$	$R_{9,16}$		
NH_4F	NH_4Cl	NH_4Br	NH_4I	AgCl	AgBr				
$R_{10,12}$	$R_{10,13}$	$R_{10,14}$	$R_{10,15}$	$R_{11,13}$	$R_{11,14}$				

Table 19: Case 7: Module PDac – Correspondence Among Salts

In matrix form $\mathbf{Ar} \leq \mathbf{R}$ where $\mathbf{A}$, $\mathbf{r}$, and $\mathbf{R}$ are defined as shown in (31).

$$
\mathbf{A} = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\quad
\mathbf{r} = \begin{pmatrix}
r_1 \\ r_2 \\ r_3 \\ r_4 \\ r_5 \\ r_6 \\ r_7 \\ r_8 \\ r_9 \\ r_{10} \\ r_{11} \\ r_{12} \\ r_{13} \\ r_{14} \\ r_{15} \\ r_{16} \\ r_{17} \\ r_{18} \\ r_{19}
\end{pmatrix}
\quad
\mathbf{R} = \begin{pmatrix}
R_{1,12} \\ R_{1,13} \\ R_{1,14} \\ R_{1,15} \\ R_{2,12} \\ R_{2,13} \\ R_{2,14} \\ R_{2,15} \\ R_{2,17} \\ R_{2,18} \\ R_{3,12} \\ R_{3,13} \\ R_{3,14} \\ R_{3,15} \\ R_{3,19} \\ R_{4,12} \\ R_{4,13} \\ R_{4,14} \\ R_{4,15} \\ R_{5,12} \\ R_{5,13} \\ R_{5,14} \\ R_{5,15} \\ R_{6,12} \\ R_{6,16} \\ R_{7,12} \\ R_{7,13} \\ R_{7,16} \\ R_{8,12} \\ R_{8,16} \\ R_{9,16} \\ R_{10,12} \\ R_{10,13} \\ R_{10,14} \\ R_{10,15} \\ R_{11,13} \\ R_{11,14}
\end{pmatrix}
\tag{31}
$$

where

$$\mathbf{R}^t = (1.996, 2.539, 2.713, 2.951, 2.295, 2.789, 2.954, 3.194, 3.2775, 3.3445, 2.648, 3.116, 3.262, 3.489, 3.25, 2.789, 3.259, 3.410, 3.628, 2.9827, 3.5150, 3.6645, 3.9018, 2.30, 2.3995, 2.51, 3.0311, 2.5698, 2.69, 2.8129, 2.1066, 2.63, 3.356, 3.516, 3.785, 2.77, 2.88)$$

Similar to Section 5.1 Table 17 shows the results obtained for $\frac{\partial r}{\partial p}$.

- T-1 fixing the following values at p_0

$$\begin{aligned} &r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{13} = \frac{R^{(0)}_{1,13}}{\sqrt{2}} \qquad r_{14} = \frac{R^{(0)}_{1,14}}{\sqrt{2}} \qquad r_{15} = \frac{R^{(0)}_{1,15}}{\sqrt{2}} \\ &r_2 = R^{(0)}_{2,12} - r_{12} \qquad r_3 = R^{(0)}_{3,12} - r_{12} \qquad r_{16} \geq 1.2 \end{aligned} \tag{32}$$

  In each maximization procedure the following values were also fixed

$$\begin{aligned} &r'_2 = \frac{R^0_{2,12} - \frac{\chi_{2,12} R^0_{2,12}}{3}(p'-p_0)}{\sqrt{2}} - r'_{12} \qquad r'_3 = \frac{R^0_{3,12} - \frac{\chi_{3,12} R^0_{3,12}}{3}(p'-p_0)}{\sqrt{2}} - r'_{12} \\ &r'_{12} = \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p'-p_0)}{\sqrt{2}} \qquad r'_{13} = \frac{R^0_{1,13} - \frac{\chi_{1,13} R^0_{1,13}}{3}(p'-p_0)}{\sqrt{2}} \\ &r'_{14} = \frac{R^0_{1,14} - \frac{\chi_{1,14} R^0_{1,14}}{3}(p'-p_0)}{\sqrt{2}} \qquad r'_{15} = \frac{R^0_{1,15} - \frac{\chi_{1,15} R^0_{1,15}}{3}(p'-p_0)}{\sqrt{2}} \end{aligned} \tag{33}$$

- T-2 fixing the following values at p_0

$$\begin{aligned} &r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{13} = \frac{R^{(0)}_{1,13}}{\sqrt{2}} \qquad r_{14} = \frac{R^{(0)}_{1,14}}{\sqrt{2}} \qquad r_{15} = \frac{R^{(0)}_{1,15}}{\sqrt{2}} \\ &r_2 = R^{(0)}_{2,12} - r_{12} \end{aligned} \tag{34}$$

- T-3 fixing the following values at p_0

$$\begin{aligned} &r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{13} = \frac{R^{(0)}_{1,13}}{\sqrt{2}} \qquad r_{14} = \frac{R^{(0)}_{1,14}}{\sqrt{2}} \qquad r_{15} = \frac{R^{(0)}_{1,15}}{\sqrt{2}} \\ &r_2 = R^{(0)}_{2,12} - r_{12} \qquad r_{16} \geq 1.2 \end{aligned} \tag{35}$$

  In each maximization procedure the following values were also fixed

$$\begin{aligned} &r'_2 = \frac{R^0_{2,12} - \frac{\chi_{2,12} R^0_{2,12}}{3}(p'-p_0)}{\sqrt{2}} - r'_{12} \\ &r'_{12} = \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p'-p_0)}{\sqrt{2}} \qquad r'_{13} = \frac{R^0_{1,13} - \frac{\chi_{1,13} R^0_{1,13}}{3}(p'-p_0)}{\sqrt{2}} \\ &r'_{14} = \frac{R^0_{1,14} - \frac{\chi_{1,14} R^0_{1,14}}{3}(p'-p_0)}{\sqrt{2}} \qquad r'_{15} = \frac{R^0_{1,15} - \frac{\chi_{1,15} R^0_{1,15}}{3}(p'-p_0)}{\sqrt{2}} \end{aligned} \tag{36}$$

- T-4 fixing the following values at p_0

$$r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{13} = \frac{R^{(0)}_{1,13}}{\sqrt{2}} \qquad r_{14} = \frac{R^{(0)}_{1,14}}{\sqrt{2}} \qquad r_{15} = \frac{R^{(0)}_{1,15}}{\sqrt{2}}$$
$$r_2 = R^{(0)}_{2,12} - r_{12} \qquad r_3 = R^{(0)}_{3,12} - r_{12} \qquad r_{16} \geq 1.2 \tag{37}$$

In each maximization procedure the following values were also fixed

$$r'_{12} = \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{13} = \frac{R^0_{1,13} - \frac{\chi_{1,13} R^0_{1,13}}{3}(p' - p_0)}{\sqrt{2}}$$
$$r'_{14} = \frac{R^0_{1,14} - \frac{\chi_{1,14} R^0_{1,14}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{15} = \frac{R^0_{1,15} - \frac{\chi_{1,15} R^0_{1,15}}{3}(p' - p_0)}{\sqrt{2}} \tag{38}$$

- T-5 fixing the following values at p_0

$$r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{13} = \frac{R^{(0)}_{1,13}}{\sqrt{2}} \qquad r_{14} = \frac{R^{(0)}_{1,14}}{\sqrt{2}} \qquad r_{15} = \frac{R^{(0)}_{1,15}}{\sqrt{2}}$$
$$r_2 = R^{(0)}_{2,12} - r_{12} \qquad r_3 = R^{(0)}_{3,12} - r_{12} \qquad r_{16} \geq 1.2 \tag{39}$$

In each maximization procedure the following values were also fixed

$$r'_2 = \frac{R^0_{2,12} - \frac{\chi_{2,12} R^0_{2,12}}{3}(p' - p_0)}{\sqrt{2}} - r'_{12}$$
$$r'_{12} = \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{13} = \frac{R^0_{1,13} - \frac{\chi_{1,13} R^0_{1,13}}{3}(p' - p_0)}{\sqrt{2}} \tag{40}$$
$$r'_{14} = \frac{R^0_{1,14} - \frac{\chi_{1,14} R^0_{1,14}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{15} = \frac{R^0_{1,15} - \frac{\chi_{1,15} R^0_{1,15}}{3}(p' - p_0)}{\sqrt{2}}$$

- T-6 fixing the following values at p_0

$$r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{13} = \frac{R^{(0)}_{1,13}}{\sqrt{2}} \qquad r_2 = R^{(0)}_{2,12} - r_{12} \qquad r_3 = R^{(0)}_{3,12} - r_{12}$$
$$r_{16} \geq 1.2 \tag{41}$$

In each maximization procedure the following values were also fixed

$$r'_2 = \frac{R^0_{2,12} - \frac{\chi_{2,12} R^0_{2,12}}{3}(p' - p_0)}{\sqrt{2}} - r'_{12} \qquad r'_3 = \frac{R^0_{3,12} - \frac{\chi_{3,12} R^0_{3,12}}{3}(p' - p_0)}{\sqrt{2}} - r'_{12}$$
$$r'_{12} = \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{13} = \frac{R^0_{1,13} - \frac{\chi_{1,13} R^0_{1,13}}{3}(p' - p_0)}{\sqrt{2}} \tag{42}$$

- T-7 fixing the following values at p_0

$$r_{12} = \frac{R^{(0)}_{1,12}}{\sqrt{2}} \qquad r_{13} = \frac{R^{(0)}_{1,13}}{\sqrt{2}}$$
$$r_2 = R^{(0)}_{2,12} - r_{12} \qquad r_3 = R^{(0)}_{3,12} - r_{12} \qquad r_{10} = R^{(0)}_{10,12} - r_{12} \qquad r_{16} \geq 1.2 \tag{43}$$

  In each maximization procedure the following values were also fixed

$$r'_2 = \frac{R^0_{2,12} - \frac{\chi_{2,12} R^0_{2,12}}{3}(p' - p_0)}{\sqrt{2}} - r'_{12} \qquad r'_3 = \frac{R^0_{3,12} - \frac{\chi_{3,12} R^0_{3,12}}{3}(p' - p_0)}{\sqrt{2}} - r'_{12}$$
$$r'_{10} = \frac{R^0_{10,12} - \frac{\chi_{10,12} R^0_{10,12}}{3}(p' - p_0)}{\sqrt{2}} - r'_{12} \tag{44}$$
$$r'_{12} = \frac{R^0_{1,12} - \frac{\chi_{1,12} R^0_{1,12}}{3}(p' - p_0)}{\sqrt{2}} \qquad r'_{13} = \frac{R^0_{1,13} - \frac{\chi_{1,13} R^0_{1,13}}{3}(p' - p_0)}{\sqrt{2}}$$

- T-8 same as T-3 but having a smaller e value

$\frac{\partial r_i}{\partial p}$	T-1		T-2		T-3		T-4	
	T-1(20)	T-1(10)	T-2(20)	T-2(10)	T-3(20)	T-3(10)	T-4(20)	T-4(10)
$\frac{\partial r_1}{\partial p}$	.2784	.2636	.0974	.0954	.2784	.2636	.2784	.2636
$\frac{\partial r_2}{\partial p}$	.8466	.8500	4.1668	4.1454	.8466	.8500	3.5193	3.5182
$\frac{\partial r_3}{\partial p}$	2.0632	2.0909	.0972	.1364	2.0632	2.0909	2.0632	2.0909
$\frac{\partial r_4}{\partial p}$	2.8707	2.8636	.0972	.1364	2.8719	2.8636	2.8707	2.8636
$\frac{\partial r_5}{\partial p}$	3.5537	3.6364	.0972	.1364	3.5537	3.6364	3.5537	3.6364
$\frac{\partial r_6}{\partial p}$	.2182	.2273	.0972	.0909	.2182	.2273	.2182	.2273
$\frac{\partial r_7}{\partial p}$	.5256	.5000	.6332	.6364	.5256	.5000	.5241	.5000
$\frac{\partial r_8}{\partial p}$	.8974	.9090	.0972	.1364	.8974	.9090	.8974	.9091
$\frac{\partial r_9}{\partial p}$	.0979	.1136	.0979	.1136	.0995	.0954	.0996	.0954
$\frac{\partial r_{10}}{\partial p}$	6.1218	6.0909	.0972	.1364	6.1218	6.0909	6.1208	6.0909
$\frac{\partial r_{11}}{\partial p}$	.0972	.0909	.4635	.0909	.0981	.0909	.0972	.0909
$\frac{\partial r_{12}}{\partial p}$	.6709	.6364	6.6971	6.6818	.6709	.6364	.6709	.6364
$\frac{\partial r_{13}}{\partial p}$	1.9148	1.8636	.0996	.0909	1.9148	1.8636	1.9148	1.8636
$\frac{\partial r_{14}}{\partial p}$	2.6866	2.6364	1.8924	2.3182	2.6866	2.6364	2.6866	2.6364
$\frac{\partial r_{15}}{\partial p}$	4.0229	4.0000	.0996	.1364	4.0229	4.0227	4.0229	4.0000
$\frac{\partial r_{16}}{\partial p}$	.4346	.4545	.3273	.3182	.3238	.3182	.3238	.3182
$\frac{\partial r_{17}}{\partial p}$	3.4175	3.4545	.0996	.0909	3.4175	3.4318	.7478	.7273
$\frac{\partial r_{18}}{\partial p}$	2.7684	2.7273	.0996	.0909	2.7684	2.7045	.1023	.0909
$\frac{\partial r_{19}}{\partial p}$	5.4953	5.5000	7.4560	7.3636	5.4953	5.5000	5.4953	5.5000
Z	26.8966		27.0580		26.8976		26.9243	
e	.9589		.7949		1.0927		1.1048	

	T-5		T-6		T-7		T-8	
	T-5(20)	T-5(10)	T-6(20)	T-6(10)	T-7(20)	T-7(10)	T-8(20)	T-8(10)
$\frac{\partial r_1}{\partial p}$	.2784	.2636	.2784	.2636	.2784	.2636	.2780	.2636
$\frac{\partial r_2}{\partial p}$	.8466	.8500	.8466	.8500	.8466	.8500	.8466	.8500
$\frac{\partial r_3}{\partial p}$	7.4560	7.4545	2.0632	2.0909	2.0632	2.0909	2.0636	2.0909
$\frac{\partial r_4}{\partial p}$	2.8719	2.8636	4.5106	4.5000	4.5106	4.5000	2.8707	2.8636
$\frac{\partial r_5}{\partial p}$	3.5525	3.6364	3.5525	3.6364	3.5525	3.6364	3.5537	3.6364
$\frac{\partial r_6}{\partial p}$	.2182	.2273	.2182	.2273	.2182	.2273	.2194	.2273
$\frac{\partial r_7}{\partial p}$	.5256	.5000	.5241	.5000	.5256	.5000	.6307	.6364
$\frac{\partial r_8}{\partial p}$	.8964	.9091	.8964	.9091	.8974	.9091	.8974	.9090
$\frac{\partial r_9}{\partial p}$	.0996	.0954	.0979	.1136	.0995	.0954	.0981	.1136
$\frac{\partial r_{10}}{\partial p}$	6.1218	6.0909	6.1208	6.0909	6.1218	6.0909	6.1218	6.0909
$\frac{\partial r_{11}}{\partial p}$	.0981	.0909	.0972	.0909	.0981	.0909	.0981	.0909
$\frac{\partial r_{12}}{\partial p}$	.6709	.6364	.6711	.6364	.6709	.6364	.6709	.6364
$\frac{\partial r_{13}}{\partial p}$	1.9148	1.8636	1.9162	1.8636	1.9148	1.8636	1.9162	1.8636
$\frac{\partial r_{14}}{\partial p}$	2.6866	2.6364	4.6434	4.6364	4.6423	4.6364	2.6866	2.6364
$\frac{\partial r_{15}}{\partial p}$	4.0229	4.0000	6.9508	6.9091	6.9507	6.9091	4.0229	4.0000
$\frac{\partial r_{16}}{\partial p}$	.3238	.3182	.4340	.4545	.3238	.3182	.3259	.3182
$\frac{\partial r_{17}}{\partial p}$	3.4175	3.4545	3.4173	3.4545	3.4175	3.4545	3.4175	3.4545
$\frac{\partial r_{18}}{\partial p}$	2.7684	2.7273	2.7684	2.7273	2.7684	2.7273	2.7684	2.7273
$\frac{\partial r_{19}}{\partial p}$	.0995	.0454	5.4947	5.5227	5.4953	5.5000	5.4953	5.5000
Z	26.8976		26.9949		26.9959		26.8965	
e	1.1123		.7146		.8861		.9589	

Table 20: Case 7: Module PDac – Absolute Values of $\frac{\partial r_i}{\partial p}$

6 Conclusions

Values of $\frac{\partial r_i}{\partial p}$ were obtained with the methods described and compared to the ones obtained with a previous method, presenting a very good agreement. In particular, more complex ions ($NH4^+$, CN^- , $ClO3^-$, $BrO3^-$) were studied. The reliability of the $\frac{\partial r_i}{\partial p}$ could be established by the reasonable agreement between values of pressure dependence of ionic polarizabilities obtained with $\frac{\partial r_i}{\partial p}$ values and those from interpolation techniques.

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7 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 [8]. It should be noted that some data was not available at LT, in those cases the missing data $*$ has been substituted by data at RT from the sane source. Observe that the PDac module only uses the data related to the values r_0 and χ_T for the salts treated.

Struct.	Salt	α_+ $10^{-24}cm^3$	α_- $10^{-24}cm^3$	r_0 $10^{-8}cm$	ε_0	ε_∞	χ_T $10^{-12}cm^2dyn^{-1}$
fcc	Li	0.030					
C=2	LiF		0.89	1.996	8.50	1.93	1.43
	LiCl		2.94	2.539	10.83	2.79	3.20
	LiBr		4.13	2.713	11.95	3.22	*4.20
	LiI		6.19	2.951	15.28	3.89	*5.7803
	Na	0.147					
	NaF		1.02	2.295	4.73	1.75	1.99
	NaCl		3.14	2.789	5.43	2.35	3.98
	NaBr		4.28	2.954	5.78	2.64	4.70
	NaI		6.35	3.194	6.62	3.08	6.45
	K	0.81					
	KF		1.20	2.648	5.11	1.86	3.10
	KCl		3.36	3.116	4.49	2.20	5.26
	KBr		4.54	3.262	4.52	2.39	6.17
	KI		6.66	3.489	4.66	2.68	7.75
	Rb	1.35					
	RbF		1.18	2.789	5.99	1.94	*3.81
	RbCl		3.45	3.259	4.53	2.20	*6.40
	RbBr		4.58	3.410	4.51	2.36	*7.69
	RbI		6.80	3.628	4.55	2.61	*9.48
	Cs	2.34					
	CsF		1.27	2.9827	7.27	2.17	*4.25
bcc	Cs	2.34					
C= $\frac{8}{3\sqrt{3}}$	CsCl		3.55	3.5150	6.68	2.67	4.5387
	CsBr		4.66	3.6645	6.38	2.83	5.4476
	CsI		6.81	3.9018	6.29	3.09	6.9396
	CaF			2.30			1.1628
	CaO			2.3995			0.9009
	SrF			2.51			1.4320
	SrO			2.5698			1.1198
	SrCl			3.0311			3.28
	BaF			2.69			1.7513
	BaO			2.8129			1.3263
	MgO			2.1066			0.606
	$NaClO_3$			3.2775			3.90625
	$NaBrO_3$			3.3445			3.24675
	NH_4F			2.63			7.75
	NH_4Cl			3.356			5.58
	NH_4Br			3.516			6.44
	NH_4I			3.785			6.62
	KCN			3.25			6.9767
	AgCl			2.77			2.2676
	AgBr			2.88			2.457

Table 21: Experimental Data at Low Temperatures

The following values of $\frac{\partial R}{\partial p}$ for different salts at Low Temperature have been obtained from the experimental values of the compressibility of each salt.

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

Salt	$\frac{\partial R}{\partial p}$	Salt	$\frac{\partial R}{\partial p}$
LiF	0.9514	KF	2.7363
LiCl	2.7083	KCl	5.4634
LiBr	3.7982	KBr	6.7088
LiI	5.6859	KI	9.0133
		KCN	7.5581
RbF	3.5420	CsF	4.2308
RbCl	6.9525	CsCl	5.3178
RbBr	8.7410	CsBr	6.6542
RbI	11.4645	CsI	9.0256
NaF	1.5224	NH4F	6.79417
NaCl	3.7000	NH4Cl	6.24216
NaBr	4.6279	NH4Br	7.54768
NaI	6.8671	NH4I	8.35223
NaCLO3	4.2676	AgCl	2.0938
NaBrO3	3.6196	AgBr	2.3587
CaF	0.8915		
CaO	0.7206		
SrF	1.1981		
SrCl	3.3128		
SrO	0.9592		
BaF	1.5703		
BaO	1.2436		
MgO	0.4255		

Table 22: Absolute Values of $\frac{\partial R}{\partial p}$ at Low Temperatures

have been used.

Anion	$\frac{\partial r_+}{\partial p}$	Cation	$\frac{\partial r_-}{\partial p}$
Li	0.2780	F	0.6709
K	2.0636	Cl	1.9148
Rb	2.8707	Br	2.6866
Na	0.8466	I	4.0229
		O^2	0.3442

Table 23: Absolute Values of $\frac{\partial r_+}{\partial p}$ and $\frac{\partial r_-}{\partial p}$ at Low Temperatures