# The *OptiSage* module

Use the ***OptiSage*** module for the assessment of Gibbs energy data.

Various types of experimental data can be utilized in order to generate optimized parameters for the Gibbs energies of stoichiometric compounds as well as the excess coefficients of a wide range of non-ideal solution models.

In the present example we will use ***OptiSage*** to treat the various phase diagram, enthalpy and activity data for the NaCl-$SrCl_2$ system in order to obtain polynomial parameters for the Gibbs energy of mixing in the liquid phase.

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# Introduction to the Data Optimization procedure

The ***OptiSage*** module is used to generate a consistent set of Gibbs energy parameters from a given set of experimental data using known Gibbs energy data from well established phases of a particular chemical system.

Typical experimental data include:

- phase diagram data: transition temperatures and pressures as well as amount and composition of the phases at equilibrium
- calorimetric data: enthalpies of formation or phase transformation, enthalpies of mixing, heat contents and heat capacity measurements
- partial Gibbs energy data: activities from vapor pressure or EMF measurements
- volumetric data: dilatometry, density measurements.

The assessor (user of ***OptiSage***) has to use his best judgement on which of the known parameters should remain fixed, which set of parameters need refinement in the optimization and which new parameters have to be introduced, especially when assessing data for non-ideal solutions.

# Overview of the data to be optimized in the NaCl-$SrCl_2$ system

Various experimental data on the binary NaCl-$SrCl_2$ system are available:

- phase diagram data (liquidus points, eutectic points)
- liquid-liquid enthalpy of mixing (at 894℃)
- activity of NaCl(liq) at 3 different temperatures (800℃, 825℃ and 850℃)

***OptiSage*** will be used to optimize the parameters for the liquid interctions ($G^E$ terms). All other data ($G°$ of the pure stoichiometric solids, as well as the pure liquid components) will be taken from the FACT database (i.e. remain fixed).
A substitutional solution model with a polynomial for the excess Gibbs energy will be used:

$$G = (X_1 G°_1 + X_2 G°_2) + RT(X_1 \ln X_1 + X_2 \ln X_2) + G^E$$

where $G^E = \Delta H - TS^E$

Using the binary excess terms:

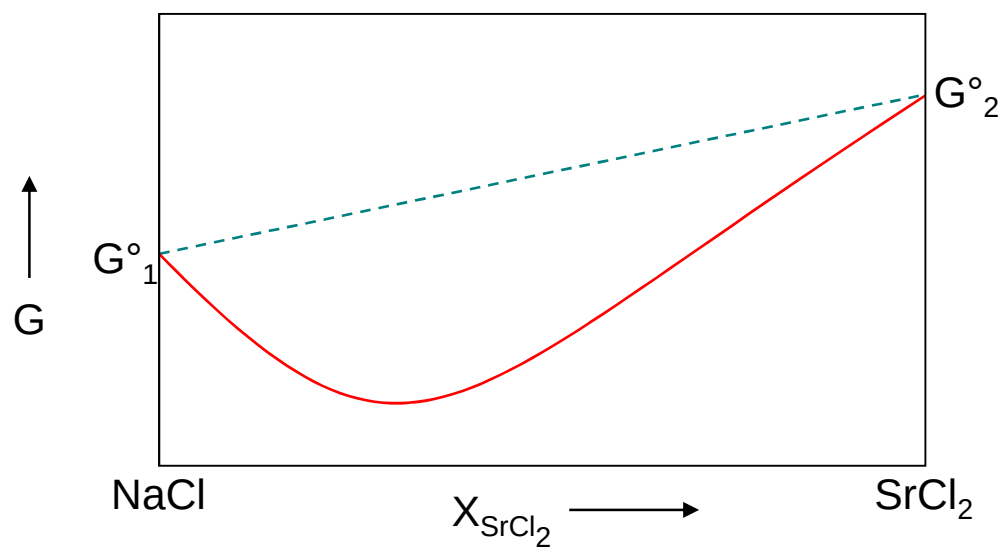
$\Delta H = X_1X_2 (A_1) + X_1^2X_2 (A_2)$

$-S^E = X_1X_2 (B_1) + X_1^2X_2 (B_2)$

one obtains:

$G^E = X_1X_2 (A_1 + B_1T) + X_1^2X_2 (A_2 + B_2T)$

Where $A_1$, $A_2$, $B_1$ and $B_2$ are the 4 parameters to be optimized.



# The 3 Steps in the Optimization Procedure

In general a three step procedure is adopted for the optimization:

Step 1. Set a thermodynamic datafile (***ChemSage*** file)

Step 2. Organise the various experimental data values (Excel file)

Step 3. Execute the optimization program interactively (run ***OptiSage***)

In order to create a ***ChemSage*** file (step 1.), it is necessary to use the ***Compound***, ***Solution*** and ***Equilib*** modules as outlined in the following slides.

# Creation of a private (r/w) compound database

- ***OptiSage*** uses a ***ChemSage*** thermodynamic datafile containing all known and unknown (to be optimized) model parameters. The ***ChemSage*** file is created by ***Equilib***.
- G° of each component of the liquid phase is taken from t he FACT database.

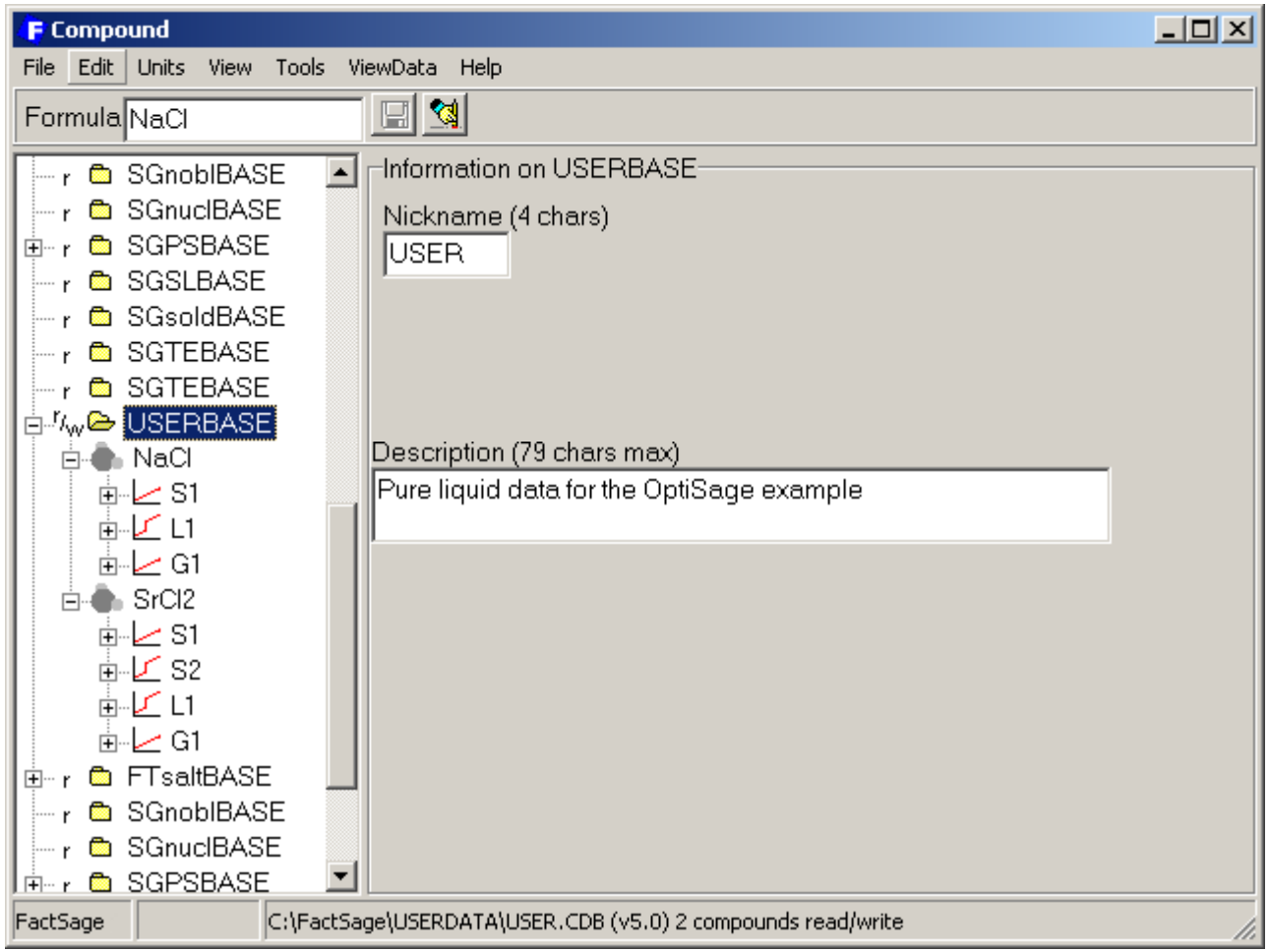
| Component | Index | G° |
|---|---|---|
| NaCl | 1 | Liquid from FACT |
| $SrCl_2$ | 2 | Liquid from FACT |

- You have to create a private r/w (read/write) COMPOUND database containing NaCl(liq) and $SrCl_2$(liq) using the ***Compound*** module. Public data (read-only) cannot be used in ***OptiSage***.

- To create a private Compound database: see ***Compound*** section 3.
- To transfer data between databases: see ***Compound*** section 11.

# Private Compound Database

A private Compound database nicknamed USER containing NaCl and $SrCl_2$ should look like:



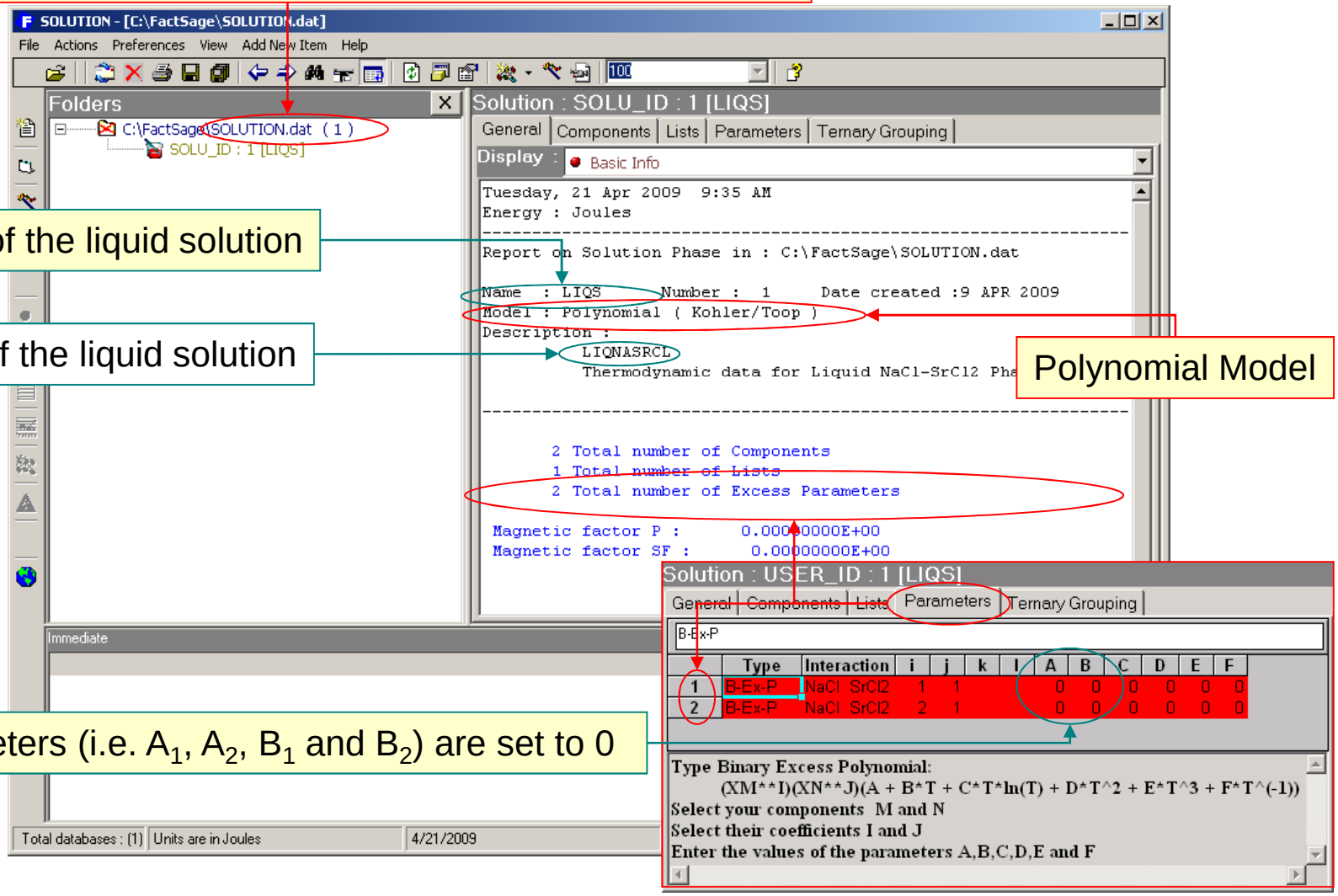

**Note:** Gaseous NaCl and $SrCl_2$ are not needed in the present example.

# Creation of a new solution database

- You have to create a private solution file containing all parameters (either known and/or to be optimized) for each solution phase to be optimized. You cannot perform an optimization using a public database (read-only) such as FACT.
- The solution file must include all parameters to be optimized (with their coefficients set to zero or to any initial value).
- For the $NaCl\text{-}SrCl_2$ system:
  - one phase is to be optimized: the liquid solution.
  - a polynomial model will be used (see slide 3).
    4 coefficients are set to zero:
    i.e. $A_1 = A_2 = B_1 = B_2 = 0$
- A solution database nicknamed **SOLUTION** has been created using the ***Solution*** module.
  - to create a private solution database: see ***Solution*** **section 5**.
- Save this solution file.

# Private Solution Database

In the ***Solution*** module, a new private solution database named **SOLUTION.dat** should look like:




Nickname of the liquid solution

**Name** of the liquid solution

Polynomial Model

Excess parameters (i.e. $A_1$, $A_2$, $B_1$ and $B_2$) are set to 0

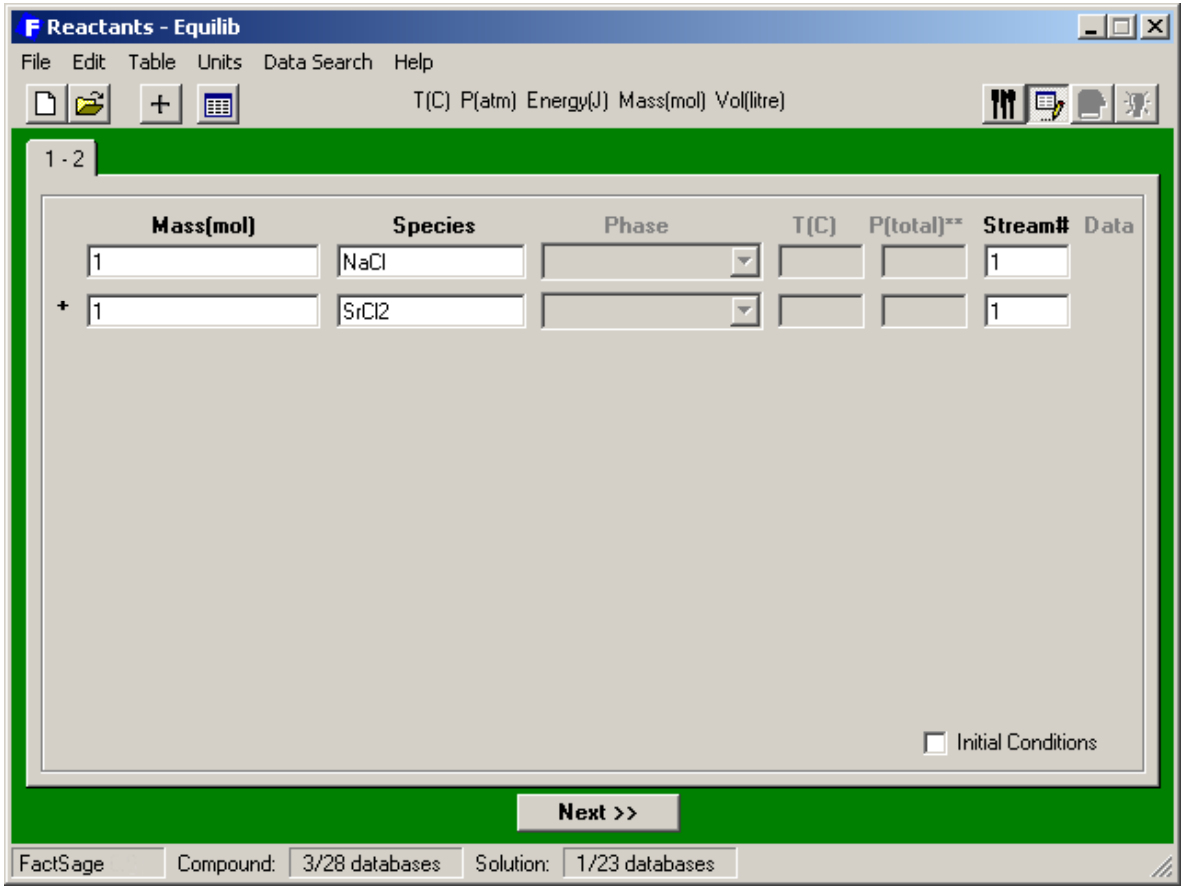
# Generation of a ***ChemSage*** file

The following four slides show how the above Compound and Solution private databases are linked with the ***Equilib*** module, and how the selection of the relevant phases in ***Equilib*** is used to generate the ***ChemSage*** file.

# Creation of a ***ChemSage*** file for the optimization

The procedure is:

- open the ***Equilib*** module
- enter the components NaCl and $SrCl_2$ in the Reactants window of ***Equilib***

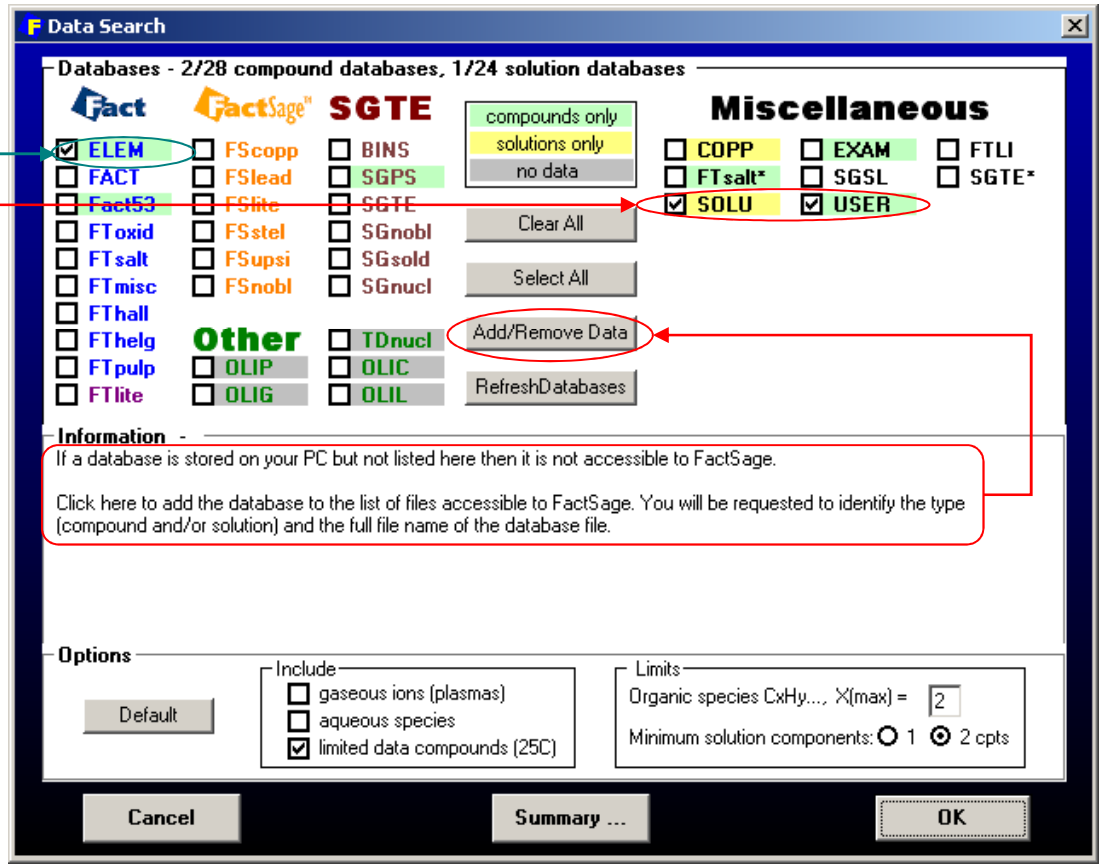


# Adding your private databases to ***FactSage*** list of databases

Do not forget to add and activate the newly created private databases to the list of databases in the ***Equilib*** module (see Equilib Advanced slide 26.3 and Phase Diagram slide 6.1).
From the Menu Bar in the Reactants-Equilib window, select: Data Search

Make sure that the **ELEM** compound database is also selected and that **no other** databases are selected.

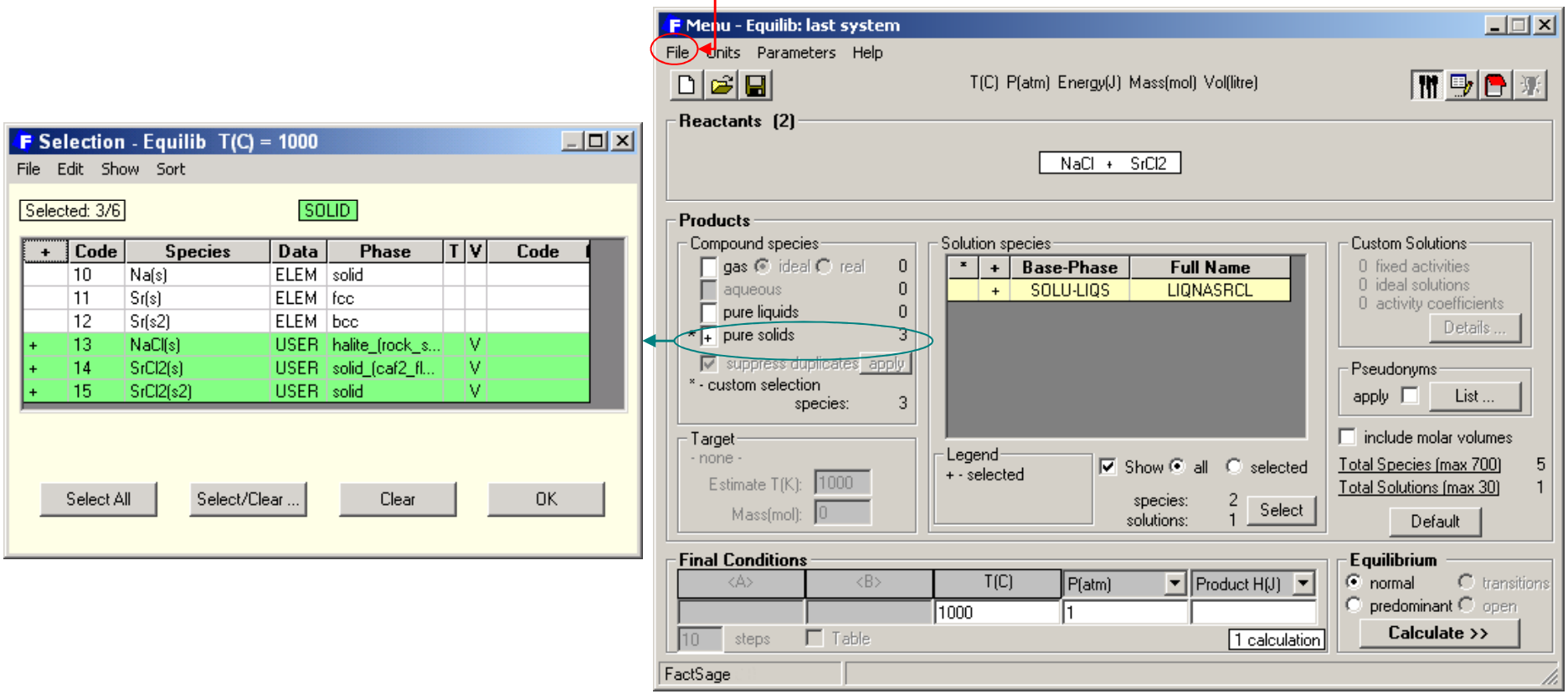
…and add your **read and write (r/w)** databases



# *Equilib* Menu window

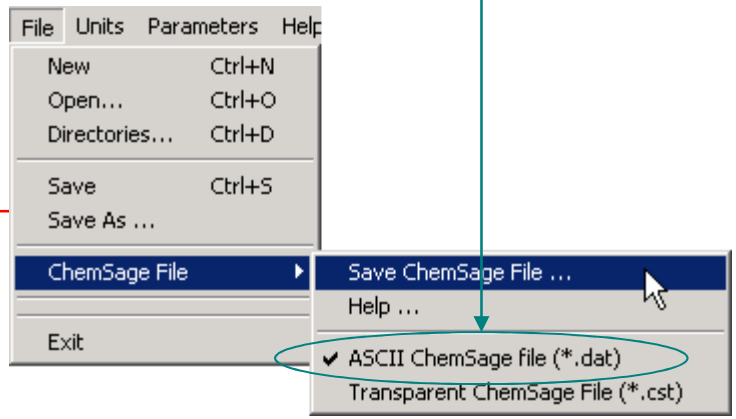
– in the Menu window of ***Equilib***, select all the species and the solutions (including the solution(s) to be optimized) involved in the actual optimization from your USER databases.

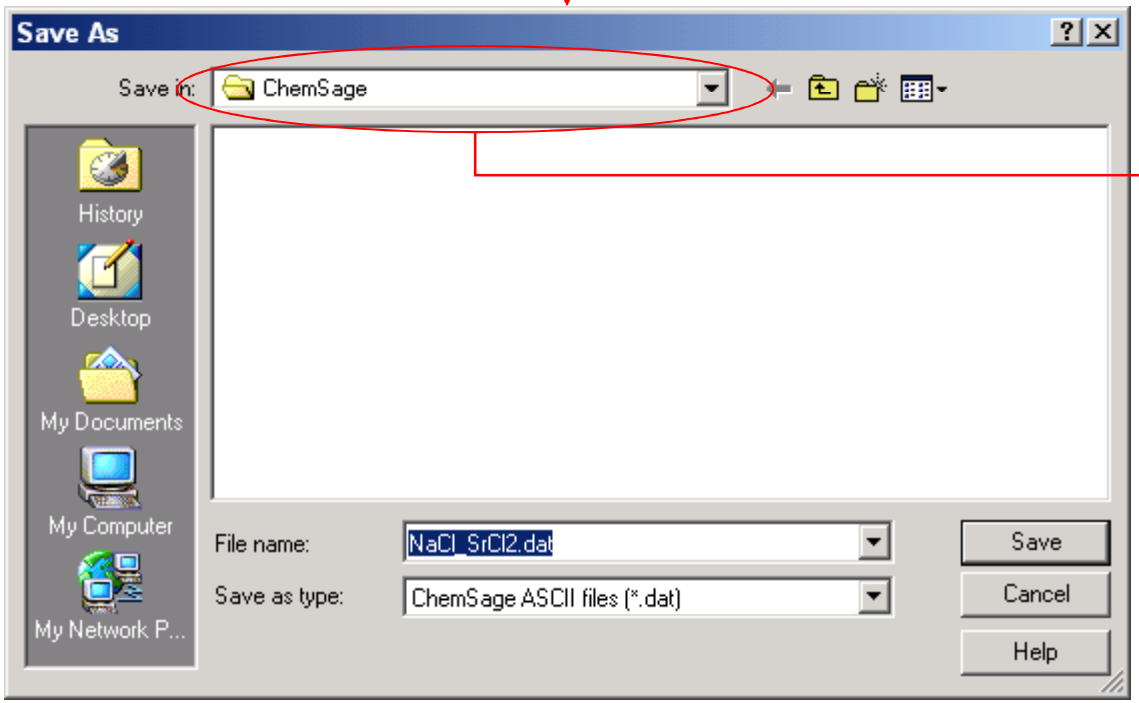
– save a ***ChemSage*** (ASCII format *.dat) file.
In the menu bar, select File > ChemSage file > Save ChemSage file…

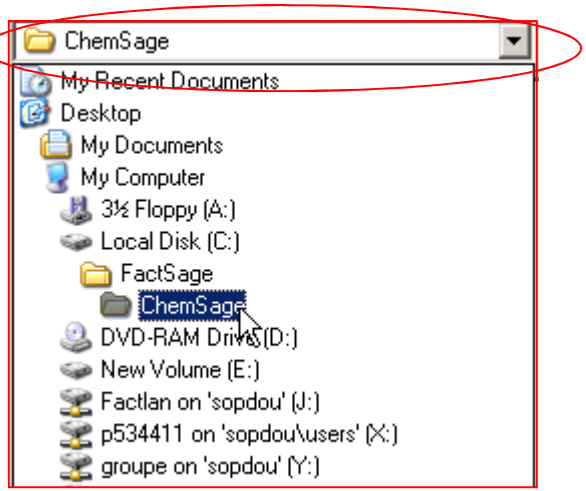


# Saving a *ChemSage* File

Saving an **ASCII *ChemSage* file (*.dat)** under the name :
**NaCl_SrCl2.dat**



# Experimental datasets to be used in the optimization

**Step 2: Organize the experimental data.**

Various types of experimental data can be used in an optimization.

In the present example activity data, enthalpies of mixing and phase diagram data will be employed. Each phase boundary will be treated as a separate dataset.

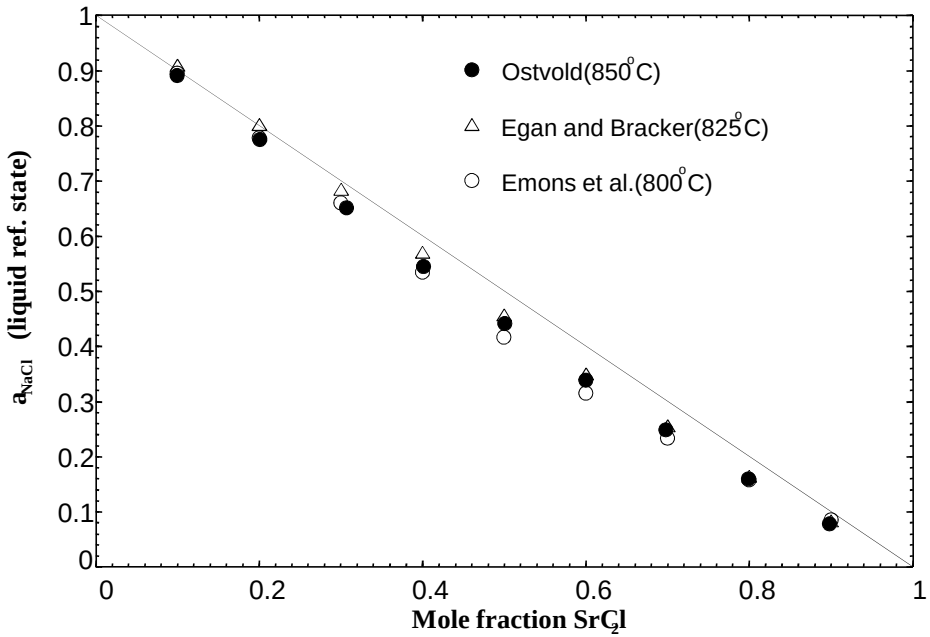
The datasets will be given the names GROUP #1, #2, …, #5. This leads to five different datasets.

The following three slides show how the five different groups are defined.

# **Group #1** – Experimental Data Points: Activity Data.

- We want to **utilize the experimental data** to **obtain optimized model parameters** for the NaCl-$SrCl_2$ liquid phase.
- Data are divided into five different groups where **each group corresponds to a specific type of *Equilib* calculation**.

- **Group #1: Activity of NaCl in the liquid phase**
  - **Experimental conditions:**
    - **Amount of NaCl in the liquid phase**
    - **Amount of $SrCl_2$ in the liquid phase**
    - **Temperature**
    - **Pressure**
  - **Measured variables:**
    - **Activity of NaCl in the liquid phase**
  - **Selected phases:**
    - **Liquid phase**



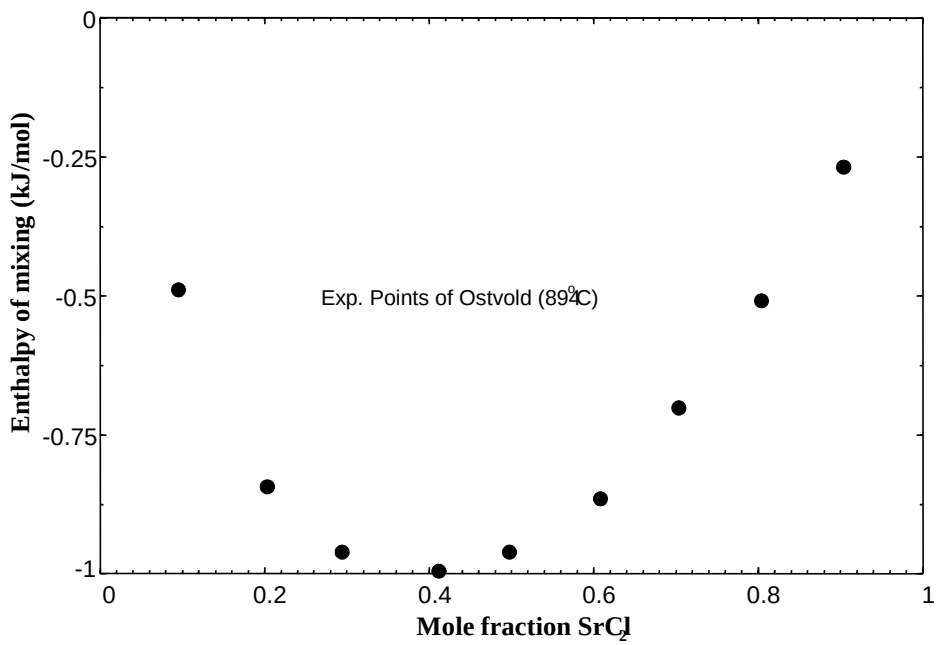
# Group #2 – Heat of mixing data

## Group #2: Enthalpy of mixing of the NaCl-$SrCl_2$ liquid mixture at 1167K (894°C).

– **Experimental conditions:**
- **Amount of NaCl(liquid)**
- **Amount of $SrCl_2$(liquid)**
- **Initial Temperature**
- **Initial Pressure**
- **Final Temperature**
- **Final Pressure**

– **Measured variables:**
- **Enthalpy of mixing (liquid)**

– **Selected phases:**
- **Liquid phase**

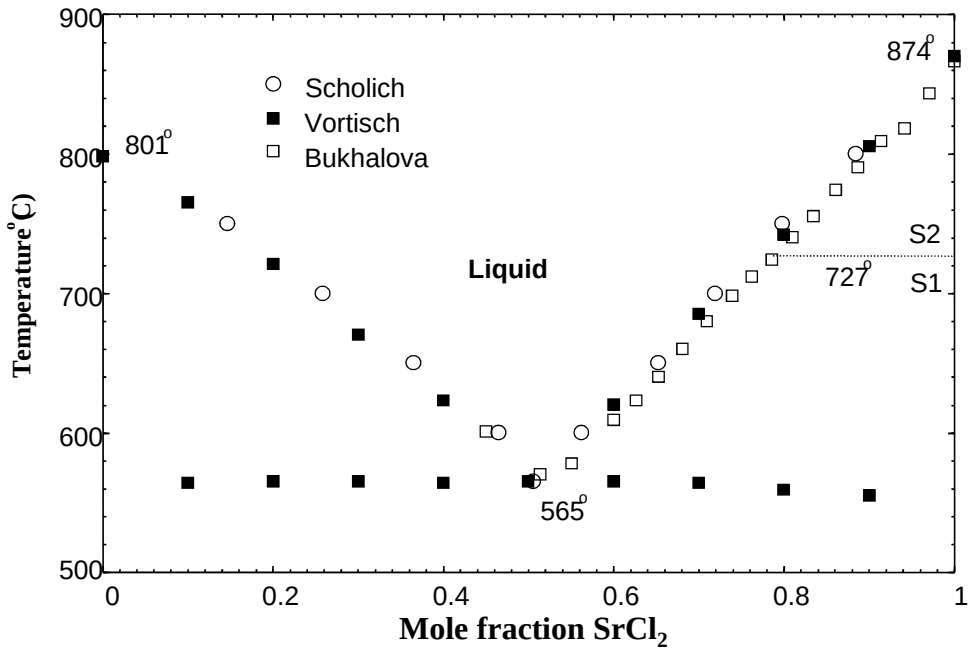


# **Groups #3, #4 and #5** – Data related to phase equilibria.

- **Group #3: Eutectic temperature**
  - **Experimental conditions:**
    - **Amount of NaCl in the liquid phase**
    - **Amount of $SrCl_2$ in the liquid phase**
    - **Pressure**
  - **Measured variables:**
    - **Temperature (*Formation Target* on liquid)**
  - **Selected phases:**
    - **Liquid phase**
    - **NaCl(s)**
    - **$SrCl_2$(s1)**

- **Group #4: NaCl liquidus data**
  - **Experimental conditions:**
    - **Amount of NaCl(s)**
    - **Amount of $SrCl_2$(s1)**
    - **Pressure**
  - **Measured variables:**
    - **Temperature (*Formation Target* on NaCl(s))**
  - **Selected phases:**
    - **Liquid phase**
    - **NaCl(s)**

- **Group #5: $SrCl_2$ liquidus data**
  - **Experimental conditions:**
    - **Amount of NaCl(s)**
    - **Amount of $SrCl_2$(s1)**
    - **Pressure**
  - **Measured variables:**
    - **Temperature (*Precipitation Target* on liquid)**
  - **Selected phases:**
    - **Liquid phase**
    - **$SrCl_2$(s1)**
    - **$SrCl_2$(s2)**



# Experimental Data

The experimental data are stored in an Excel spreadsheet.

Microsoft Excel - NaCl_SrCl2.xls

| Activity of NaCl in the liquid phase | | | | | |
|---|---|---|---|---|---|
| Experimental Conditions | | | | Measured Variable | |
| P | moles | moles | T | activity | error |
| | SrCl2 | NaCl | K | NaCl | (estimated at 1%) |
| atm | liquid | liquid | | liquid | |
| 1 | 0.2 | 0.8 | 1073.15 | 0.777 | 0.00777 |
| 1 | 0.3 | 0.7 | 1073.15 | 0.659 | 0.00659 |
| 1 | 0.4 | 0.6 | 1073.15 | 0.533 | 0.00533 |
| 1 | 0.9 | 0.1 | 1098 | 0.0808 | 0.000808 |
| 1 | 0.8 | 0.2 | 1098 | 0.162 | 0.00162 |
| 1 | 0.5 | 0.5 | 1098 | 0.454 | 0.00454 |
| 1 | 0.3 | 0.7 | 1098 | 0.682 | 0.00682 |
| 1 | 0.401 | 0.599 | 1123 | 0.5437 | 0.005437 |
| 1 | 0.6 | 0.4 | 1123 | 0.3381 | 0.003381 |
| 1 | 0.799 | 0.201 | 1123 | 0.1593 | 0.001593 |
| 1 | 0.46 | 0.54 | 1123 | 0.53 | 0.0053 |

Group #1 / Group #2 / Group #3 / Group #4 / Group #5

Ready NUM

# Executing the ***OptiSage*** module

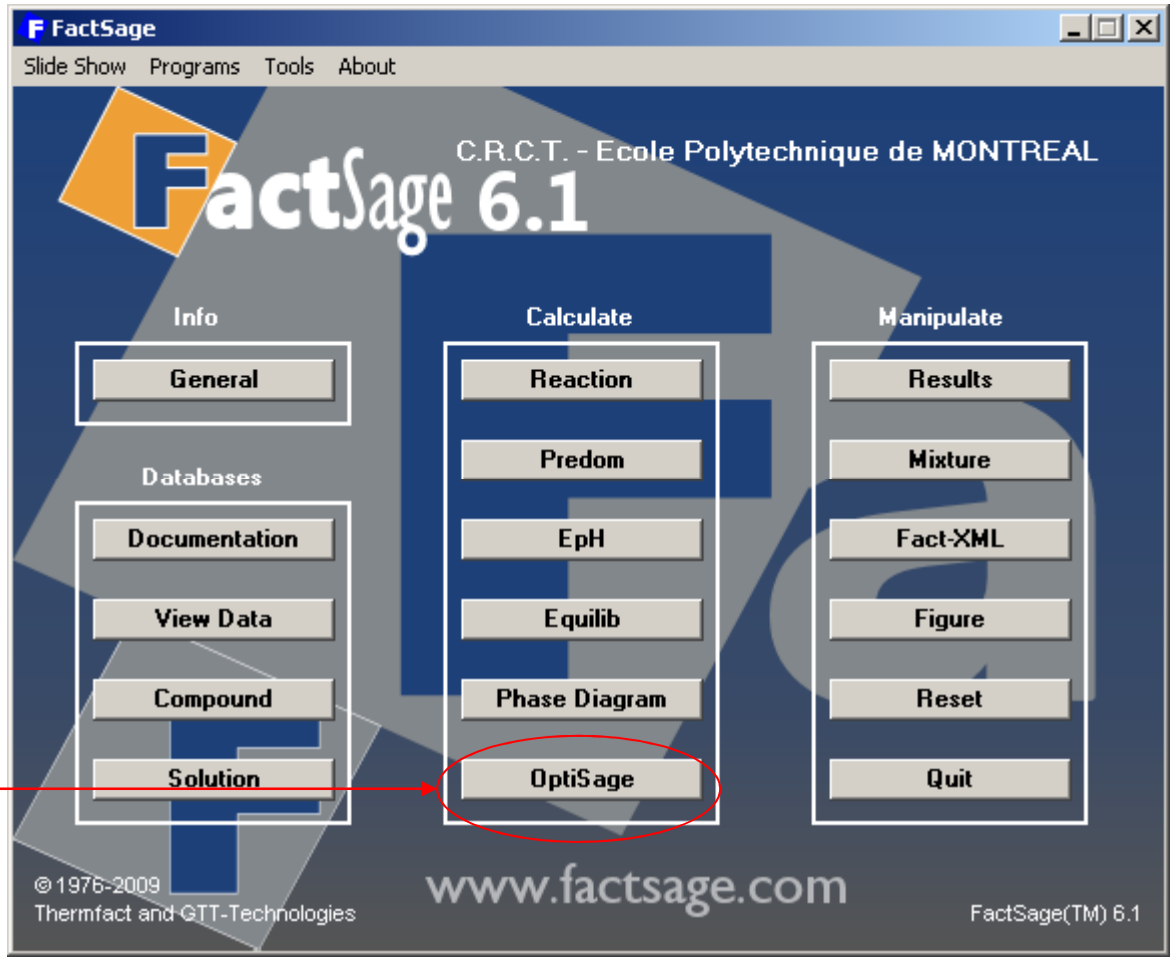
**Step 3. Execute the optimization program interactively.**

When the thermodynamic datafile (***ChemSage*** file) has been created (Step 1.) and the numerical values of the experimental data to be used in the optimization have been organised into groups (Step 2.), the ***OptiSage*** module can be executed and the ***ChemSage*** file loaded.

The following two slides show how to initiate ***OptiSage***.

# The *OptiSage* Module

- After creating :
  - a compound database
  - a solution database
  - a ***ChemSage*** file
- and organising the experimental data into groups
- ***OptiSage*** is ready to be employed

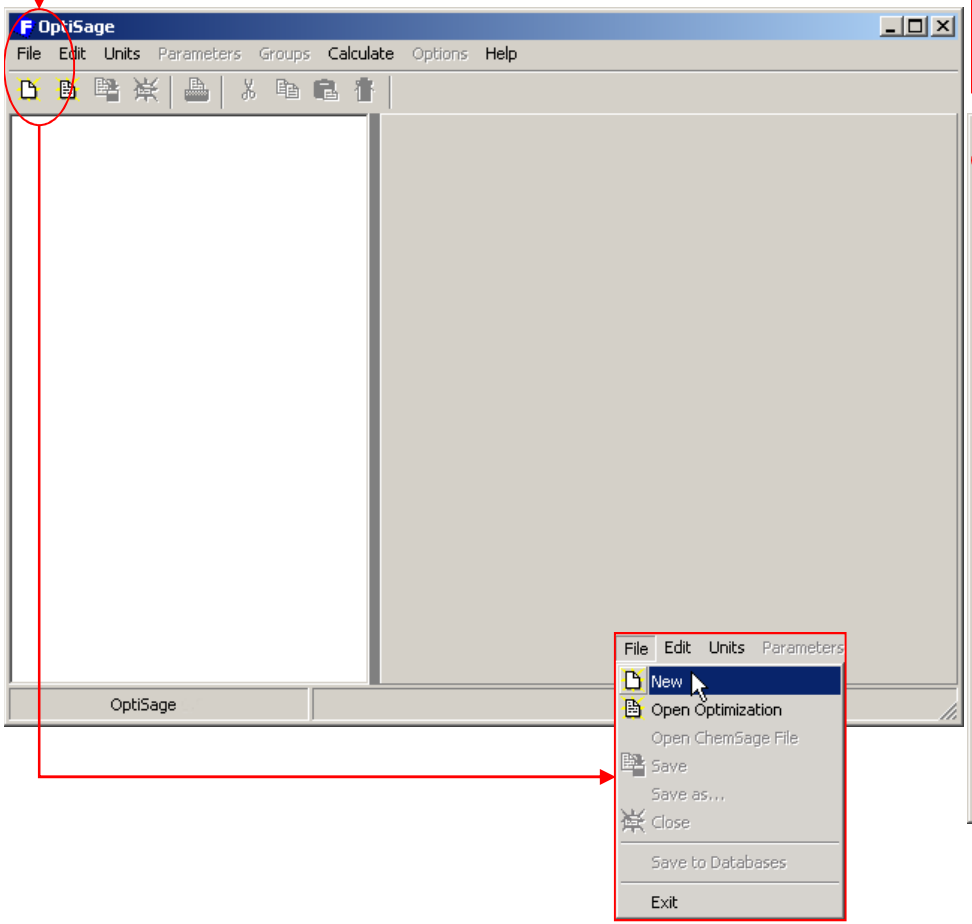


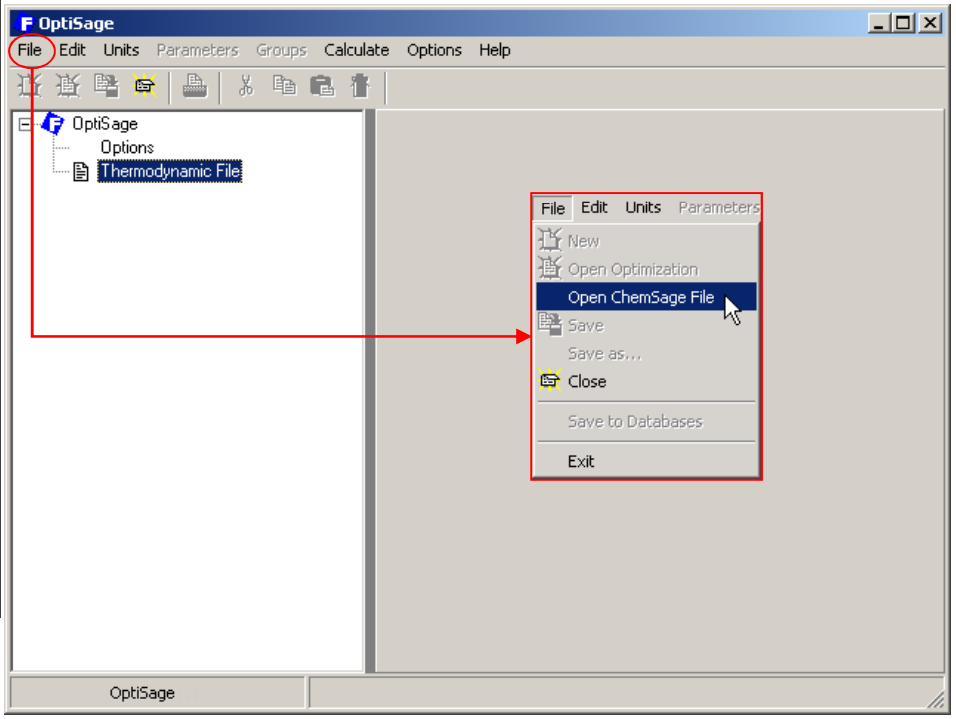
# *OptiSage* main window: New optimization

- Open a new optimization.
- Select File > New from the Menu bar or click on from the toolbar to open a **New** optimization.

Then open your ***ChemSage*** file by selecting:

1. File > Open ChemSage File from the Menu bar, or
2. Thermodynamic File from the treeview and double-click to select an input ChemSage thermodynamic file.



# Creating ***OptiSage*** input for the experimental data

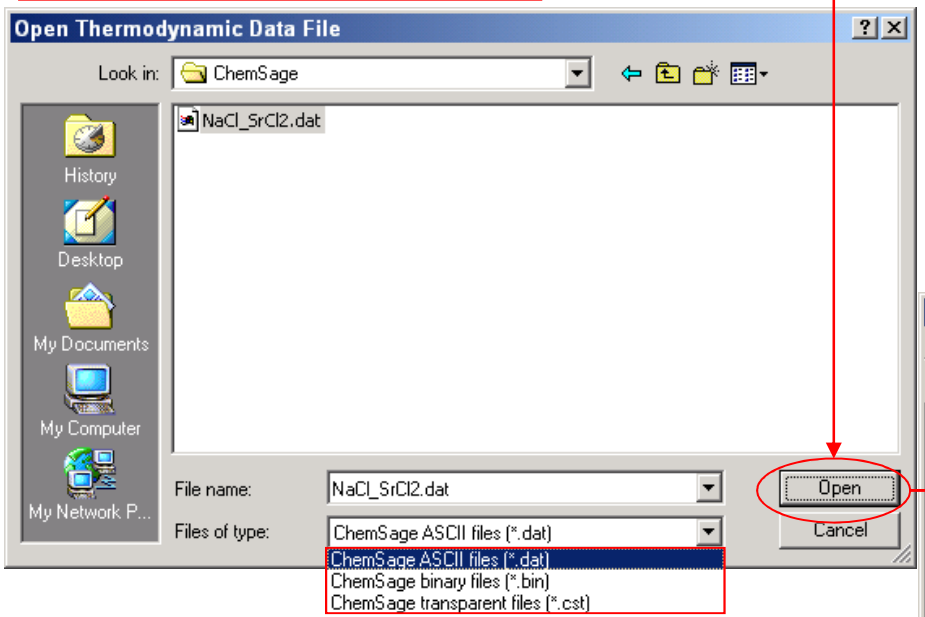
The thermodynamic data of the system are already stored. Since the thermodynamic datafile also contains the names of the phases and their constituents these names are also available in ***OptiSage*.**

The following eight slides show how the data for experimental Group #1, Activities of the components in the liquid phase at a given temperature, are entered into the calculation.

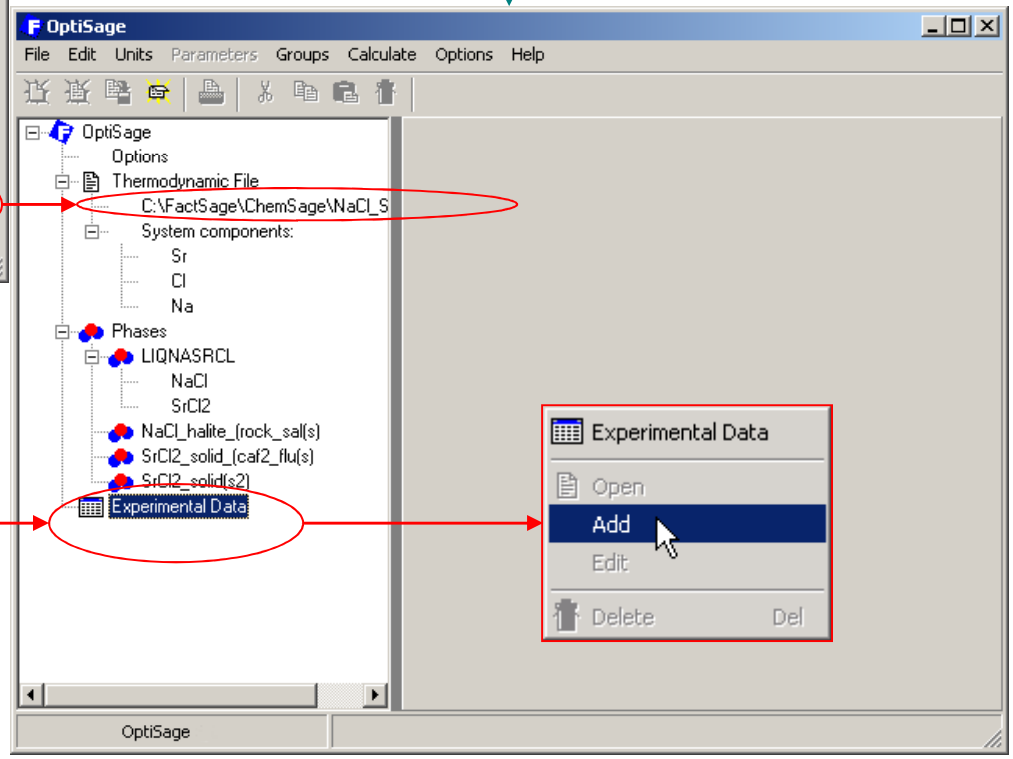
NOTE: For all experimental input, there is a distinction made between the experimental conditions and the measured variables. In the present case, activities have been measured as function of temperature and composition. Thus temperature and composition (as well as total pressure) are experimental conditions and the measured activities are the measured variables. Different parts of the input window are used for these different data.

# Importing the data into Group #1

Open the ***ChemSage*** file previously created.




At this point, the ***OptiSage*** window shows the tree view (fully expanded) and we are ready to enter the **experimental data** that will be used in the optimization.

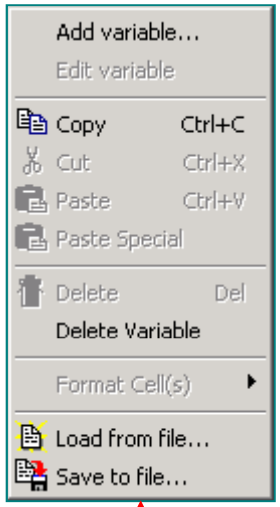


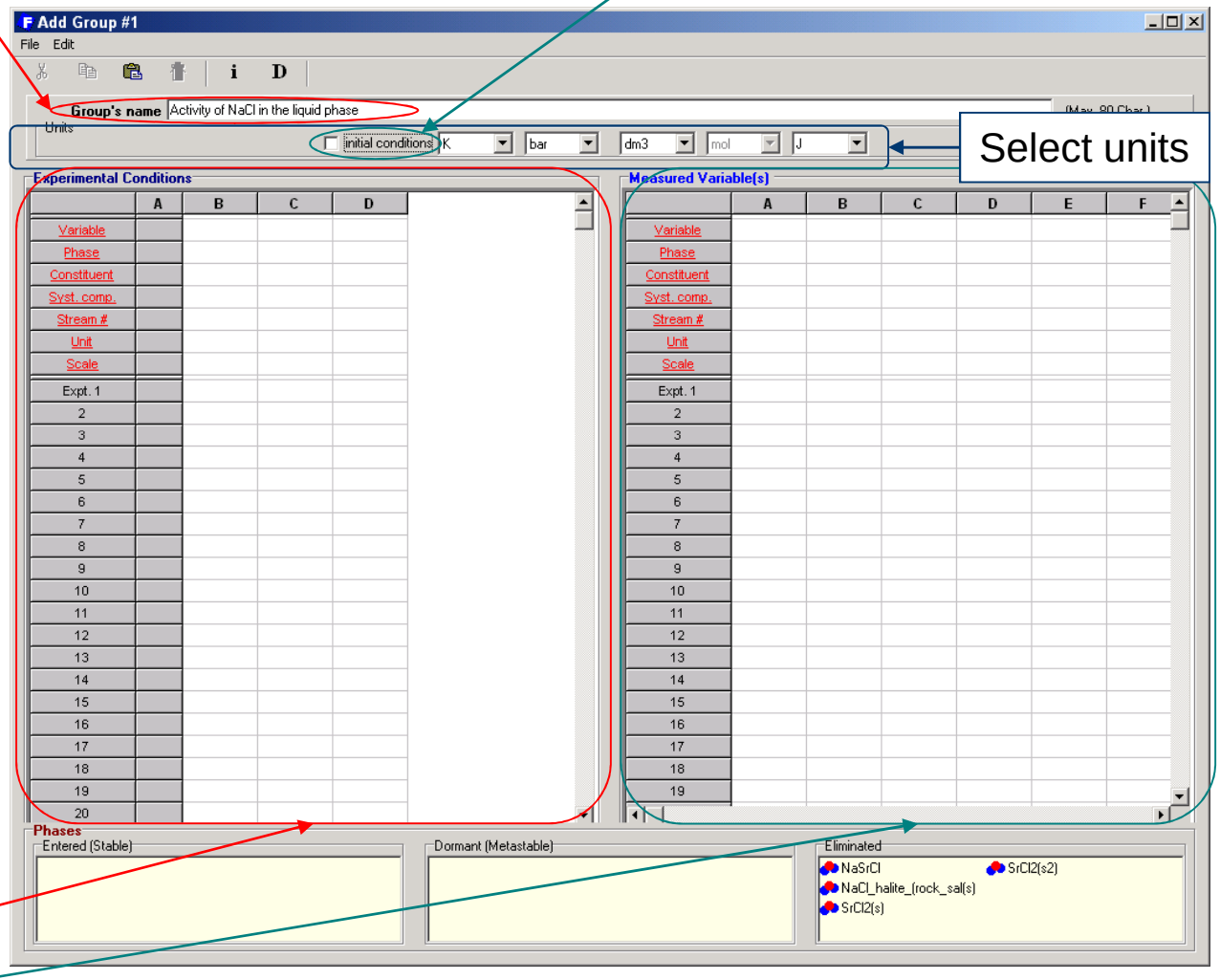

A **right-click** on **Experimental Data** opens the pop-up menu. Select **<Add>** to open the **'Add Group'** window.

# The **Add Group** window

Enter the description of group #1: **Activity of NaCl in the liquid phase**

Check «**initial conditions**» only when ΔH, ΔG, ΔV, ΔS or $\Delta C_p$ are calculated. (ex: adiabatic T, $\Delta H_{mix}$, etc…)




Select units

A **right-click** in each spreadsheet opens a **pop-up menu** where you can add, edit, delete, load from a file, save to a file either the **Experimental Conditions** or the **Measured Variable(s)**

# Adding new **Experimental Conditions**

- **Group #1: Activity of NaCl in the liquid phase**

1. **Experimental conditions:**
   1. **Amount of NaCl in the liquid phase**
   2. **Amount of $SrCl_2$ in the liquid phase**
   3. **Temperature**
   4. **Pressure**

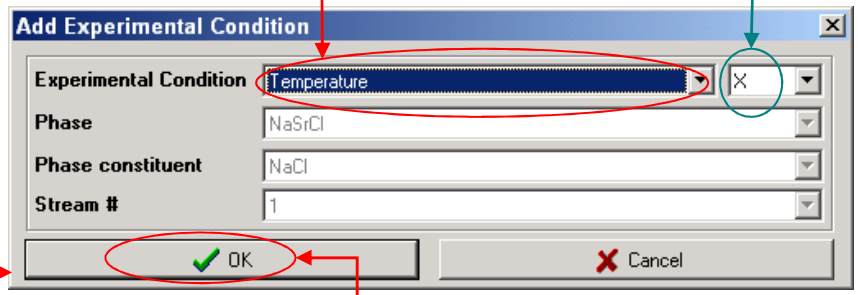
2. **Measured variables:**
   1. **Activity of NaCl in the liquid phase**

3. **Selected phases:**
   1. **Liquid phase**

| Activity of NaCl in the liquid phase | | | | | |
|---|---|---|---|---|---|
| Experimental conditions | | | | Measured variable | |
| P | moles SrCl2 | moles NaCl | T | activity NaCl | error |
| | | | K | | (estimated at 1%) |
| atm | liquid | liquid | | liquid | |
| 1 | 0.2 | 0.8 | 1073.15 | 0.777 | 0.00777 |
| 1 | 0.3 | 0.7 | 1073.15 | 0.659 | 0.00659 |
| 1 | 0.4 | 0.6 | 1073.15 | 0.533 | 0.00533 |
| 1 | 0.9 | 0.1 | 1098 | 0.0808 | 0.000808 |
| 1 | 0.8 | 0.2 | 1098 | 0.162 | 0.00162 |
| 1 | 0.5 | 0.5 | 1098 | 0.454 | 0.00454 |
| 1 | 0.3 | 0.7 | 1098 | 0.682 | 0.00682 |
| 1 | 0.401 | 0.599 | 1123 | 0.5437 | 0.005437 |
| 1 | 0.6 | 0.4 | 1123 | 0.3381 | 0.003381 |
| 1 | 0.799 | 0.201 | 1123 | 0.1593 | 0.001593 |
| 1 | 0.46 | 0.54 | 1123 | 0.53 | 0.0053 |

1. **Right-click** in the **Experimental Conditions** spreadsheet and select **Add variable…** from the pop-up menu or click on the i button in the menu bar to open the **Add Experimental Conditions** window.

2. **Enter** an **experimental condition**. For example, **temperature**, on a **linear scale X**.



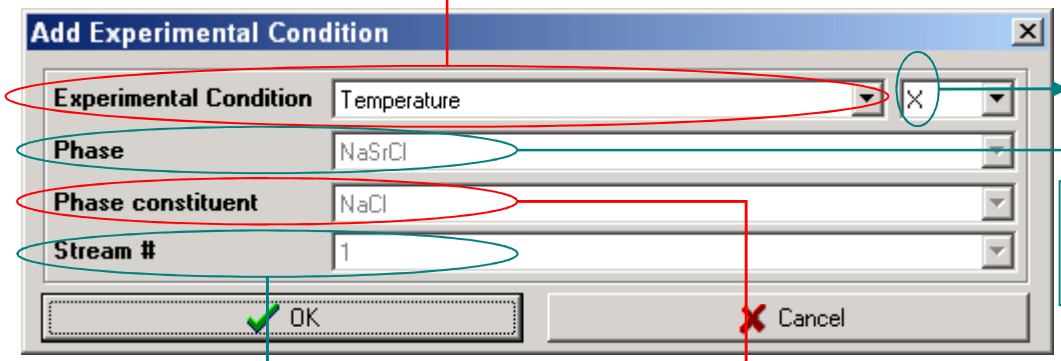

3. **Click** OK.

4. **Repeat** for the 3 other **experimental conditions**.

# The «Add Experimental Condition» Window

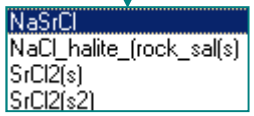
**Note:** **Choosing** the **experimental conditions is equivalent to** entering **reactants** and fixing **final conditions** in ***Equilib***.

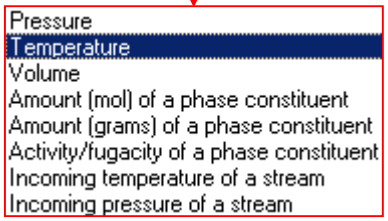
List of the **experimental conditions** you can declare.




List of **scales** available

List of the **phases** available (when the option is enabled)



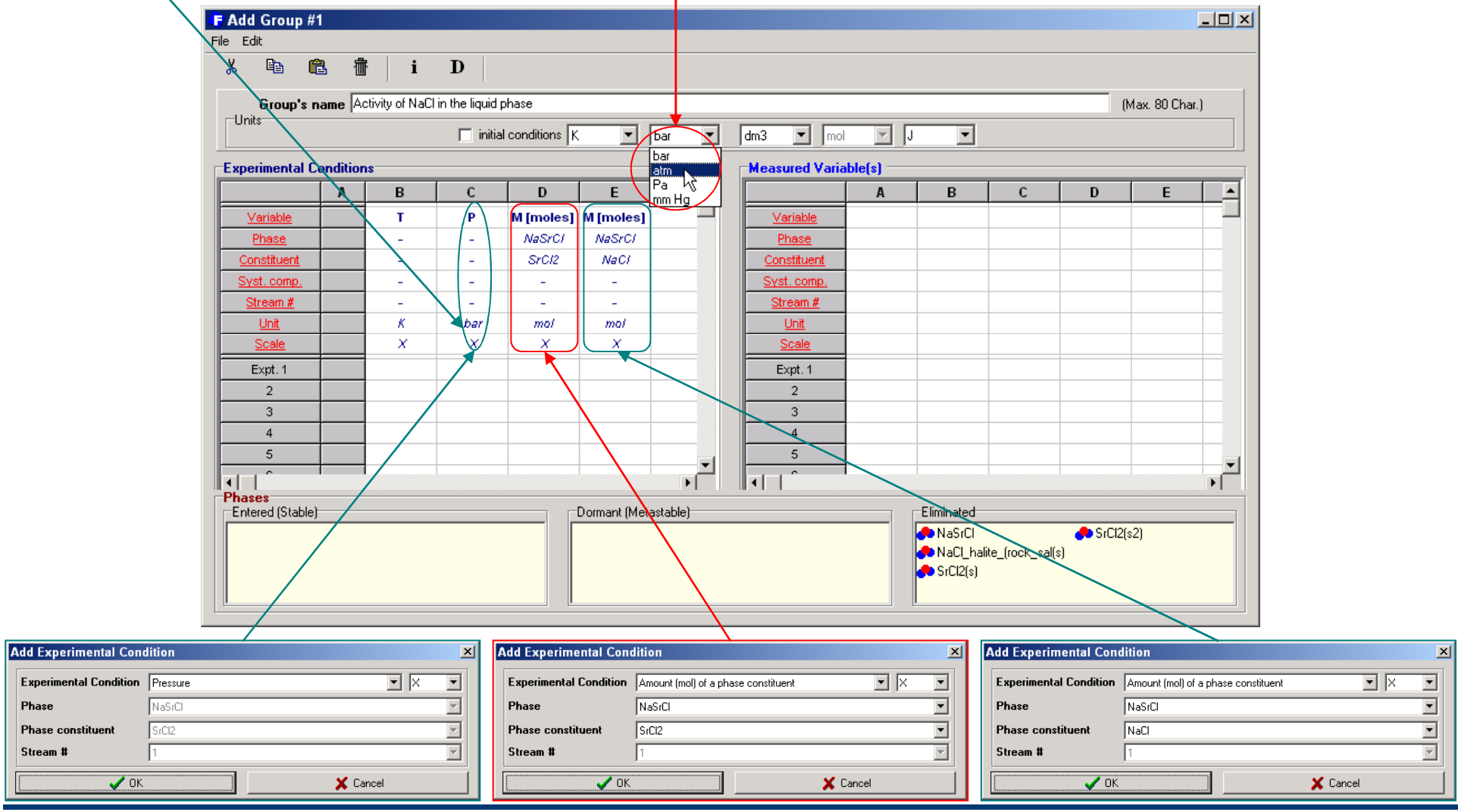

List of the **phase constituents** available when needed.

List of **streams** (max. 20)
**Enabled** if the «**initial conditions**» checkbox in the unit frame of the **Add Group** window is checked and needed when there is any difference between the initial and the final conditions

# Adding the 3 other **experimental conditions** of Group #1

**Changing Units**

**Pressures** are in **bar** and your data are in **atm**. **Select** the appropriate unit.



# Adding new **Measured Variables**

- **Group #1: Activity of NaCl in the liquid phase**

**1. Experimental conditions:**

- **Amount of NaCl in the liquid phase**
- **Amount of $SrCl_2$ in the liquid phase**
- **Temperature**
- **Pressure**

**2. Measured variables:**

**Activity of NaCl in the liquid phase**

**3. Selected phases:**

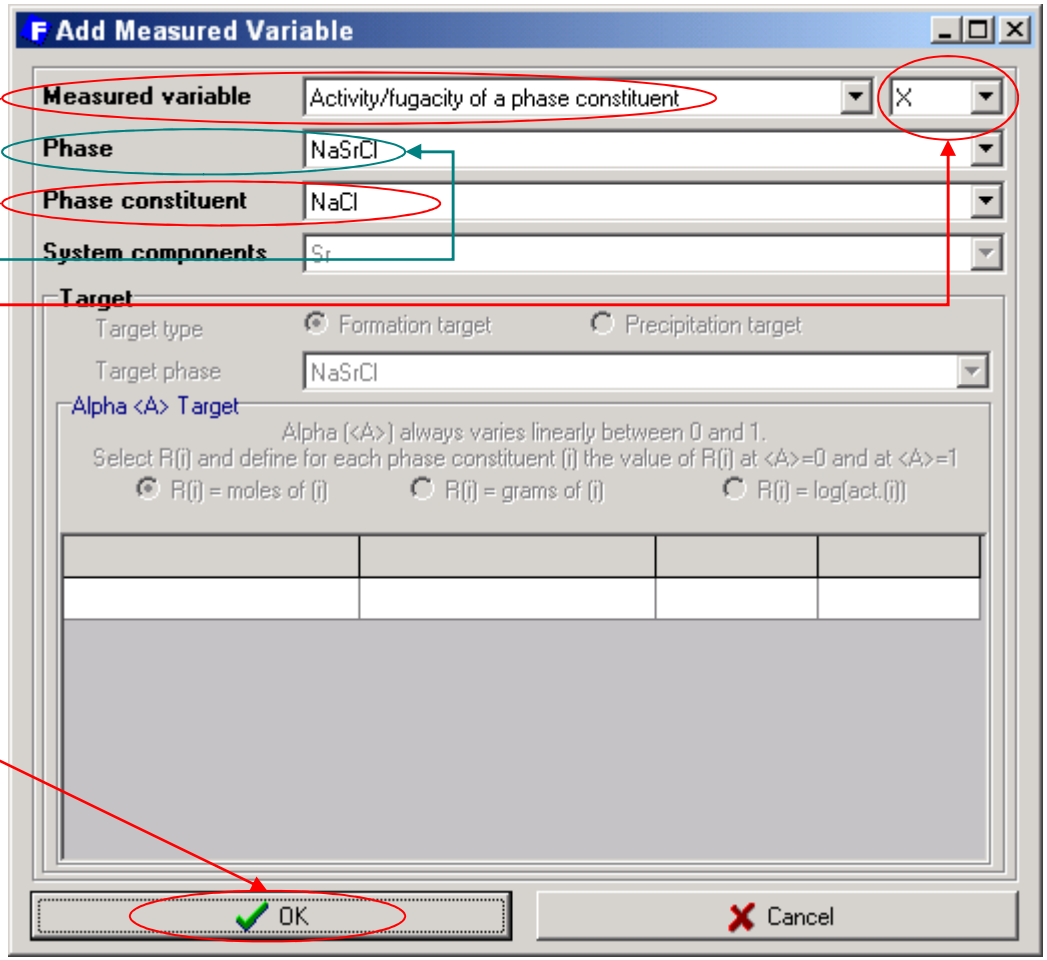
**Liquid phase**

| Activity of NaCl in the liquid phase | | | | | |
|---|---|---|---|---|---|
| Experimental Conditions | | | | Measured Variable | |
| P | moles | moles | T | activity | error |
| | SrCl2 | NaCl | K | NaCl | (estimated at 1%) |
| atm | liquid | liquid | | liquid | |
| 1 | 0.2 | 0.8 | 1073.15 | 0.777 | 0.00777 |
| 1 | 0.3 | 0.7 | 1073.15 | 0.659 | 0.00659 |
| 1 | 0.4 | 0.6 | 1073.15 | 0.533 | 0.00533 |
| 1 | 0.9 | 0.1 | 1098 | 0.0808 | 0.000808 |
| 1 | 0.8 | 0.2 | 1098 | 0.162 | 0.00162 |
| 1 | 0.5 | 0.5 | 1098 | 0.454 | 0.00454 |
| 1 | 0.3 | 0.7 | 1098 | 0.682 | 0.00682 |
| 1 | 0.401 | 0.599 | 1123 | 0.5437 | 0.005437 |
| 1 | 0.6 | 0.4 | 1123 | 0.3381 | 0.003381 |
| 1 | 0.799 | 0.201 | 1123 | 0.1593 | 0.001593 |
| 1 | 0.46 | 0.54 | 1123 | 0.53 | 0.0053 |

# Adding a **Measured Variable**

1. **Right-click** in the **Measured Variable(s)** spreadsheet and select **Add variable…** from the pop-up menu or click on the D button in the menu bar to open the **Add Measured Variable** window.

2. **Enter** a **measured variable**.
   Here, the **activity**
   of **NaCl**
   in the **NaSrCl (liquid)** phase
   on a **linear scale X**.

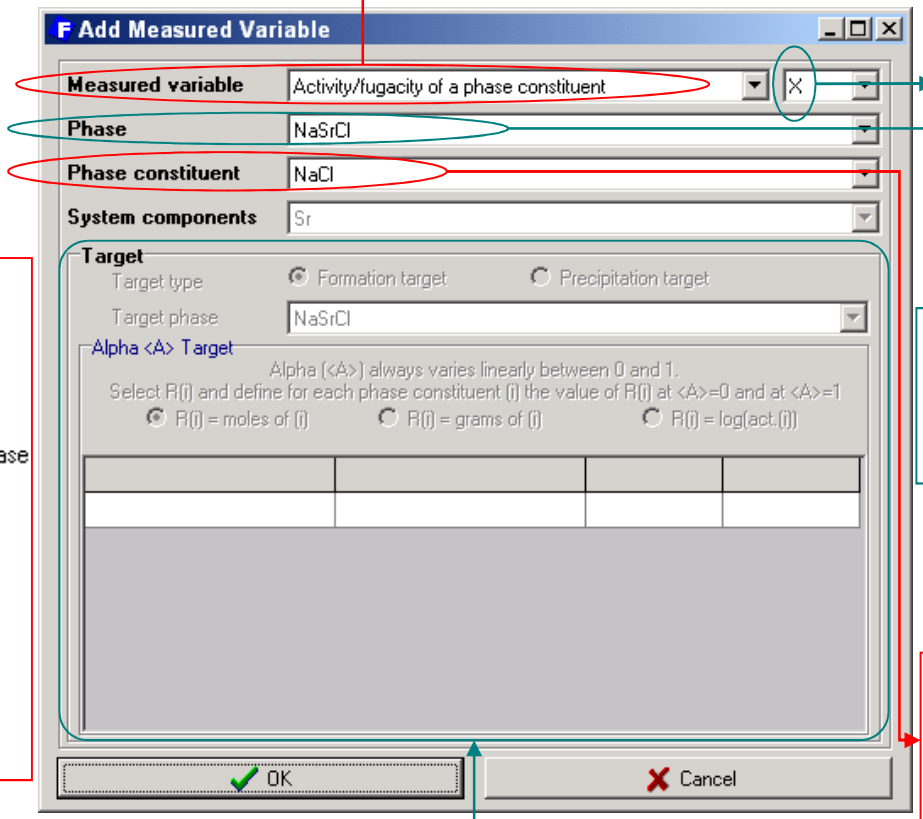



3. **Click** OK.

4. **Repeat** for the other **measured variables if necessary**.

# The «Add Measured Variable» Window

List of the **measured variables** you can declare.




List of **scales** available

X
1/X
ln X
log X

List of the **phases** available (when the option is enabled)

NaSrCl
NaCl_halite_(rock_sal(s)
SrCl2(s)
SrCl2(s2)

List of the **phase constituents** available when needed.

NaCl
SrCl2

Pressure
Temperature
Alpha <A>
Amount (mol) of a phase constituent
Amount (grams) of a phase constituent
Activity/fugacity of a phase constituent
Mole fraction of a phase constituent
Mole fraction of a system component in a mixture phase
Activity of a mixture phase
Heat capacity of a phase constituent
Enthalpy of a phase constituent
Entropy of a phase constituent
Gibbs energy of a phase constituent
Volume of a phase constituent
Heat capacity of the system
Enthalpy of the system
Entropy of the system
Gibbs energy of the system
Volume of the system
Density of the system

More are available for **aqueous** systems.

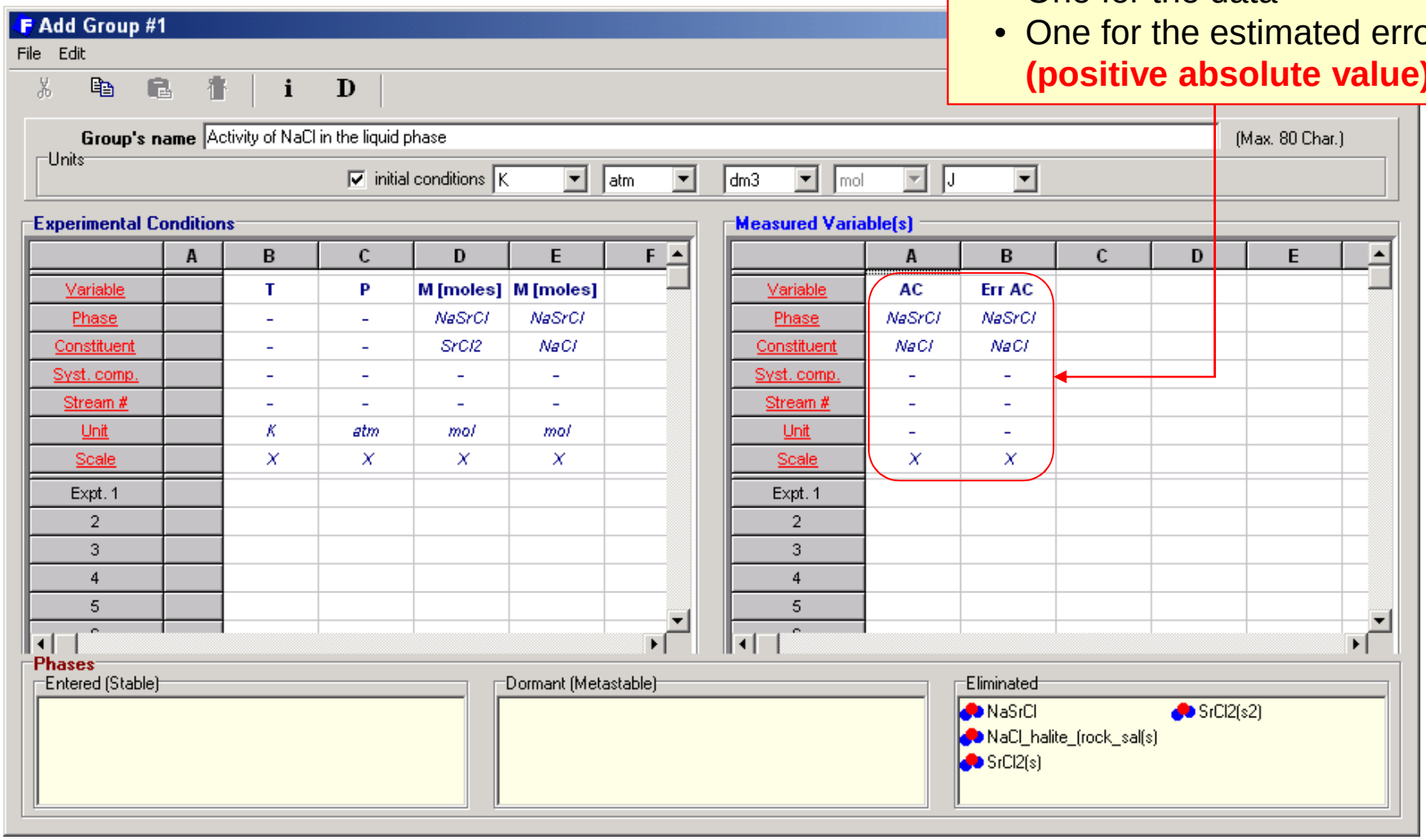
The **Target** frame is enabled if the final T (P or <A>) is **not** specified but generated by way of a Target calculation. See slide 7.22.

# Group #1: **declaration of variables**

The declaration of all variables is completed.
The «Add Group» window should look like:

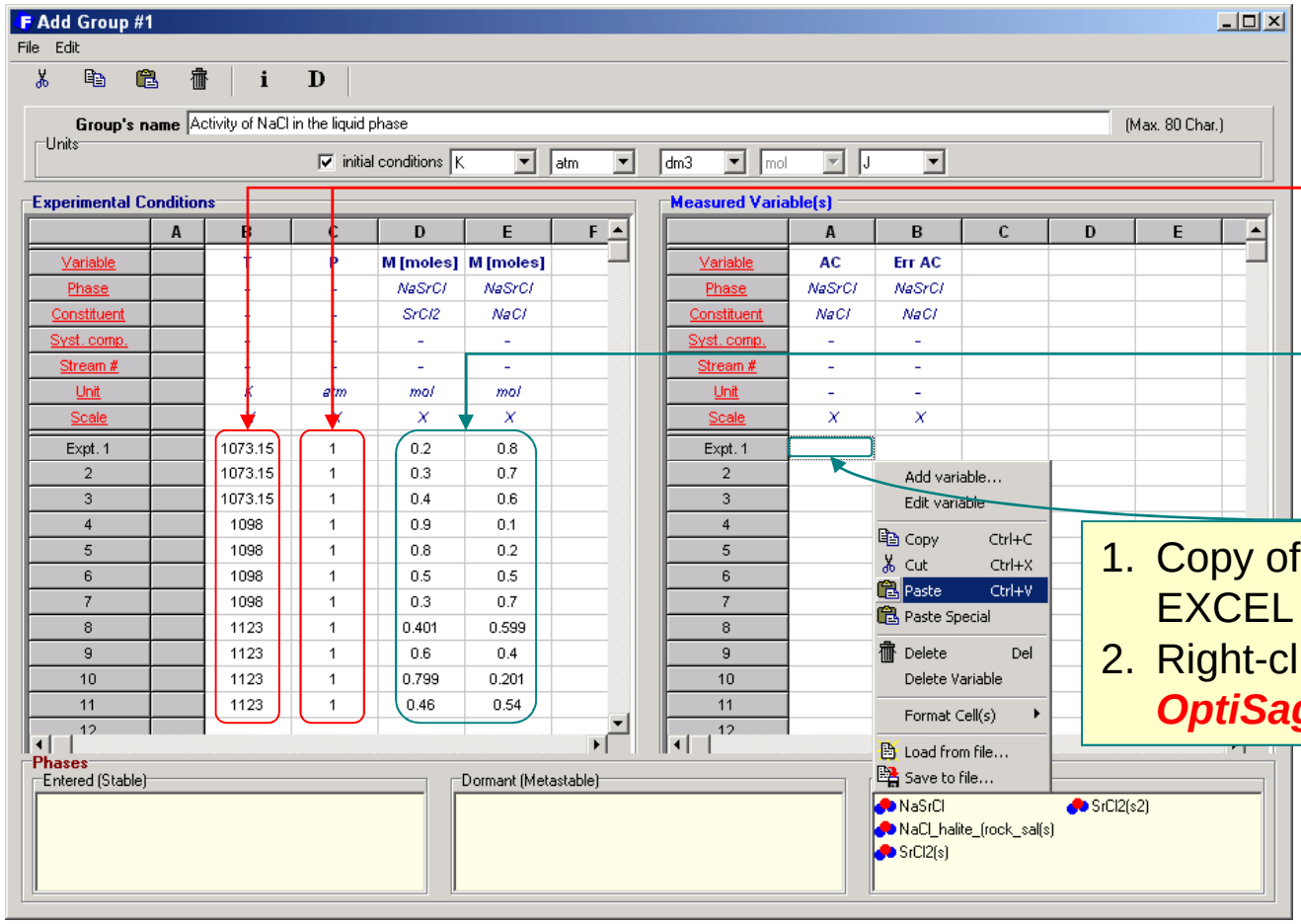
Each Measured Variables declaration creates 2 columns:

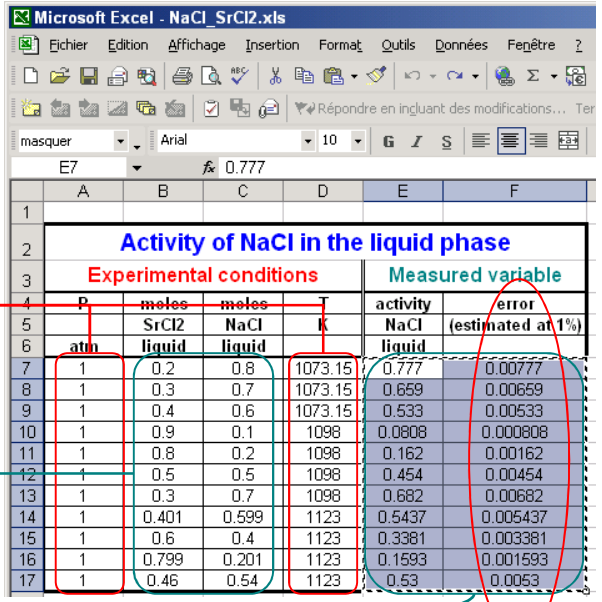
- One for the data
- One for the estimated error **(positive absolute value)**



# Import the data into Group #1

You can enter your data manually or, if your data are in a spreadsheet, copy and paste them in the «**Add Group**» window.




1. Copy of 2 colums of data in EXCEL
2. Right-click in the first cell in ***OptiSage*** to select **Paste**.

Experimental or estimated error must be entered if date are to be considered in the optimization. If a cell is blank or has a value of zero the corresponding data will be ignored.

# Group #1, Selection of the phases

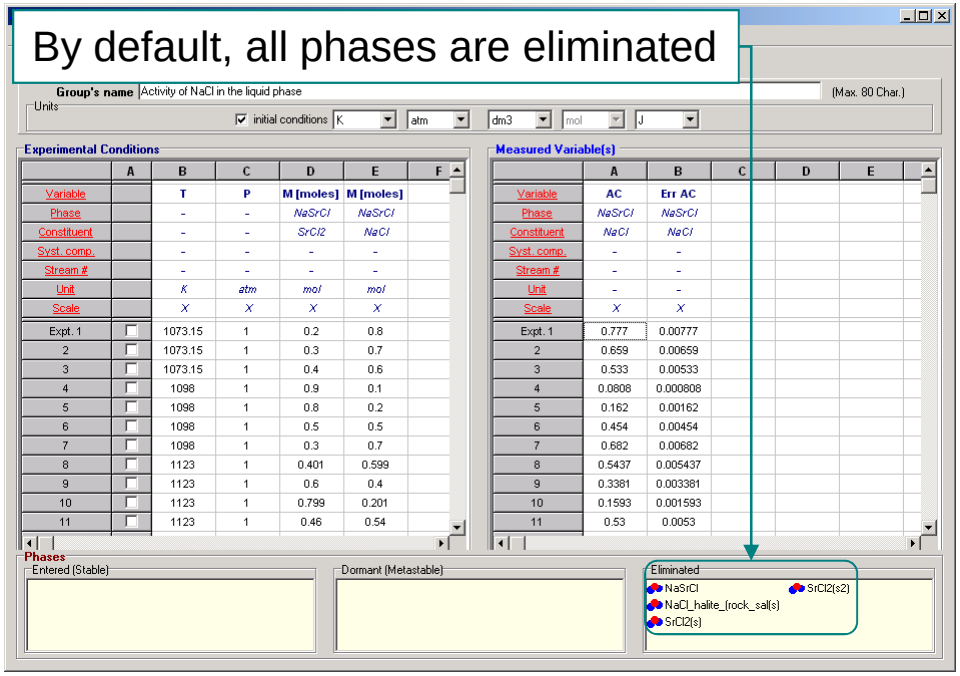
1. **Experimental conditions:**
   - **Amount of NaCl in the liquid phase**
   - **Amount of $SrCl_2$ in the liquid phase**
   - **Temperature**
   - **Pressure**
2. **Measured variables:**

   **Activity of NaCl in the liquid phase**
3. **Selected phases:**

   **Liquid phase (NaSrCl)**

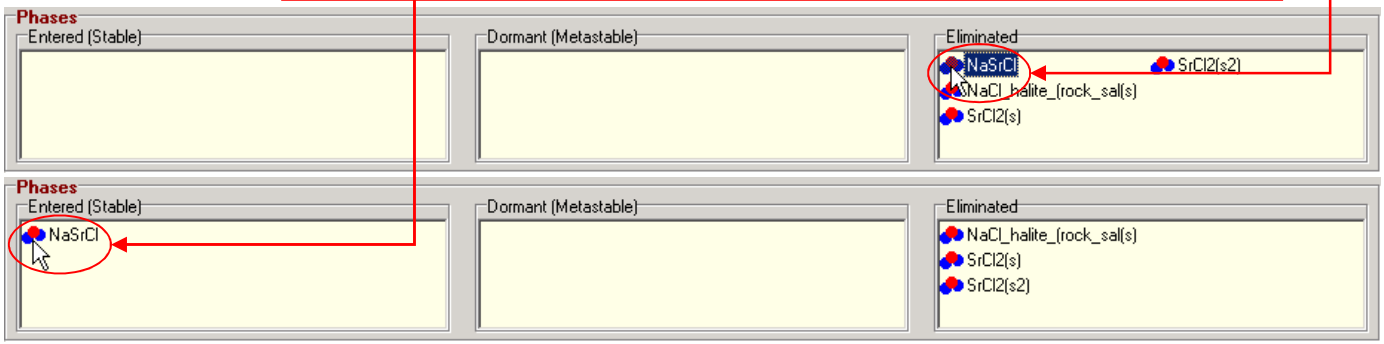
This is equivalent to species selection in ***Equilib***

By default, all phases are eliminated




To select a phase:

1. **Click** on a phase in the **Eliminated** frame and
2. **Drag** it in the **Entered(Stable)** frame

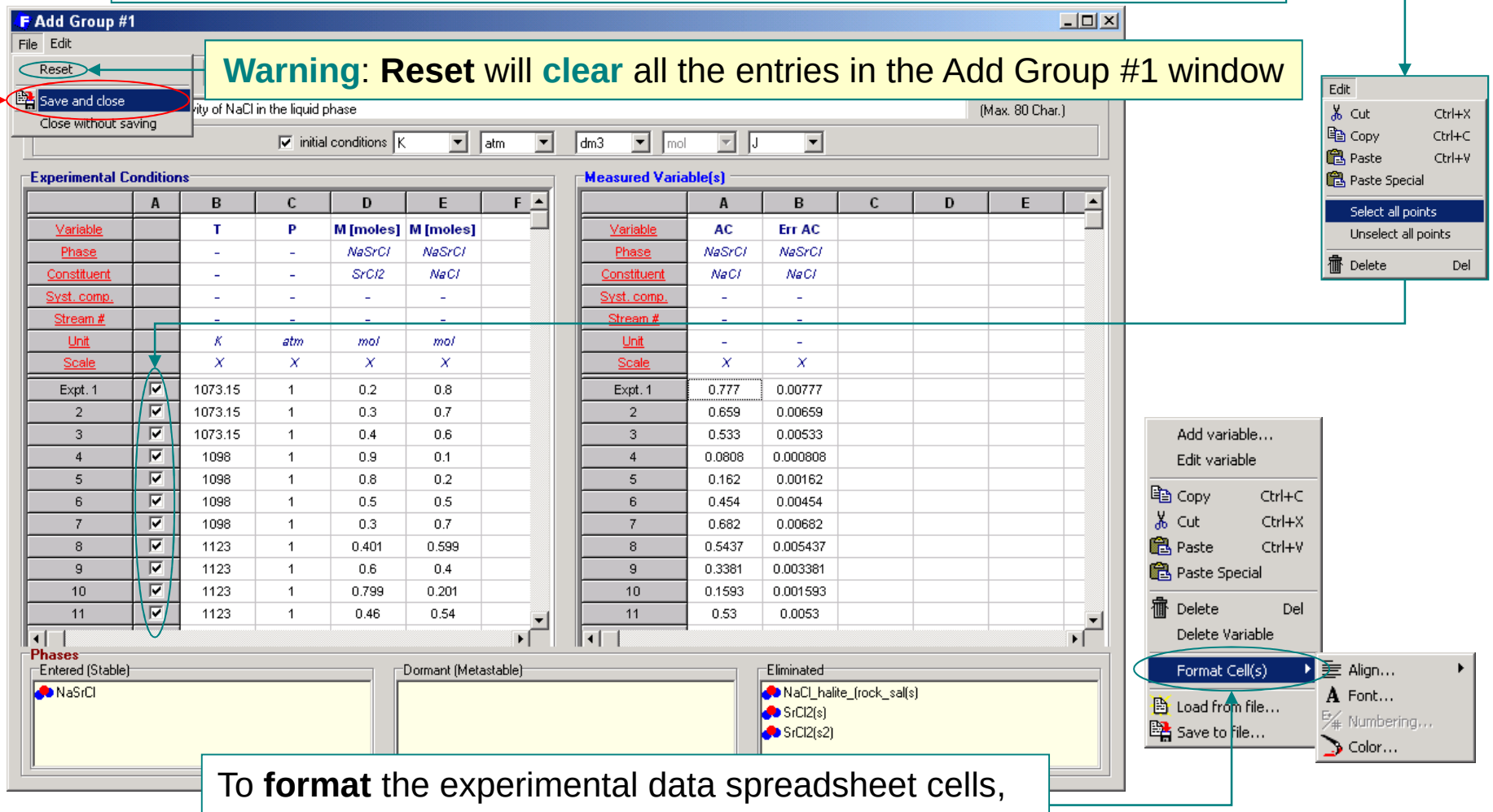


# **Saving** experimental data and **closing** Group #1

To save data and return to the ***OptiSage*** main window, select **File > Save and close**

To select or unselect all points, use **Edit > Select** (or **Unselect**) **all points**

**Warning**: **Reset** will **clear** all the entries in the Add Group #1 window

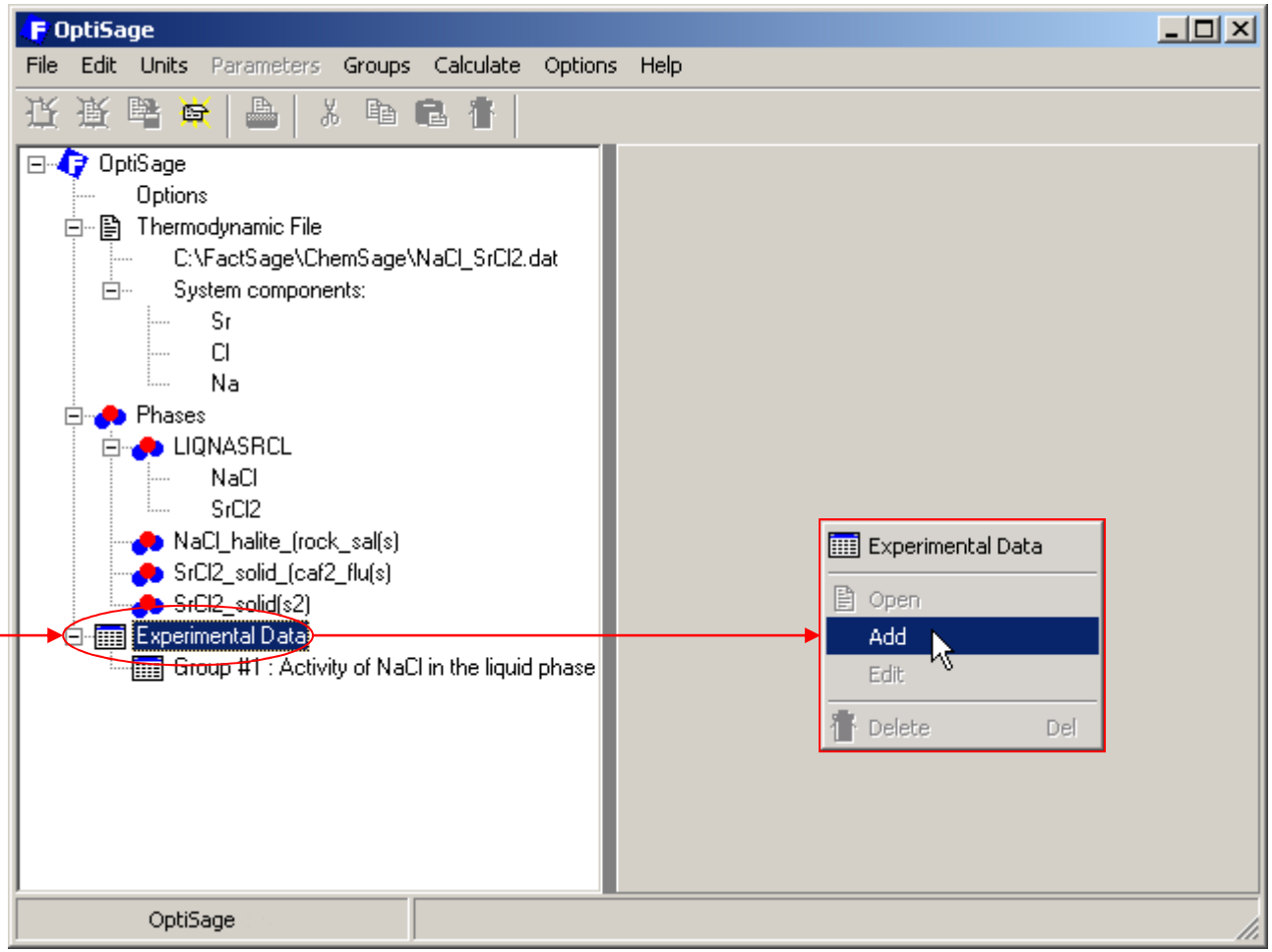



To **format** the experimental data spreadsheet cells, use the pop-up menu (right-click in the spreadsheet)

# Importing the data into Group #2

## Group #2: Enthalpy of mixing of the NaCl-$SrCl_2$ liquid mixture at 1167K (894℃).

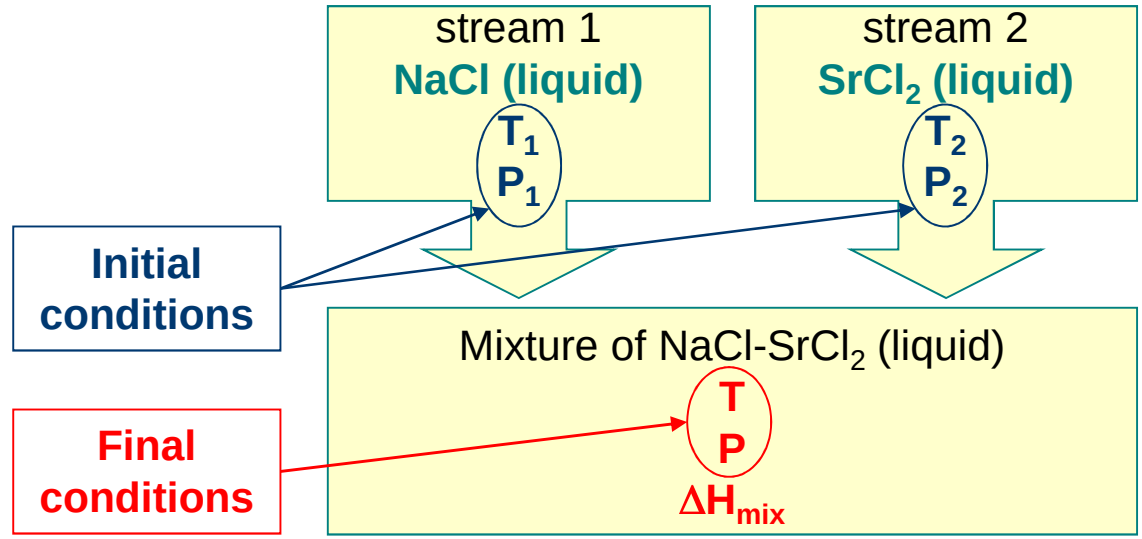
A **right-click** on **Experimental Data** opens the pop-up menu.
Select **<Add>** to open the **'Add Group'** window.

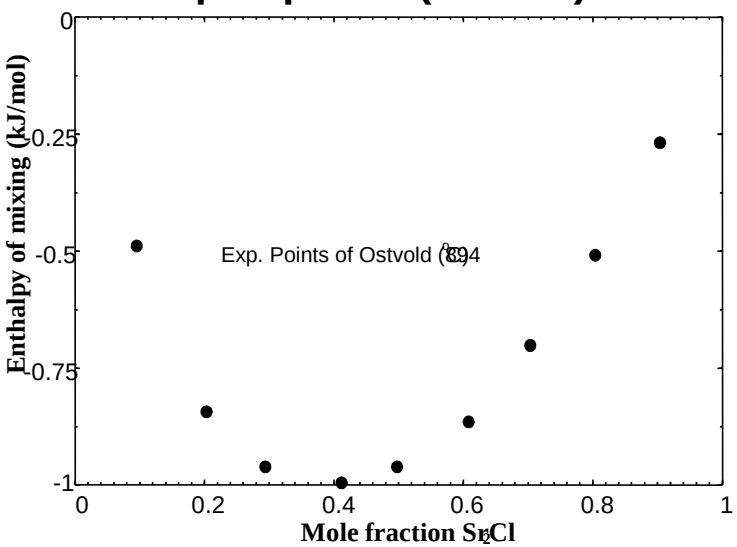


# Group #2: Heat of mixing data

## Enthalpy of mixing of the NaCl-$SrCl_2$ liquid mixture at 1167K (894°C)

1. **Experimental conditions:**
   - Amount of NaCl(liquid)
   - Amount of $SrCl_2$(liquid)
   - Initial Temperature
   - Initial Pressure
   - Final Temperature
   - Final Pressure
2. **Measured variables:**
   - Enthalpy of mixing (liquid)
3. **Selected phases:**
   - Liquid phase (NaSrCl)



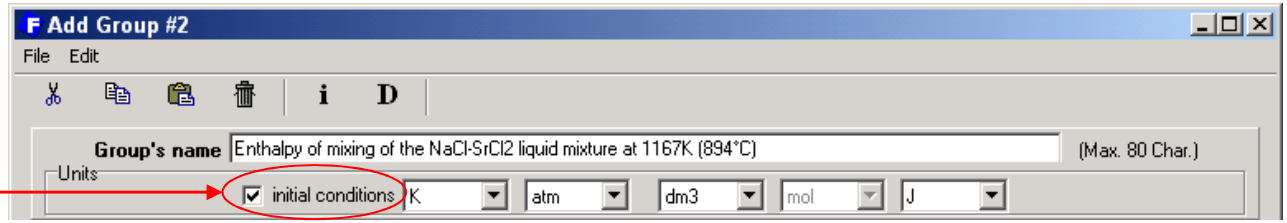

Here,
$P=P_1=P_2=$ 1 atm
$T=T_1=T_2=$ 1167 K

**Enthalpy of mixing in binary liquid mixture of NaCl-SrCl2 at 1167K**

| Experimental Conditions | | | | Measured Variable | |
|---|---|---|---|---|---|
| P | moles | moles | T | H | error |
| | SrCl2 | NaCl | K | J | J |
| atm | liquid | liquid | | | |
| 1 | 0.095 | 0.905 | 1167 | -490 | 50 |
| 1 | 0.204 | 0.796 | 1167 | -845 | 50 |
| 1 | 0.294 | 0.706 | 1167 | -962 | 50 |
| 1 | 0.412 | 0.588 | 1167 | -996 | 50 |
| 1 | 0.498 | 0.502 | 1167 | -962 | 50 |
| 1 | 0.608 | 0.392 | 1167 | -703 | 50 |
| 1 | 0.704 | 0.296 | 1167 | -510 | 50 |
| 1 | 0.904 | 0.096 | 1167 | -269 | 50 |

# Group #2: Declaration of **Experimental Conditions**

1. **Enter** a group description
2. **Select** the units
3. **Check** the initial conditions




4. **Declare all Experimental Conditions**

**Experimental Conditions:**

- **Amount of NaCl(liquid)**
- **Amount of $SrCl_2$(liquid)**
- **Final Temperature (T)**
- **Final Pressure (P)**
- **Initial Temperature [ $T_1$ , $T_2$ ]**
- **Initial Pressure [ $P_1$ , $P_2$ ]**

**[ Initial conditions ]**

**[ $T_1$ ]** **[ $T_2$ ]** **[ $P_1$ ]** **[ $P_2$ ]**

Experimental Conditions

| | A | B | C | D | E | F | G | H | I |
|---|---|---|---|---|---|---|---|---|---|
| Variable | | T | IT [incoming T] | IT [incoming T] | P | IP [incoming P] | IP [incoming P] | M [moles] | M [moles] |
| Phase | | - | - | - | - | - | - | NaSrCl | NaSrCl |
| Constituent | | - | - | - | - | - | - | NaCl | SrCl2 |
| Syst. comp. | | - | - | - | - | - | - | - | - |
| Stream # | | - | 1 | 2 | - | 1 | 2 | 1 | 2 |
| Unit | | K | K | K | atm | atm | atm | mol | mol |
| Scale | | X | X | X | X | X | X | X | X |

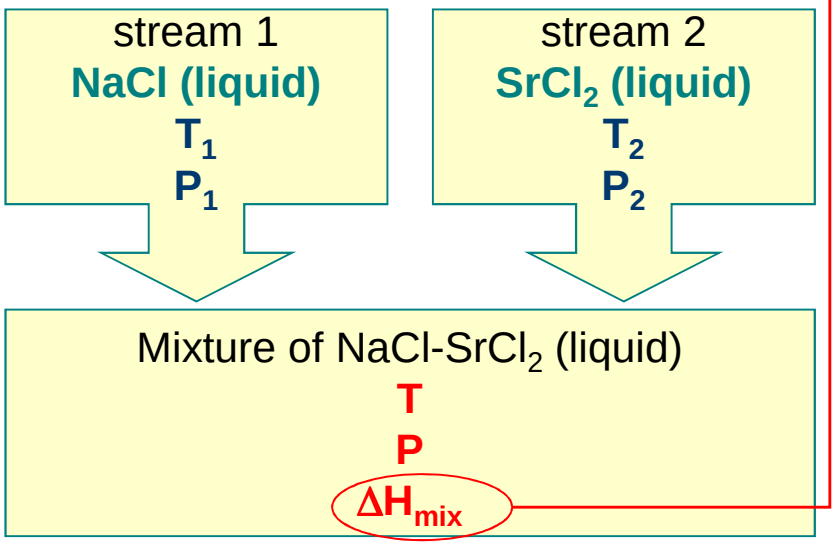
**Amount of NaCl(liquid)**

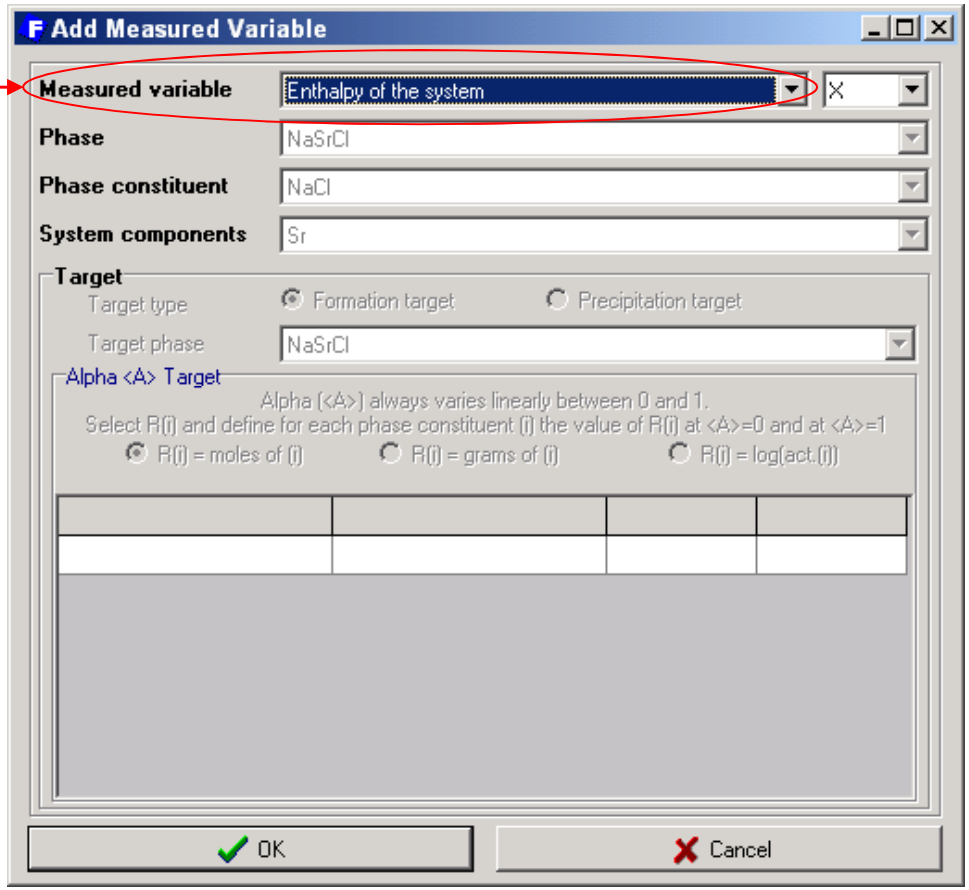
**Amount of $SrCl_2$(liquid)**

**(T)** **(P)** **(Final conditions)**

# Group #2: Declaration of the **Measured Variable**

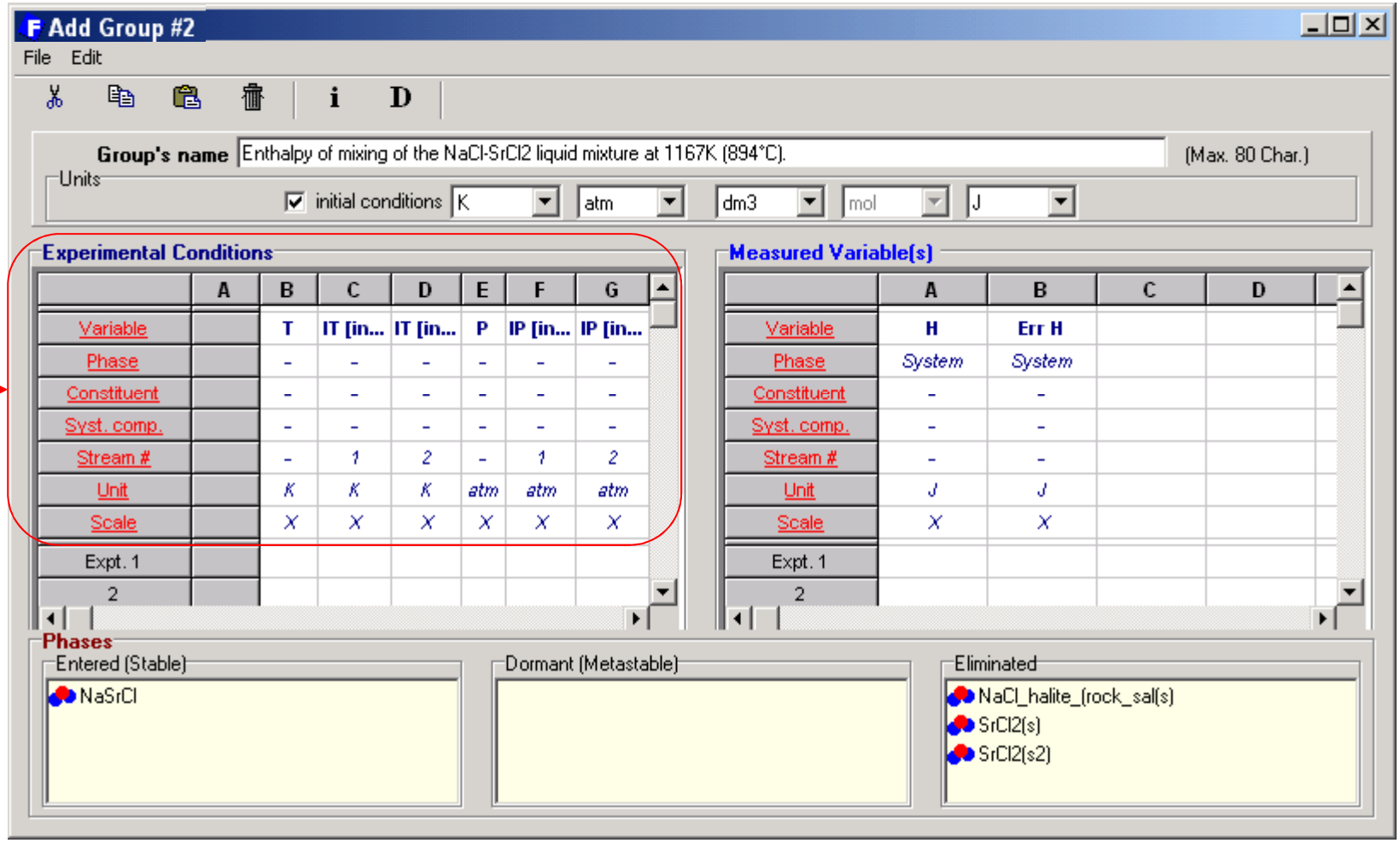
1. **Experimental conditions:**
   - **Amount of NaCl(liquid)**
   - **Amount of $SrCl_2$(liquid)**
   - **Initial Temperature**
   - **Initial Pressure**
   - **Final Temperature**
   - **Final Pressure**
2. **Measured variables:**
   - **Enthalpy of mixing (liquid)**
3. **Selected phases:**
   - **Liquid phase (NaSrCl)**



# Group #2: Summary of the variables

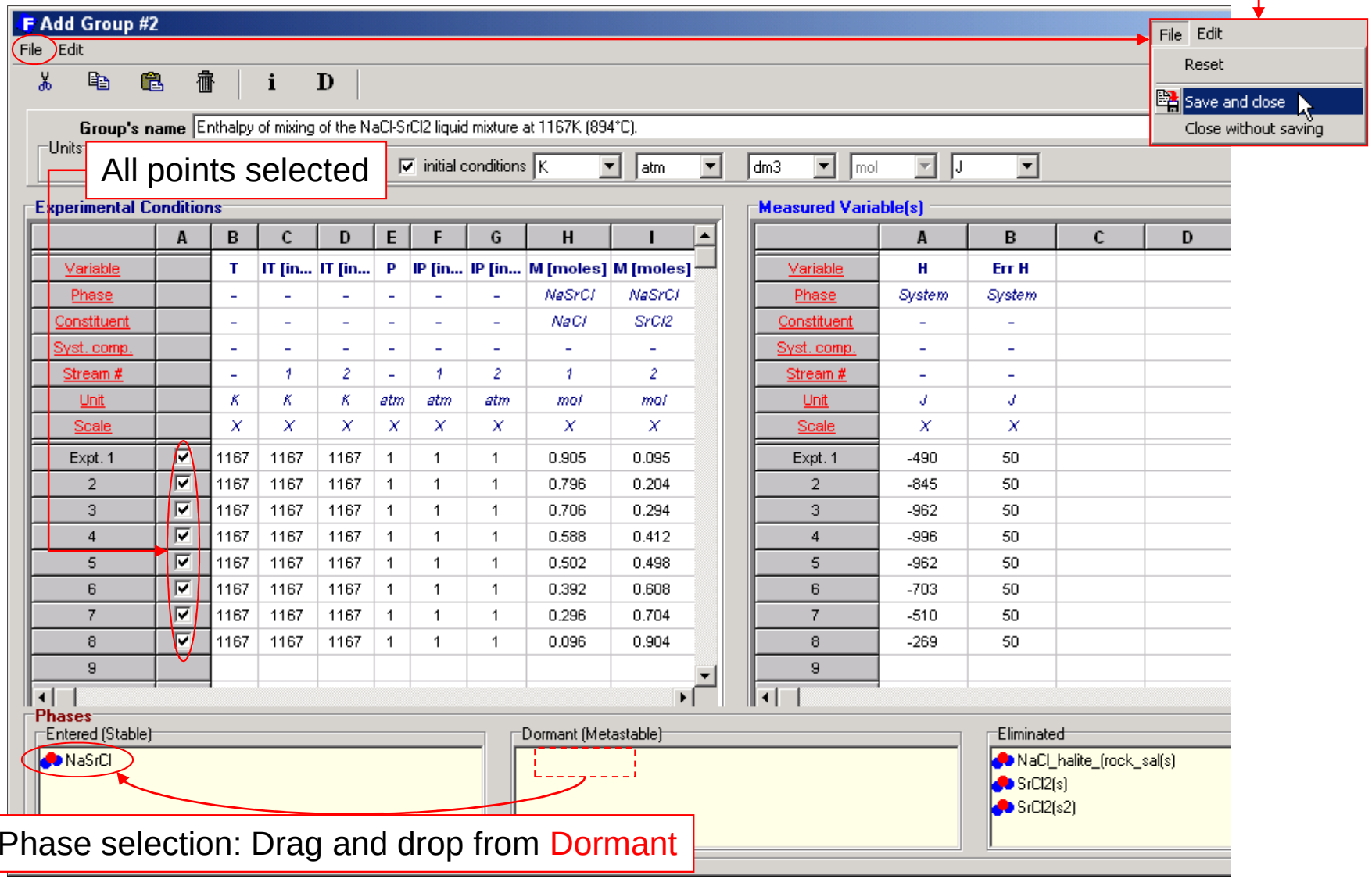
The «Add Group #2» window when the declaration of all variables is finished




Please see slide 7.15 for the complete declaration of **Experimental Conditions**

# Import the experimental data into Group #2 window

Finally, **save** data and return to the ***OptiSage*** main window, select **File > Save and close**




| | A | B | C | D | E | F | G | H | I |
|---|---|---|---|---|---|---|---|---|---|
| Variable | | T | IT [in... | IT [in... | P | IP [in... | IP [in... | M [moles] | M [moles] |
| Phase | | - | - | - | - | - | - | NaSrCl | NaSrCl |
| Constituent | | - | - | - | - | - | - | NaCl | SrCl2 |
| Syst. comp. | | - | - | - | - | - | - | - | - |
| Stream # | | - | 1 | 2 | - | 1 | 2 | 1 | 2 |
| Unit | | K | K | K | atm | atm | atm | mol | mol |
| Scale | | X | X | X | X | X | X | X | X |
| Expt. 1 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.905 | 0.095 |
| 2 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.796 | 0.204 |
| 3 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.706 | 0.294 |
| 4 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.588 | 0.412 |
| 5 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.502 | 0.498 |
| 6 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.392 | 0.608 |
| 7 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.296 | 0.704 |
| 8 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.096 | 0.904 |
| 9 | | | | | | | | | |

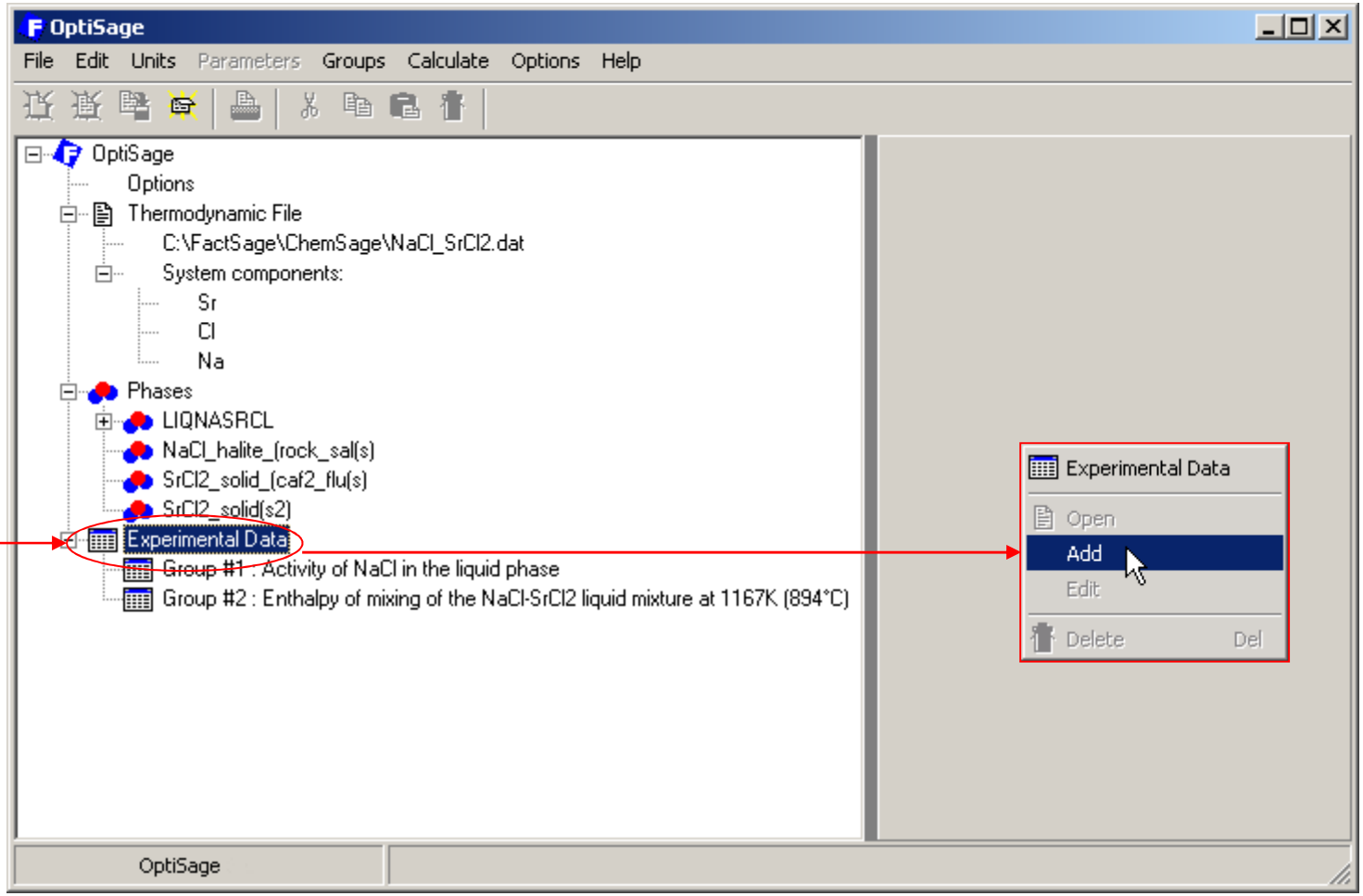
| | A | B | C | D |
|---|---|---|---|---|
| Variable | H | Err H | | |
| Phase | System | System | | |
| Constituent | - | - | | |
| Syst. comp. | - | - | | |
| Stream # | - | - | | |
| Unit | J | J | | |
| Scale | X | X | | |
| Expt. 1 | -490 | 50 | | |
| 2 | -845 | 50 | | |
| 3 | -962 | 50 | | |
| 4 | -996 | 50 | | |
| 5 | -962 | 50 | | |
| 6 | -703 | 50 | | |
| 7 | -510 | 50 | | |
| 8 | -269 | 50 | | |
| 9 | | | | |

Phase selection: Drag and drop from Dormant

# Importing data into Group #3

## Group #3: Eutectic Temperature

A **right-click** on **Experimental Data** opens the pop-up menu. Select **<Add>** to open the **'Add Group'** window.

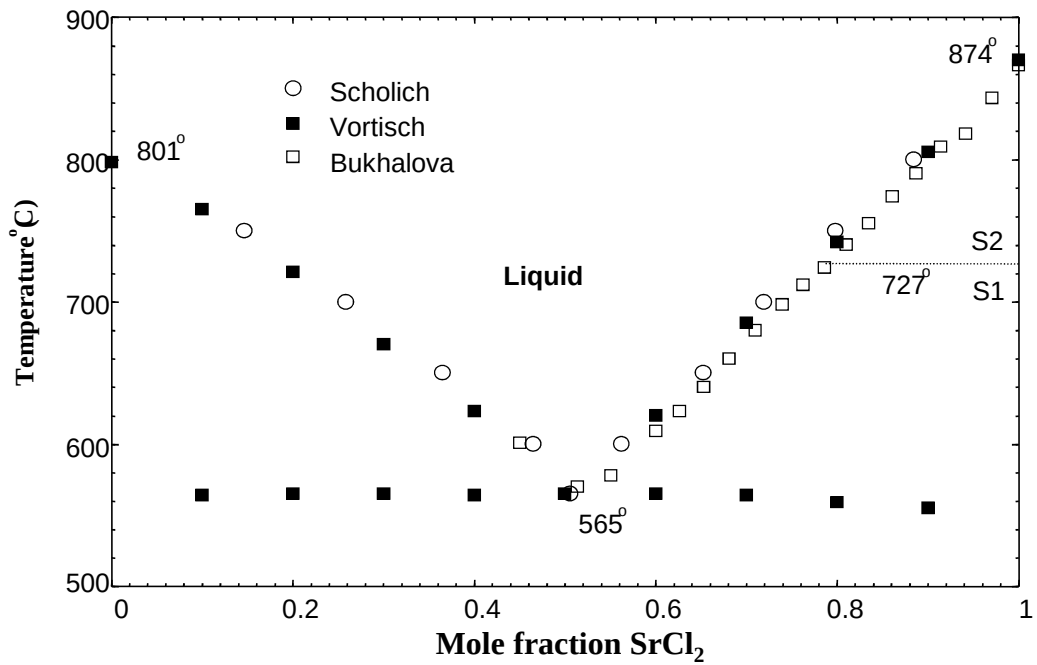


# Group #3: **Eutectic Temperature**

1. **Experimental conditions:**
   - **Amount of NaCl(liquid)**
   - **Amount of $SrCl_2$(liquid)**
   - **Pressure**

2. **Measured variables:**
   - **Temperature (used in *Formation Target* for liquid phase (NaSrCl))**

3. **Selected phases:**
   - **Liquid phase (NaSrCl)**
   - **NaCl(s)**
   - **SrCl2(s1)**




| Eutectic Temperature | | | | |
|---|---|---|---|---|
| Experimental Conditions | | | Measured Variable | |
| P | moles SrCl2 | moles NaCl | T(K) formation target | error (K) |
| atm | liquid | liquid | liquid | |
| 1 | 0.5 | 0.5 | 838 | 2 |
| 1 | 0.4 | 0.6 | 837 | 2 |

# Declaration and input of the **Experimental Conditions**

Group's name entered, units selected

F Add Group #3

File Edit

Group's name: Eutectic Temperature (formation target of the liquid phase). (Max. 80 Char.)

Units: initial conditions K atm dm3 mol J

**Experimental Conditions**

| | A | B | C | D | E |
|---|---|---|---|---|---|
| Variable | | P | M [moles] | M [moles] | |
| Phase | | - | NaSrCl | NaSrCl | |
| Constituent | | - | NaCl | SrCl2 | |
| Syst. comp. | | - | - | - | |
| Stream # | | - | - | - | |
| Unit | | atm | mol | mol | |
| Scale | | X | X | X | |
| Expt. 1 | | 1 | 0.5 | 0.5 | |
| 2 | | 1 | 0.6 | 0.4 | |
| 3 | | | | | |

**Measured Variable(s)**

| | A | D |
|---|---|---|
| Variable | | |
| Phase | | |
| Constituent | | |
| Syst. comp. | | |
| Stream # | | |
| Unit | | |
| Scale | | |
| Expt. 1 | | |
| 2 | | |
| 3 | | |

Add variable...
Edit variable
Copy Ctrl+C
Cut Ctrl+X
Paste Ctrl+V
Paste Special
Delete Del
Delete Variable
Format Cell(s)
Load from file...
Save to file...

**Phases**

Entered (Stable)

Dormant (Metastable)

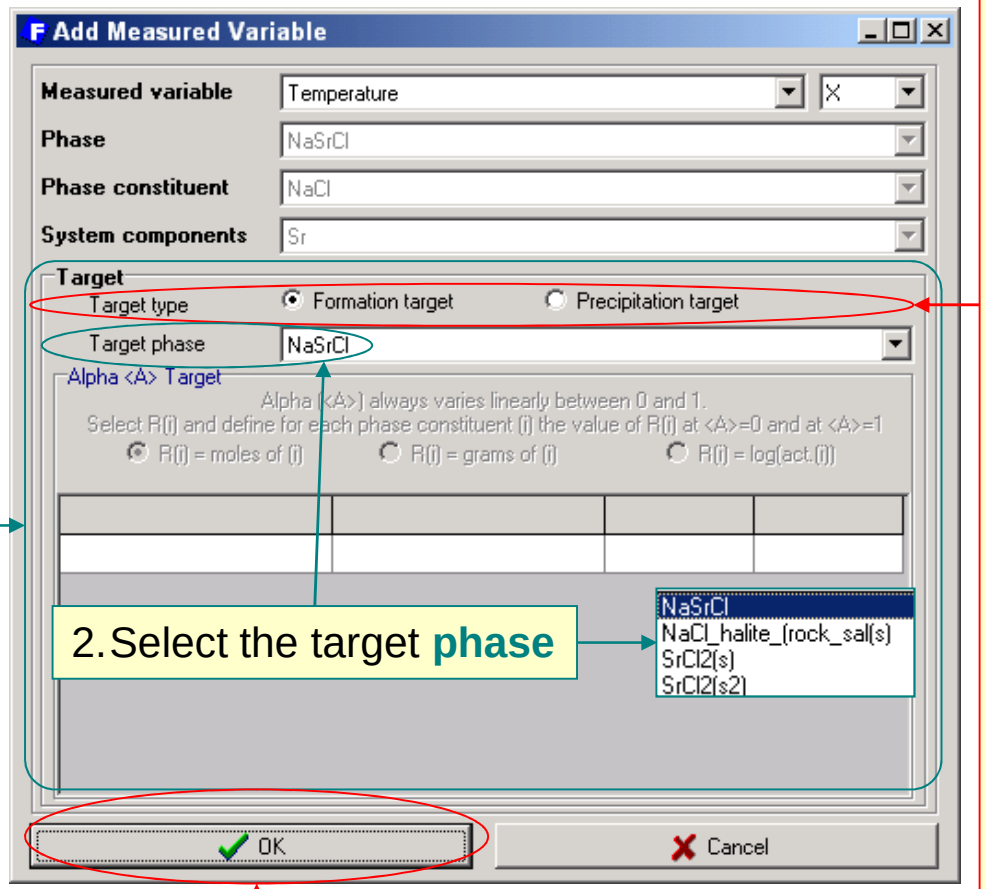
Eliminated: NaSrCl, SrCl2(s2), NaCl_halite_(rock_sal(s), SrCl2(s)

Experimental Conditions variables and data entered

We will select a formation target of the **liquid** phase for the eutectic **temperature measurements**

# Measured variable: **formation** and **precipitation** target features

The **Target** frame is enabled because the final T is **not** specified.



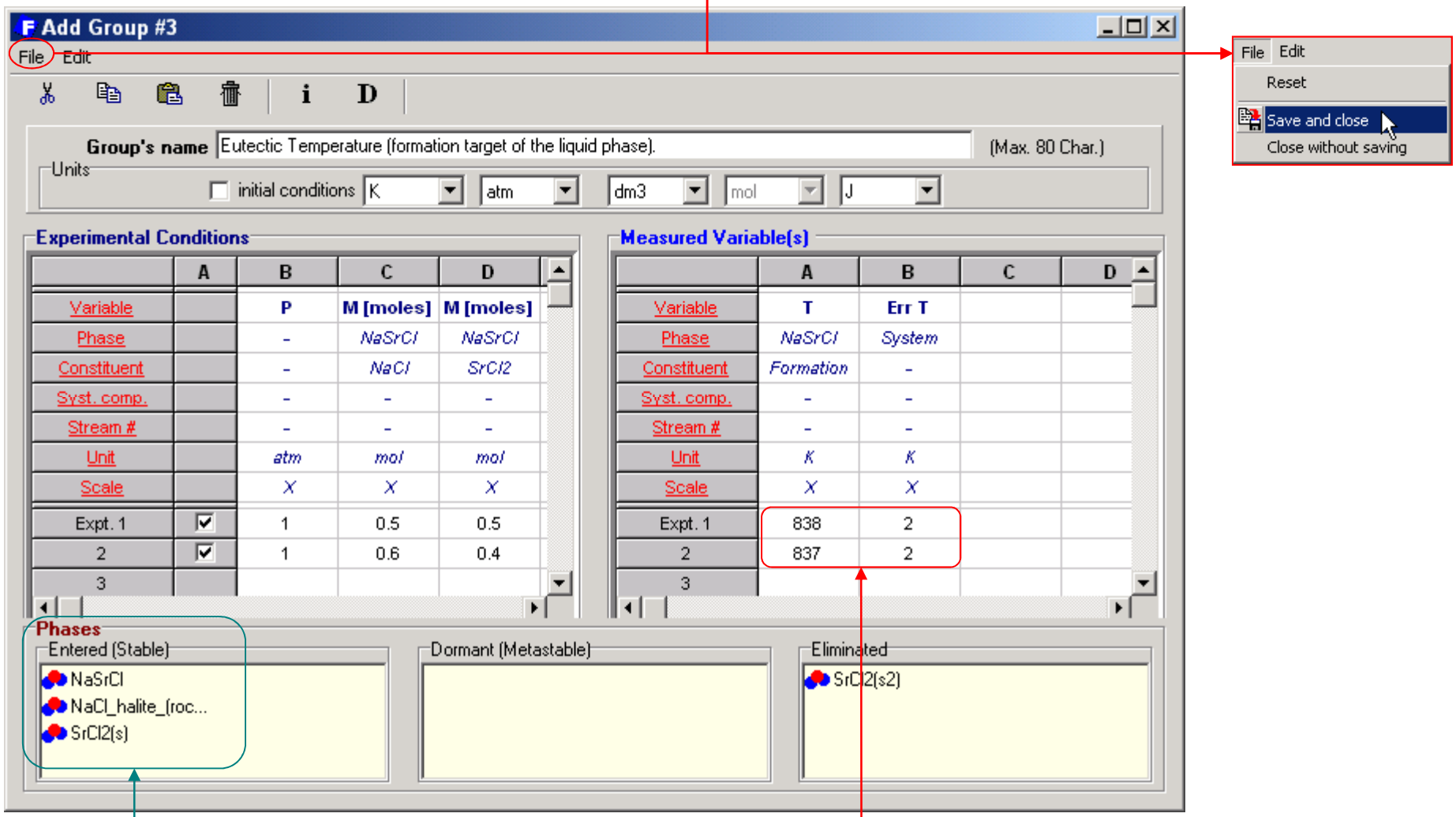

2. Select the target **phase**

3. Press **OK**.

1. Select the target **type**:
   - **Formation Target:** The program calculates when this phase first forms (activity = 1, and normally zero mass). Note that one of T, P or alpha (<A>) must not be specified (i.e. blank) so that ***OptiSage*** can calculate the limiting T (P or <A>) when the **formation target** phase first forms. The formation target phase may be a compound species (for example a pure solid or liquid) or a solution phase (gas phase or real solution). (See also ***Equilib Advanced*** slides 3.1 to 3.6).
   - **Precipitation Target:** The program calculates when a second phase first starts to precipitate (activity = 1, zero mass) from this target solution phase (activity = 1, 100% mass). Note that one of T, P or alpha (<A>) must not be specified (i.e. blank) so that ***OptiSage*** can calculate the limiting T (P or <A>) when the second phase precipitates. The precipitate target phase must be a solution phase. (See also ***Equilib Advanced*** slides 3.7 to 3.11).

# Declaration and input of **Measured Variable**, **phases' selection**

3. Finally, **save** data and return to the ***OptiSage*** main window, select **File > Save and close**



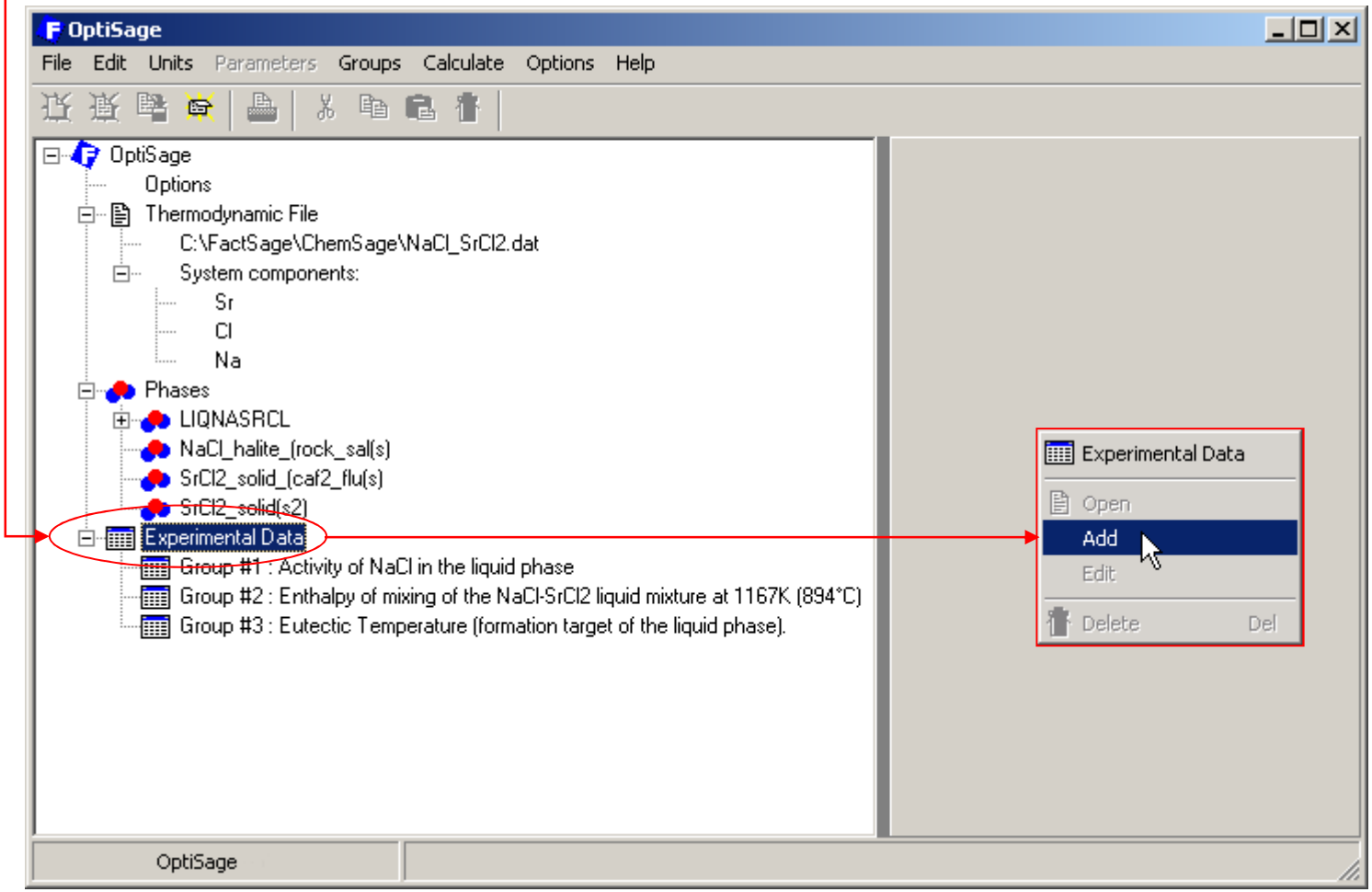

1. Select the phases

2. Enter the data for the measured variables

# Importing the data into Group #4

## Group #4: NaCl Liquidus Data

A **right-click** on **Experimental Data** opens the pop-up menu. Select **<Add>** to open the **'Add Group'** window.

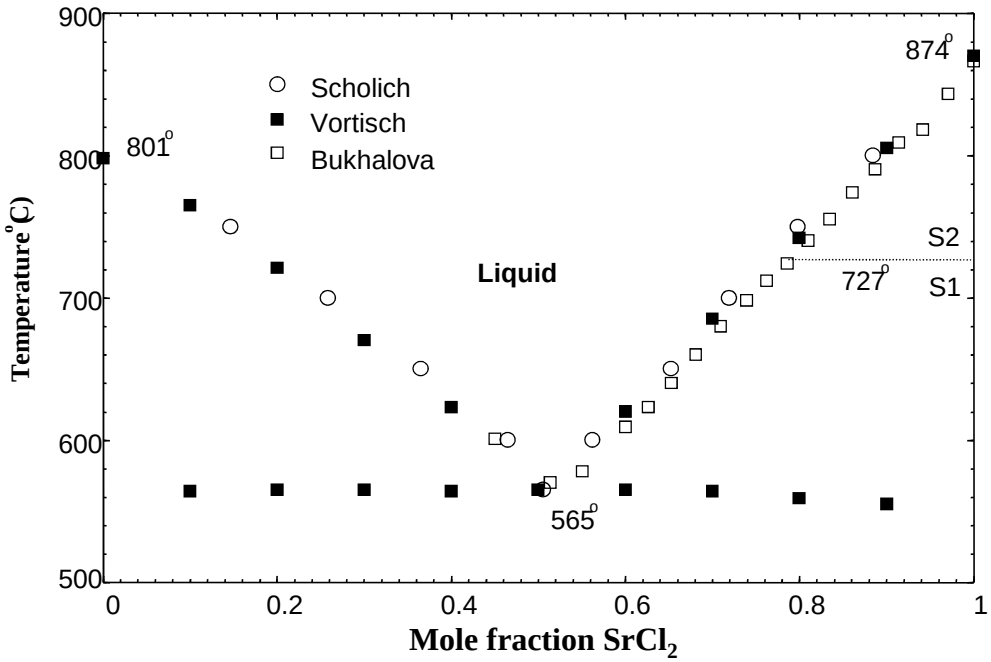


# Group #4: NaCl Liquidus Data

1. **Experimental conditions:**
   - Amount of NaCl(s)
   - Amount of $SrCl_2$(s1)
   - Pressure

2. **Measured variables:**
   - Temperature (used in *Formation Target* for NaCl(s))

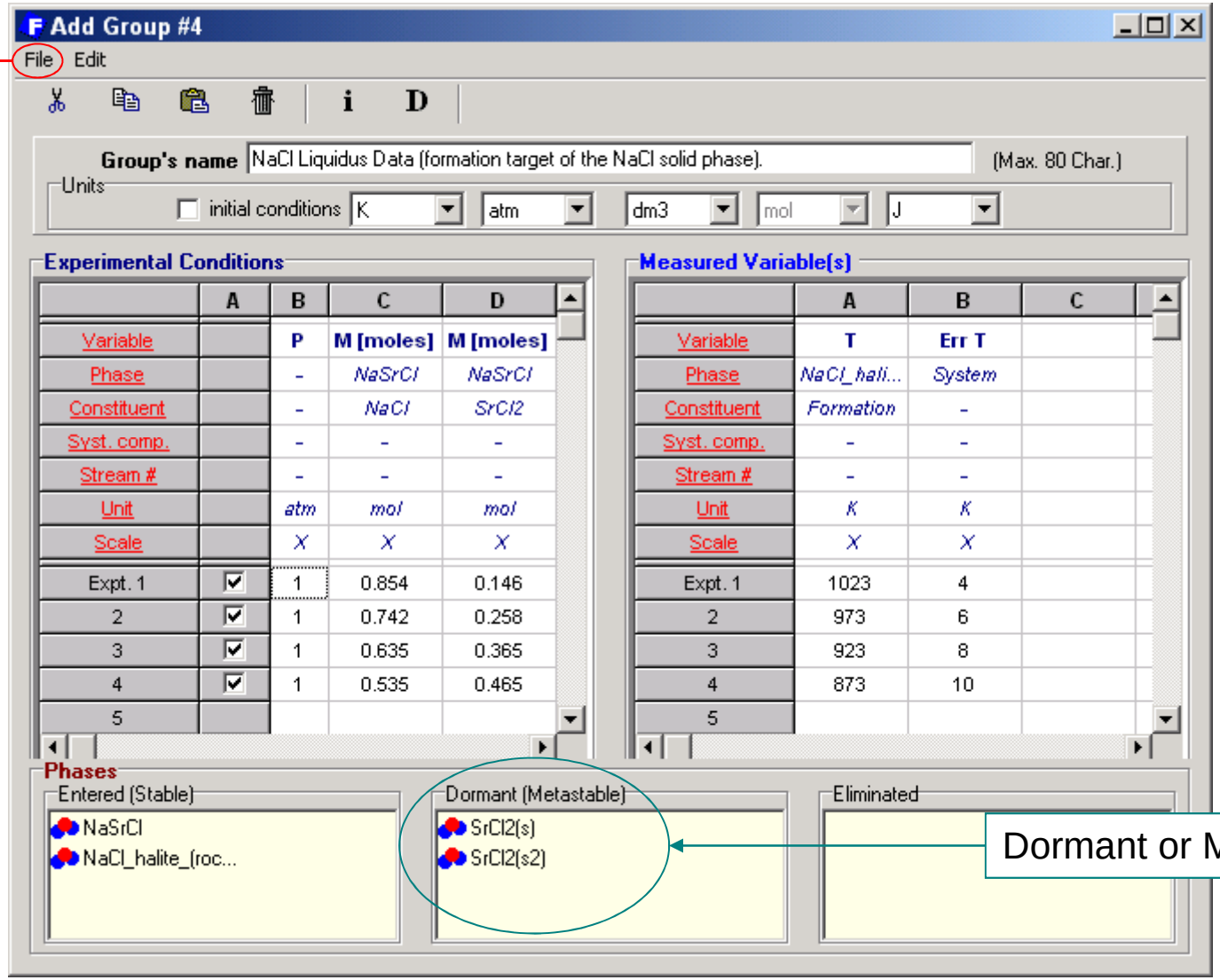
3. **Selected phases:**
   - Liquid phase (NaSrCl)
   - NaCl(s)

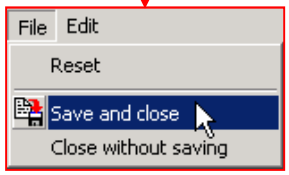



| NaCl Liquidus Data | | | | |
|---|---|---|---|---|
| Experimental Conditions | | | Measured Variable | |
| P | moles | moles | T(K) | error |
| | SrCl2 | NaCl | Formation Target | (K) |
| atm | liquid | liquid | NaCl(s) | |
| 1 | 0.146 | 0.854 | 1023 | 4 |
| 1 | 0.258 | 0.742 | 973 | 6 |
| 1 | 0.365 | 0.635 | 923 | 8 |
| 1 | 0.465 | 0.535 | 873 | 10 |

# Metastable Phases (Filling the Add Group #4 window)

Do not forget to **save** your data (select **File > Save and close**)



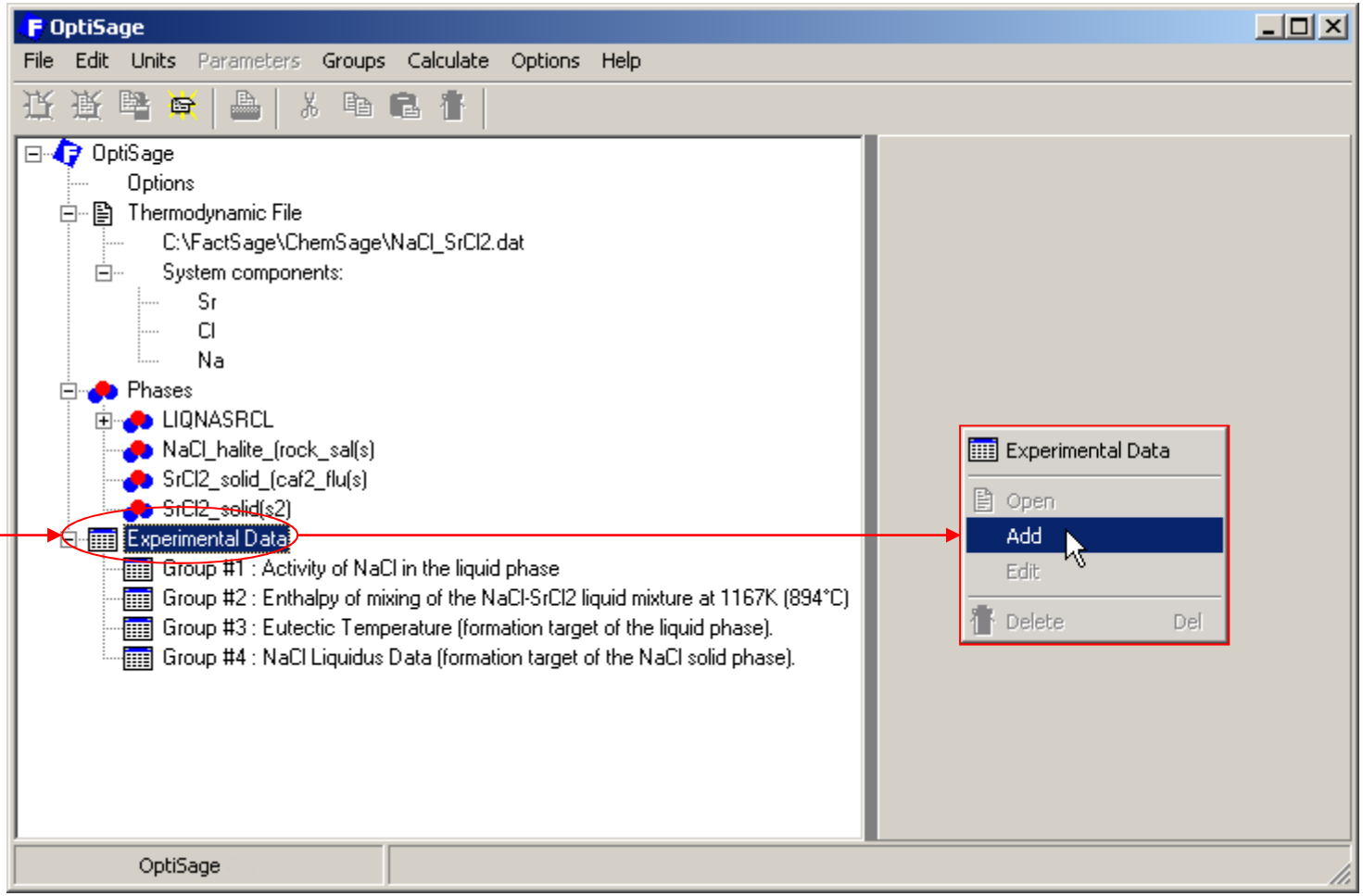




Dormant or Metastable phases

# Importing the data into Group #5

## Group #5: $SrCl_2$ Liquidus Data

A **right-click** on **Experimental Data** opens the pop-up menu. Select **<Add>** to open the **'Add Group'** window.

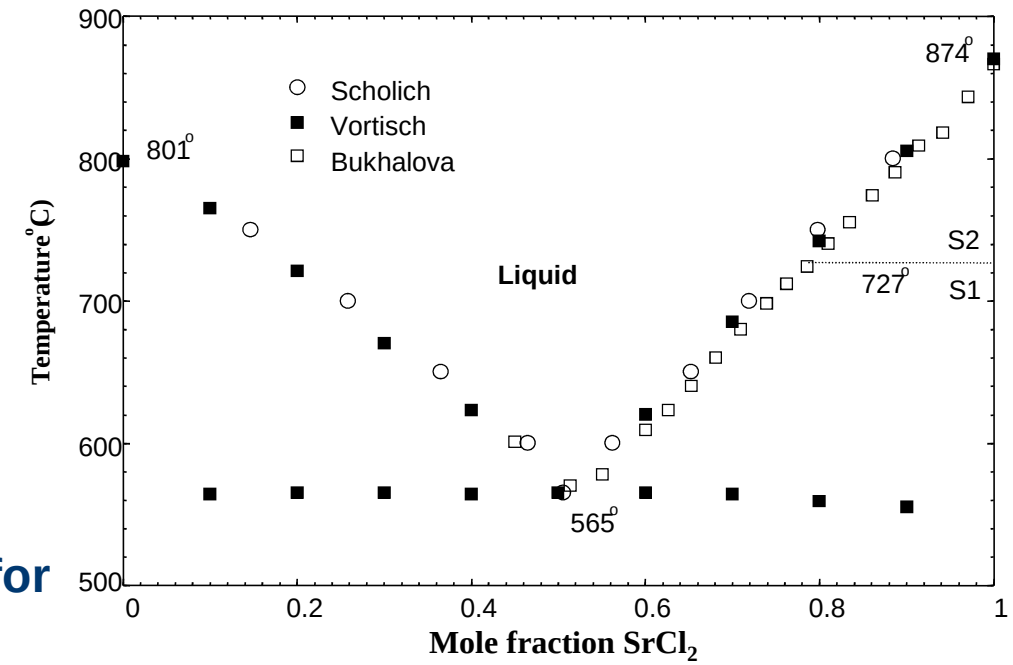


# Group #5: $SrCl_2$ liquidus data

1. **Experimental conditions:**
   - Amount of NaCl(s)
   - Amount of $SrCl_2$(s1)
   - Pressure

2. **Measured variables:**
   - Temperature (used in *Precipitation Target* for liquid phase (NaSrCl))

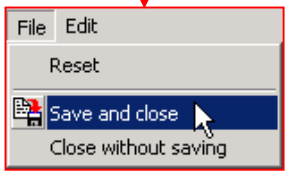
3. **Selected phases:**
   - Liquid phase (NaSrCl)
   - $SrCl_2$(s1)
   - $SrCl_2$(s2)




| SrCl2 Liquidus Data | | | | |
|---|---|---|---|---|
| Experimental Conditions | | | Measured Variable | |
| P | moles SrCl2 | moles NaCl | T(K) Precipitation Target | error (K) |
| atm | liquid | liquid | liquid | |
| 1 | 0.97 | 0.03 | 1116 | 5 |
| 1 | 0.914 | 0.086 | 1082 | 5 |
| 1 | 0.86 | 0.14 | 1047 | 5 |
| 1 | 0.81 | 0.19 | 1013 | 5 |
| 1 | 0.762 | 0.238 | 985 | 5 |
| 1 | 0.68 | 0.32 | 933 | 5 |
| 1 | 0.6 | 0.4 | 882 | 5 |
| 1 | 0.513 | 0.487 | 843 | 5 |

# Add Group #5 with data entered and phases selected

Do not forget to **save** your data.




**Add Group #5**

File Edit

**Group's name** SrCl2 Liquidus Data (precipitation target of the liquid phase). (Max. 80 Char.)

Units: initial conditions K atm dm3 mol J

**Experimental Conditions**

| | A | B | C | D | E |
|---|---|---|---|---|---|
| Variable | | P | M [moles] | M [moles] | |
| Phase | | - | NaSrCl | NaSrCl | |
| Constituent | | - | NaCl | SrCl2 | |
| Syst. comp. | | - | - | - | |
| Stream # | | - | - | - | |
| Unit | | atm | mol | mol | |
| Scale | | X | X | X | |
| Expt. 1 | ☑ | 1 | 0.03 | 0.97 | |
| 2 | ☑ | 1 | 0.086 | 0.914 | |
| 3 | ☑ | 1 | 0.14 | 0.86 | |
| 4 | ☑ | 1 | 0.19 | 0.81 | |
| 5 | ☑ | 1 | 0.238 | 0.762 | |
| 6 | ☑ | 1 | 0.32 | 0.68 | |
| 7 | ☑ | 1 | 0.4 | 0.6 | |
| 8 | ☑ | 1 | 0.487 | 0.513 | |
| 9 | | | | | |

**Measured Variable(s)**

| | A | B | C | D |
|---|---|---|---|---|
| Variable | T | Err T | | |
| Phase | NaSrCl | System | | |
| Constituent | Precipitation | | | |
| Syst. comp. | - | - | | |
| Stream # | - | - | | |
| Unit | K | K | | |
| Scale | X | X | | |
| Expt. 1 | 1116 | 5 | | |
| 2 | 1082 | 5 | | |
| 3 | 1047 | 5 | | |
| 4 | 1013 | 5 | | |
| 5 | 985 | 5 | | |
| 6 | 933 | 5 | | |
| 7 | 882 | 5 | | |
| 8 | 843 | 5 | | |
| 9 | | | | |

This time, it is a ***precipitation*** target

**Phases**

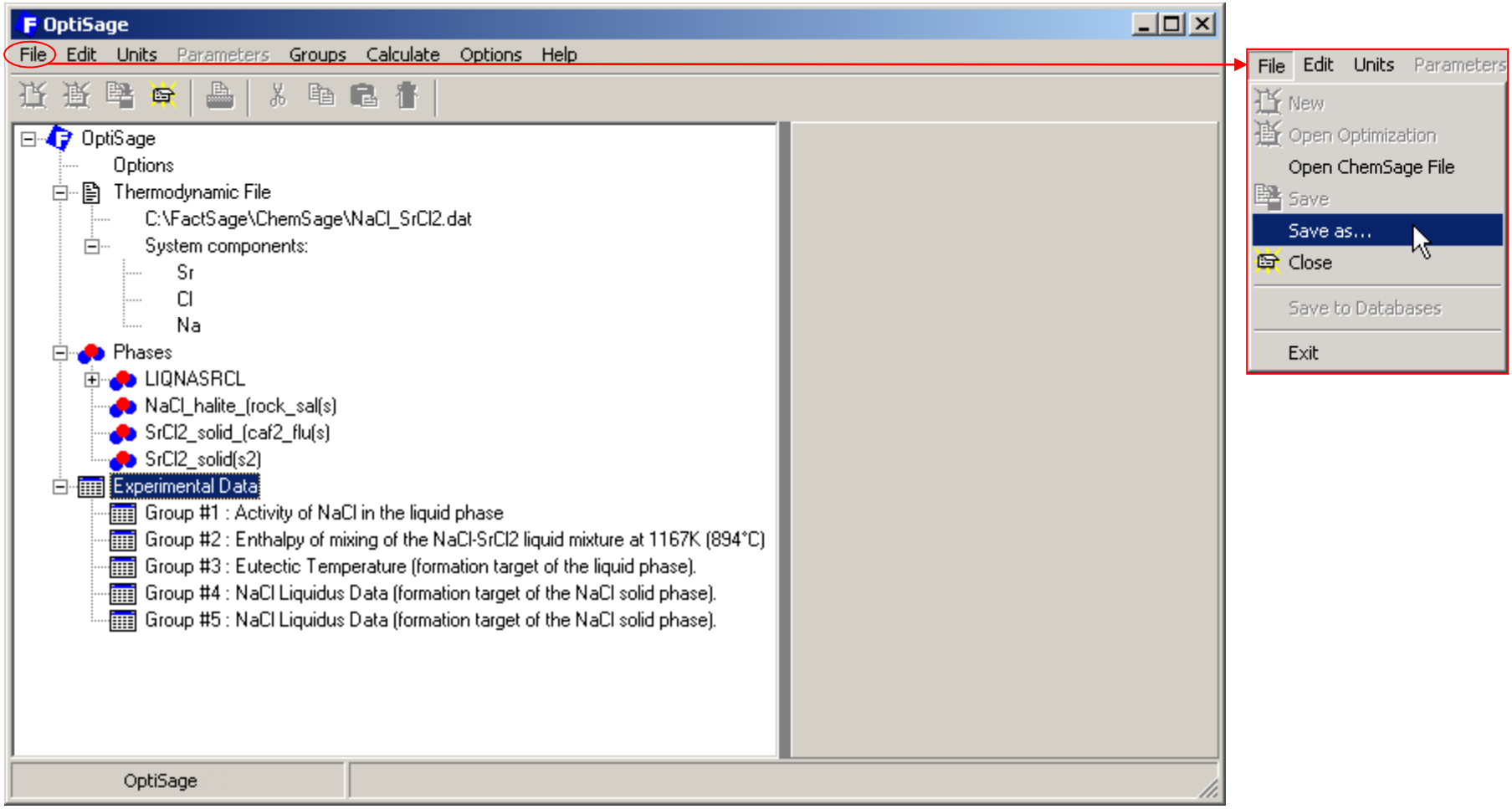
Entered (Stable): NaSrCl, SrCl2(s), SrCl2(s2)

Dormant (Metastable): NaCl_halite_(roc...

Eliminated

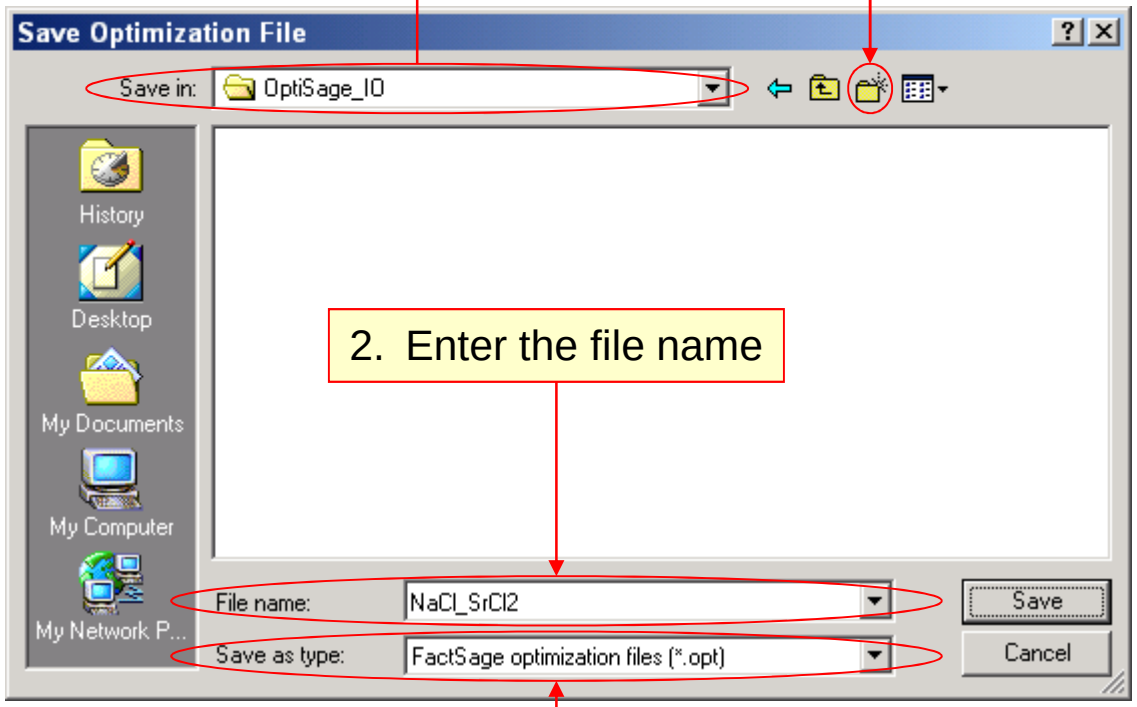
# Creation of (Save as…) a ***FactSage*** optimization file

Your Experimental Data are saved in a default folder (FACT-51\OptIO\Default, in the present case).
The next step is to create a ***FactSage*** optimization file.
Select **File > Save as…** to open the **Save Optimization File** dialog box.



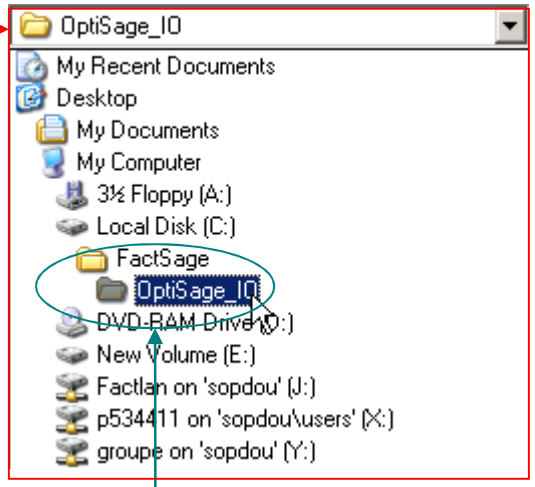
# Saving a ***FactSage*** optimization file

1. Browse or create your own folder




2. Enter the file name

3. Save your optimization file (*.opt)



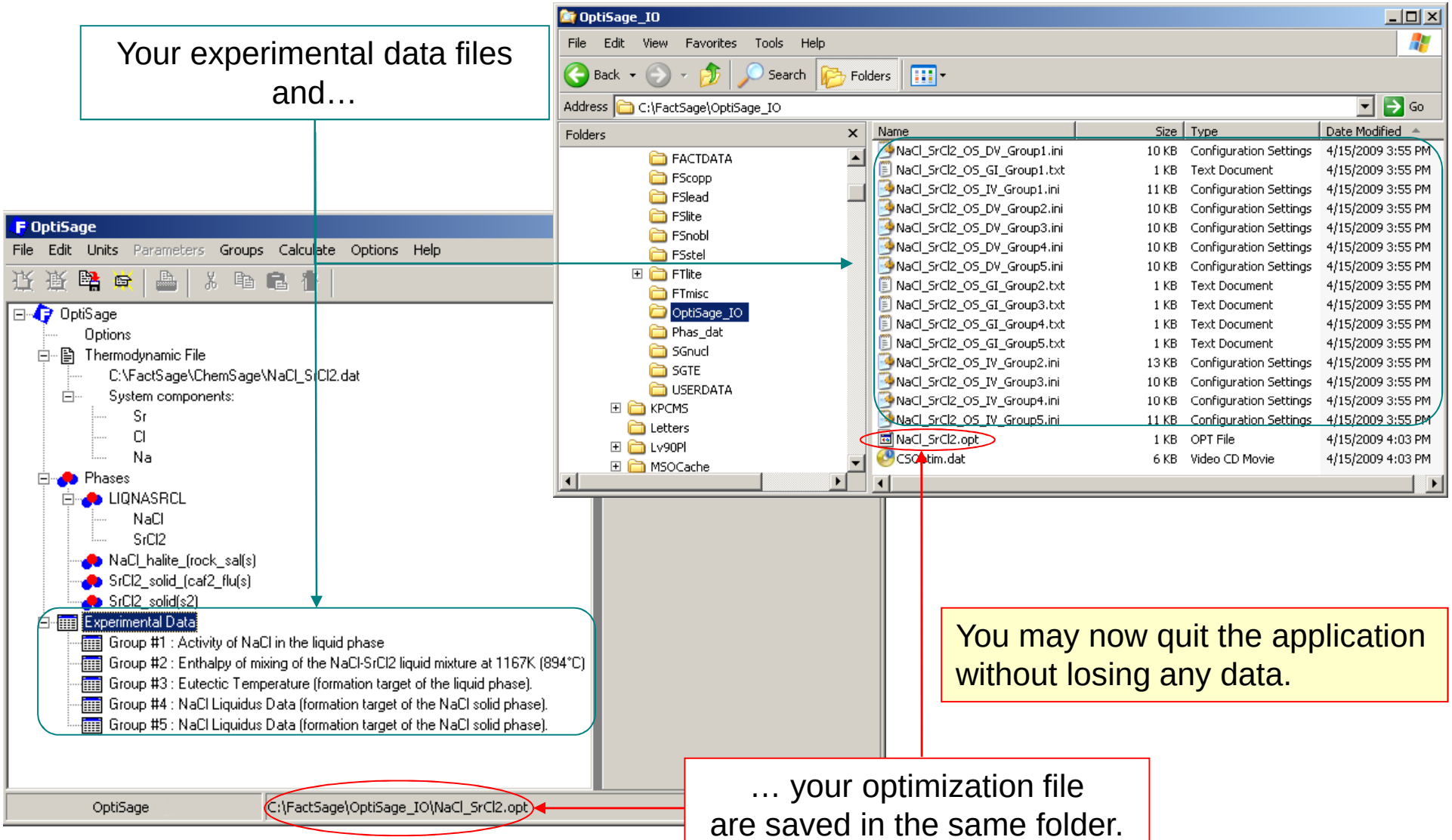

Folder **OptiSage_IO** created in **FactSage**

**Warning:**
You must save an optimization file before closing the application. Failing to do that operation will result in the loss of your experimental data files.

Note: You can save your file after adding a group of experimental data.

# Location of your files

Your experimental data files and…




You may now quit the application without losing any data.

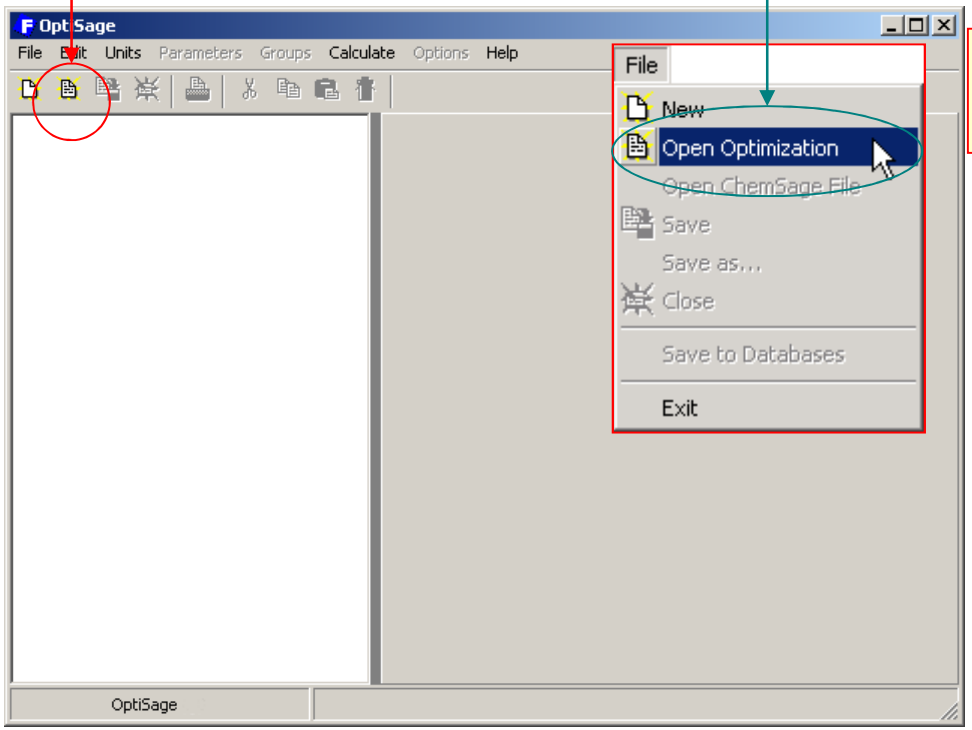
… your optimization file are saved in the same folder.

# Opening an OptiSage file

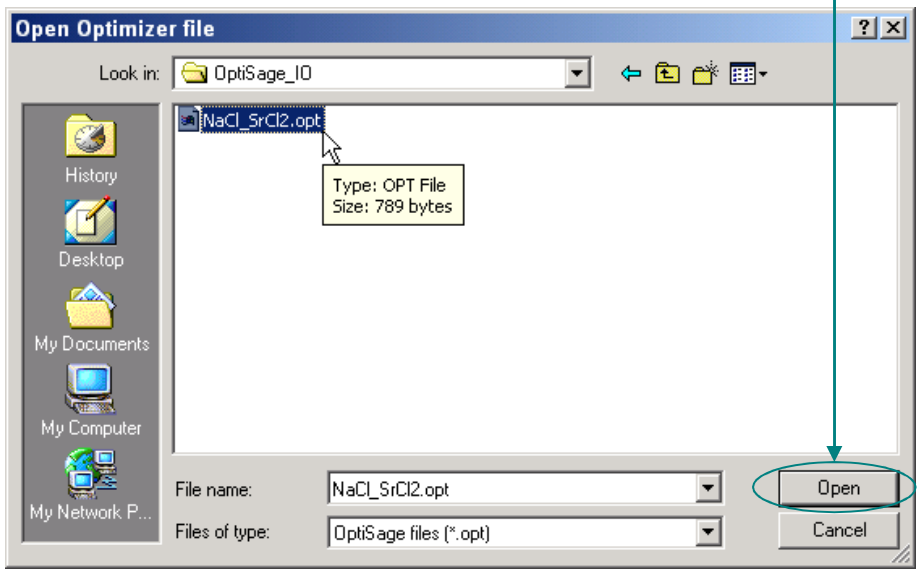
The next time you want to work on your optimization, just open your file in the ***OptiSage*** main window by:

**clicking** on the « Open OptiSage file » button or

**selecting** the menu File > Open Optimization




…to open the « Open Optomizer file » window. select your *.opt file and press **Open**



# Execution of an optimization

The actual execution of the optimization consists of several actions which a user has to go through one after the other.

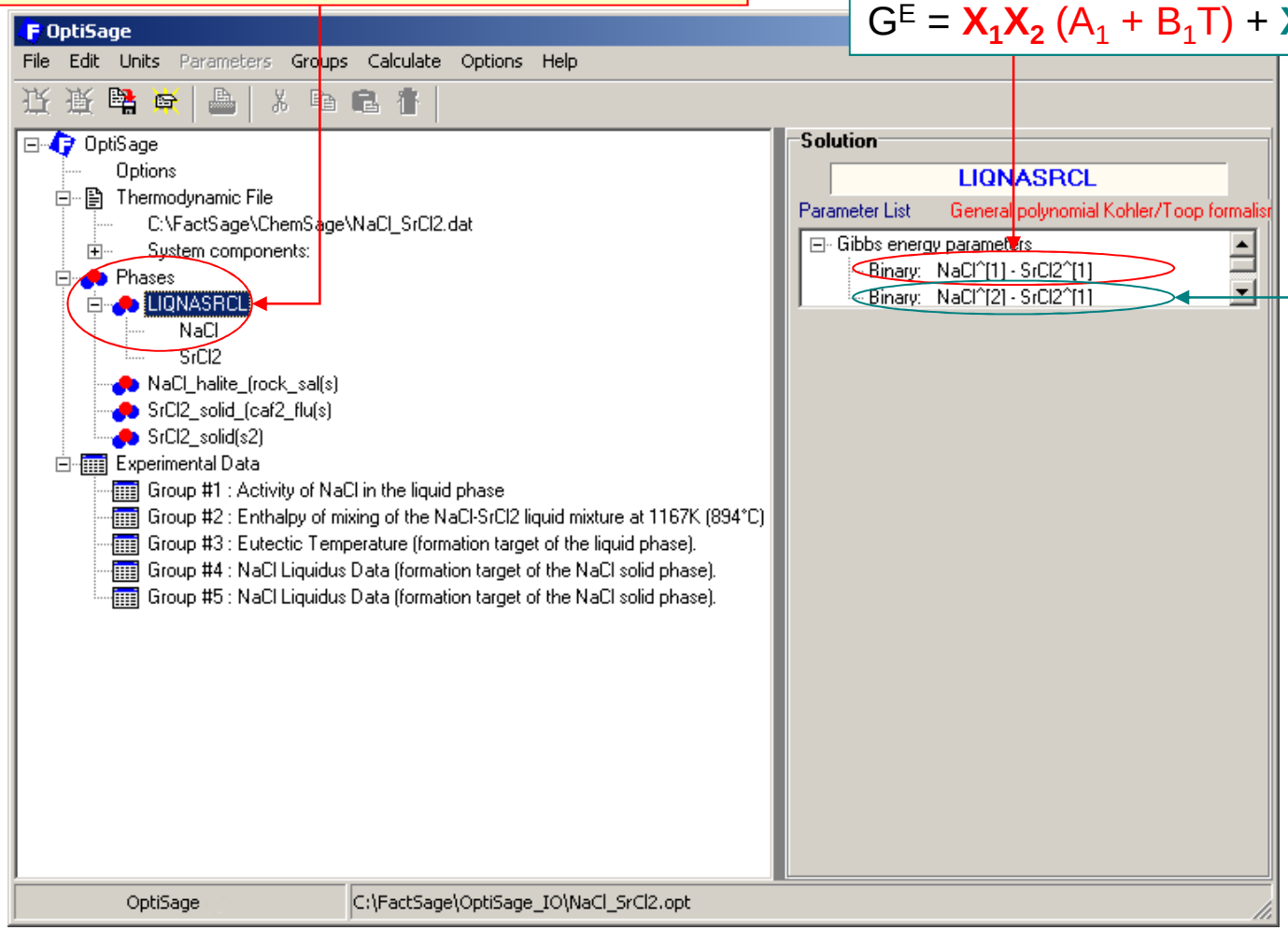
- The parameters that shall be optimized have to be selected.
- Initial values for these parameters have to be entered and estimated values for the errors of the parameters have to be defined.
- In some cases it is necessary to provide numerical relationships between the parameters if they are not mathematically independent.

After that the optimization calculation can be started.

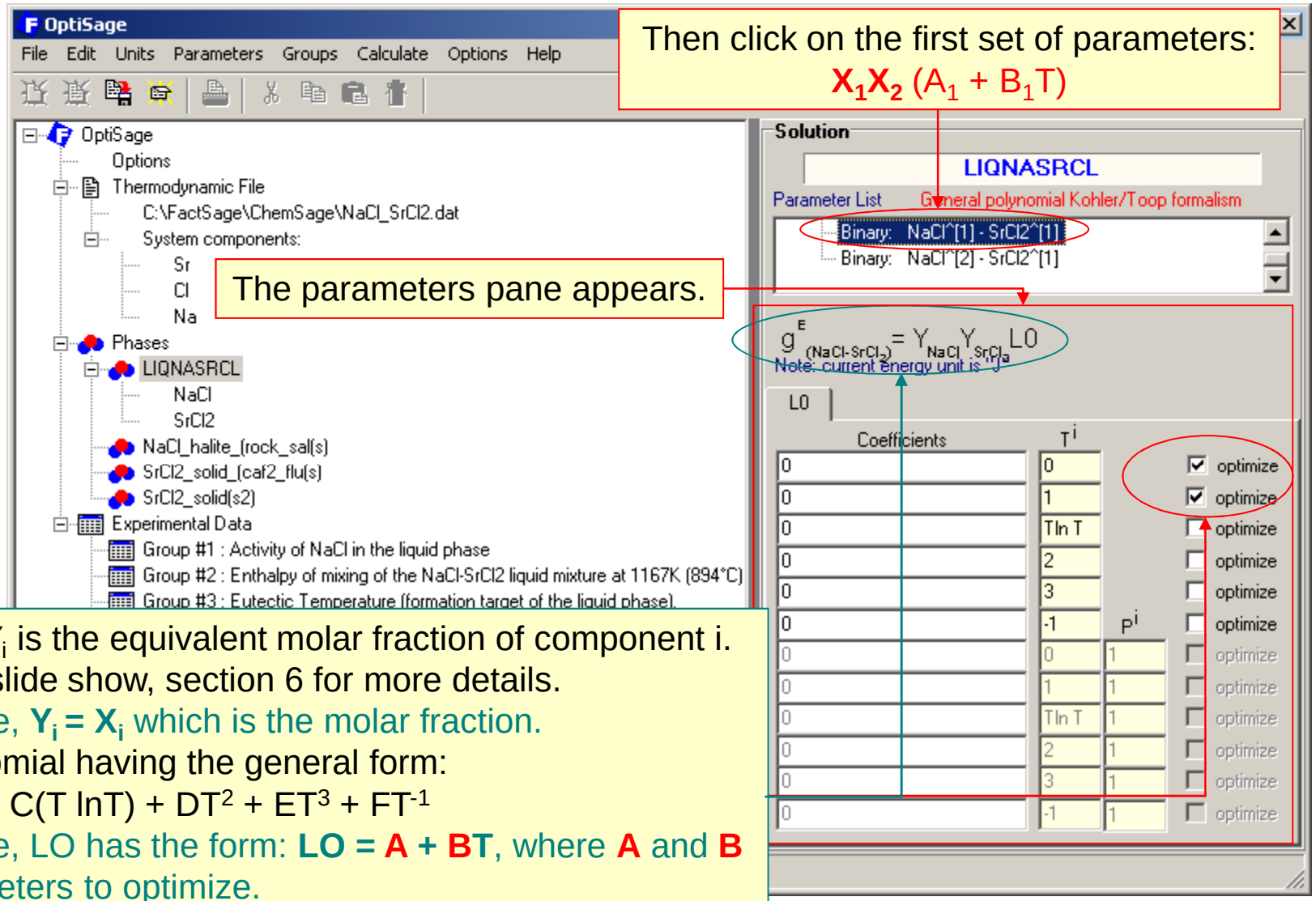
# Selection of the phase to optimize

To select the phase to optimize, **click** on its name and the **Solution** (or phase component) panel appears.

In our example, we want to optimize the parameters of the liquid phase. Please review slide 2.2 where we define $G^E$ as $G^E = \mathbf{X_1X_2}\,(A_1 + B_1T) + \mathbf{X_1^2X_2}\,(A_2 + B_2T)$



# Selection of the first set of parameters to optimize

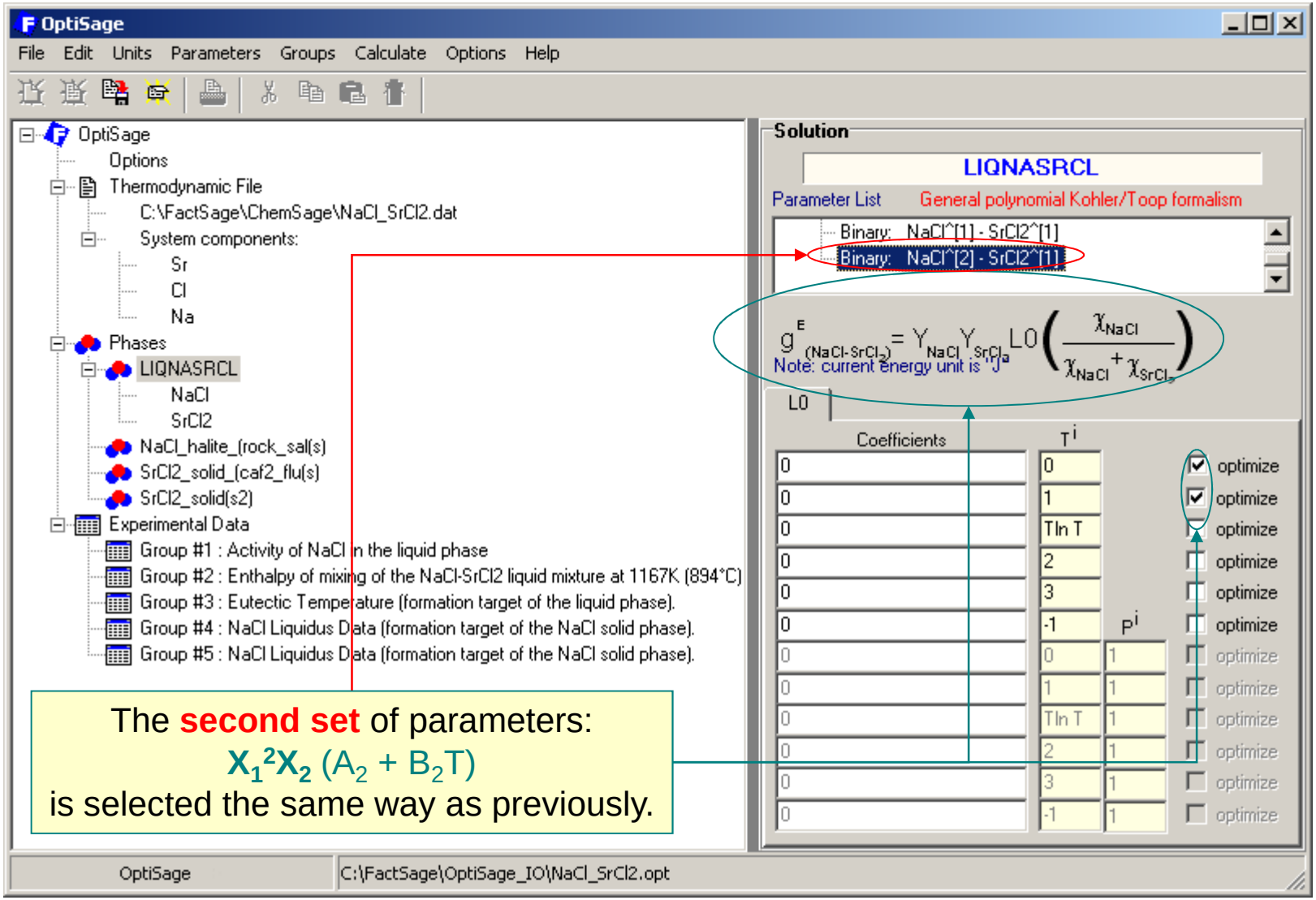



Then click on the first set of parameters:
$X_1X_2\ (A_1 + B_1T)$

The parameters pane appears.

The variable $Y_i$ is the equivalent molar fraction of component i.
See Solution slide show, section 6 for more details.
In our example, $Y_i = X_i$ which is the molar fraction.
LO is a polynomial having the general form:
$LO = A + BT + C(T \ln T) + DT^2 + ET^3 + FT^{-1}$
In our example, LO has the form: **LO = A + BT**, where **A** and **B** are the parameters to optimize.
**Check the optimize check boxes for these two parameters.**

# Selection of the second set of parameters to optimize




The **second set** of parameters:

$X_1^2X_2\ (A_2 + B_2T)$

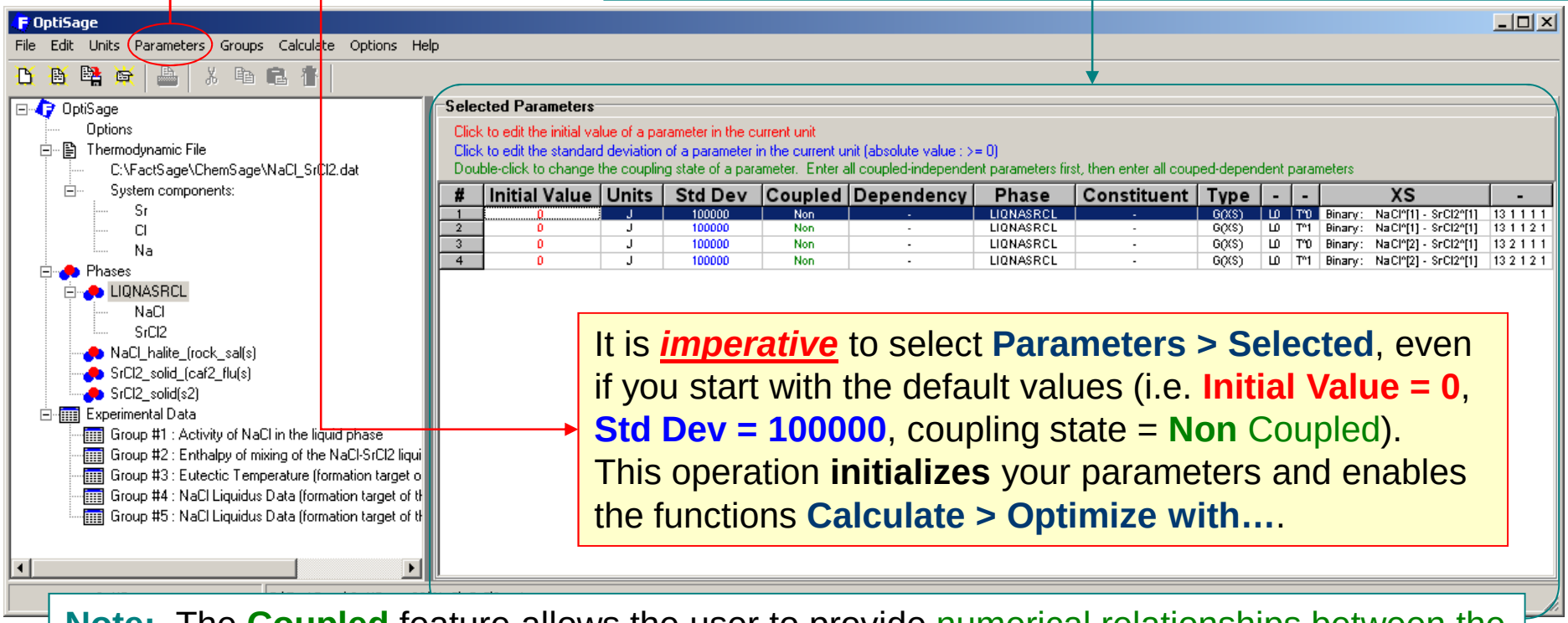
is selected the same way as previously.

# Parameters menu and edition of selected parameters

**Clears** your selection

**Opens** the **Selected Parameters** pane where you can edit:

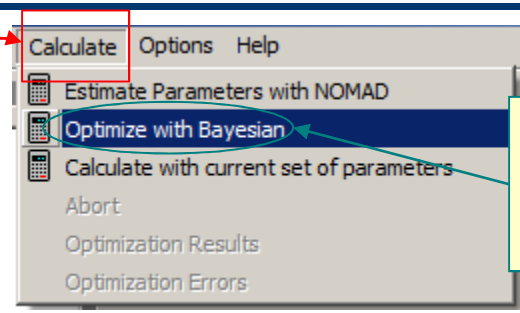
- the initial value of a parameter
- the standard deviation (i.e. error) of a parameter
- the coupling state of a parameter



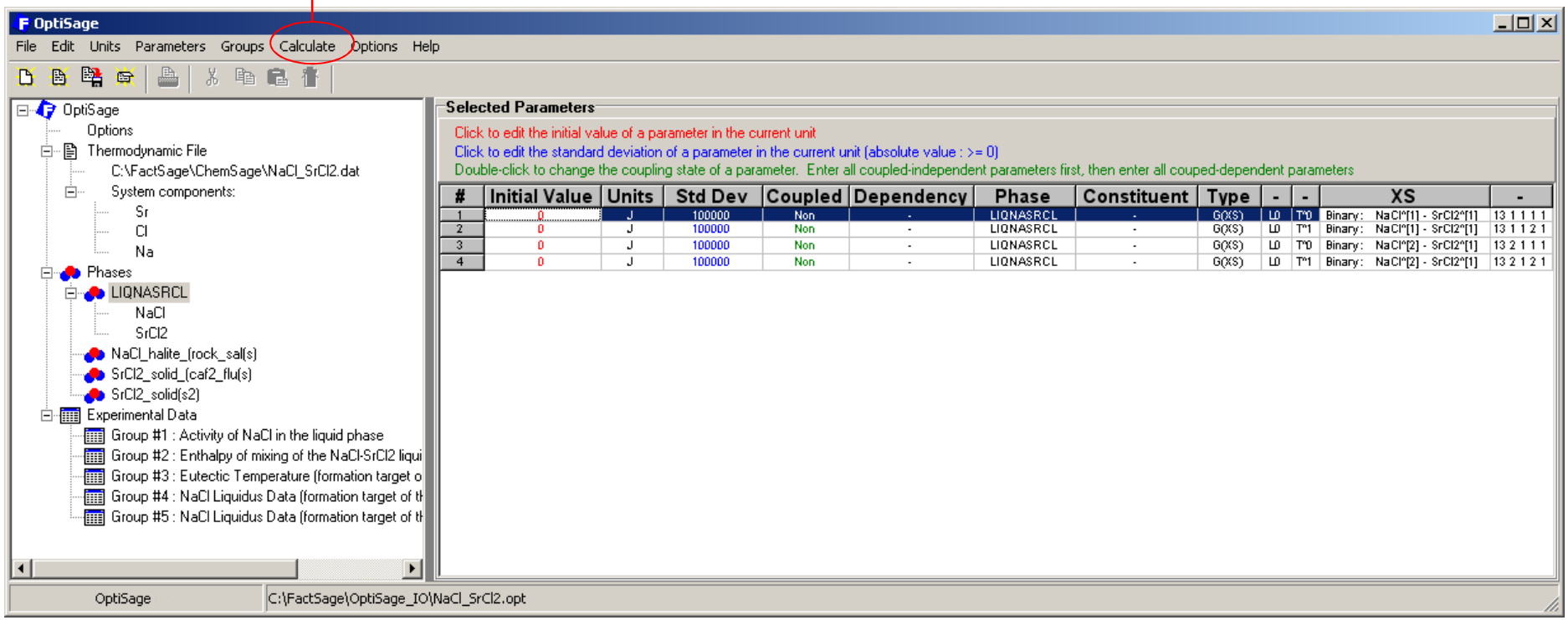

It is ***imperative*** to select **Parameters > Selected**, even if you start with the default values (i.e. **Initial Value = 0**, **Std Dev = 100000**, coupling state = **Non** Coupled). This operation **initializes** your parameters and enables the functions **Calculate > Optimize with…**.

**Note:** The **Coupled** feature allows the user to provide numerical relationships between the parameters if they are not mathematically independent. It is an advanced feature of the ***Optisage*** module and will be demonstrated during ***FactSage*** workshops.

# Initiating an optimization



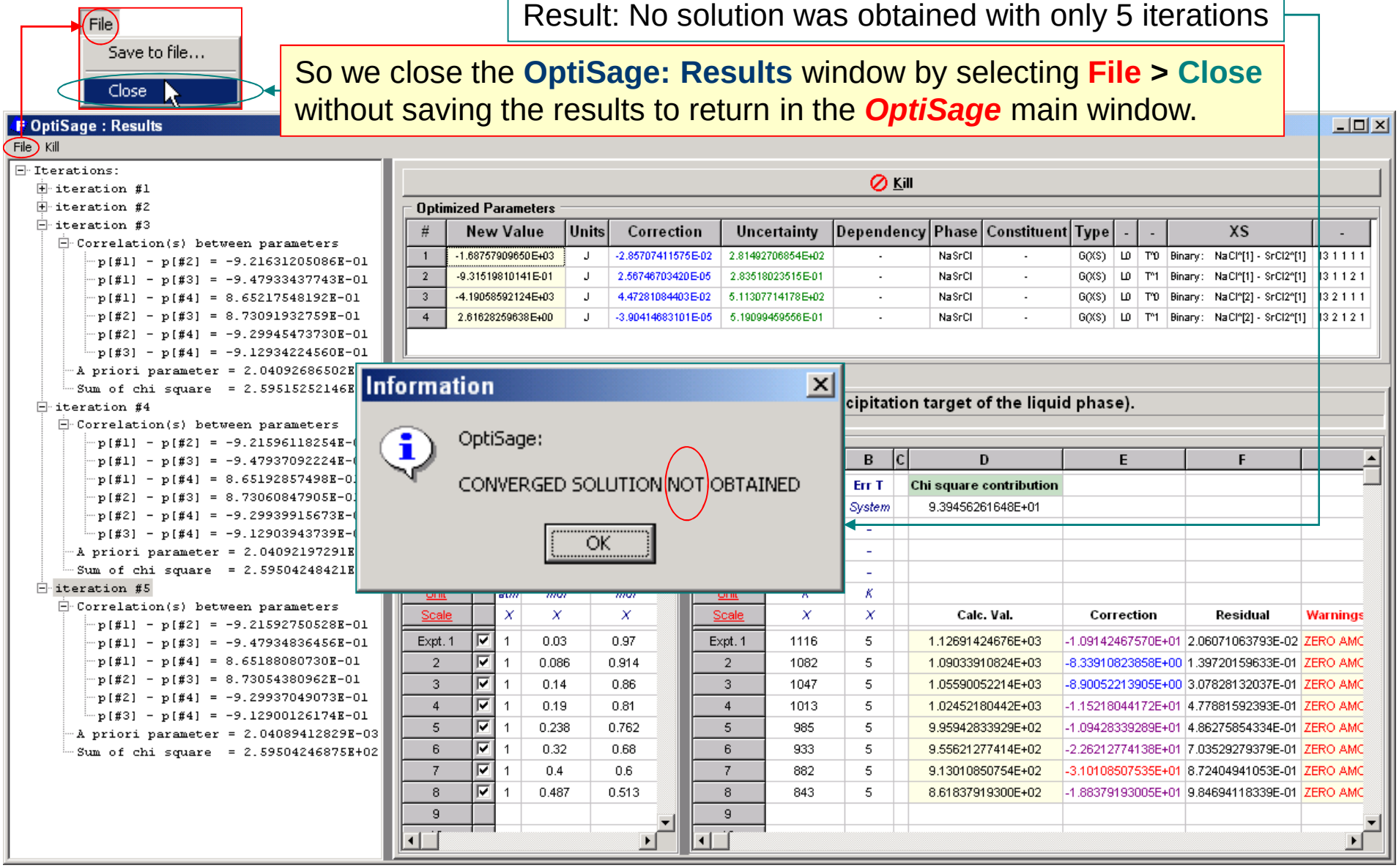

From the menu bar, select **Calculate** > **Optimize with Bayesian** to start calculation of your first optimization using the Bayesian technique.



# Optimization results after 5 iterations

Result: No solution was obtained with only 5 iterations

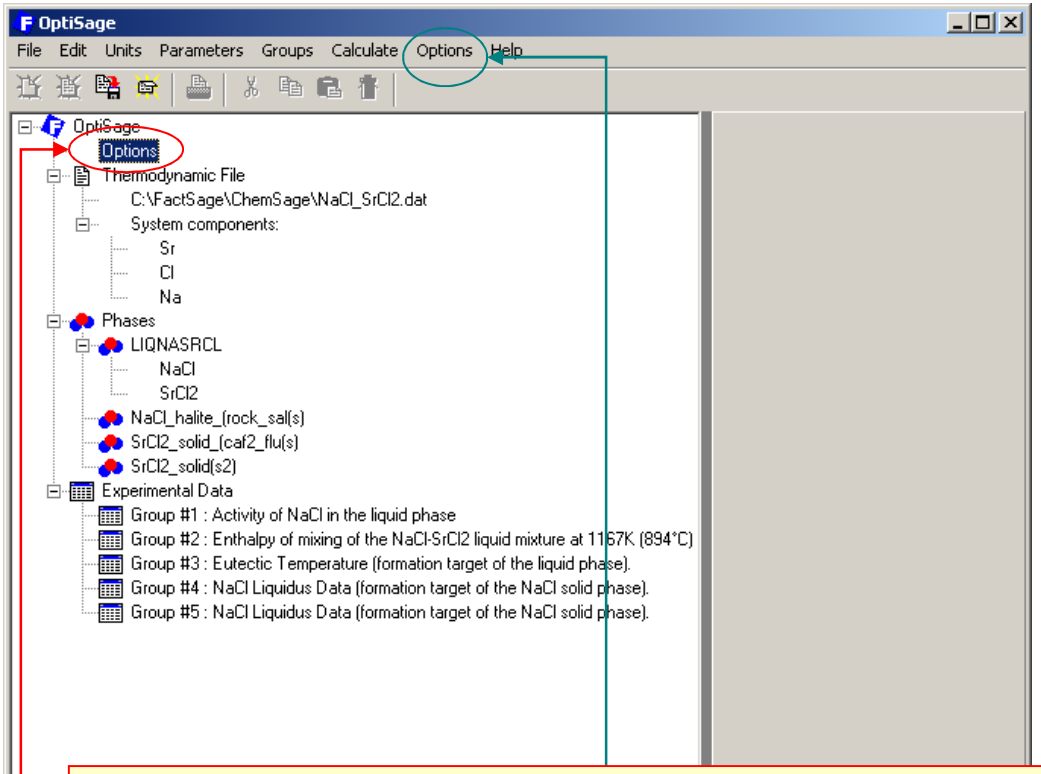
So we close the **OptiSage: Results** window by selecting **File > Close** without saving the results to return in the ***OptiSage*** main window.



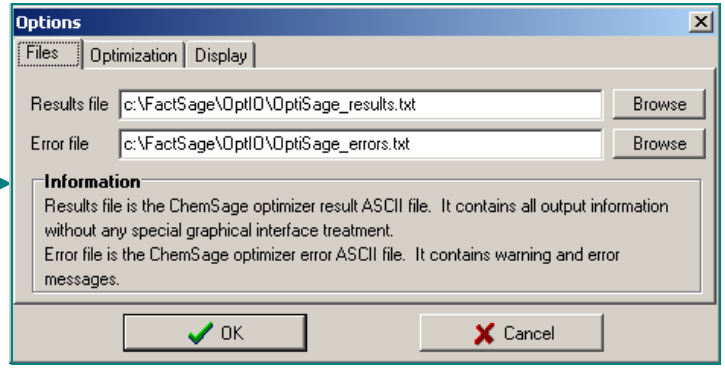
# **Options** Features

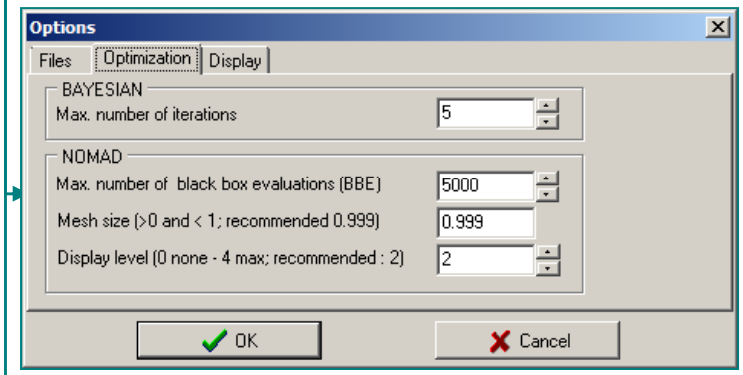
Different options are available in ***OptiSage***, you can select:

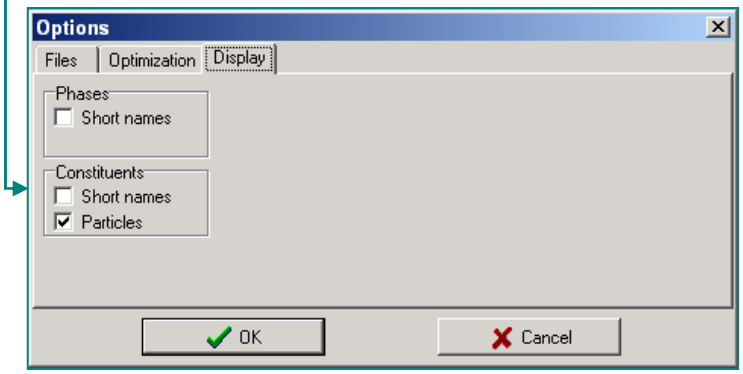
1. The directories for your results and errors files;
2. Optimization options;
3. The way to display the phases and the constituents.



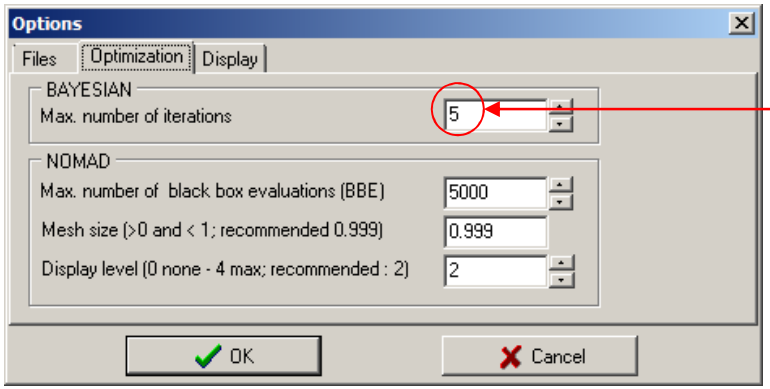

To open the **Options** window, double click on **Options** in the tree view or select **Options** in the Menu bar.



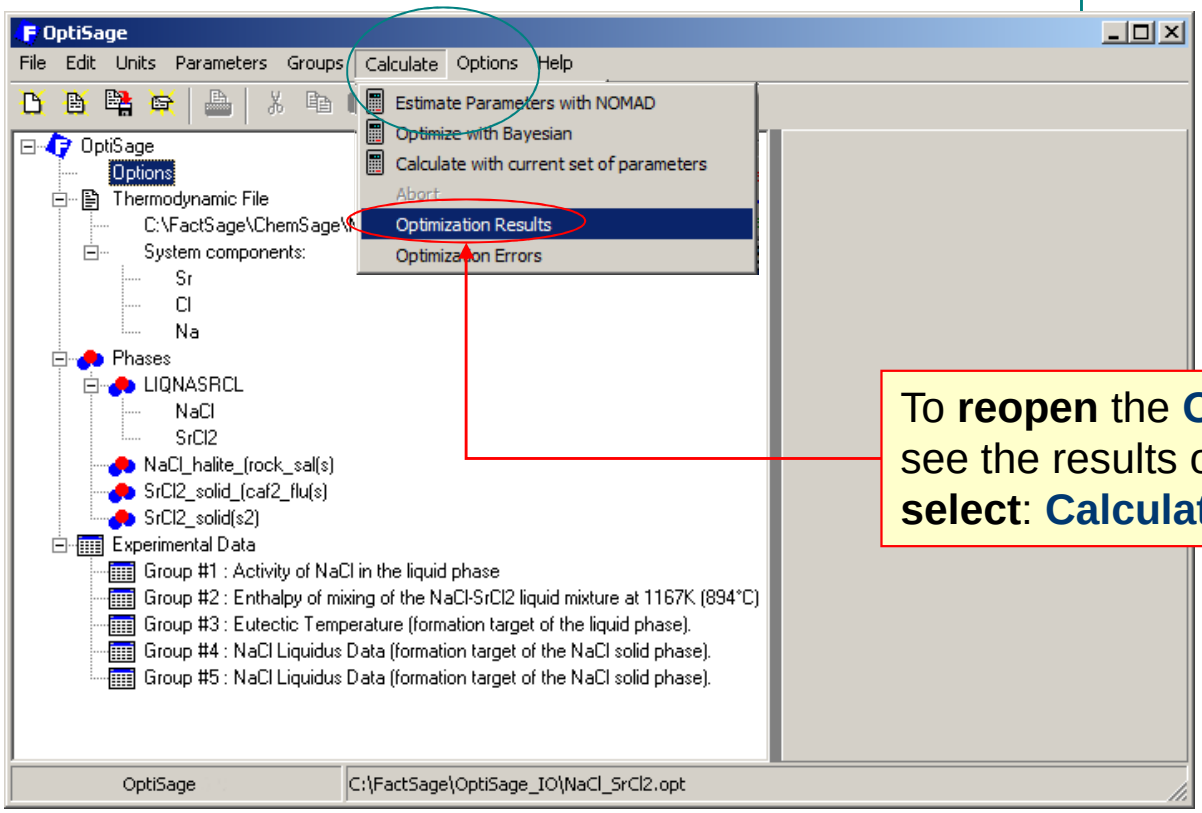



# Changing **optimization** options




In our case, we want a larger number of iterations. The default value is 5. Let's put **8** as the maximum number of iterations.

We can now start a new optimization




To **reopen** the **OptiSage: Results** window and see the results of the previous optimization, **select**: **Calculate > Optimization Results**.

# Convergent solution of the 2nd optimization

We have a convergent solution after **7** iterations

**Information**

OptiSage:

CONVERGED SOLUTION OBTAINED AFTER 7 ITERATIONS

OK

**OptiSage : Results**

File Kill

```
Iterations:
  iteration #1
  iteration #2
  iteration #3
  iteration #4
  iteration #5
    Correlation(s) between parameters
      p[#1] - p[#2] = -9.21594122072E-01
      p[#1] - p[#3] = -9.47935654231E-01
      p[#1] - p[#4] = 8.65189611378E-01
      p[#2] - p[#3] = 8.73056665015E-01
      p[#2] - p[#4] = -9.29938153378E-01
      p[#3] - p[#4] = -9.12900935544E-01
    A priori parameter = 1.69193005338E-12
    Sum of chi square  = 2.59502205984E+02
  iteration #6
    Correlation(s) between parameters
      p[#1] - p[#2] = -9.21594026729E-01
      p[#1] - p[#3] = -9.47936105759E-01
      p[#1] - p[#4] = 8.65190312269E-01
      p[#2] - p[#3] = 8.73057191302E-01
      p[#2] - p[#4] = -9.29938596255E-01
      p[#3] - p[#4] = -9.12901456348E-01
    A priori parameter = 4.61335051951E-13
    Sum of chi square  = 2.59502205959E+02
  iteration #7
    Correlation(s) between parameters
      p[#1] - p[#2] = -9.21598047309E-01
      p[#1] - p[#3] = -9.47938945257E-01
      p[#1] - p[#4] = 8.65197078272E-01
      p[#2] - p[#3] = 8.73063514763E-01
      p[#2] - p[#4] = -9.29942076872E-01
      p[#3] - p[#4] = -9.12905382882E-01
    A priori parameter = 5.45836284914E-13
    Sum of chi square  = 2.59502205935E+02
```

Kill

**Optimized Parameters**

| # | New Value | Units | Correction | Uncertainty | Dependency | Phase | Constituent | Type | - | - | XS | - |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -1.68754432123E+03 | J | 3.18645102773E-03 | 2.81502663602E+02 | - | NaSrCl | - | G(XS) | L0 | T^0 | Binary: NaCl^[1] - SrCl2^[1] | 13 1 1 1 1 |
| 2 | -9.31551010206E-01 | J | -2.62786304479E-06 | 2.83527218209E-01 | - | NaSrCl | - | G(XS) | L0 | T^1 | Binary: NaCl^[1] - SrCl2^[1] | 13 1 1 2 1 |
| 3 | -4.19065110589E+03 | J | -5.05568159506E-03 | 5.11323998802E+02 | - | NaSrCl | - | G(XS) | L0 | T^0 | Binary: NaCl^[2] - SrCl2^[1] | 13 2 1 1 1 |
| 4 | 2.61633848012E+00 | J | 4.09815249977E-06 | 5.19114426112E-01 | - | NaSrCl | - | G(XS) | L0 | T^1 | Binary: NaCl^[2] - SrCl2^[1] | 13 2 1 2 1 |

Group #1 | Group #2 | Group #3 | Group #4 | Group #5

**SrCl2 Liquidus Data (precipitation target of the liquid phase).**

**Experimental Conditions**

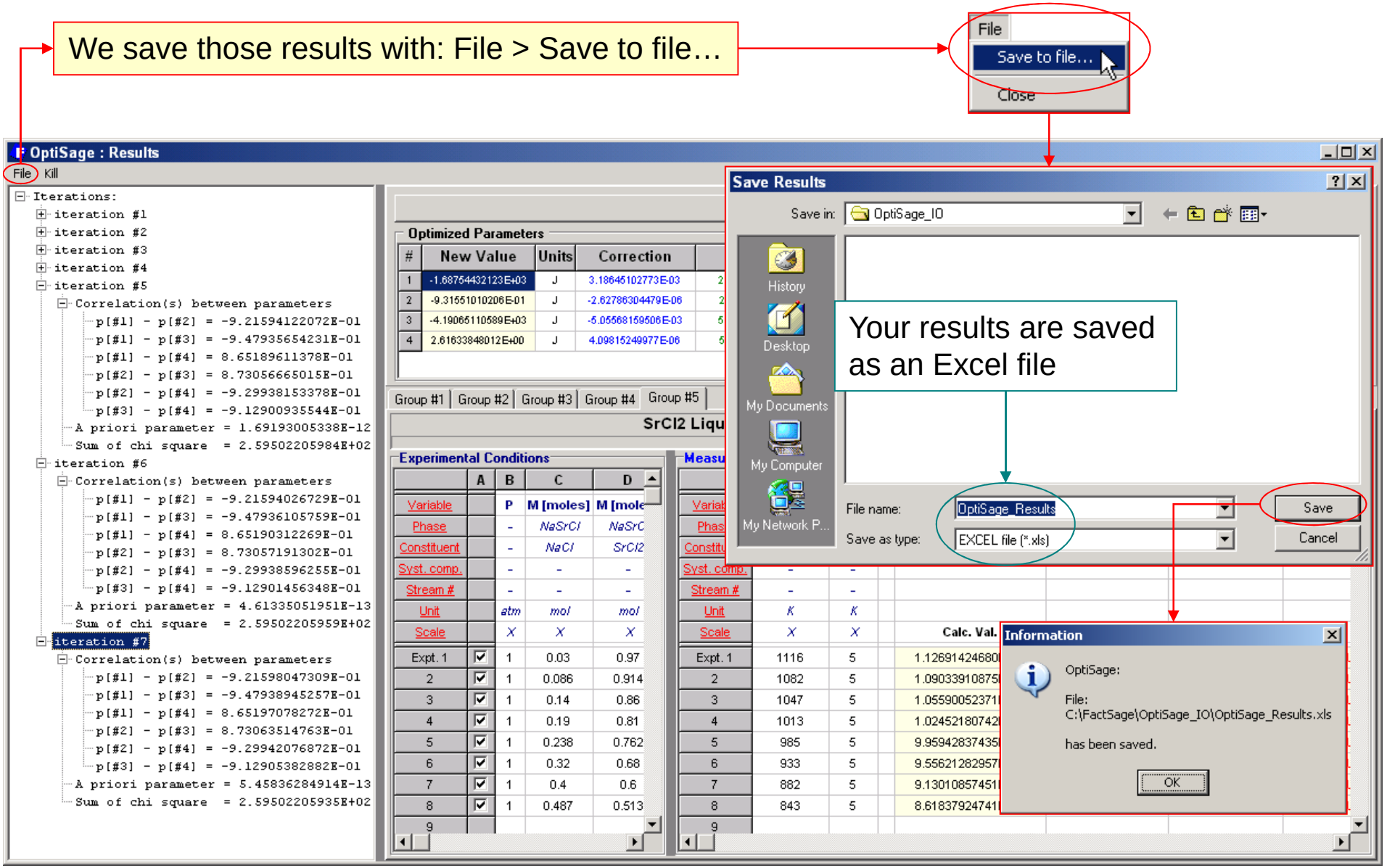
| | A | B | C | D |
|---|---|---|---|---|
| Variable | | P | M [moles] | M [mole |
| Phase | | - | NaSrCl | NaSrC |
| Constituent | | - | NaCl | SrCl2 |
| Syst. comp. | | - | - | - |
| Stream # | | - | - | - |
| Unit | | atm | mol | mol |
| Scale | | X | X | X |
| Expt. 1 | ☑ | 1 | 0.03 | 0.97 |
| 2 | ☑ | 1 | 0.086 | 0.914 |
| 3 | ☑ | 1 | 0.14 | 0.86 |
| 4 | ☑ | 1 | 0.19 | 0.81 |
| 5 | ☑ | 1 | 0.238 | 0.762 |
| 6 | ☑ | 1 | 0.32 | 0.68 |
| 7 | ☑ | 1 | 0.4 | 0.6 |
| 8 | ☑ | 1 | 0.487 | 0.513 |
| 9 | | | | |

**Measured Variable(s)**

| | A | B | C | D | E | F | |
|---|---|---|---|---|---|---|---|
| Variable | T | Err T | | Chi square contribution | | | |
| Phase | NaSrCl | System | | 9.39456683482E+01 | | | |
| Constituent | Precipitation | - | | | | | |
| Syst. comp. | - | - | | | | | |
| Stream # | - | - | | | | | |
| Unit | K | K | | | | | |
| Scale | X | X | | Calc. Val. | Correction | Residual | Warnings |
| Expt. 1 | 1116 | 5 | | 1.12691424680E+03 | -1.09142468016E+01 | 2.06071257188E-02 | ZERO AMOU |
| 2 | 1082 | 5 | | 1.09033910875E+03 | -8.33910875446E+00 | 1.39720165215E-01 | ZERO AMOU |
| 3 | 1047 | 5 | | 1.05590052371E+03 | -8.90052370758E+00 | 3.07828053221E-01 | ZERO AMOU |
| 4 | 1013 | 5 | | 1.02452180742E+03 | -1.15218074204E+01 | 4.77881440795E-01 | ZERO AMOU |
| 5 | 985 | 5 | | 9.95942837435E+02 | -1.09428374345E+01 | 4.86275873567E-01 | ZERO AMOU |
| 6 | 933 | 5 | | 9.55621282957E+02 | -2.26212829572E+01 | 7.03530016811E-01 | ZERO AMOU |
| 7 | 882 | 5 | | 9.13010857451E+02 | -3.10108574508E+01 | 8.72407553784E-01 | ZERO AMOU |
| 8 | 843 | 5 | | 8.61837924741E+02 | -1.88379247412E+01 | 9.84700324780E-01 | ZERO AMOU |
| 9 | | | | | | | |

# Convergent solution of the 2nd optimization, saving the results

We save those results with: File > Save to file…



# Optimization results, EXCEL file

Microsoft Excel - OptiSage_Results.xls

OPTIMIZED PARAMETERS (iteration #7)

| # | New Value | Units | Correction | Uncertainty | Dependency | Phase | Constituent | Type | - | - | XS | - |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -1.68754432123E+03 | J | 3.18645102773E-03 | 2.81502663602E+02 | - | NaSrCl | - | G(XS) | L0 | T^0 | Binary: NaCl^[1] - SrCl2^[1] | 131111 |
| 2 | -9.31551010206E-01 | J | -2.62786304479E-06 | 2.83527218209E-01 | - | NaSrCl | - | G(XS) | L0 | T^1 | Binary: NaCl^[1] - SrCl2^[1] | 131121 |
| 3 | -4.19065110589E+03 | J | -5.05568159506E-03 | 5.11323998802E+02 | - | NaSrCl | - | G(XS) | L0 | T^0 | Binary: NaCl^[2] - SrCl2^[1] | 132111 |
| 4 | 2.61633848012E+00 | J | 4.09815249977E-06 | 5.19114426112E-01 | - | NaSrCl | - | G(XS) | L0 | T^1 | Binary: NaCl^[2] - SrCl2^[1] | 132121 |

Values of the optimized parameters ($A_1$, $A_2$, $B_1$ and $B_2$). See slide 9.15 for more details.

Activity of NaCl in the liquid

| | A | B | C | D | E |
|---|---|---|---|---|---|
| - | | | | | |
| Variable | | T | P | M [moles] | M [moles] |
| Phase | | - | - | NaSrCl | NaSrCl |
| Constituent | | - | - | SrCl2 | NaCl |
| Syst. comp. | | - | - | - | - |
| Stream # | | - | - | - | - |
| Unit | | K | atm | mol | mol |
| Scale | | X | X | X | X |
| - | | | | | |
| Expt. 1 | | 1073.15 | 1 | 0.2 | 0.8 |
| 2 | | 1073.15 | 1 | 0.3 | 0.7 |
| 3 | | 1073.15 | 1 | 0.4 | 0.6 |
| 4 | | 1098 | 1 | 0.9 | 0.1 |
| 5 | | 1098 | 1 | 0.8 | 0.2 |
| 6 | | 1098 | 1 | 0.5 | 0.5 |
| 7 | | 1098 | 1 | 0.3 | 0.7 |
| 8 | | 1123 | 1 | 0.401 | 0.599 |
| 9 | | 1123 | 1 | 0.6 | 0.4 |
| 10 | | 1123 | 1 | 0.799 | 0.201 |
| 11 | | 1123 | 1 | 0.46 | 0.54 |

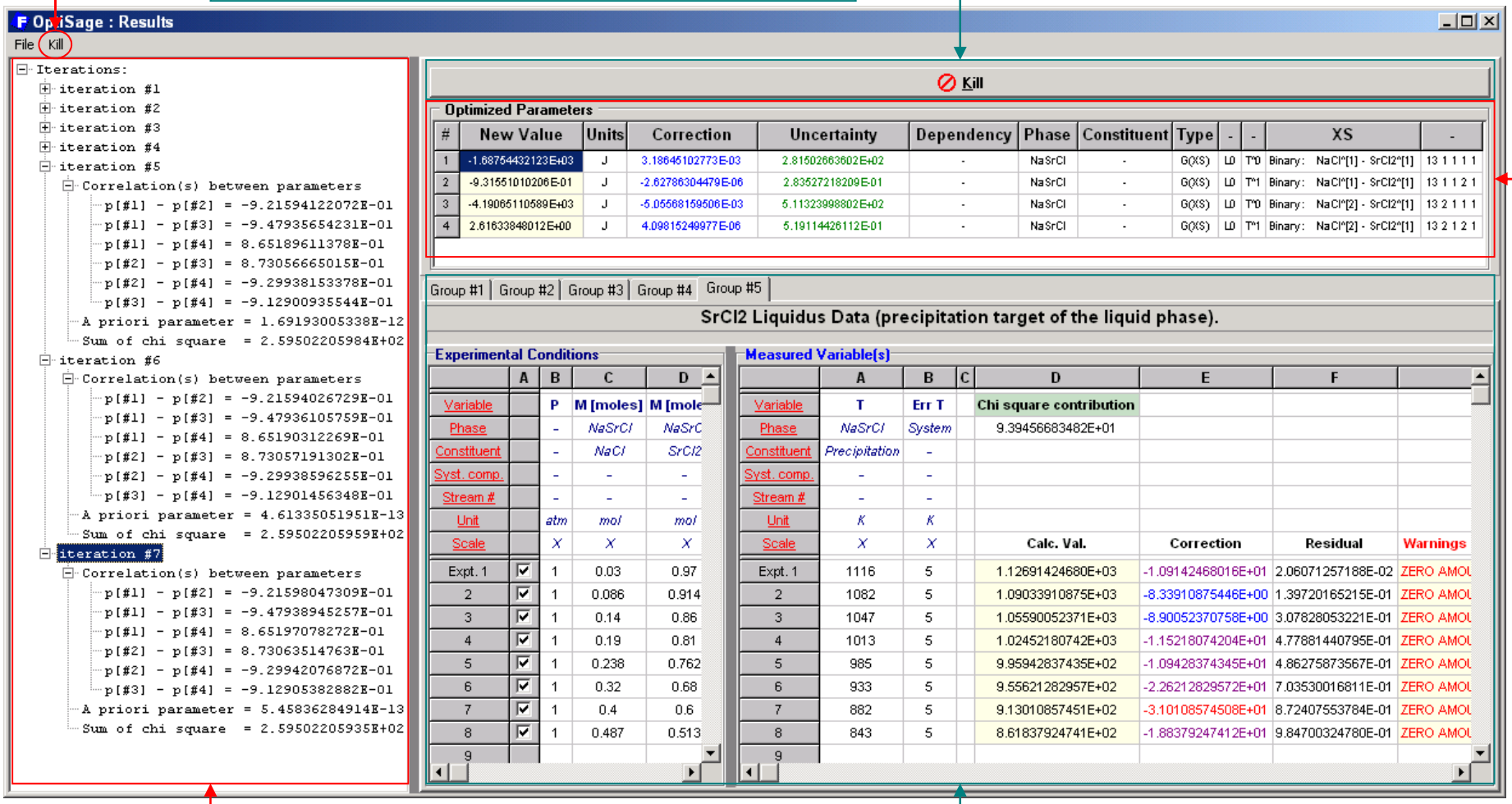
| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| - | | | | | | | |
| Variable | AC | Err AC | | Chi square contribution | | | |
| Phase | NaSrCl | NaSrCl | | 1.15708051190E+02 | | | |
| Constituent | NaCl | NaCl | | | | | |
| Syst. comp. | - | - | | | | | |
| Stream # | - | - | | | | | |
| Unit | - | - | | | | | |
| Scale | X | X | | Calc. Val. | | | |
| - | | | | | | | |
| Expt. 1 | 0.777 | 0.00777 | | 7.82618755115E-01 | 5.61875511509E-03 | 9.55267671615E-04 | - |
| 2 | 0.659 | 0.00659 | | 6.68105787552E-01 | -9.10578755223E-03 | 1.53866515704E-03 | - |
| 3 | 0.533 | 0.00533 | | 5.55009242708E-01 | -2.20092427077E-02 | 1.84229038126E-03 | - |
| 4 | 0.0808 | 0.00081 | | 7.68076855919E-02 | 3.99231440808E-03 | 5.83641995659E-04 | - |
| 5 | 0.162 | 0.00162 | | 1.59389832054E-01 | 2.81016794581E-03 | 7.39178122779E-04 | - |
| 6 | 0.454 | 0.00454 | | 4.47777350950E-01 | 6.22264904956E-03 | 1.79881681719E-03 | - |
| 7 | 0.682 | 0.00682 | | 6.69258954546E-01 | 1.27410454539E-02 | 1.54214635001E-03 | - |
| 8 | 0.5437 | 0.00544 | | 5.56875968183E-01 | -1.31759681833E-02 | 1.85864688424E-03 | - |
| 9 | 0.3381 | 0.00338 | | 3.46344409878E-01 | -8.24440987787E-03 | 1.46506413083E-03 | - |
| 10 | 0.1593 | 0.00159 | | 1.61091553306E-01 | 1.79155330565E-03 | 7.46157126390E-04 | - |
| 11 | 0.53 | 0.0053 | | 4.92238522589E-01 | 3.77614774114E-02 | 1.87021482508E-03 | - |

Calculated values of the measured variables with the optimized parameters. See slides 9.17 to 9.20 and 9.22 for more details.

# The OptiSage window: general view

To abort an optimization: click on **Kill** in the menu bar or press the **Kill** button

The **Optimize Parameters** frame




The **tree view** frame

The **Groups** frame

# The OptiSage window: the tree view frame

```
Iterations:
  iteration #1
  iteration #2
  iteration #3
  iteration #4
  iteration #5
    Correlation(s) between parameters
      p[#1] - p[#2] = -9.21594122072E-01
      p[#1] - p[#3] = -9.47935654231E-01
      p[#1] - p[#4] = 8.65189611378E-01
      p[#2] - p[#3] = 8.73056665015E-01
      p[#2] - p[#4] = -9.29938153378E-01
      p[#3] - p[#4] = -9.12900935544E-01
    A priori parameter = 1.69193005338E-12
    Sum of chi square  = 2.59502205984E+02
  iteration #6
    Correlation(s) between parameters
      p[#1] - p[#2] = -9.21594026729E-01
      p[#1] - p[#3] = -9.47936105759E-01
      p[#1] - p[#4] = 8.65190312269E-01
      p[#2] - p[#3] = 8.73057191302E-01
      p[#2] - p[#4] = -9.29938596255E-01
      p[#3] - p[#4] = -9.12901456348E-01
    A priori parameter = 4.61335051951E-13
    Sum of chi square  = 2.59502205959E+02
  iteration #7
    Correlation(s) between parameters
      p[#1] - p[#2] = -9.21598047309E-01
      p[#1] - p[#3] = -9.47938945257E-01
      p[#1] - p[#4] = 8.65197078272E-01
      p[#2] - p[#3] = 8.73063514763E-01
      p[#2] - p[#4] = -9.29942076872E-01
      p[#3] - p[#4] = -9.12905382882E-01
    A priori parameter = 5.45836284914E-13
    Sum of chi square  = 2.59502205935E+02
```

Indicates that the results of the iteration #7 are viewed in the Optimized Parameters and the Groups frames. To see the results of a previous iteration, click on it.

# The OptiSage window: Review of the Optimized Parameters

**Remember** (see slide 2.2) that ***OptiSage*** is used to optimize the parameters for the liquid Gibbs energy model (XS terms) and that a polynomial model for the Gibbs energy of the liquid was used:

$G = (X_1 G°_1 + X_2 G°_2) + RT(X_1 \ln X_1 + X_2 \ln X_2) + G^E$

where $G^E = \Delta H - TS^E$

Using the binary excess terms: $\Delta H = X_1X_2 (A_1) + X_1^2X_2 (A_2)$ and $-S^E = X_1X_2 (B_1) + X_1^2X_2 (B_2)$

Hence: $G^E = X_1X_2 (A_1 + B_1T) + X_1^2X_2 (A_2 + B_2T)$

Where $A_1$, $A_2$, $B_1$ and $B_2$ are the 4 parameters to be optimized and the subscript 1 and 2 are respectively for NaCl and $SrCl_2$. We have 2 sets of parameters, one in $\mathbf{X_1X_2}$ and one in $\mathbf{X_1^2X_2}$.

OptiSage uses a more general form for the expressions of these excess energies, $G^E = \Sigma g^E$ where:

$$g^E_{(NaCl-SrCl_2)} = Y_{NaCl} Y_{SrCl_2} LO$$

and

$$g^E_{(NaCl-SrCl_2)} = Y_{NaCl} Y_{SrCl_2} LO \left( \frac{\chi_{NaCl}}{\chi_{NaCl} + \chi_{SrCl_2}} \right)$$

where the variable $Y_i$ is the equivalent molar fraction of component i.
See Solution slide show, section 6 for more details.
In our example, $\mathbf{Y_i = X_i}$ which is the molar fraction.
LO is a polynomial having the general form:
$LO = A + BT + C(T \ln T) + DT^2 + ET^3 + FT^{-1}$
In our example, LO has the form: **LO = A + BT**, where **A** and **B** are the parameters to optimize.
Then,

$$g^E_{(NaCl-SrCl_2)} = X_{NaCl} X_{SrCl_2} (A_1 + B_1T)$$

and

$$g^E_{(NaCl-SrCl_2)} = X_{NaCl} X_{SrCl_2} (A_2 + B_2T)(X_{NaCl})$$
$$= X^2_{NaCl} X_{SrCl_2} (A_2 + B_2T)$$

# The OptiSage window: the Optimized Parameters frame

$$g^{E}_{(NaCl-SrCl_2)} = X^{1}_{NaCl} X^{1}_{SrCl_2} \left( A_1 T^0 + B_1 T^1 \right)$$

**Optimized Parameters**

| # | New Value | Units | Correction | Uncertainty | Dependency | Phase | Constituent | Type | - | | XS | - |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -1.68754432123E+03 | J | 3.18645102773E-03 | 2.81502663602E+02 | - | NaSrCl | - | G(XS) | L0 | T^0 | Binary: NaCl^[1] - SrCl2^[1] | 13 1 1 1 1 |
| 2 | -9.31551010206E-01 | J | 2.62786304479E-06 | 2.83527218209E-01 | - | NaSrCl | - | G(XS) | L0 | T^1 | Binary: NaCl^[1] - SrCl2^[1] | 13 1 1 2 1 |
| 3 | -4.19065110589E+03 | J | -5.05568159506E-03 | 5.11323998802E+02 | - | NaSrCl | - | G(XS) | L0 | T^0 | Binary: NaCl^[2] - SrCl2^[1] | 13 2 1 1 1 |
| 4 | 2.61633848012E+00 | J | 4.09815249977E-06 | 5.19114426112E-01 | - | NaSrCl | - | G(XS) | L0 | T^1 | Binary: NaCl^[2] - SrCl2^[1] | 13 2 1 2 1 |

$$g^{E}_{(NaCl-SrCl_2)} = X^{2}_{NaCl} X^{1}_{SrCl_2} \left( A_2 T^0 + B_2 T^1 \right)$$

The **Correction** value is the difference between the New Value of the Optimized Parameter (obtained in this iteration) and it's value obtained in the previous iteration.

The **Uncertainty** term is the error on the new value of the optimized parameter.

# *OptiSage* main window: another view of the optimized parameters

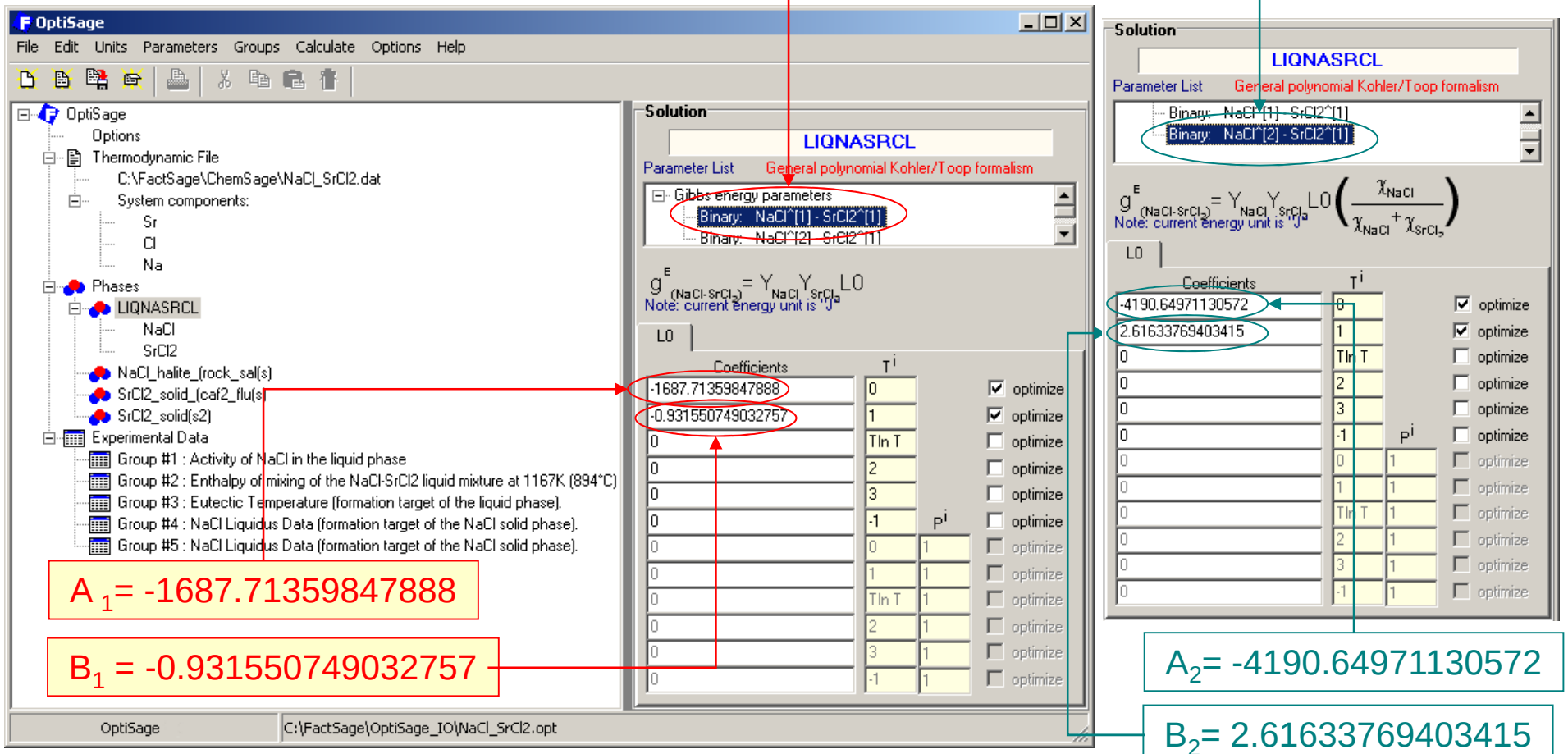
Return to the ***OptiSage*** main window to have another view of the optimized parameters.

First set of parameters:

$$g^{E}_{(NaCl-SrCl_2)} = X^{1}_{NaCl} X^{1}_{SrCl_2} \left(A_1 T^0 + B_1 T^1\right)$$

Second set of parameters:

$$g^{E}_{(NaCl-SrCl_2)} = X^{2}_{NaCl} X^{1}_{SrCl_2} \left(A_2 T^0 + B_2 T^1\right)$$




$A_1$= -1687.71359847888

$B_1$ = -0.931550749032757

$A_2$= -4190.64971130572

$B_2$= 2.61633769403415

# The OptiSage window: the Groups frame, group #1 tab

Measured value = Calculated Value + Correction

Group #1 | Group #2 | Group #3 | Group #4 | Group #5

**Activity of NaCl in the liquid phase.**

**Experimental Conditions**

| | A | B | C | D | E |
|---|---|---|---|---|---|
| Variable | | T | P | M [moles] | M [moles] |
| Phase | | - | - | NaSrCl | NaSrCl |
| Constituent | | - | - | SrCl2 | NaCl |
| Syst. comp. | | - | - | - | - |
| Stream # | | - | - | - | - |
| Unit | | K | atm | mol | mol |
| Scale | | X | X | X | X |
| Expt. 1 | ☑ | 1073.15 | 1 | 0.2 | 0.8 |
| 2 | ☑ | 1073.15 | 1 | 0.3 | 0.7 |
| 3 | ☑ | 1073.15 | 1 | 0.4 | 0.6 |
| 4 | ☑ | 1098 | 1 | 0.9 | 0.1 |
| 5 | ☑ | 1098 | 1 | 0.8 | 0.2 |
| 6 | ☑ | 1098 | 1 | 0.5 | 0.5 |
| 7 | ☑ | 1098 | 1 | 0.3 | 0.7 |
| 8 | ☑ | 1123 | 1 | 0.401 | 0.599 |
| 9 | ☑ | 1123 | 1 | 0.6 | 0.4 |
| 10 | ☑ | 1123 | 1 | 0.799 | 0.201 |
| 11 | ☑ | 1123 | 1 | 0.46 | 0.54 |
| 12 | | | | | |

**Measured Variable(s)**

| | A | B | C | D | | | |
|---|---|---|---|---|---|---|---|
| Variable | AC | Err AC | | Chi square contribution | | | |
| Phase | NaSrCl | NaSrCl | | 1.15708051190E+02 | | | |
| Constituent | NaCl | NaCl | | | | | |
| Syst. comp. | - | - | | | | | |
| Stream # | - | - | | | | | |
| Unit | - | - | | | | | |
| Scale | X | X | | Calc. Val. | Correction | Residual | Warnings |
| Expt. 1 | 0.777 | 0.00777 | | 7.82618755115E-01 | -5.61875511509E-03 | 9.55267671615E-04 | - |
| 2 | 0.659 | 0.00659 | | 6.68105787552E-01 | -9.10578755223E-03 | 1.53866515704E-03 | - |
| 3 | 0.533 | 0.00533 | | 5.55009242708E-01 | -2.20092427077E-02 | 1.84229038126E-03 | - |
| 4 | 0.0808 | 0.000808 | | 7.68076855919E-02 | 3.99231440808E-03 | 5.83641995659E-04 | - |
| 5 | 0.162 | 0.00162 | | 1.59389832054E-01 | 2.61016794581E-03 | 7.39178122779E-04 | - |
| 6 | 0.454 | 0.00454 | | 4.47777350950E-01 | 6.22264904956E-03 | 1.79881681719E-03 | - |
| 7 | 0.682 | 0.00682 | | 6.69258954546E-01 | 1.27410454539E-02 | 1.54214635001E-03 | - |
| 8 | 0.5437 | 0.005437 | | 5.56875968183E-01 | -1.31759681833E-02 | 1.85864688424E-03 | - |
| 9 | 0.3381 | 0.003381 | | 3.46344409878E-01 | -8.24440987787E-03 | 1.46506413083E-03 | - |
| 10 | 0.1593 | 0.001593 | | 1.61091553306E-01 | -1.79155330565E-03 | 7.46157126390E-04 | - |
| 11 | 0.53 | 0.0053 | | 4.92238522589E-01 | 3.77614774114E-02 | 1.87021482508E-03 | - |
| 12 | | | | | | | |

Color code for correction term C:

- Less than Err: black
- 1 × Err < C < 2 ×Err: blue
- 2 × Err < C < 3 ×Err: mauve
- More than 3 ×Err: red

**Calculated values** of the **measured variables** with the optimized parameters.

# The OptiSage window: the Groups frame, Group #2 tab

To view the results of a group, press on its tab

Group #1 | Group #2 | Group #3 | Group #4 | Group #5

**Enthalpy of mixing of the NaCl-SrCl2 liquid mixture at 1167K (894°C).**

**Experimental Conditions**

| | A | B | C | D | E | F | G | H | I |
|---|---|---|---|---|---|---|---|---|---|
| Variable | | T | IT [in... | IT [in... | P | IP [in... | IP [in... | M [moles] | M [moles] |
| Phase | | - | - | - | - | - | - | NaSrCl | NaSrCl |
| Constituent | | - | - | - | - | - | - | NaCl | SrCl2 |
| Syst. comp. | | - | - | - | - | - | - | - | - |
| Stream # | | - | 1 | 2 | - | 1 | 2 | 1 | 2 |
| Unit | | K | K | K | atm | atm | atm | mol | mol |
| Scale | | X | X | X | X | X | X | X | X |
| Expt. 1 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.905 | 0.095 |
| 2 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.796 | 0.204 |
| 3 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.706 | 0.294 |
| 4 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.588 | 0.412 |
| 5 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.502 | 0.498 |
| 6 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.392 | 0.608 |
| 7 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.296 | 0.704 |
| 8 | ☑ | 1167 | 1167 | 1167 | 1 | 1 | 1 | 0.096 | 0.904 |
| 9 | | | | | | | | | |

**Measured Variable(s)**

| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| Variable | H | Err H | | Chi square contribution | | | |
| Phase | System | System | | 1.09823928513E+01 | | | |
| Constituent | - | - | | | | | |
| Syst. comp. | - | - | | | | | |
| Stream # | - | - | | | | | |
| Unit | J | J | | | | | |
| Scale | X | X | | Calc. Val. | Correction | Residual | Warnings |
| Expt. 1 | -490 | 50 | | -4.71150065755E+02 | -1.88499342454E+01 | 1.85225119661E+01 | - |
| 2 | -845 | 50 | | -8.15703833625E+02 | -2.92961663745E+01 | 2.70174484579E+01 | - |
| 3 | -962 | 50 | | -9.64372154224E+02 | 2.37215422365E+00 | 2.69829247930E+01 | - |
| 4 | -996 | 50 | | -1.00576148896E+03 | 9.76148895701E+00 | 2.32106566687E+01 | - |
| 5 | -962 | 50 | | -9.47797791114E+02 | -1.42022088863E+01 | 2.25546469807E+01 | - |
| 6 | -703 | 50 | | -7.93725795221E+02 | 9.07257952214E+01 | 2.65888878538E+01 | - |
| 7 | -510 | 50 | | -6.10143921456E+02 | 1.00143921456E+02 | 3.04653082822E+01 | - |
| 8 | -269 | 50 | | -1.81365501656E+02 | -8.76344983443E+01 | 2.04363249461E+01 | - |
| 9 | | | | | | | |

These are the values entered previously (see slide 7.18)

# The OptiSage window: the Groups frame, Group #3 tab

Group #1 | Group #2 | Group #3 | Group #4 | Group #5

**Eutectic Temperature (formation target of the liquid phase).**

**Experimental Conditions**

| | A | B | C | D |
|---|---|---|---|---|
| Variable | | P | M [moles] | M [moles] |
| Phase | | - | *NaSrCl* | *NaSrCl* |
| Constituent | | - | *NaCl* | *SrCl2* |
| Syst. comp. | | - | - | - |
| Stream # | | - | - | - |
| Unit | | *atm* | *mol* | *mol* |
| Scale | | *X* | *X* | *X* |
| Expt. 1 | ☑ | 1 | 0.5 | 0.5 |
| 2 | ☑ | 1 | 0.6 | 0.4 |
| 3 | | | | |

**Measured Variable(s)**

| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| Variable | T | Err T | | Chi square contribution | | | |
| Phase | *NaSrCl* | *System* | | 3.34476564656E+01 | | | |
| Constituent | *Formation* | - | | | | | |
| Syst. comp. | - | - | | | | | |
| Stream # | - | - | | | | | |
| Unit | *K* | *K* | | | | | |
| Scale | *X* | *X* | | Calc. Val. | Correction | Residual | Warnings |
| Expt. 1 | 838 | 2 | | 8.45663658061E+02 | -7.66365806064E+00 | 4.85772622141E-01 | - |
| 2 | 837 | 2 | | 8.45663658061E+02 | -8.66365806065E+00 | 4.85772620792E-01 | - |
| 3 | | | | | | | |

If you want to have a better view of your results, you can slide the barrier between the **Experimental Conditions** and the Measured Variable(s) spreadsheets.

# The OptiSage window: the Groups frame, Group #4 tab

Group #1 | Group #2 | Group #3 | Group #4 | Group #5

**NaCl Liquidus Data (formation target of the NaCl solid phase).**

**Experimental Conditions**

| | A | B | C | D |
|---|---|---|---|---|
| Variable | | P | M [moles] | M [moles] |
| Phase | | - | *NaSrCl* | *NaSrCl* |
| Constituent | | - | *NaCl* | *SrCl2* |
| Syst. comp. | | - | - | - |
| Stream # | | - | - | - |
| Unit | | *atm* | *mol* | *mol* |
| Scale | | *X* | *X* | *X* |
| Expt. 1 | ☑ | 1 | 0.854 | 0.146 |
| 2 | ☑ | 1 | 0.742 | 0.258 |
| 3 | ☐ | 1 | 0.635 | 0.365 |
| 4 | ☑ | 1 | 0.535 | 0.465 |
| 5 | | | | |

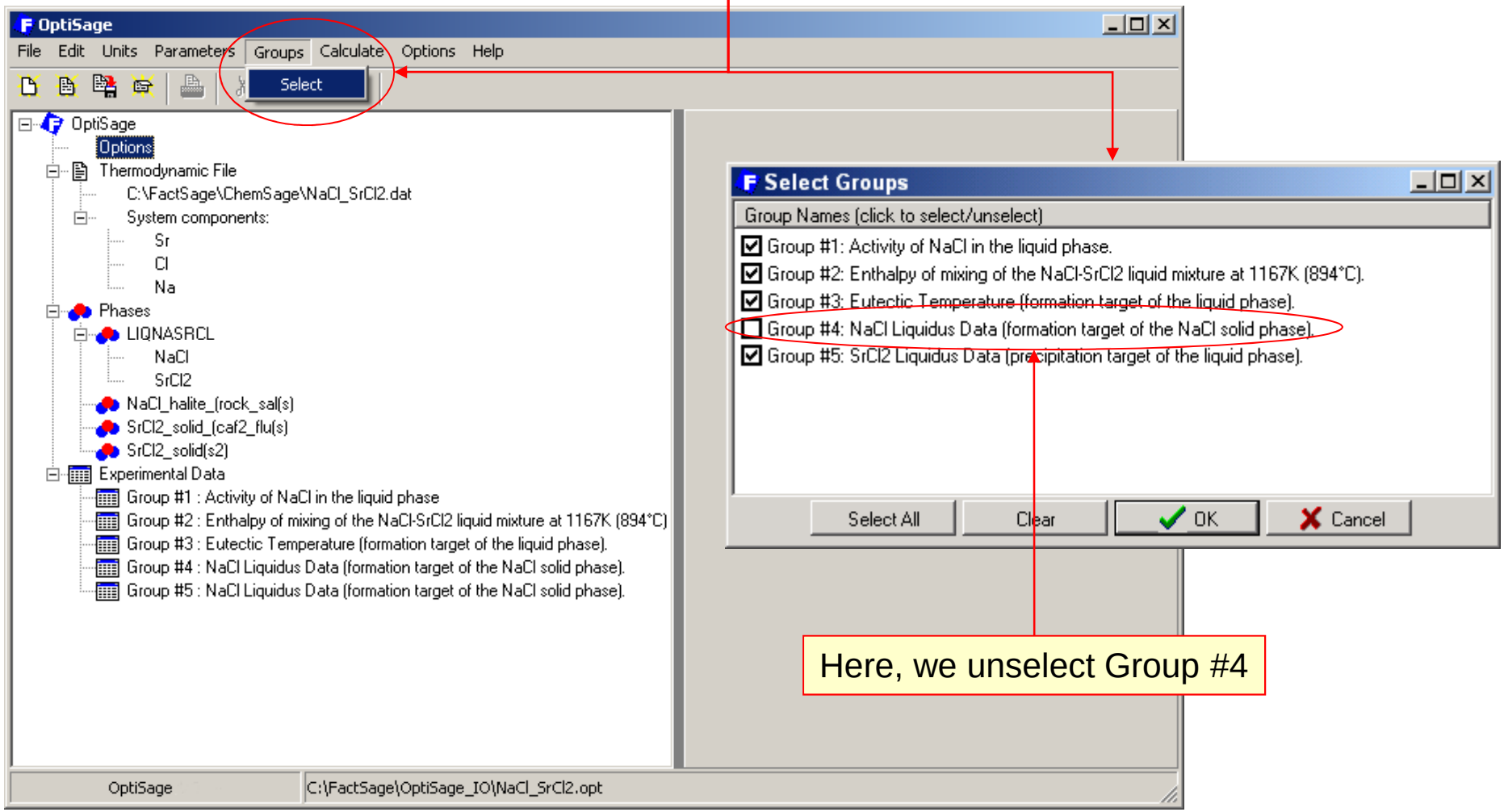
**Measured Variable(s)**

| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| Variable | T | Err T | | Chi square contribution | | | |
| Phase | *NaCl_halite_(rock_sal(s)* | *System* | | 5.41843708011E+00 | | | |
| Constituent | *Formation* | - | | | | | |
| Syst. comp. | - | - | | | | | |
| Stream # | - | - | | | | | |
| Unit | *K* | *K* | | | | | |
| Scale | *X* | *X* | | Calc. Val. | Correction | Residual | Warnings |
| Expt. 1 | 1023 | 4 | | 1.01820359657E+03 | 4.79640342777E+00 | 2.22753690429E-01 | - |
| 2 | 973 | 6 | | 9.67935167242E+02 | 5.06483275807E+00 | 5.48246161407E-01 | - |
| 3 | 923 | 8 | | 9.14077612750E+02 | 8.92238724967E+00 | 8.48769941534E-01 | - |
| 4 | 873 | 10 | | 8.58772795854E+02 | 1.42272041464E+01 | 1.04051187430E+00 | - |
| 5 | | | | | | | |

If you want to remove a data before making another optimization, simply unselect it. Here, we remove experimental data point 3.

# Selection of a group of data

To **select** or **unselect** a group of data for an optimization, go to the ***OptiSage* main** window menu bar and click on **Groups > Select** to open the **Select Groups** window.




Here, we unselect Group #4

# The OptiSage window: the Groups frame, Group #5 tab

Group #1 | Group #2 | Group #3 | Group #4 | Group #5

**SrCl2 Liquidus Data (precipitation target of the liquid phase).**

**Experimental Conditions**

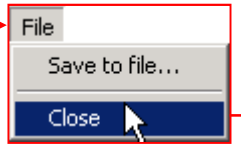
| | A | B | C | D |
|---|---|---|---|---|
| Variable | | P | M [moles] | M [moles] |
| Phase | | - | *NaSrCl* | *NaSrCl* |
| Constituent | | - | *NaCl* | *SrCl2* |
| Syst. comp. | | - | - | - |
| Stream # | | - | - | - |
| Unit | | *atm* | *mol* | *mol* |
| Scale | | *X* | *X* | *X* |
| Expt. 1 | ☑ | 1 | 0.03 | 0.97 |
| 2 | ☑ | 1 | 0.086 | 0.914 |
| 3 | ☑ | 1 | 0.14 | 0.86 |
| 4 | ☑ | 1 | 0.19 | 0.81 |
| 5 | ☑ | 1 | 0.238 | 0.762 |
| 6 | ☑ | 1 | 0.32 | 0.68 |
| 7 | ☑ | 1 | 0.4 | 0.6 |
| 8 | ☑ | 1 | 0.487 | 0.513 |
| 9 | | | | |

**Measured Variable(s)**

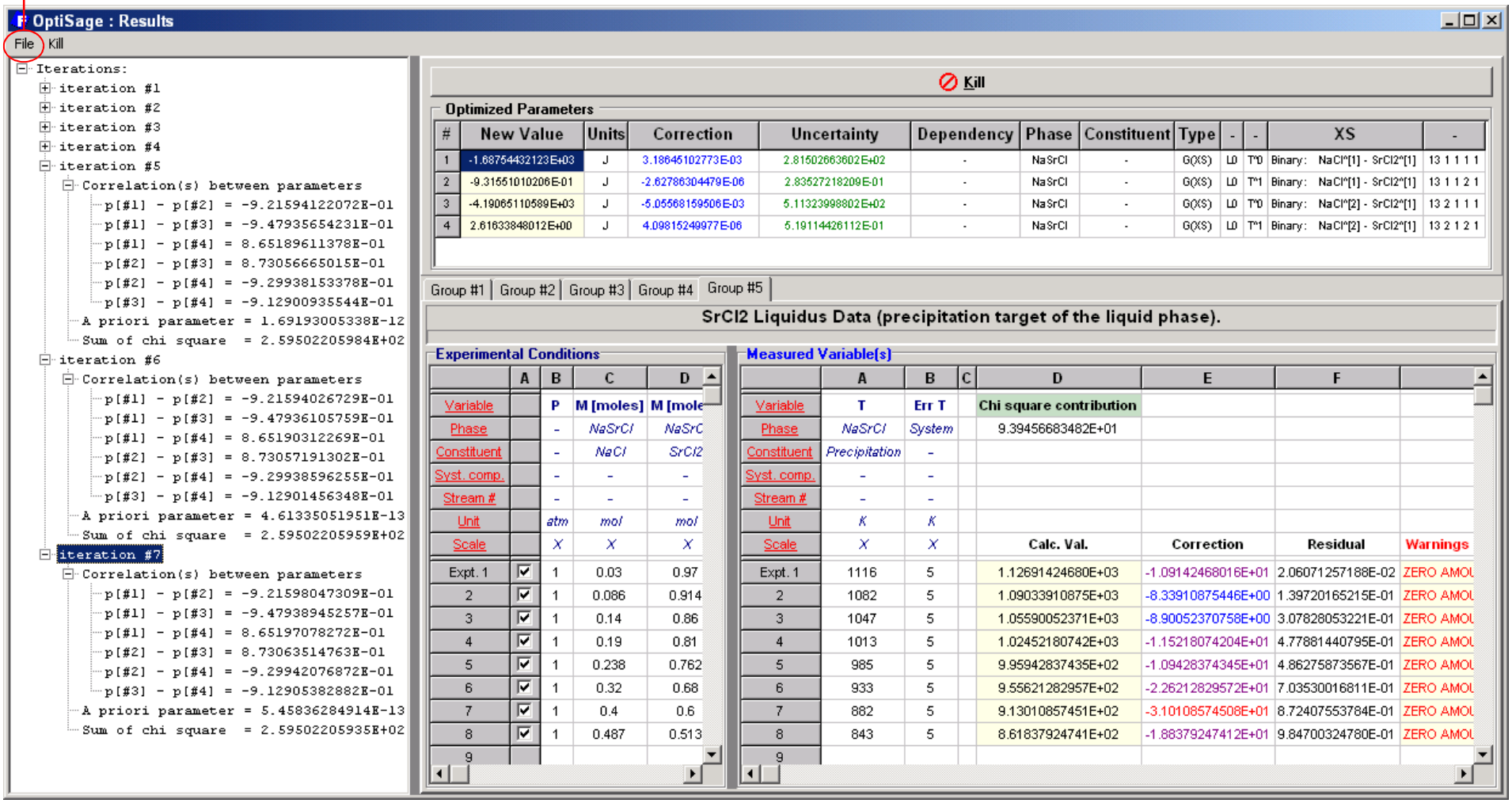
| | A | B | C | D | E | F | G |
|---|---|---|---|---|---|---|---|
| Variable | T | Err T | | Chi square contribution | | | |
| Phase | *NaSrCl* | *System* | | 9.39456683482E+01 | | | |
| Constituent | *Precipitation* | - | | | | | |
| Syst. comp. | - | - | | | | | |
| Stream # | - | - | | | | | |
| Unit | *K* | *K* | | | | | |
| Scale | *X* | *X* | | Calc. Val. | Correction | Residual | Warnings |
| Expt. 1 | 1116 | 5 | | 1.12691424680E+03 | -1.09142468016E+01 | 2.06071257188E-02 | ZERO AMOUNT OF SrCl2(s) |
| 2 | 1082 | 5 | | 1.09033910875E+03 | -8.33910875446E+00 | 1.39720165215E-01 | ZERO AMOUNT OF SrCl2(s) |
| 3 | 1047 | 5 | | 1.05590052371E+03 | -8.90052370758E+00 | 3.07828053221E-01 | ZERO AMOUNT OF SrCl2(s) |
| 4 | 1013 | 5 | | 1.02452180742E+03 | -1.15218074204E+01 | 4.77881440795E-01 | ZERO AMOUNT OF SrCl2(s) |
| 5 | 985 | 5 | | 9.95942837435E+02 | -1.09428374345E+01 | 4.86275873567E-01 | ZERO AMOUNT OF SrCl2(s2) |
| 6 | 933 | 5 | | 9.55621282957E+02 | -2.26212829572E+01 | 7.03530016811E-01 | ZERO AMOUNT OF SrCl2(s2) |
| 7 | 882 | 5 | | 9.13010857451E+02 | -3.10108574508E+01 | 8.72407553784E-01 | ZERO AMOUNT OF SrCl2(s2) |
| 8 | 843 | 5 | | 8.61837924741E+02 | -1.88379247412E+01 | 9.84700324780E-01 | ZERO AMOUNT OF SrCl2(s2) |
| 9 | | | | | | | |

A colored background indicates a warning

# Close OptiSage: Results window

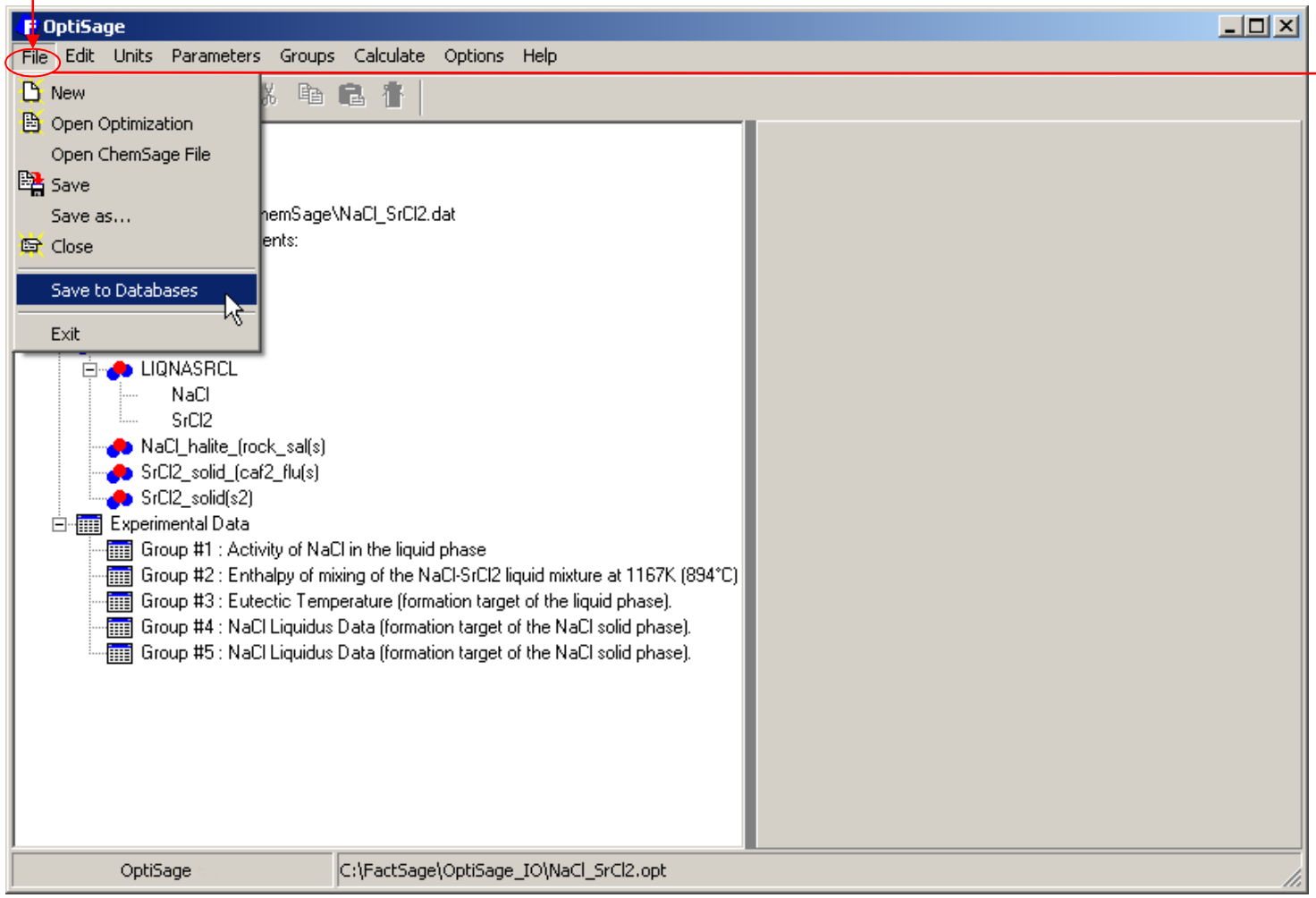


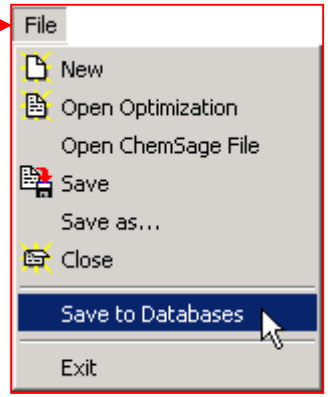

**Close** the **OptiSage: Results** window to return to the main window



# Creation (Save data to databases) of an optimized **Database**

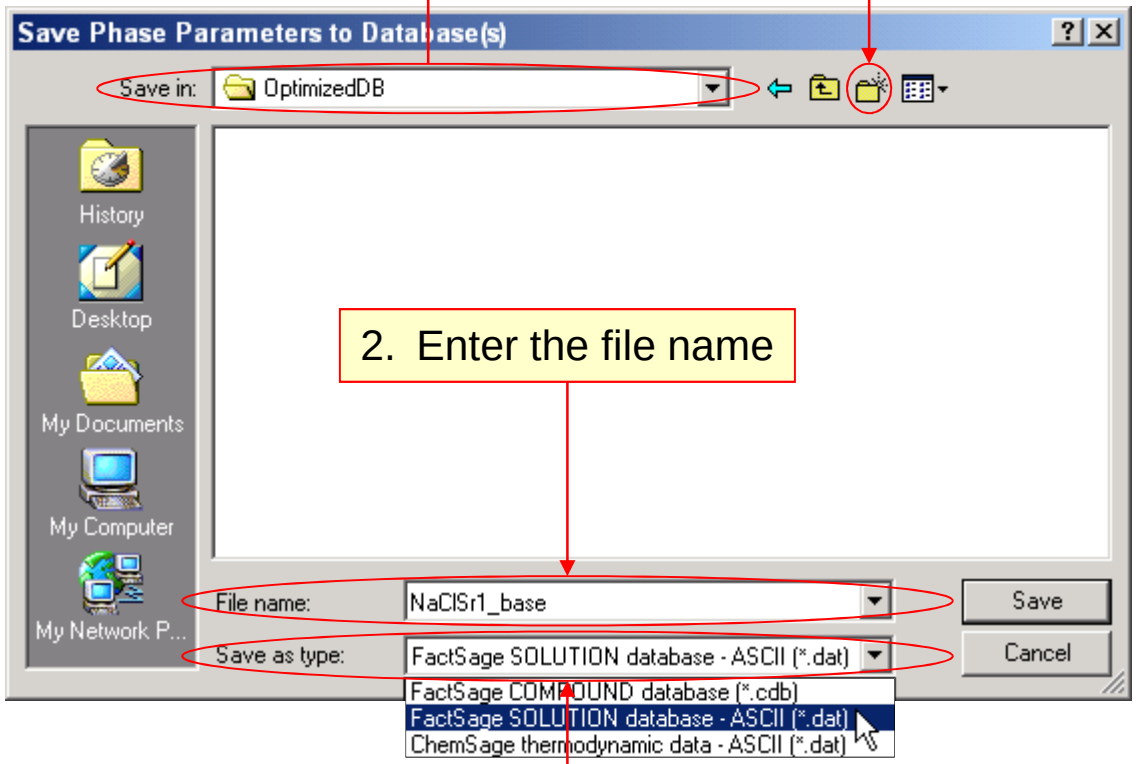
You can save your data to a database.
In the OptiSage main window, select **File > Save to databases** to open the **Save Phase Parameters to Database(s)** dialog box.



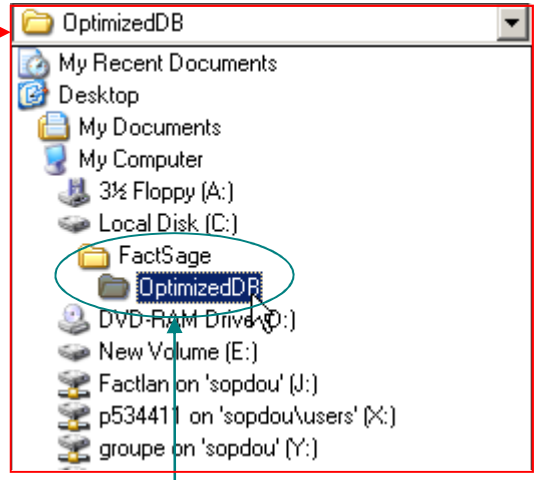



# Saving Phase parameters to a database

1. Browse or create your own folder

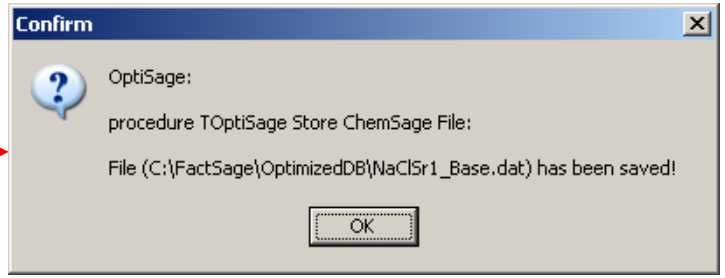



2. Enter the file name




Folder **Optimized DB** created in **FactSage**

3. Save your database.
   In our example, we save a Solution database.




Note: You can save your parameters manually.

## **Generation of diagrams:** comparison between **experimental** and **calculated** curves

The ***OptiSage*** module has no own calculational capabilities for thermodynamic properties or phase diagrams. From our newly created private database, ***Equilib*** and ***Phase Diagram*** can extract the data for appropriate calculations. To add your database to your list of databases available, please see slide 4.2.

The graphical comparison between calculated and experimental data can be made by use of overlays in the ***Figure*** module. For the addition of experimental points into a calculated diagram please see the **section 8** of the Slide Show on the ***Figure*** module.

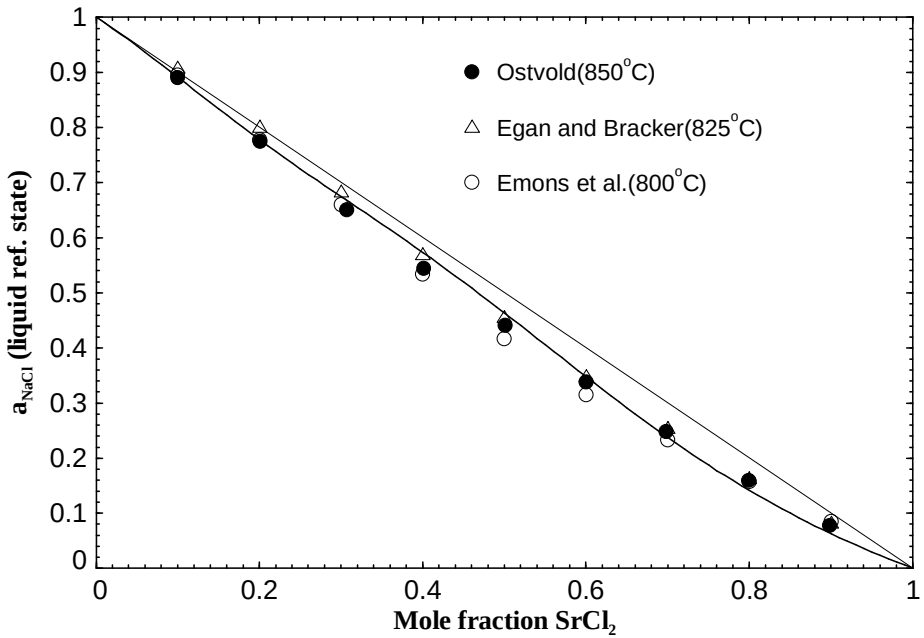
# Comparison between **experimental** and **calculated** curves

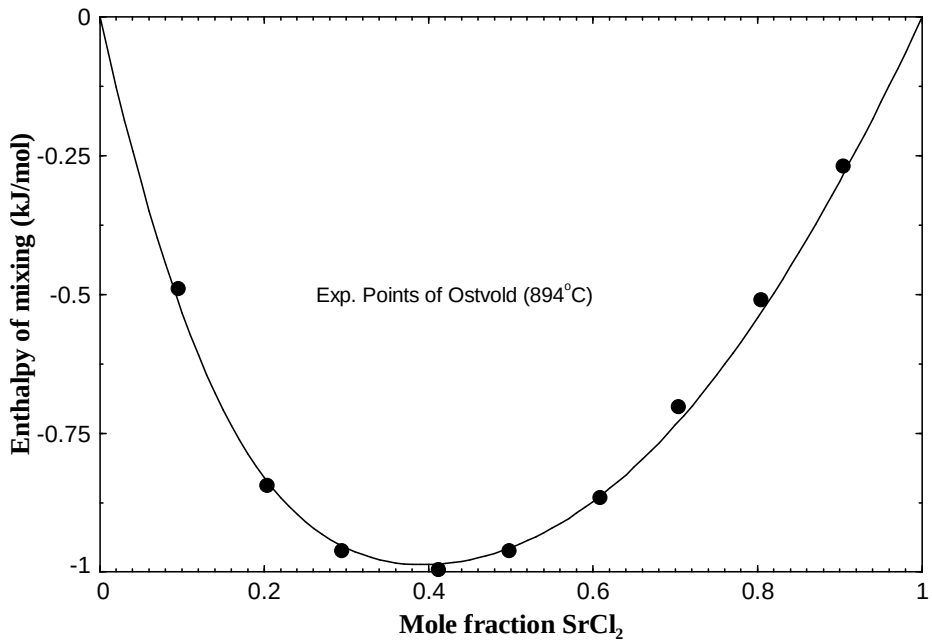
Use the ***Equilib*** module to calculate **activity curves for NaCl in the liquid phase**, then overlay the experimental data from an appropriate FIG-file that was prepared earlier.

Also use the ***Equilib*** module to calculate the **enthalpy of mixing curve** from the new database. Make sure you use the correct „initial conditions“ in the reactants screen:

<A> NaCl(liq, 894 ℃) + <1-A> SrCl2(liq, 894 ℃)

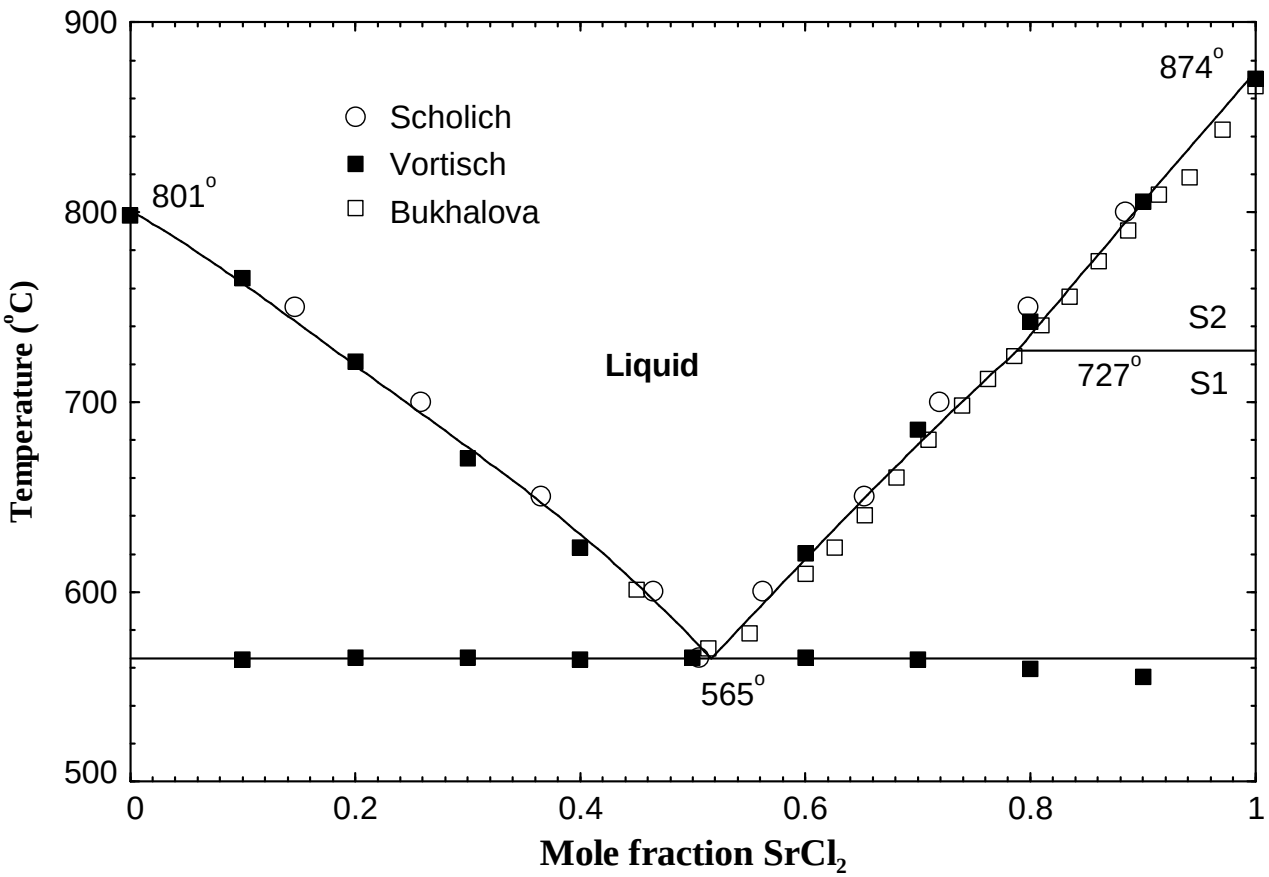
Thus only the mixing enthalpy is calculated and not the full enthalpy of the liquid.



# Comparison between **experimental** and **calculated** curves

Use the ***Phase Diagram*** module to generate a **phase diagram** with the appropriate temperature and composition range. Then overlay the FIG-file which contains the experimental points, the legend etc.



# Estimation of parameters with **NOMAD** (version 6.2+)

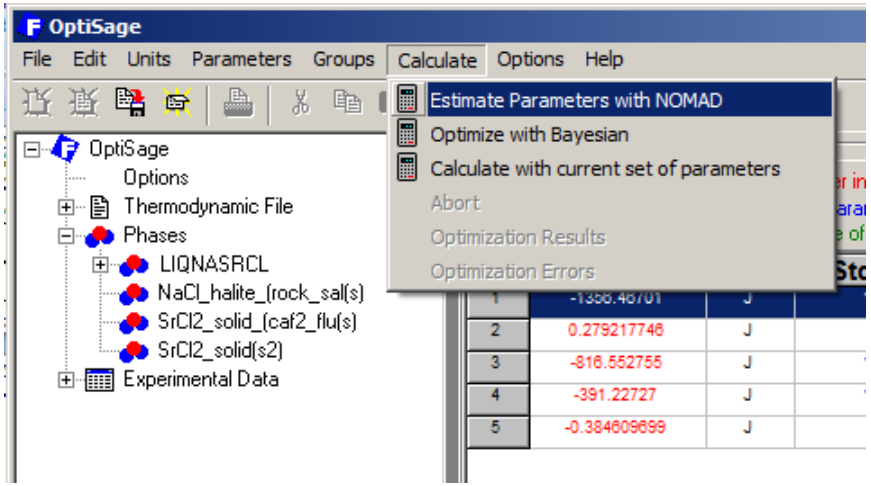
**NOMAD** is a **Non-linear Optimiser with Mesh Adaptive Direct search** algorithm developed at **GERAD** (www.gerad.com/nomad). It permits the minimisation of an objective function (like the sum of squared-errors in OptiSage) without involving any derivatives (black-box optimisation).

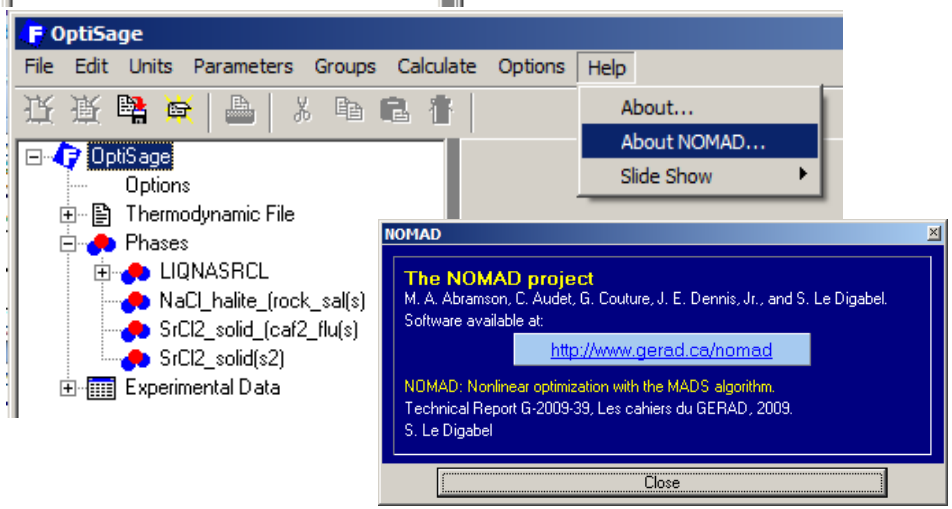
**NOMAD** has been integrated in ***OptiSage*** from ***version 6.2*** to give the user the option of estimating the selected optimized parameters from scratch (starting with 0 values). Every iteration of **NOMAD** is usually quite fast, and several hundreds of iterations can be performed.

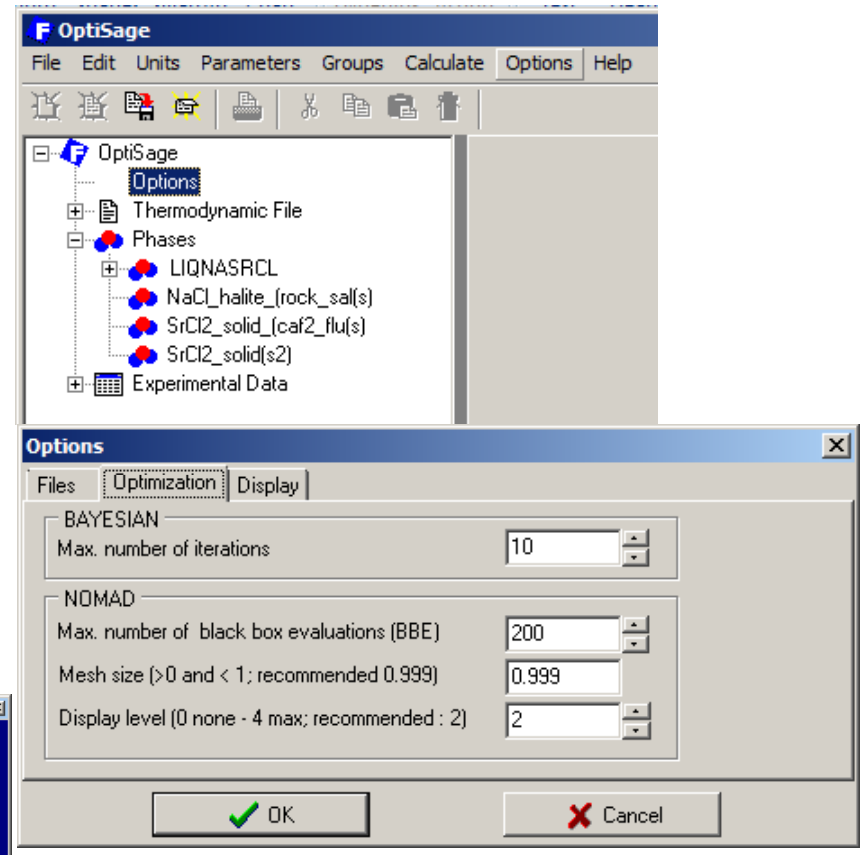
At any point, the ***OptiSage*** user can kill the **NOMAD** window, and the latest best solution of estimated parameters is kept and transfered automatically to ***OptiSage***, so the user can perform a Bayesian optimisation from this initial estimated set of parameters.

# Estimation of parameters with **NOMAD** (version 6.2+)

The new features associated to **NOMAD** in ***OptiSage*** are:



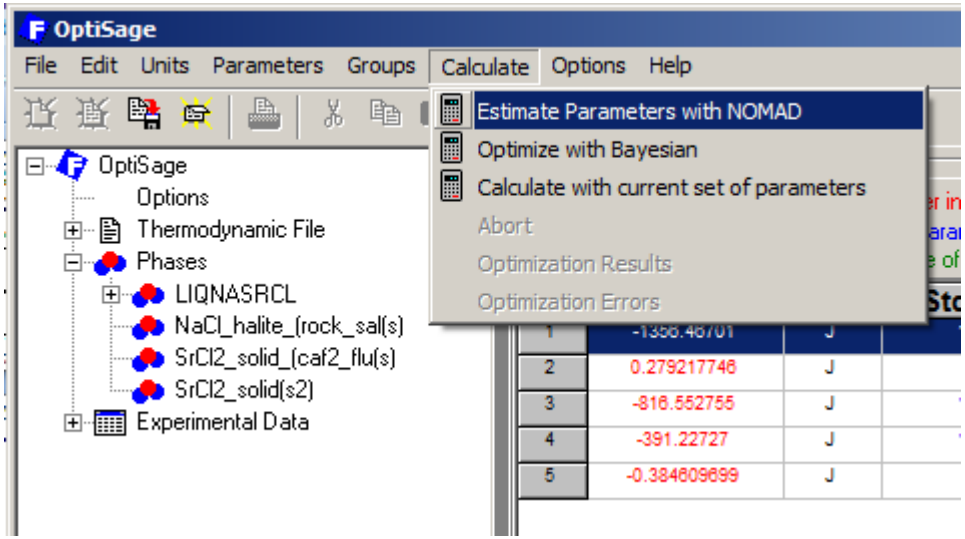



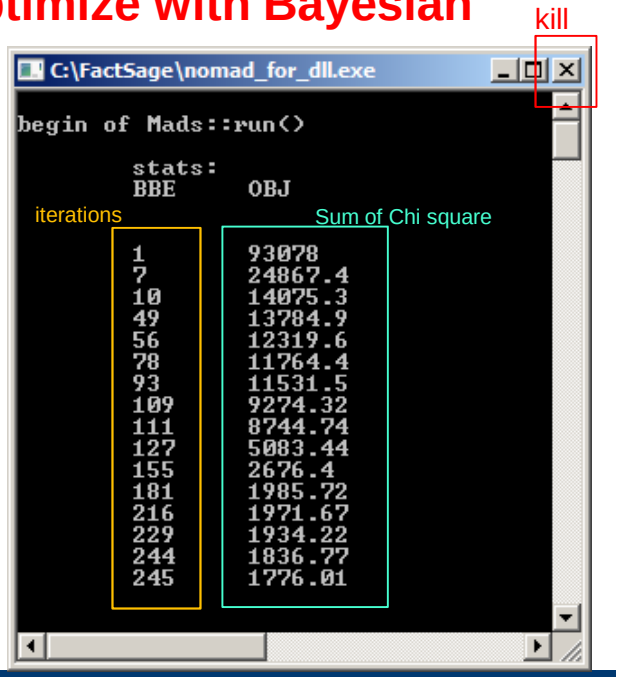
# Estimation of parameters with **NOMAD** (version 6.2+)

The new features associated to **NOMAD** in ***OptiSage*** are:

- **Calculate > Estimate Parameters with NOMAD**

  Run this option to have **NOMAD** performing an optimisation with its MESH ADAPTIVE DIRECT SEARCH algorithm.
  The recommended procedure is to run a few hundred of iterations in **NOMAD**, kill the DOS-type window, and then use the current set of estimated parameters to run a complete Bayesian optimisation using **Calculate > Optimize with Bayesian**



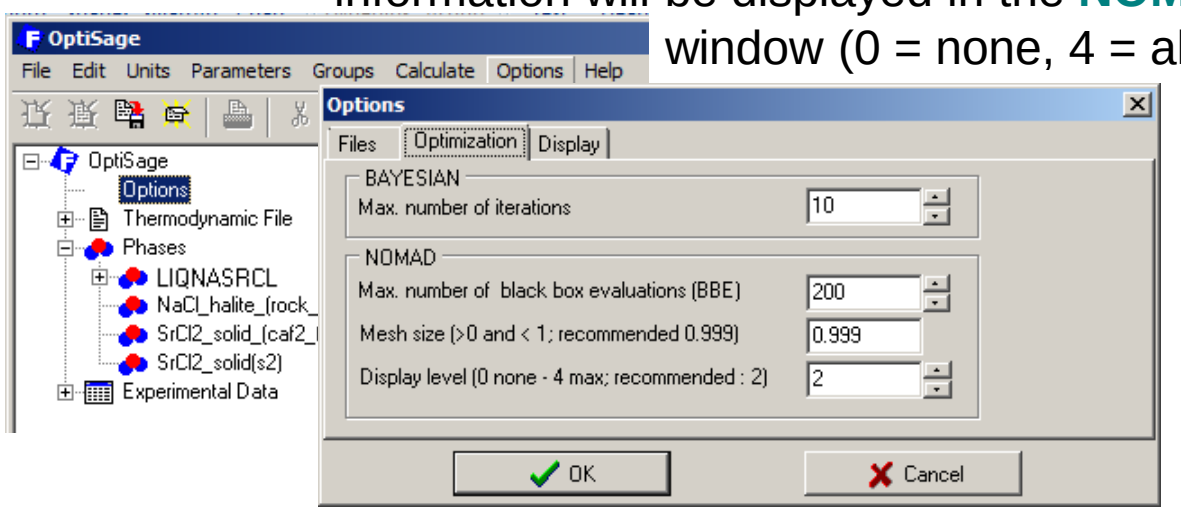
# Estimation of parameters with **NOMAD** (version 6.2+)

The new features associated to **NOMAD** in ***OptiSage*** are:

- **Options | Optimization...**

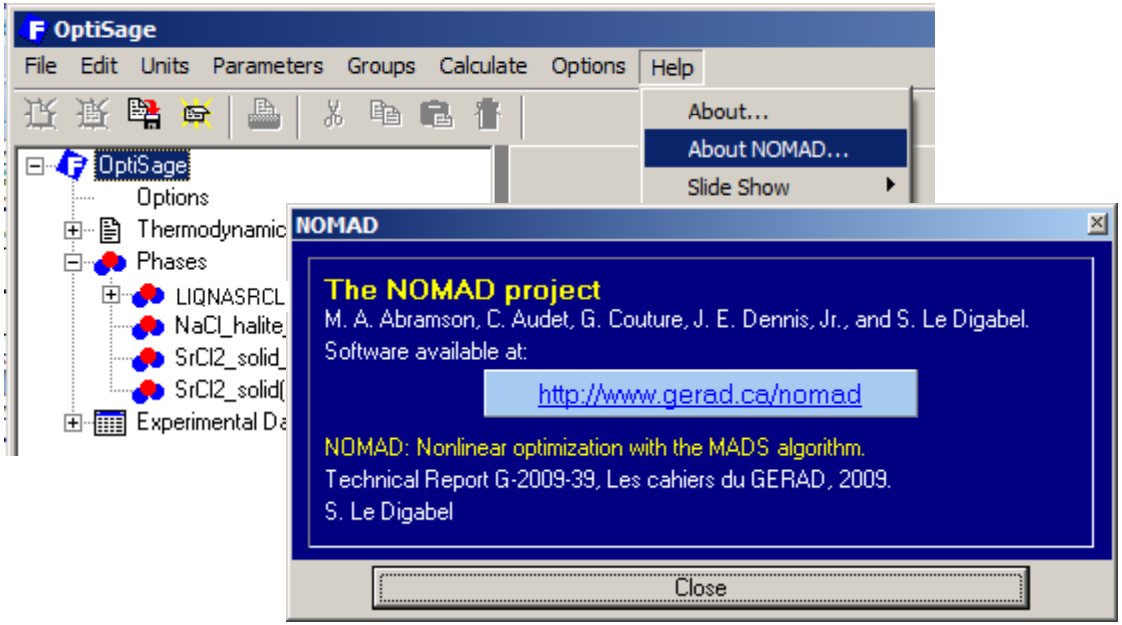
  1- The "max. number of iterations" now applies to the standard Bayesian method.

  2- **NOMAD** optimization options are "Max. number of black box evaluations (BBE)" (in fact the max. number of iterations for **NOMAD**); the "Mesh size" (up to 0.999 to cover the complete range of error of all parameters; or down to 0.001 if your starting estimates are excellent); "Display level" is how much information will be displayed in the **NOMAD** DOS-type window (0 = none, 4 = all; 2 = recommended).



# Estimation of parameters with **NOMAD** (version 6.2+)

The new features associated to **NOMAD** in ***OptiSage*** are:

- **Help > About NOMAD...**

  Gives a link to the **NOMAD** Website (www.gerad.com/nomad) and information about its developpers.