

# The **Solution** module

Use **Solution** to enter non-ideal mixing properties in your private solution databases.

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**NOTE: Use the HOME/Pos1 button to return to the table of contents.**

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NOTE: Use the HOME/Pos1 button to return to the table of contents.

# The *Solution* module



Click on *Solution* in the main *FactSage* window.

# Toolbars and menus

The following two slides explain the **use of the *Solution* module** from its Main window. There are **three** main **sub-windows** from which information on a the **phase tree** of a database, detailed **information** on particular data items, and results of data **searches** can be read.

Furthermore there are **several option menus** and **toolbars** available.

# Solution Main Window

**Treeview Window** lists all the databases, solution phases and functions

**Information Window** provides detailed information on the current item selected in the Treeview Window

The screenshot shows the Solution software interface. The main window title is "SOLUTION - [C:\Models\Data\Facttext.dat]". The menu bar includes "File", "Actions", "Preferences", "View", "Add New Item", and "Help". The toolbar contains various icons for file operations and a search box with "100" entered. The "Folders" window on the left shows a tree structure of databases and solution phases. The "Database : C:\Models\Data\Facttext.dat ( 108 )" window on the right displays a table of phases. The "Immediate" window at the bottom shows search results for "FeS". The status bar at the bottom indicates "Total databases : (2) Units are in Calories" and the date "20/02/01".

Phase	Nickname	Date	Model	Info-(Line 1)
1	FES	WED JAN 25, 1989	1	FeS-liq (solvent) with Fe, FeO, MgS, MnS,...
2	ILME	DEC 19, 1996	4	Ilmenite containing Ti2O3 with MgTiO3, F...
3	CATI	MON MAR 12, 1990	1	Ca3Ti2O7-Ca3Ti2O6 solid solution
4	PERO	MON MAR 12, 1990	1	Perovskite Ca2Ti2O6-Ca2Ti2O5 solid solut...
5	PSEU	DEC 19, 1996	4	Pseudobrookite containing Ti3O5 with Mg...
6	ZROC	MON APR 27, 1992	1	ZrO2-cubic solution, valid only when ZrO2...
7	ZROT	WED APR 29, 1992	1	ZrO2-tetragonal solution, valid only when ..
8	REAL	FRI MAY 01, 1992	3	Re2O3+Al2O3 liquid (Re = rare earths) w...
9	TISP	DEC 19, 1996	4	MTi2O4-spinel only valid above 1050 K, M...
10	TIO2	THU MAY 21, 1992	1	Rutile with Ti2O3 in solution and also with..
11	ALSP	THU MAY 21, 1992	1	Al2O3-spinel (Fe,Mg,Mn)Al2O4-Al2O3
12	MONO	SAT APR 22, 1995	1	Monoxide AO (rocksalt) Al2O3,CaO,Cu2O,...
14	MULL	MON MAR 15, 1993	6	Mullite non-stoichiometric compound. Unl...

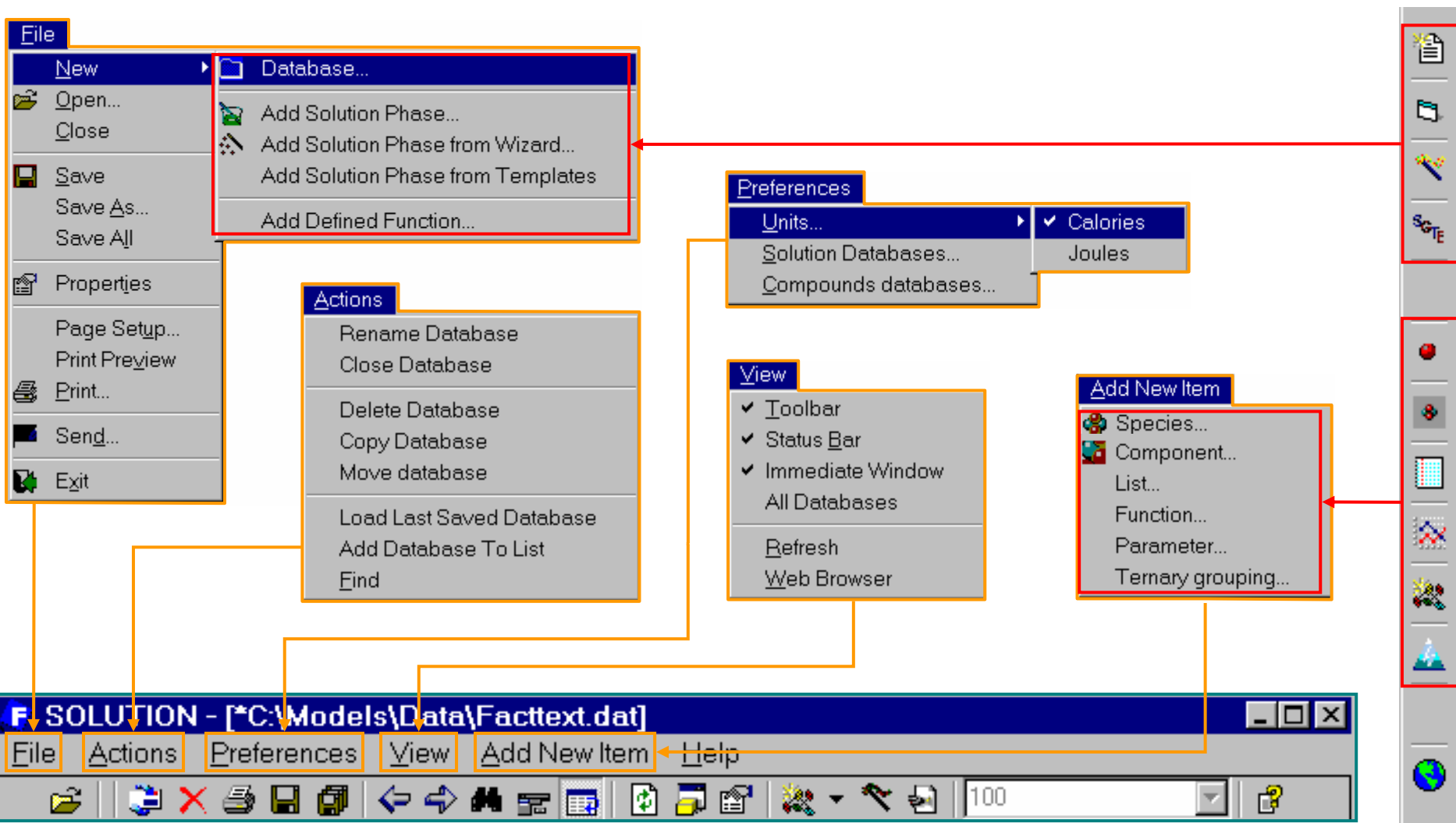
index	Compound	SOLN_ID	Database
2	FeS	1	C:\Models\Data\Facttext.dat
15	FeS	27	C:\Models\Data\Facttext.dat
35	FeS	101	C:\Models\Data\Facttext.dat
2	FeS	152	C:\Models\Data\Facttext.dat
2	FeS	153	C:\Models\Data\Facttext.dat

**Status Bar:** indicate the actual state of your session

**Immediate Window** displays search results, click on an item and the treeview jumps to it

The **Solution** program permits you to enter parameters defining the Gibbs Energy Surfaces of non-ideal solutions. (Data management: creating, listing, loading and modifying databases.)

# Toolbars and menus



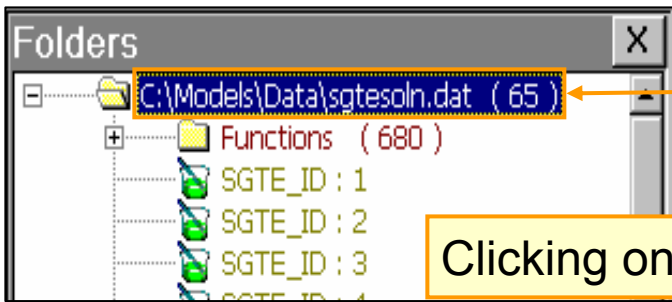
Features of the program are accessible through program menu at the top of the window, toolbars and also context menus available by right-clicking on various objects.

# Obtaining **information** on an **existing database**

The following three slides show how **information** on a particular **database** that **already exists** can be obtained using the **features** of the ***Solution*** module.

As an example the **SGTE solution database** was used.

# List of **Solution** Phases



To display the list of solution phases in the “SGTESOLN.dat” database, click on the specific database in the code explorer Treeview

Clicking on the column heading sorts the list on that field

Database :C:\Models\Data\sgtesoln.dat ( 65 )

Phase	Nickname	Date	Model	Info-(Line 1)	Info-(Line 2)
1	<None>	MAY 28, 1998	20	FCC_A1	This is also the MC(1-x) carbide or nitride!
2	<None>	MAY 28, 1998	20	BCC_A2	
3	<None>	MAY 28, 1998	20	HCP_A3	to the M2C carbide and M2N nitride !
4	<None>	APR 23, 1998	20	CBCC_A12	-Mn phase !
5	<None>	APR 23, 1998	20	CUB_A13	-Mn phase !
6	<None>	APR 23, 1998	20	SIGMA	
7	<None>	APR 24, 1998	20	P_PHASE	
8	<None>	APR 24, 1998	20	MU_PHASE	
9	<None>	APR 24, 1998	20	R_PHASE	
10	<None>	APR 24, 1998	20		
11	<None>	APR 24, 1998	20		
12	<None>	APR 23, 1998	20		

Right-click on an item for a context sensitive menu (other options if many items are selected)

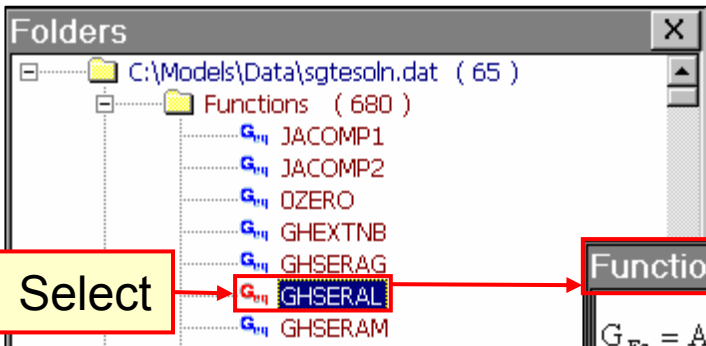
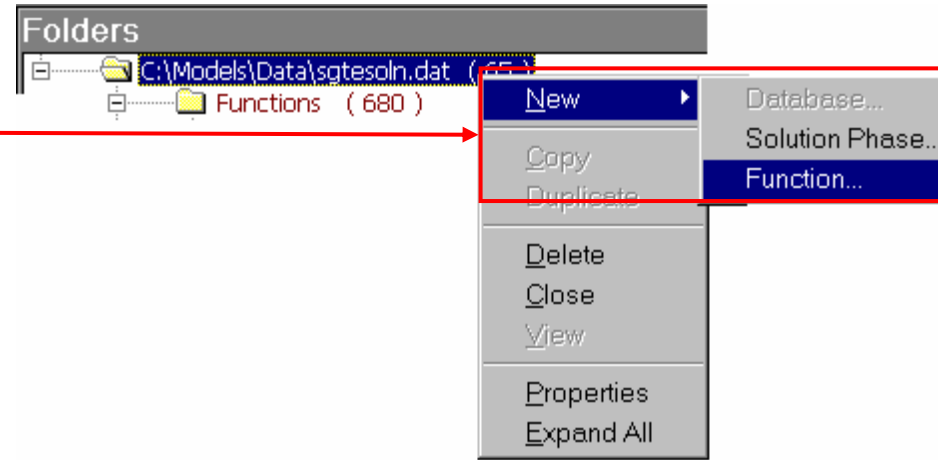
## Columns displayed are:

- **Phase number:** becomes the solution phase number SOLN\_N when the database is used by **Equilib**;
- **Nickname:** appears when the database is used by **Equilib**;
- **Date** of creation of the phase;
- Solution **model:** code number for the phase type (e.g., Compound Energy Model);
- **Two lines** of description.



# List of Gibbs Energy Expression of **GHSERAL** Function

Context sensitive menu:  
Entry of a new function can be done by right-click on the corresponding database. Click on «New» and «Function».



Note: GHSERAL has 3 ranges

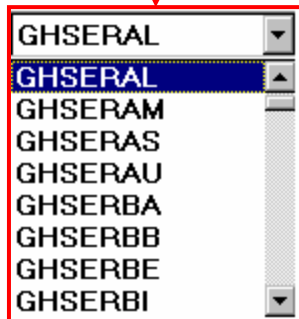
Function : GHSERAL

$$G_{B_1} = A + BT + CTLnT + DT^2 + ET^3 + \frac{F}{T} + \sum_1^6 G_i T^{P_i}$$

Select : GHSERAL 3 [Add] [Delete] [Update]

	1	2	3
T	700	933.6	2900
A	-1906.3456	-2695.08604	-2695.43093
B	32.7608848	53.30472036	45.09129708
C	-5.8239	-9.2219	-7.588
D	-0.000450445029	0.00442925	0
E	-0.00000020976673	-0.00000137768332	0
F	17708.413	17708.413	0
G1	0	0	-2.94996176E+27
Pw1			

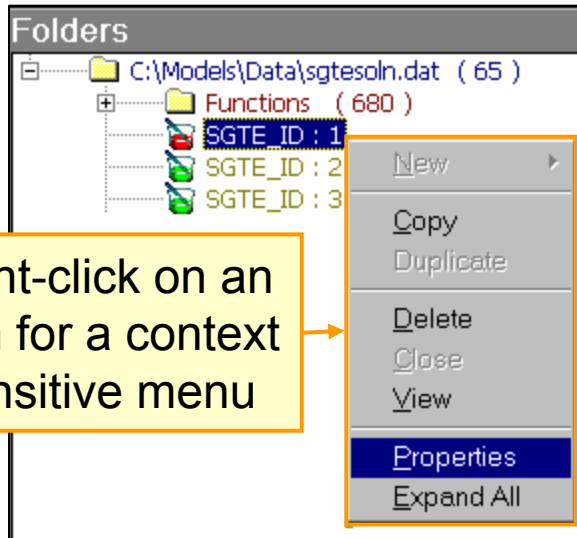
You can scroll for other functions



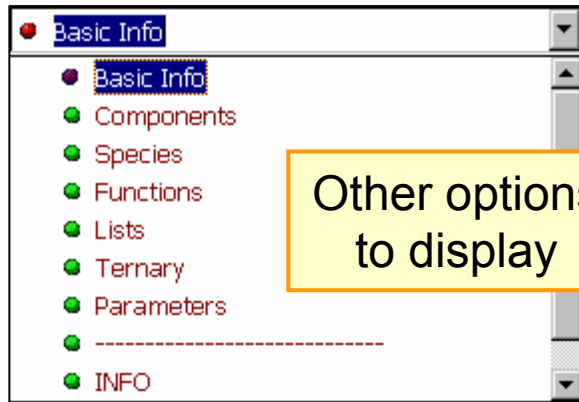
You can add, remove or modify the ranges values then press on the update button to save all modifications.

# Inspection of the phase **SGTE\_1** alias **FCC\_A1**

Your solution phase is now ready for a new entry or modification



Right-click on an item for a context sensitive menu



Other options to display

Solution : SGTE\_ID : 1

General | Species | Components | Functions | Parameters | Ternary Grouping

Display : Basic Info

Tuesday, 20 Feb 2001 2:59 PM  
Energy : Calories

-----  
Report on Solution Phase in : C:\Models\Data\sgtesoln.dat

Name :           Number : 1       Date created :MAY 28, 1998  
Model : Compound Energy Formalism with SGTE Format  
Description :  
      FCC\_A1  
      This is also the MC(1-x) carbide or nitride!

-----

59 Total number of Species  
168 Total number of Components  
0 Total number of Lists  
288 Total number of Excess Parameters ( 9 Not defined )  
117 Total number of Defined Functions  
2 Total number of Sublattices  
      Lattice : 1       56 Species( Site ratio = 1)  
      Lattice : 2       3 Species( Site ratio = 1)

Magnetic factor P :       2.80000000E-01  
Magnetic factor SF :      3.00000000E+00

The information window is a tabbed display containing details of the currently selected phase in the Treeview Window. Number of tabs displayed and their contents depend upon the solution model chosen.

# Generation of a database (Example: **NaCl-SrCl<sub>2</sub> liquid**)

The following fourteen slides show how a **private solution database is built**.

As an example the entry of the data for the **liquid phase in the NaCl-SrCl<sub>2</sub> system** are used.

The **basic data** that need to be stored are **explained first** and in the following thirteen slides the **entry of each data item** is shown in detail.

(This phase has also already been stored in Factdata/Examsoln.dat under the phasename LIQS. You may open and edit this file.)

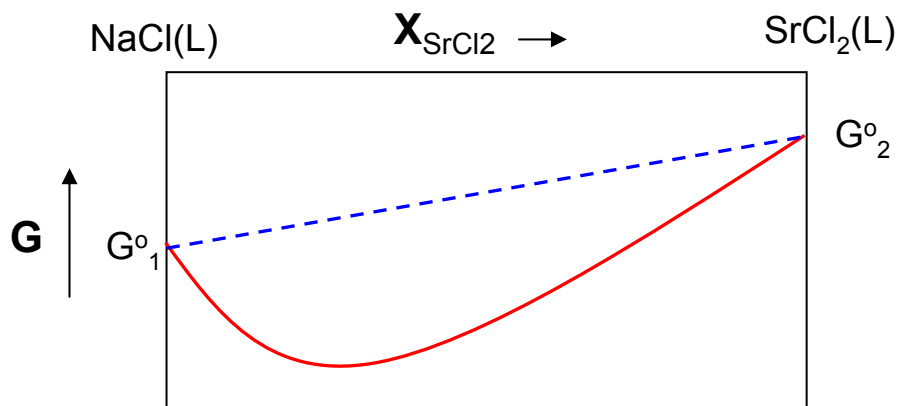
**Example of use of *Solution* program Parameter Entry for a simple Type-1 Polynomial Solution**

**Description:** Thermodynamic data for binary liquid  $\text{NaCl-SrCl}_2$  phase

**Entry:** Joules

**Model:** Polynomial

Components	Index	$G^\circ$
NaCl	1	L From FACTBASE
SrCl2	2	L From FACTBASE



**Gibbs energy:**  $G = (X_1G^\circ_1 + X_2G^\circ_2) + RT(X_1\ln(X_1) + X_2\ln(X_2)) + G^E$

**Binary Excess mixing terms**

$$\Delta H = X_1X_2(-11128.649) + X_1^2X_2(-9547.7573)$$

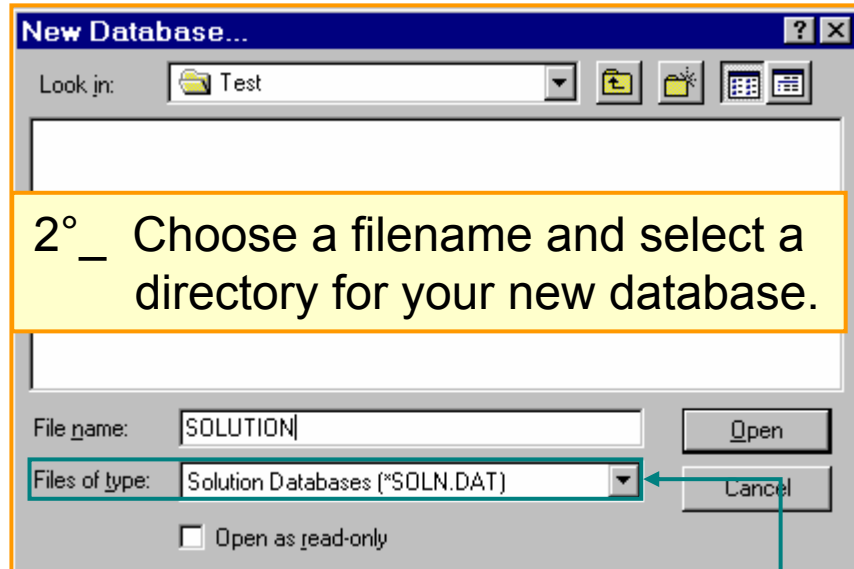
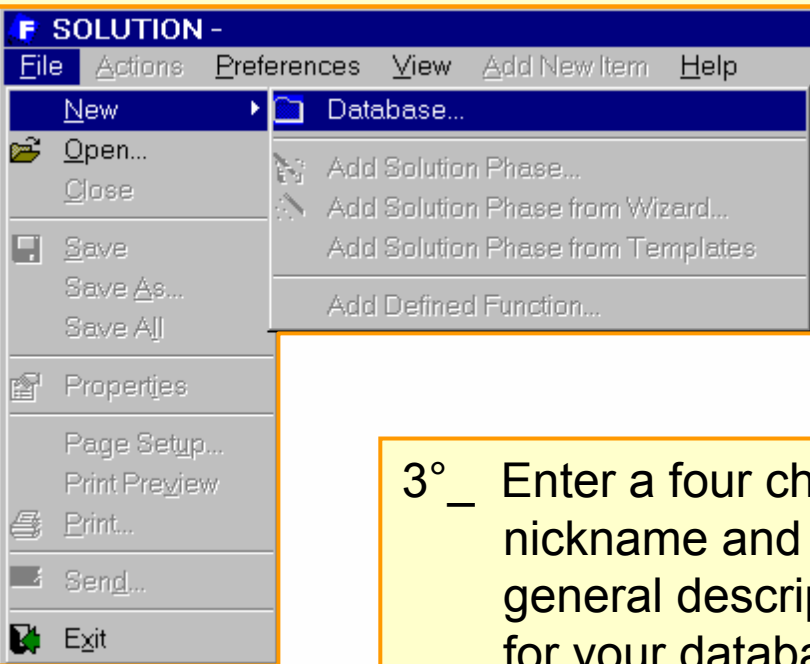
$$S^E = X_1X_2(-8.9242) + X_1^2X_2(-8.92971)$$

**Hence:**

$$G^E = X_1X_2(-11128.649 + 8.9242 T) + X_1^2X_2(-9547.7573 + 8.92971 T)$$

# Creation of a Private Solution Database **USERSOLN**

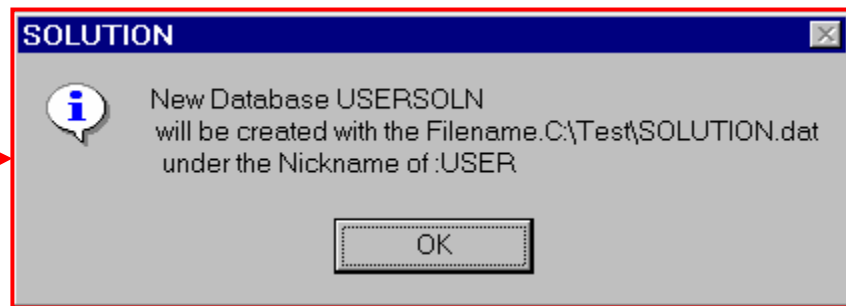
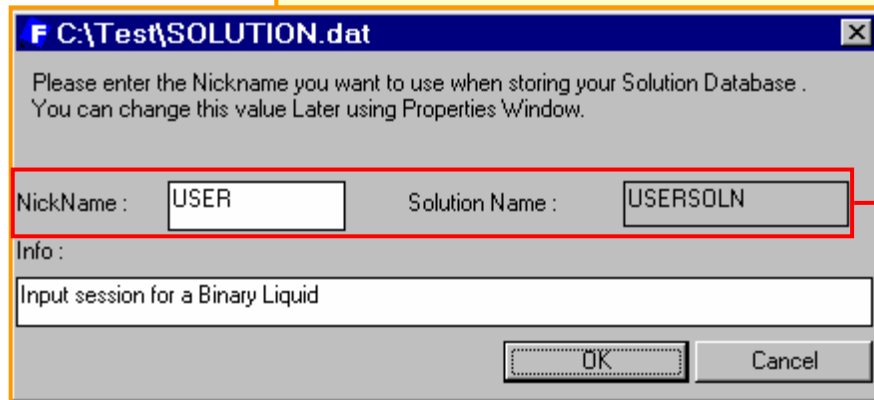
1°\_ Click on «New»; «Database...» from the «File» menu.



2°\_ Choose a filename and select a directory for your new database.

3°\_ Enter a four character nickname and a general description for your database (optional).

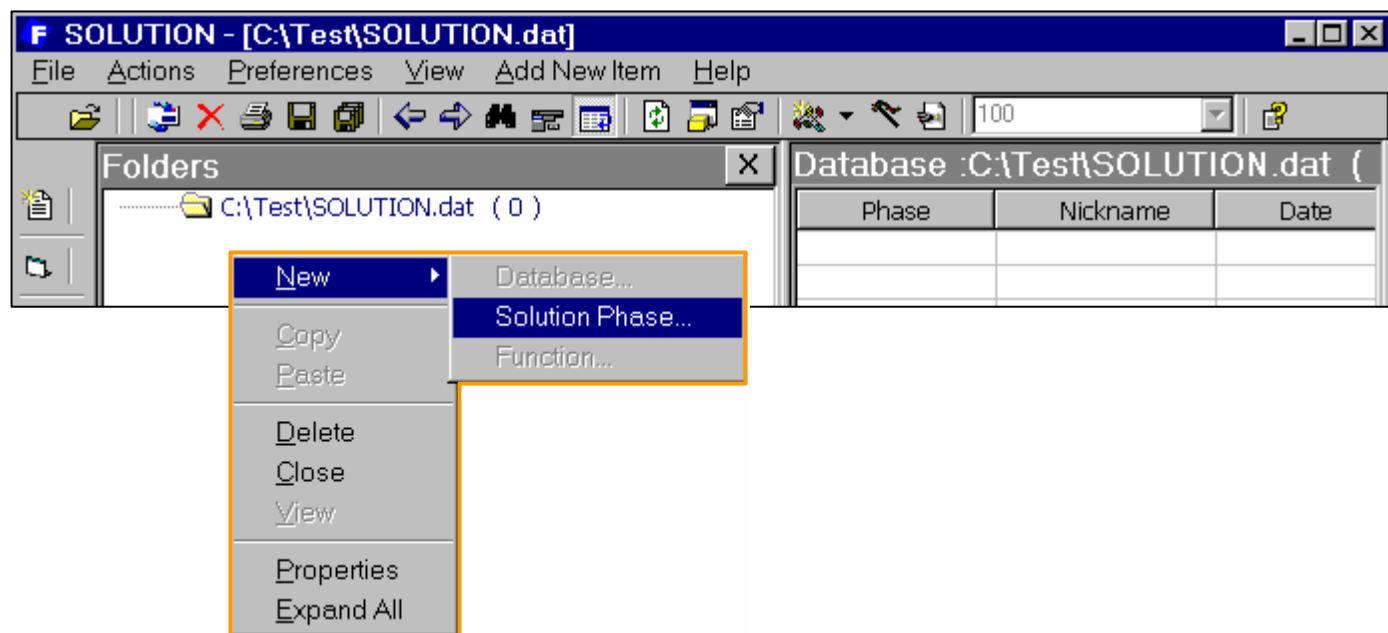
Different database formats



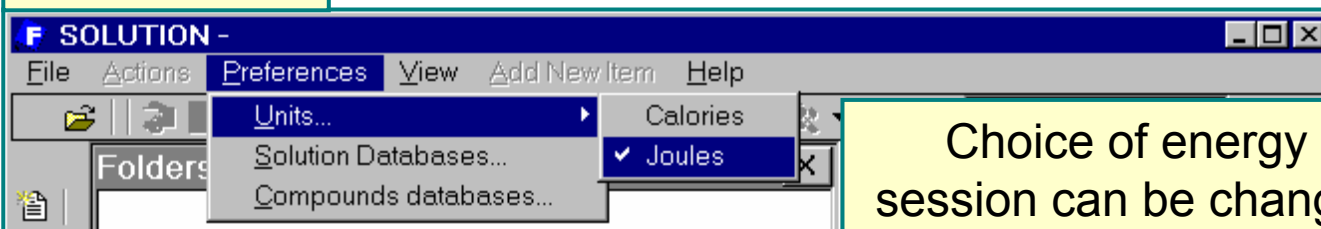
# Creation of a **Solution Phase** (Entry for a Simple Polynomial Solution)

To create a solution phase:

1° Click on «New» and «Solution Phase...» from the «File» menu or the context sensitive menu



By the way...



Choice of energy units for the session can be changed at any time

...Creation of a **Solution Phase** (Input session for the binary NaCl-SrCl<sub>2</sub> solution)

...To create a solution phase:

2°\_ Enter a four-character nickname for your new solution phase;

3°\_ Select / Identify the solution model;

4°\_ Enter a description of your solution phase (2 lines);

5°\_ Select the magnetic contributions.

**F Add New Solution**

Properties | Attributes

20 FEB 2001

Number

Nickname :

Model Type :

- Polynomial (Kohler/Toop)**
- Polynomial (Kohler/Toop)
- Wagner Interaction Formalism
- Quasi-Chemical
- Sublattice (Kohler/Toop)
- Pitzer
- Polynomial (Muggianu)
- Sublattice (MUGGIANU)
- Sublattice (QUASI-CHEMICAL)

**F Add New Solution**

Properties | Attributes

INFO [Line-1 ]

INFO [Line-2 ]

Additional contribution from magnetic ordering :

Type phase FCC\_A1: P=0.28 and SF=3.00

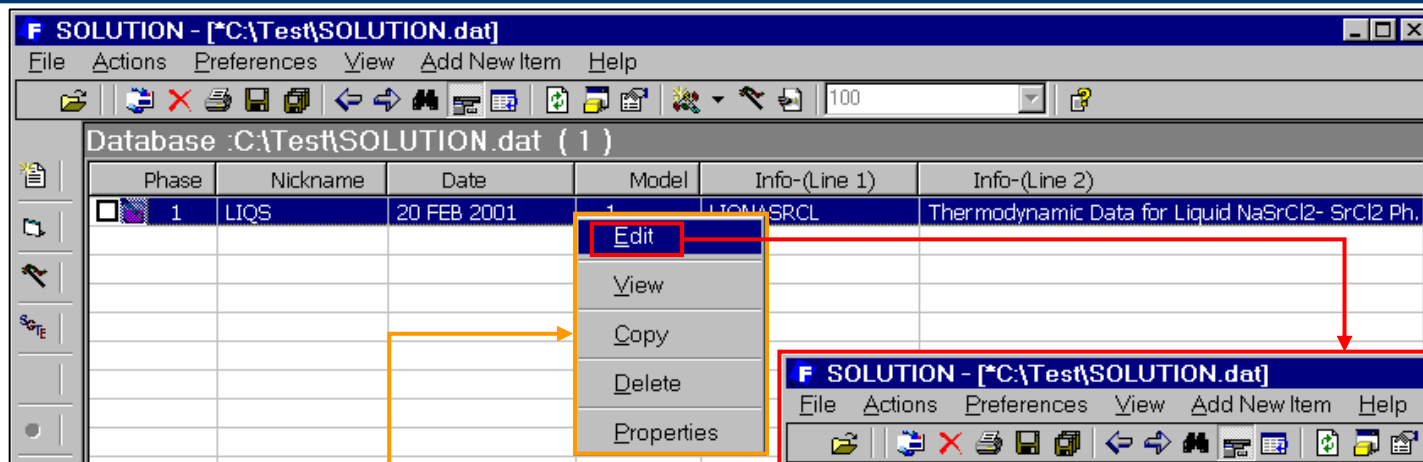
Type phase BCC\_A2: P=0.40 and SF=1.00

Type phase HCP\_A3: P=0.28 and SF=3.00

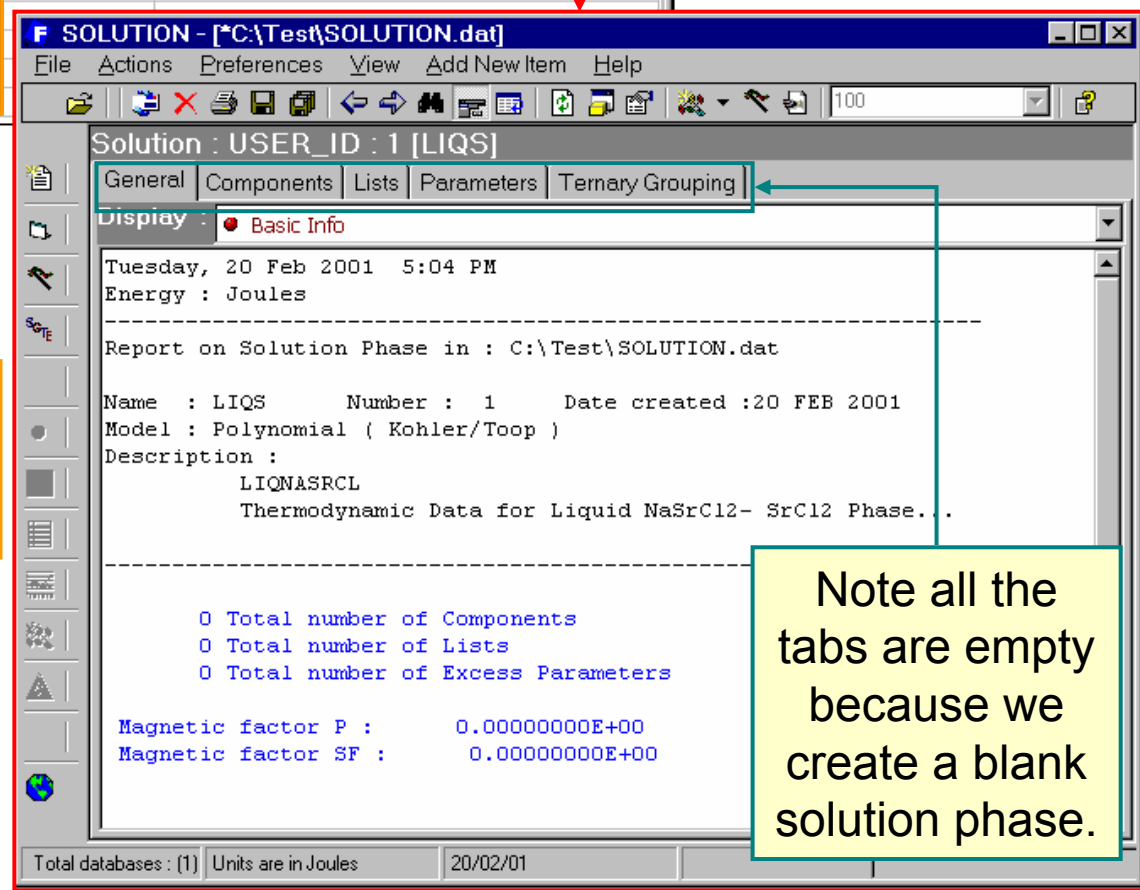
Cancel OK

(Kohler / Toop) interpolation method used for ternary and higher-order systems

# Basics of Entering Components, Lists and Parameters



Right-click on your solution in the information window for a context menu, then click on «Edit».



Note all the tabs are empty because we create a blank solution phase.



For **NaCl** we enter the **standard Gibbs energy** of the liquid from the **FACT** Compound database

Retrieval of data for NaCl from the main FACT database

The components' tab provides an example of entering a new component

NaCl has 3 phases S1, L1 and G1

Number	Formula	Database	Cp-ranges	Phase	Description	Particles	Fract
	NaCl	C:\FACTWIN\FACTDATA\FACTBASE.CDB (version: 3)--[FACTBASE]		Liquid	Sodium Chloride		

Available phases:			
NaCl	Sodium Chloride	Halite	S1
NaCl	Sodium Chloride	Liquid	L1
NaCl	Sodium Chloride	Gas	G1

For  $\text{SrCl}_2$  we enter the **standard Gibbs energy** of the liquid from the **FACT** Compound database

Retrieval of data for  $\text{SrCl}_2$  from the main FACT database

**New Component Entry...**

Formula :

Databases :

Available phases:

SrCl2	Strontium Chloride	Solid	S1
SrCl2	Strontium Chloride	Solid	S2
SrCl2	Strontium Chloride	Liquid-1	L1
SrCl2	Strontium Chloride	Gas-1	G1

SrCl<sub>2</sub> has 4 phases S1, S2, L1 and G1

# Alternate way to enter thermodynamic data

If  $G^\circ_{(added)}$  is defined then:  $G^\circ_{SrCl_2} = G^\circ_{ref}(L1) + G^\circ_{(added)}$   
 (If  $G^\circ_{ref} = 0$ , you must respect the convention that  $H^\circ_{298} = 0$  for elements).

The Properties + G(Added) tab displays certain variables for the component and some advanced properties.

Solution : USER\_ID : 1 [LIQS]

General Components Lists Parameters Ternary Grouping

Number	Formula	Database	C.	P...	Description
1	NaCl	... FACTBA...	2	L1	Sodium Chloride
2	SrCl2	... FACTBA...	2	L1	Srtrium Chloride

Edit

- Add New Component...
- Add User Data
- Insert
- Delete

Property Pages - SrCl2

Reset Import User Data

G (Reference) Properties + G(Added)

Select the range: 1

Cp expression for the range number 1

$$C_p = \sum_i C(i) * T^{P(i)}$$

i	C(i)	P(i)
1	-1.58910237E+02	0.0
2	1.05680040E-01	1.0
3	0.00000000E+00	-2.0
4	0.00000000E+00	2.0
5	-5.16605183E+04	-1.0
6	6.49638483E+03	-0.5
7	0.00000000E+00	0.0

DH298: -80.53832370E+04 J/mol  
 S298: 13.57315693E+01 J/mol.K  
 T\_Max: 80.00100000E+01 K  
 Density: 3.1 g/cc  
 P\_magnetic: 0.00000000E+00  
 SF\_magnetic: 0.00000000E+00  
 T\_magnetic: 0.00000000E+00 K  
 B\_magnetic: 0.00000000E+00

Help OK Cancel

The G(Reference) tab displays  $C_p$  values and other «extended properties»

Property Pages - SrCl2

Reset Import User Data

G (Reference) Properties + G(Added)

+ Summary :

+ G(Added) in Joules

\* Properties :

Description :	Srtrium Chloride
Group :	1
Particles :	1.000
Equivalent :	1.00000
Composition limit :	1.00E+00
Status :	0 - None
CLIM :	(Default value is 1.00E+07)

$$A + B * T + C * T^2 + D * T^U + E * T^V + F * T * \ln(T) + G * T^{(-1)} + H * T^W + I * T^X$$

Help OK Cancel

Default values are chosen regarding "Particles", "Equivalent", "Composition limits" and "Acid/Base (Kohler-Toop)" groupings

# Entry of Model Parameters for Excess Mixing Properties (Solution Polynomial)

Entry can also be expressed as Redlich-Kister or Legendre Polynomials

Solution : USER\_ID : 1 [LIQS]

General | Components | Lists | Parameters | Ternary Grouping

Type	Interaction	i	j	k	l	A	B	C
1								

**F New Parameter Entry...**

Select: Binary Excess Polynomial

Type Binary Excess Polynomial:  
 $(X_M^{**I})(X_N^{**J})(A + B*T + C*T*\ln(T) + D*T^2 + E*T^3 + F*T^{(-1)})$   
 Select your components M and N  
 Select their coefficients I and J  
 Enter the values of the parameters A,B,C,D,E and F

Components and Coefficients:  $X_{NaCl}^1 \times X_{SrCl2}^1 (-1128.649 + 8.92422T)$

M	NaCl	I	1
N	SrCl2	J	1

A =	-1.11286490E+04
B =	8.92422000E+00
C =	0.00000000E+00
D =	0.00000000E+00
E =	0.00000000E+00
F =	0.00000000E+00

Brief reminder of how to enter parameters

Enter your parameter values then press «Apply»

The Gibbs energy of mixing is given by  $\Delta G = RT (X_1 \ln X_1 + X_2 \ln X_2) + G^E$

# Entry of the Second Parameter for **Excess Mixing Properties** of the solution

$$X_{\text{NaCl}}^2 \times X_{\text{SrCl}_2}^1 (-9547.7573 + 8.92971T)$$

SOLUTION - [C:\Test\SOLUTION.dat]

File Actions Preferences View Add New Item Help

Solution : USER\_ID : 1 [LIQS]

General Components Lists Parameters Ternary Grouping

	Type	Interaction	i	j	k	l	A	B	C
1	B-Ex-P	NaCl SrCl2	1	1			-1.11E+04	8.92E+00	0.00E-01

Add New Interaction...  
Delete Interaction NaCl SrCl2  
Edit Interaction NaCl SrCl2  
Sort Interactions  
Refresh

**New Parameter Entry...**

Select: Binary Excess Polynomial

Type Binary Excess Polynomial:  
 $(X_M^{**I})(X_N^{**J})(A + B*T + C*T*\ln(T) + D*T^2 + E*T^3 + F*T^{(-1)})$

Select your components M and N  
 Select their coefficients I and J  
 Enter the values of the parameters A,B,C,D,E and F

Components and Coefficients:

M	I
NaCl	2
N	J
SrCl2	1

A =	-9.54775730E+03
B =	8.92971000E+00
C =	0.00000000E+00
D =	0.00000000E+00
E =	0.00000000E+00
F =	0.00000000E+00

Apply Close

Enter your parameter values then press «Apply»

# Summarize, Edit and View the Excess Parameters

A grid showing the existing excess interactions

The screenshot displays the FactSage software interface. The main window title is "SOLUTION - [C:\Test\SOLUTION.dat]". The menu bar includes "File", "Actions", "Preferences", "View", "Add New Item", and "Help". The toolbar contains various icons for file operations and navigation. The main area shows the "Parameters" tab for "Solution : USER\_ID : 1 [LIQS]". A search box contains "B-Ex-P". Below it is a table of interactions:

	Type	Interaction	i	j	A	B	C	D	E	F
1	B-Ex-P	NaCl SrCl2	1	1	-1.11E+04	8.92E+00	0.00E-01	0.00E-01	0.00E-01	0.00E-01
2	B-Ex-P	NaCl SrCl2	2	1	-9.55E+03	8.93E+00	0.00E-01	0.00E-01	0.00E-01	0.00E-01

A context menu is open over the second row, with options: "Add New Interaction...", "Delete Interaction NaCl SrCl2", "Edit Interaction NaCl SrCl2", "Sort Interactions", and "Refresh".

Annotations include:

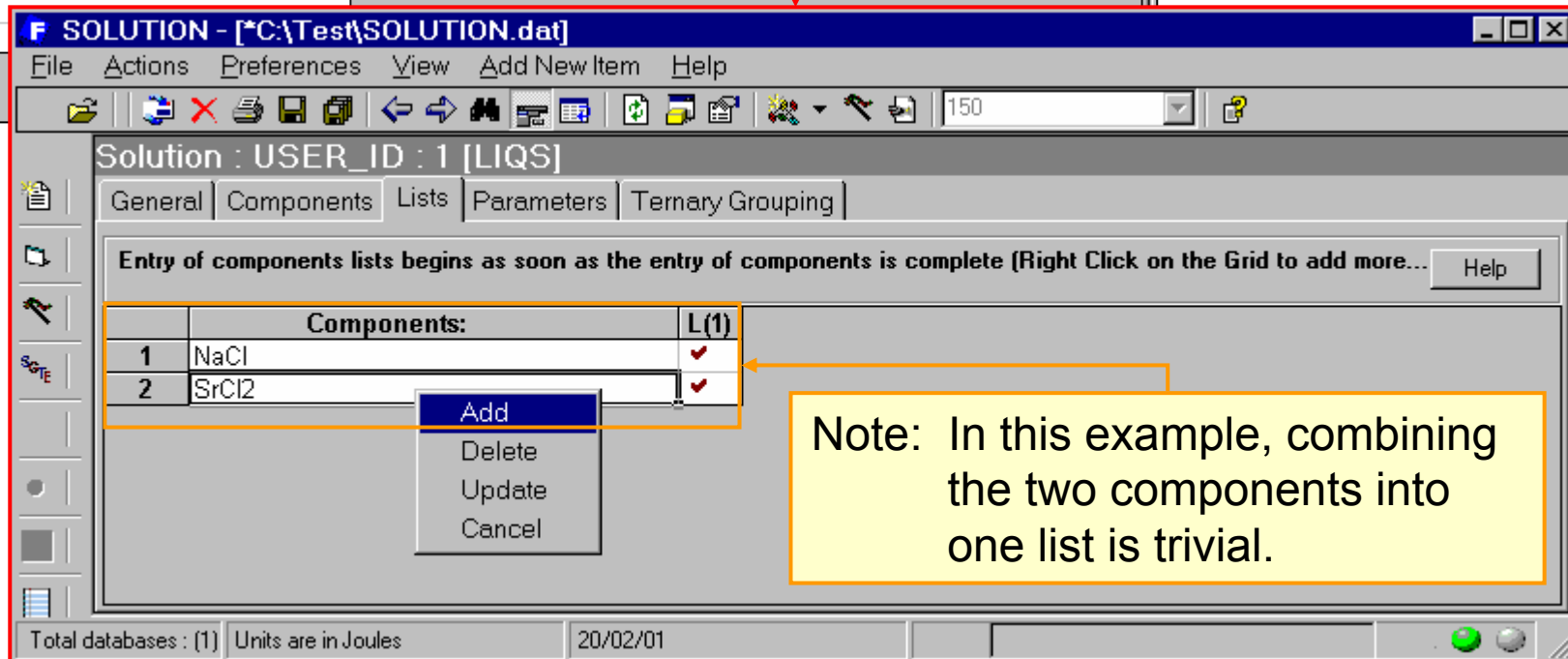
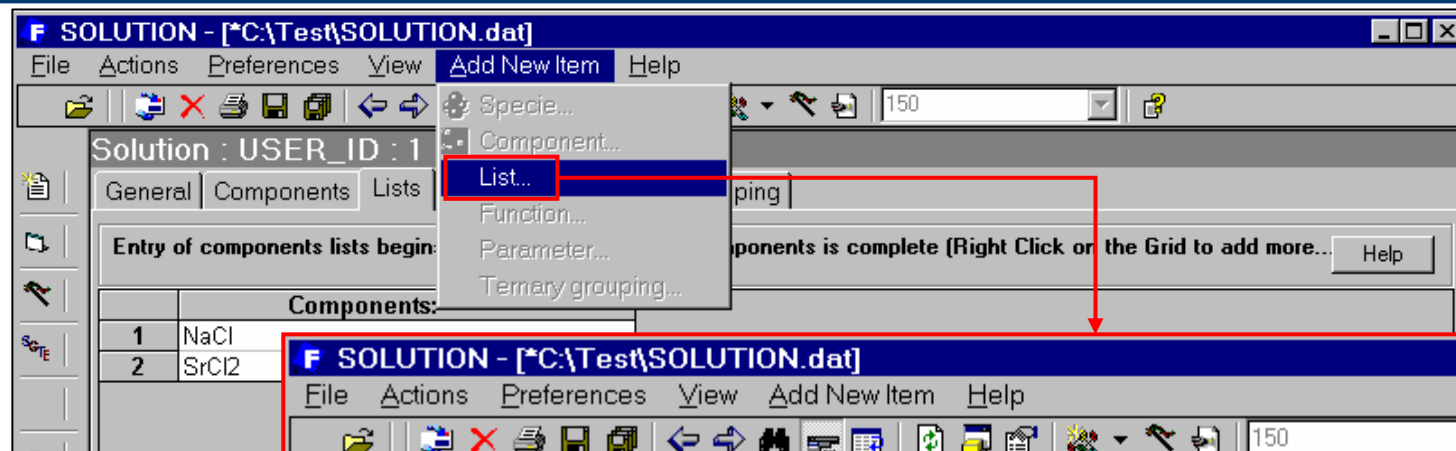
- A yellow box at the top left points to the table with the text "A grid showing the existing excess interactions".
- A yellow box at the bottom center points to the table columns with the text "Components, powers and parameters for the selected interaction".
- A yellow box at the bottom right points to the text area with the text "A Help Window explaining the above entered excess interaction parameters".

At the bottom of the window, the status bar shows "Total databases : (1)", "Units are in Joules", and the date "20/02/01".

Components, powers and parameters for the selected interaction

A Help Window explaining the above entered excess interaction parameters

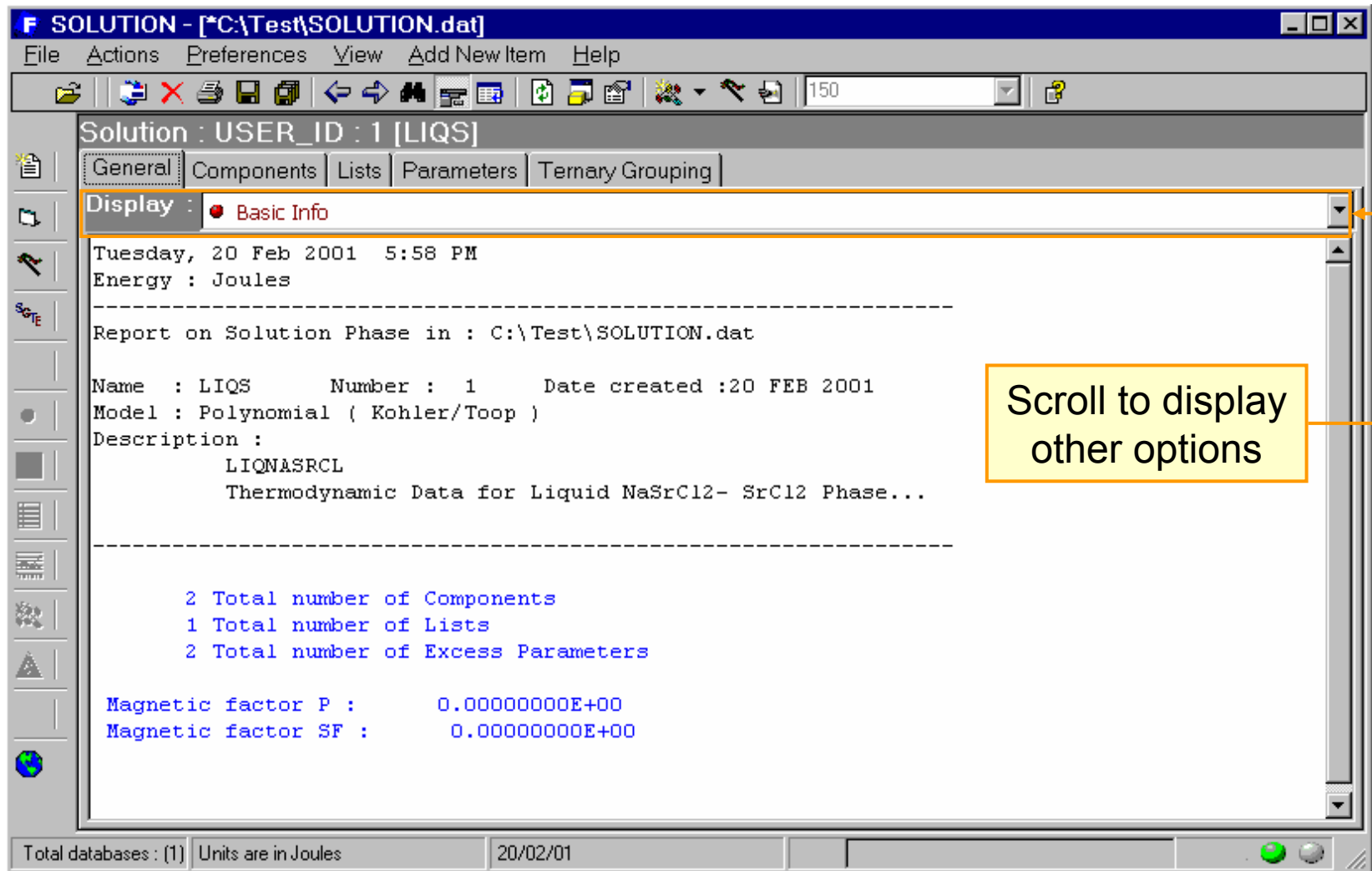
# Entry of Component Lists



A solution phase may contain one or more lists of components which have been assessed together to form a multi-component solution. Only the use of such combinations is safe (in *Equilib*).

# Inspecting the Solution File

Note that the parameters ( $H^{\circ}_{298}$ ,  $S^{\circ}_{298}$ ,  $C_p$ ) in the expression for  $G^{\circ}_{(ref)}$ ,  $G_{(added)}$  and  $G_{(excess)}$  can also be displayed using other display options.



The screenshot shows the FactSage SOLUTION application window. The title bar reads "F SOLUTION - [\*C:\Test\SOLUTION.dat]". The menu bar includes "File", "Actions", "Preferences", "View", "Add New Item", and "Help". The toolbar contains various icons for file operations and a numerical input field set to "150". The main window title is "Solution : USER\_ID : 1 [LIQS]". Below the title bar, there are tabs for "General", "Components", "Lists", "Parameters", and "Ternary Grouping". A "Display" dropdown menu is open, showing "Basic Info" selected. A scroll bar on the right side of the main content area is highlighted with an orange box, and a callout box points to it with the text "Scroll to display other options". The main content area displays the following text:

```
Tuesday, 20 Feb 2001  5:58 PM
Energy : Joules
-----
Report on Solution Phase in : C:\Test\SOLUTION.dat

Name : LIQS      Number : 1      Date created :20 FEB 2001
Model : Polynomial ( Kohler/Toop )
Description :
    LIQNASRCL
    Thermodynamic Data for Liquid NaSrCl2- SrCl2 Phase...
-----

  2 Total number of Components
  1 Total number of Lists
  2 Total number of Excess Parameters

Magnetic factor P :      0.00000000E+00
Magnetic factor SF :     0.00000000E+00
```

The status bar at the bottom shows "Total databases : (1)", "Units are in Joules", and the date "20/02/01".



# Saving Solution Database

Saving a database can be done by clicking on «Save» from the «File» menu or by pressing the «Save» button.

The screenshot shows the FactSage Solution software interface. The main window is titled "SOLUTION - [C:\Test\SOLUTION.dat]". The menu bar includes "File", "Actions", "Preferences", "View", "Add New Item", and "Help". The toolbar contains various icons, including a "Save" icon (floppy disk). The "Folders" pane on the left shows the directory structure: "C:\Test\SOLUTION.dat (1)" containing "USER\_ID : 1 [LIQS]". The "File" menu is open, and the "Save" option is highlighted. The main display area shows the "Solution : USER\_ID : 1 [LIQS]" details, including the date and time (Tuesday, 20 Feb 2001 6:03 PM), energy units (Joules), and a report on the solution phase. The report includes the name (LIQS), number (1), date created (20 FEB 2001), model (Polynomial ( Kohler/Toop )), and description (LIQNASRCL Thermodynamic Data for Liquid NaSrCl2- SrCl2 Phase...). A confirmation dialog box titled "SOLUTION" is displayed in the foreground, stating "Database C:\Test\SOLUTION.dat successfully saved!" with an "OK" button.

# Examples of data entries in solution database

The following 11 slides show **4 different examples** of the data needed to describe non-ideal solutions according to different Gibbs energy models.

These files are stored in your Factdata directory in Examsoln.dat. You can open this file using the **Solution** module in order to see how the data have been entered.

The **first example** shows the data for a simple substitutional solution treated with polynomials in the mole fractions and using the Kohler method for extrapolation into the ternary, here the **Liquid LiCl-KCl-CsCl Phase**.

The phase name used in the **Factdata/Examsoln.dat** database is **AkCl**.

# First example from **Factdata/ExamsoIn.dat**

Thermodynamic Data for **Liquid LiCl-KCl-CsCl Phase**

Phase Nickname: **AkCl**

Entry in **joules**  
**Kohler** interpolation method

	<b>Component No.</b>	<b>G°</b>
LiCl	1	L from FACT database
KCl	2	S1 from FACT database + $\Delta G_{\text{fusion}}^{\circ}$ where: $\Delta G_{\text{fusion}}^{\circ} = 26284 - 25.176 T$
CsCl	3	L from FACT database

## Binary excess mixing terms:

$$\text{LiCl-KCl system: } \Delta H = X_1 X_2 (-17570 - 377 X_1)$$

$$S^E = X_1 X_2 (-7.627 - 4.958 X_1)$$

$$\text{Hence: } G^E = X_2 X_1 (-17570 + 7.267 T) + X_2 X_1^2 (-377 - 4.958 T)$$

$$\text{LiCl-CsCl system: } \Delta H = X_1 X_3 (-19456 - 7448 X_1 - 9080 X_1 X_3)$$

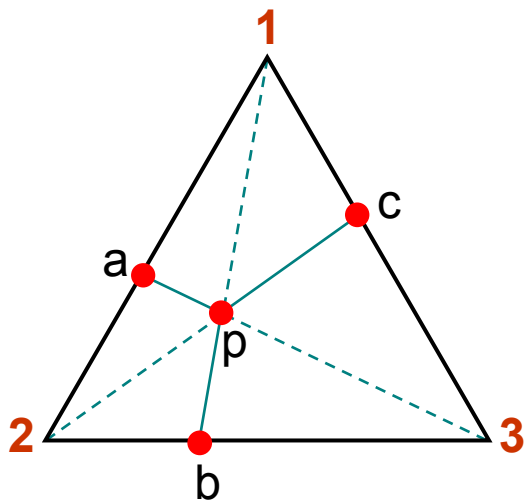
$$S^E = X_1 X_3 (-20.541 + 3.285 X_1)$$

$$\text{KCl-CsCl system: } G^E = X_2 X_3 (795)$$

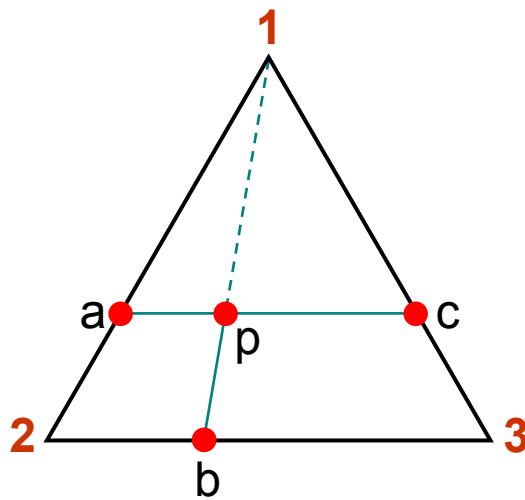
$$\text{Ternary terms: } G^E = X_1 X_2 X_3 (-20000)$$

# Kohler, Toop and Muggianu interpolation methods

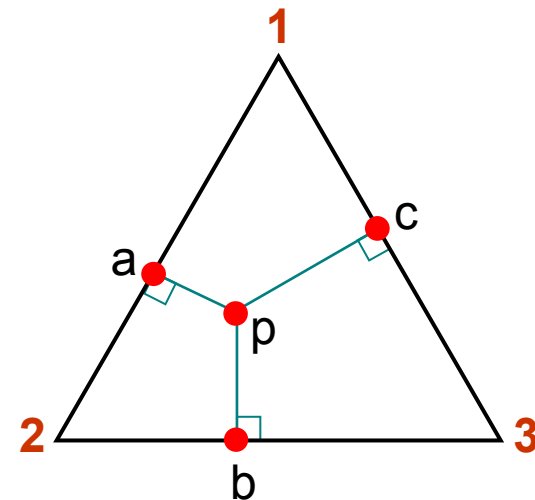
Kohler



Toop



Muggianu



**Kohler, Toop** and **Muggianu** methods of including binary polynomial terms in ternary **Gibbs Energy Equations**.

**Reference:**

P. Chartrand and A.D. Pelton, «On the choice of “Geometric” Thermodynamic Models», J. Phase Equilibria, 21, 141-147 (2000).

The **second example** shows the data used for the description of a dilute metallic solution, here **Liquid Fe-C-Mn-O Solution**.

The phase name used in **Factdata/Examsoln.dat** is **IRON**.

# Second example from **Factdata/ExamsoIn.dat**

Thermodynamic Data for **Liquid Fe-C-Mn-O Solution**

Phase Nickname: **IRON**

Entered Component	Component number	G° (ref)	N (Particles/mol)	Actual Component	Composition Limit (X)
Fe (solvent)	1	FACT L	1	Fe	–
C	2	FACT S1	1	C	0.1
Mn	3	FACT L	1	Mn	0.1
O <sub>2</sub>	4	FACT G	2	O	0.1

Actual Component	i	$\ln \gamma_i^\circ$
C	2	$2073/T - 1.727$
Mn	3	$672/T$
O	4	$-14086/T + 2.948$

i	j	$\epsilon_{ij}$
2	2	$23974/T$
2	3	$-3502/T$
2	4	$-38209/T$
3	4	$-8803$

**Reference:** (Unified interaction parameter formalism)

A.D. Pelton, «The Polynomial Representation of Thermodynamic Properties in Dilute Solutions», Met. Trans., 28B, 869-76 (1997).

## Third example from **Factdata/Examsoln.dat**

The **third example** shows the data used for the description of the **Liquid Li, Na, K / F, SO<sub>4</sub> Solution**.

The dataset is given the name **SALT** in the **Factdata/Examsoln.dat** database.

# Third example from **Factdata/Examsoln.dat**

Thermodynamic Data for **Liquid Li, Na, K / F, SO<sub>4</sub> Solution**

Phase Nickname: **SALT**

## (Sublattice Model)

	Species Number	Lattice	Absolute Charge	Kohler/Toop Group
Li	1	cationic	1	1
Na	2	cationic	1	1
K	3	cationic	1	1
F	4	anionic	1	(1)
SO <sub>4</sub>	5	anionic	2	(2)

**G° of all liquid salts from FACT database**

**X<sub>i</sub> = ionic site fractions:**

$$X_{\text{Li}} = \frac{n_{\text{Li}}}{(n_{\text{Li}} + n_{\text{Na}} + n_{\text{K}})} \quad \text{etc}$$

$$X_{\text{F}} = \frac{n_{\text{F}}}{(n_{\text{F}} + n_{\text{SO}_4})} \quad \text{etc}$$

**Y<sub>i</sub> = equivalent ionic fractions:**

$$Y_{\text{Li}} = X_{\text{Li}} \quad \text{etc}$$

$$Y_{\text{F}} = \frac{n_{\text{F}}}{(n_{\text{F}} + 2n_{\text{SO}_4})}$$

$$Y_{\text{SO}_4} = \frac{2n_{\text{SO}_4}}{(n_{\text{F}} + 2n_{\text{SO}_4})}$$

### References: (Sublattice Model)

A.D. Pelton «A Database and Sublattice Model for Molten Salt Solutions», Calphad J., 12, 127-142 (1988).

### (Quasichemical Sublattice Model)

Y. Dessureault and A.D. Pelton, «Contribution to the Quasichemical Model of Reciprocal Molten Salt Solutions», J. Chim. Phys., 88, 1811-1830 (1991).



# Excess terms (Joules/equivalent)

## Binary Common-Anion Systems

$$\text{LiF} - \text{NaF}: G^E = Y_1 Y_2 (-7565 + 1.607T) + Y_1 Y_2^2 (-368 + 1.124T)$$

$$\text{LiF} - \text{KF}: G^E = Y_1 Y_3 (-19251 + 1.375T) + Y_1 Y_3^2 (-1205) + Y_1 Y_3^3 (4732) + Y_1^2 Y_3 (3.146T)$$

$$\text{NaF} - \text{KF}: G^E = Y_2 Y_3 (-335 + 2.541T)$$

$$\text{Li}(\text{SO}_4)_{1/2} - \text{Na}(\text{SO}_4)_{1/2}: G^E = Y_1 Y_2 (-4247) + Y_1^2 Y_2 (-1444)$$

$$\text{Li}(\text{SO}_4)_{1/2} - \text{K}(\text{SO}_4)_{1/2}: G^E = Y_1 Y_3 (-10712 + 4.700T) + Y_1^2 Y_3 (-3891 - 1.000T)$$

$$\text{Na}(\text{SO}_4)_{1/2} - \text{K}(\text{SO}_4)_{1/2}: G^E = Y_2 Y_3 (-2197)$$

## Binary Common-Cation Systems

$$\text{LiF} - \text{Li}(\text{SO}_4)_{1/2}: G^E = Y_4 Y_5 (-988 - 2.352T) + Y_4 Y_5 (Y_5 - Y_4)(-359)$$

$$\text{NaF} - \text{Na}(\text{SO}_4)_{1/2}: G^E = Y_4 Y_5 (56 - 1.214T) + Y_4 Y_5 (Y_5 - Y_4)(-217 + 2.044T)$$

$$\text{KF} - \text{K}(\text{SO}_4)_{1/2}: G^E = Y_4 Y_5 (-1263 - 1.522T) + Y_4 Y_5 (Y_5 - Y_4)(486)$$

## Ternary Common-Anion Terms

$$\text{LiF} - \text{NaF} - \text{KF}: Y_1 Y_2 Y_3 (-300)$$

$$\text{Li}(\text{SO}_4)_{1/2} - \text{Na}(\text{SO}_4)_{1/2} - \text{K}(\text{SO}_4)_{1/2}: Y_1 Y_2 Y_3^2 (400)$$

## Reciprocal Terms

$$Y_1 Y_2 Y_4 Y_5 (-8483 + 3.069T)$$

$$Y_1 Y_3 Y_4 Y_5 (-29893 + 14.017T)$$

$$Y_2 Y_3 Y_4 Y_5 (-6338 + 3.588T)$$

The **fourth example** shows the data stored for the **Fe-Cr system**. The data are given in **the form** that is used in the **SGTE Solution database**.

**Functions** are used to define the Gibbs energies of the components of the solution phases.

The excess Gibbs energy of liquid, FCC and BCC is treated with the **Redlich-Kister polynomial**.

For the SIGMA phase a **three-sublattice ideal solution** approach is used.

# Fourth example from **Factdata/ExamsoIn.dat**

Thermodynamic properties of the **Cr-Fe System**

Entry in **joules**

Excess Model: Redlich-Kister-Muggianu

Phase	Nickname	Number of Sublattices	Sites	Constituents on sublattice numbers		
				1	2	3
LIQUID	LIQU	1	1	Cr, Fe	–	–
BCC_A2	BCC	2	1:3	Cr, Fe	Va	–
FCC_A1	FCC	2	1:1	Cr, Fe	Va	–
SIGMA	SIGM	3	8:4:18	Fe	Cr	Cr, Fe

Thermodynamic parameters of the **elements** and **solution phases**

**LIQUID:**

$${}^{\circ}G_{\text{Cr}}^{\text{LIQUID}} = \text{LIQU015}$$

$${}^{\circ}G_{\text{Fe}}^{\text{LIQUID}} = \text{GFELIQ}$$

$${}^{\circ}L_{\text{Cr,Fe}}^{\text{LIQUID}} = -14550 + 6.65T$$

**BCC\_A2** (Additional contribution from magnetic ordering):

$${}^{\circ}G_{Cr}^{BCC} = GHSERCR$$

$${}^{\circ}G_{Fe}^{BCC} = GHSEFFE$$

$$T_C^{BCC} = -311.5y_{Cr} + 1043y_{Fe} + y_{Cr}y_{Fe} [1650 + 550(y_{Cr} - y_{Fe})]$$

$$\beta^{BCC} = -0.01y_{Cr} + 2.22y_{Fe} - 0.85y_{Cr}y_{Fe}$$

$${}^{\circ}L_{Cr,Fe:Va}^{BCC} = 20500 - 9.68T$$

**FCC\_A1** (Additional contribution from magnetic ordering):

$${}^{\circ}G_{Cr}^{FCC} = GCRFCC$$

$${}^{\circ}G_{Fe}^{FCC} = GFEFCC$$

$$T_C^{FCC} = -1109y_{Cr} - 201y_{Fe}$$

$$\beta^{FCC} = -2.46y_{Cr} - 2.1y_{Fe}$$

$${}^{\circ}L_{Cr,Fe:Va}^{FCC} = 10833 - 7.477T$$

$${}^1L_{Cr,Fe:Va}^{FCC} = 1410$$

**SIGMA:**

$$G_{Fe:Cr:Cr}^{SIGMA} = 8 GFEFCC + 22 GHSERCR + SIGM034$$

$$G_{Fe:Cr:Fe}^{SIGMA} = 8 GFEFCC + 4 GHSERCR + 18 GHSEFFE + SIGM035$$

# Thermodynamic parameters of the **elements** and **solution phases** (continued)

$$\text{LIQU015} = \begin{cases} \text{GHSECR} + 24339.955 - 11.420225T + 2.37615 \times 10^{-21}T^7 & \text{for } T < 2180\text{K} \\ \text{GHSECR} + 18409.36 - 8.563683T + 2.88526 \times 10^{32}T^{-9} & \text{for } T > 2180\text{K} \end{cases}$$

$$\text{GHSECR} = \begin{cases} \left\{ \begin{array}{l} -8856.94 + 157.48T - 26.908T \ln T + 1.89435 \times 10^{-3}T^2 \\ -1.47721 \times 10^{-6}T^3 + 139250T^{-1} \end{array} \right\} & \text{for } T < 2180\text{K} \\ -34869.344 + 344.18T - 50T \ln T - 2.88526 \times 10^{32}T^{-9} & \text{for } T > 2180\text{K} \end{cases}$$

$$\text{GHSEFE} = \begin{cases} \left\{ \begin{array}{l} 1225.7 + 124.34T - 23.5143T \ln T - 4.39752 \times 10^{-3}T^2 \\ -5.8927 \times 10^{-8}T^3 + 77359T^{-1} \end{array} \right\} & \text{for } T < 1811\text{K} \\ -25383.581 + 299.31255T - 46T \ln T + 2.29603 \times 10^{31}T^{-9} & \text{for } T > 1811\text{K} \end{cases}$$

$$\text{GFELIQ} = \begin{cases} 12040.17 - 6.55843T - 3.6751551 \times 10^{-21}T^7 + \text{GHSEFE} & \text{for } T < 1811\text{K} \\ -10839.7 + 291.302T - 46T \ln T & \text{for } T > 1811\text{K} \end{cases}$$

$$\text{GCRFCC} = 7284 + 0.163T + \text{GHSECR}$$

$$\text{GFEFCC} = \begin{cases} -1462.4 + 8.282T - 1.15T \ln T + 6.4 \times 10^{-4}T^2 + \text{GHSEFE} & \text{for } T < 1811\text{K} \\ -27098.266 + 300.25256T - 46T \ln T + 2.78854 \times 10^{31}T^{-9} & \text{for } T > 1811\text{K} \end{cases}$$

$$\text{SIGM034} = 92300 - 95.96T$$

$$\text{SIGM035} = 117300 - 95.96T$$

# References for the fourth example

- **Compound Energy Formalism**

- M.Hillert and M.Jarl, Calphad Vol 2(1978) p 227-238
- J.O. Anderson, A.Fernandez Guillermet, M.Hillert, B.Jansson, B.Sundman, Acta Metall., 34(1986) p 437-445.

- **Cr-Fe system**

- Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15(1991) p 317-425.
- J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92.