The *Compound* module

- Use ***Compound*** for the administration of a private compound database, i.e. enter, edit, delete pure substance data in a database.

Table of Contents

The *Compound* module

- **Click** on ***Compound*** in the main ***FactSage*** window to activate this module.

Create a private *Compound* database

Before you can start entering compound data in a private database you must first create the database file with the basic information.

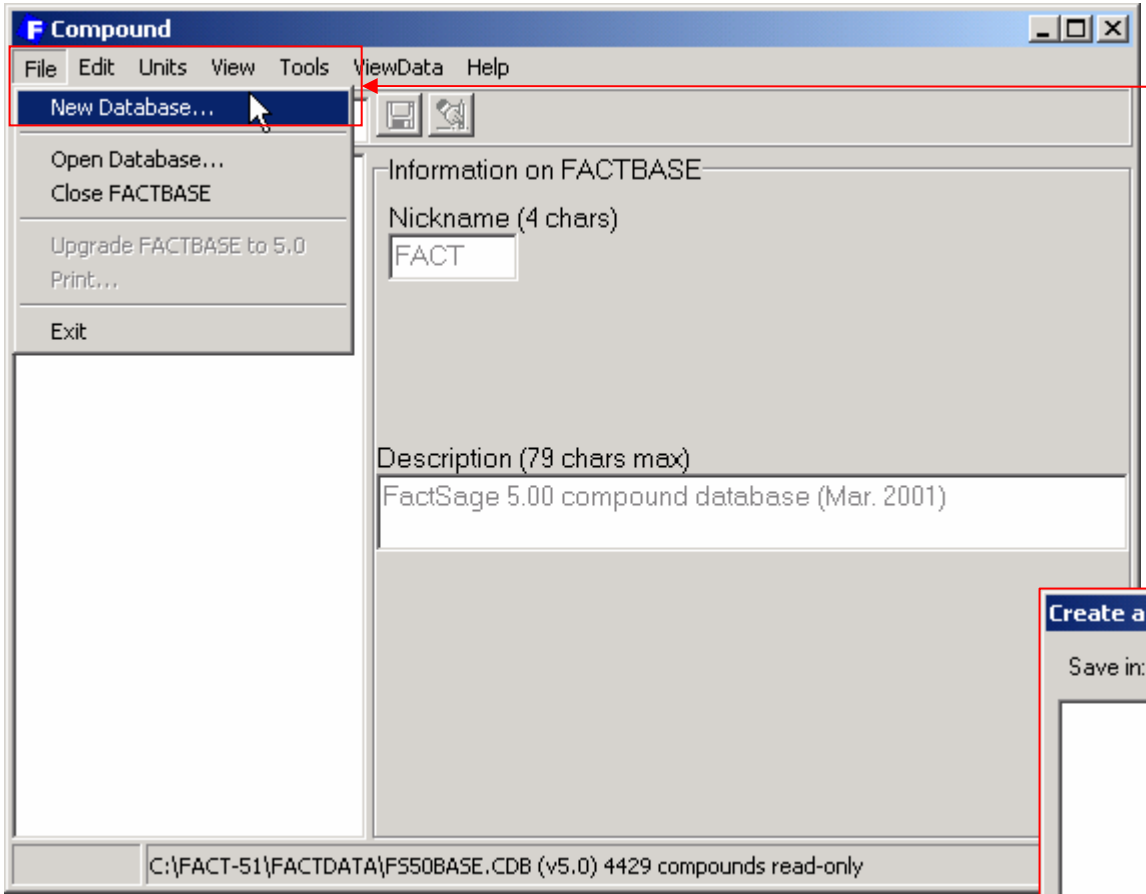
A directory must be chosen and a file name be given, a nick name must be defined and a short database description may be entered.

At the end of this procedure the Compound module will give a status of the new database showing

- its location: **path\name**
- the number of compounds it contains: **0 compound(s)** initially;
- the ***FactSage*** version it goes with: **5.0**
- and its access permission: **read/write**.

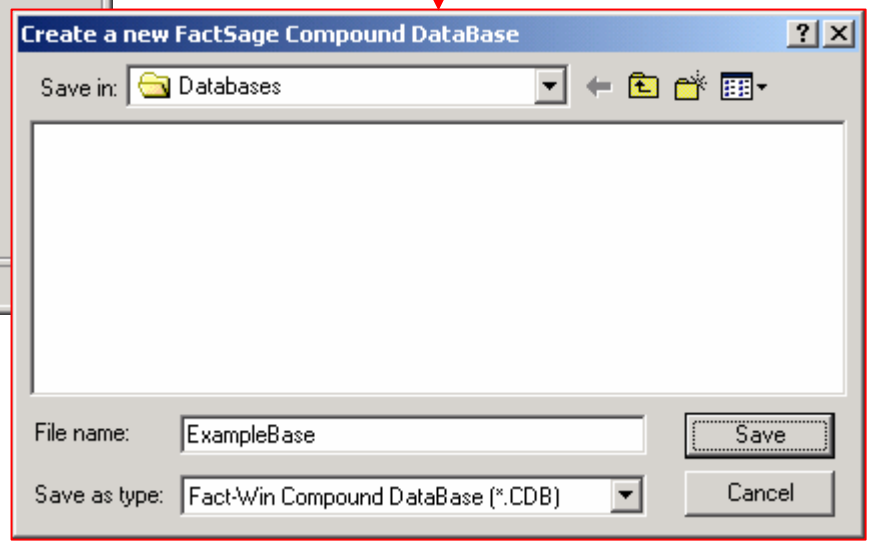
Create a private *Compound* database, I

To create a read and write ($^{r}/_{w}$) database:

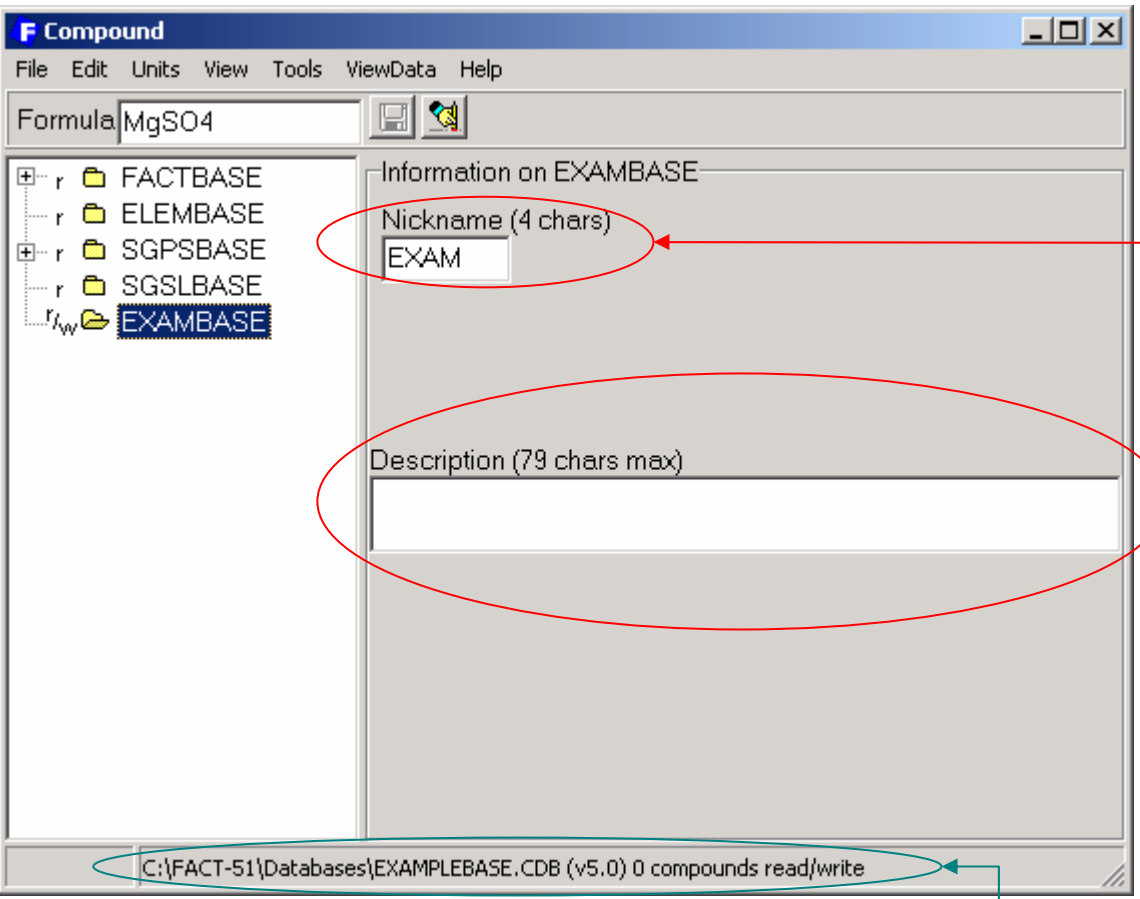


1. Click on «**New Database…**» from the «**File**» Menu

2. Choose a **filename** and select a **directory** for your new database



Create a private ***Compound*** database, II



The program selects automatically a four character nickname and adds the suffix -**BASE** to complete the name of your private database. You can edit the nickname.

You can enter a short description of your private database (with a maximum of 79 characters).

The status bar provides information on the database:

- its location: **C:\FACT-51\DATABASE\EXAMPLEBASE.CDB**;
- the number of compounds it contains: **0 compound(s)** (for now);
- its version: **5.0**;
- and its access permission: **read/write**.

Add a **compound** to the database

The following 20 slides (sections 4 to 9) show how to enter the data for a new compound with three phases (solid, liquid, gas) into a private database.

$MgCl_2$ is taken as an example. The data for this compound are summarized in slide 4.3. All entries are made using the values in this figure.

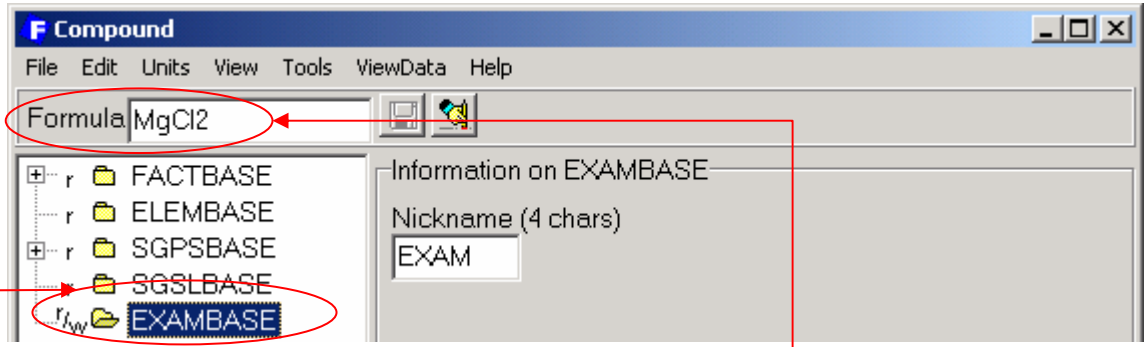
The two different variants of entering data are demonstrated:

1) H_{298}, S_{298} and C_p with transition data for the high temperature phase (using data for solid and liquid $MgCl_2$)
2) H_{298}, S_{298} and C_p for the high temperature phase itself (using data for the gas).

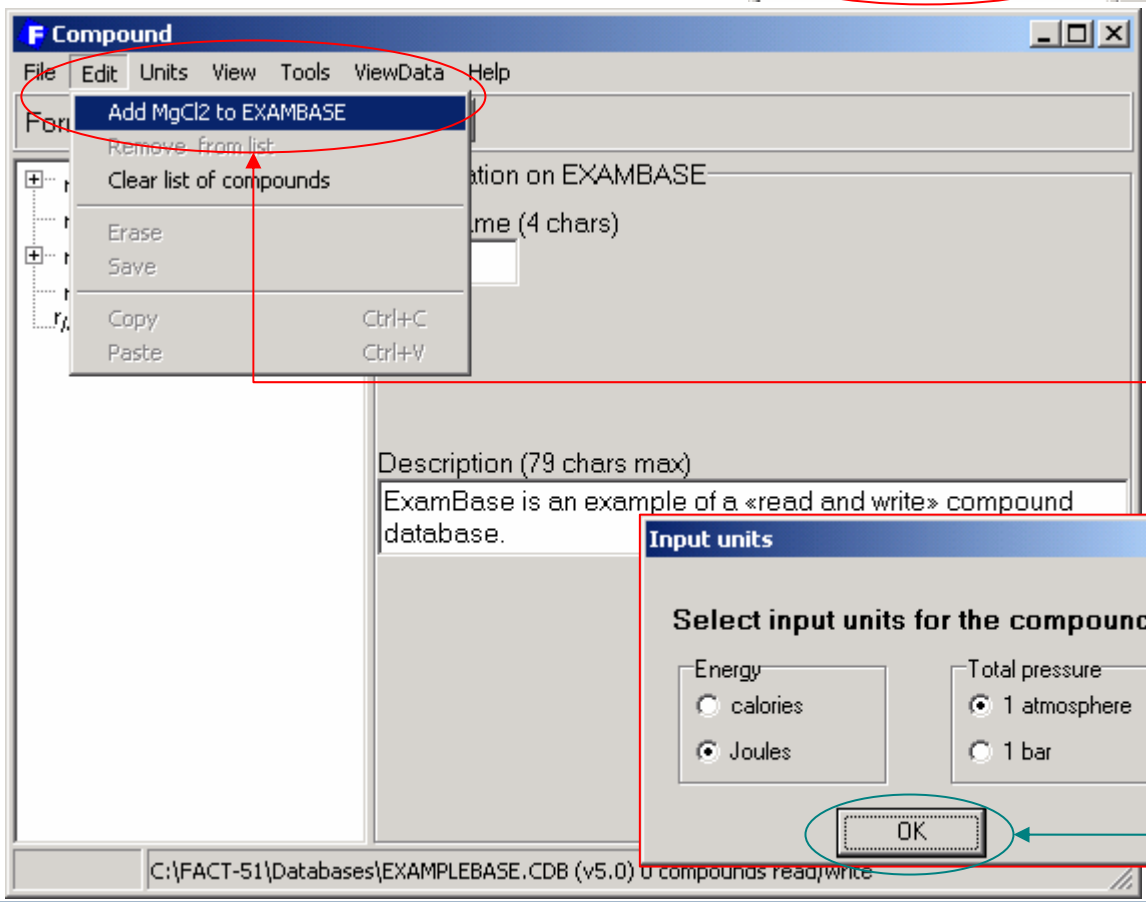
Add a **compound** to the database, I

To enter a new compound, for example **$MgCl_2$**, in the **EXAMBASE**:

1. Select **EXAMBASE** database



2. Type the chemical formula of the compound: **$MgCl_2$**, in the **Formula** input box



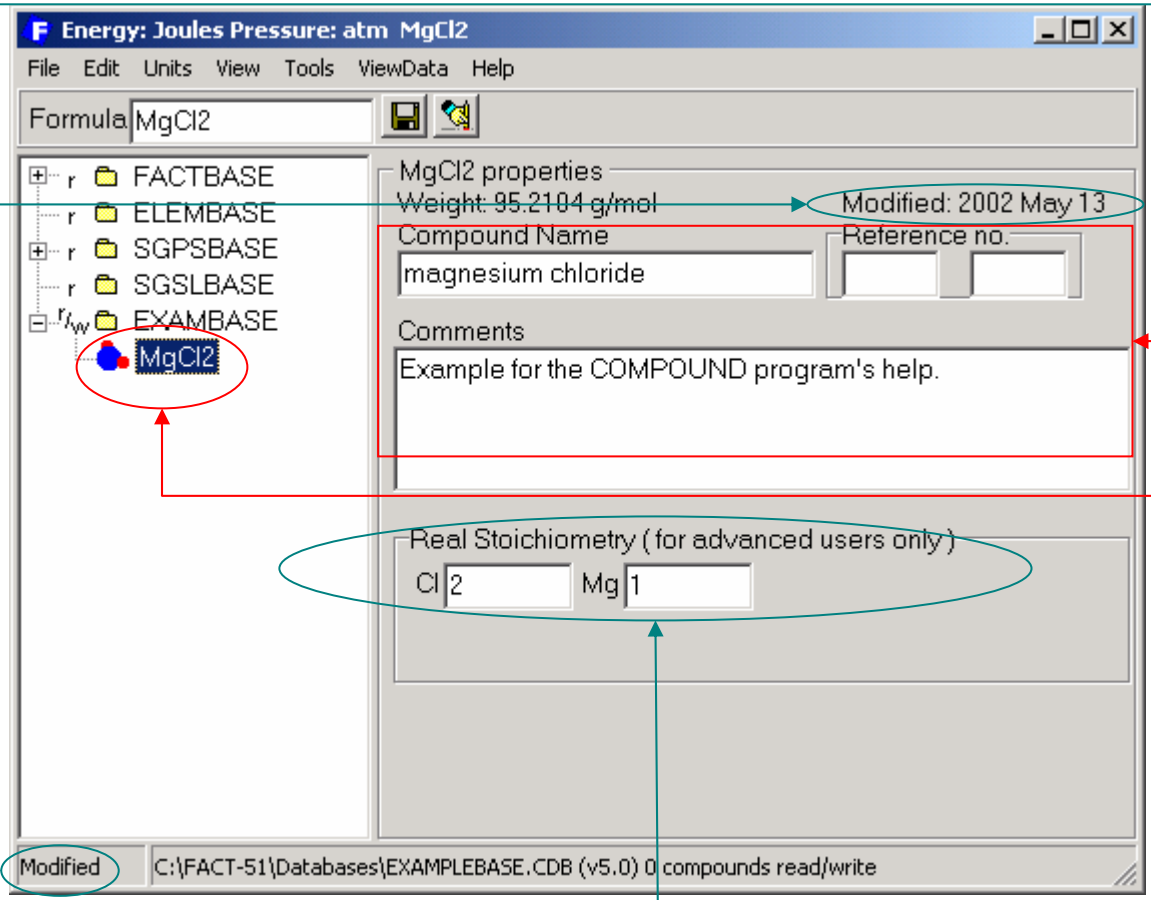
3. Select the function «**Add $MgCl_2$ to EXAMBASE**» from the **Edit** Menu.

4. Select **input units** for the compound.

5. Press «**OK**»

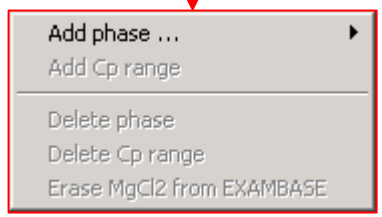
Add a **compound** to the database, II

Your database is now ready for a new entry or for a modification of a compound's data.

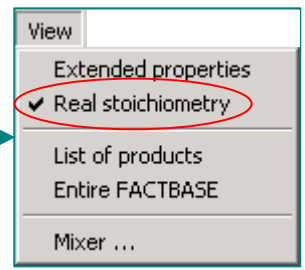


6. If you want, you can enter:
   - the **compound name**;
   - **reference number(s)**;
   - and **comments**.

7. Right click on **MgCl2** to access the following pop-up menu.

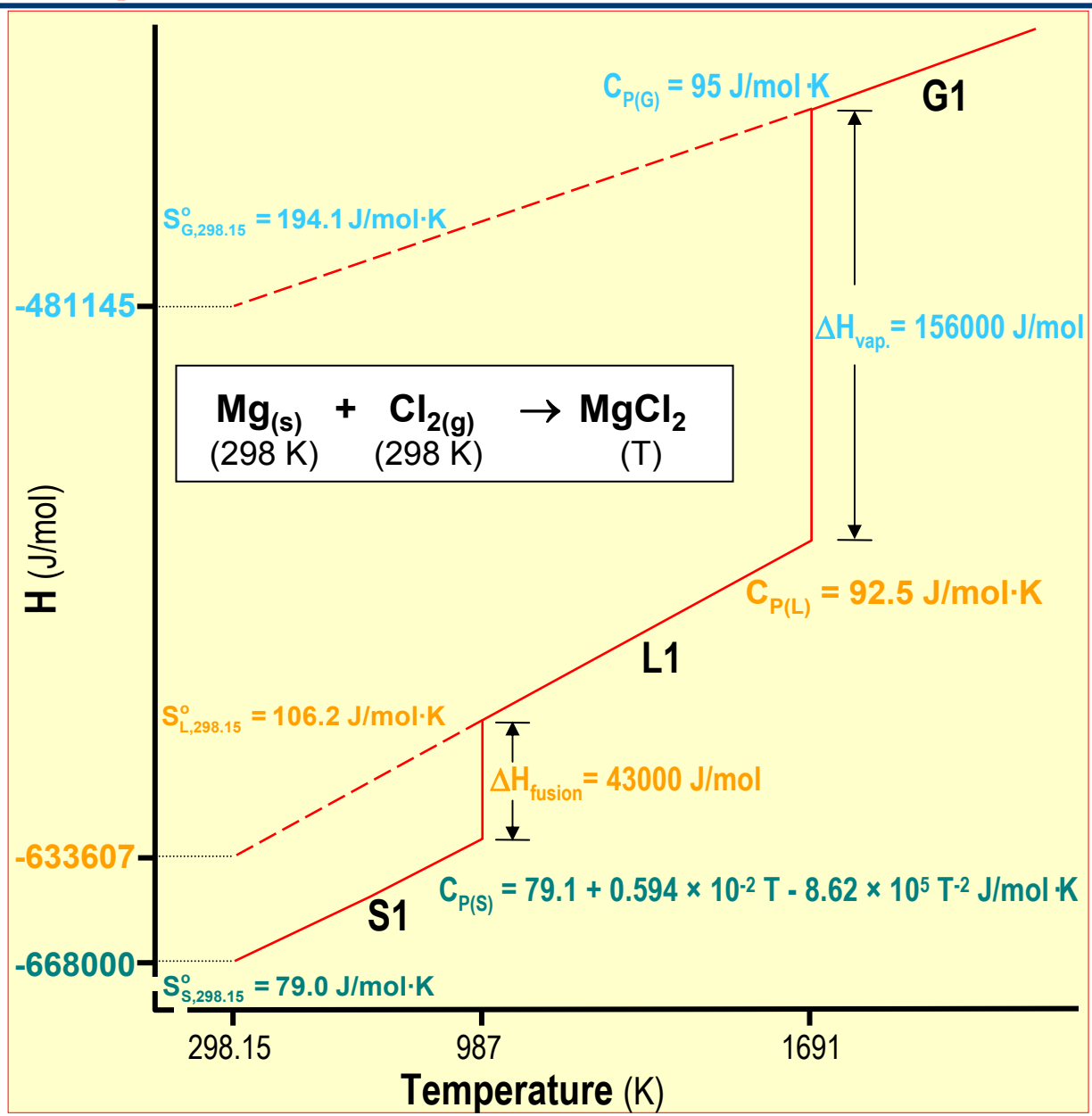


The **Real Stoichiometry** input box appears if you have checked «Real stoichiometry» in the menu **View**. This feature is for **advanced users only** and applies to **every phase of the compound** (it does not apply to elements).

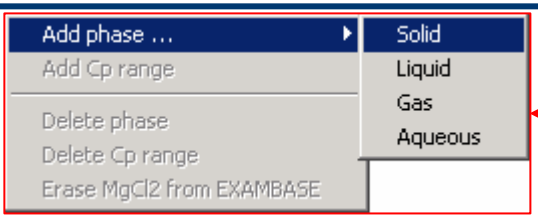


Add a **compound** to the database, III

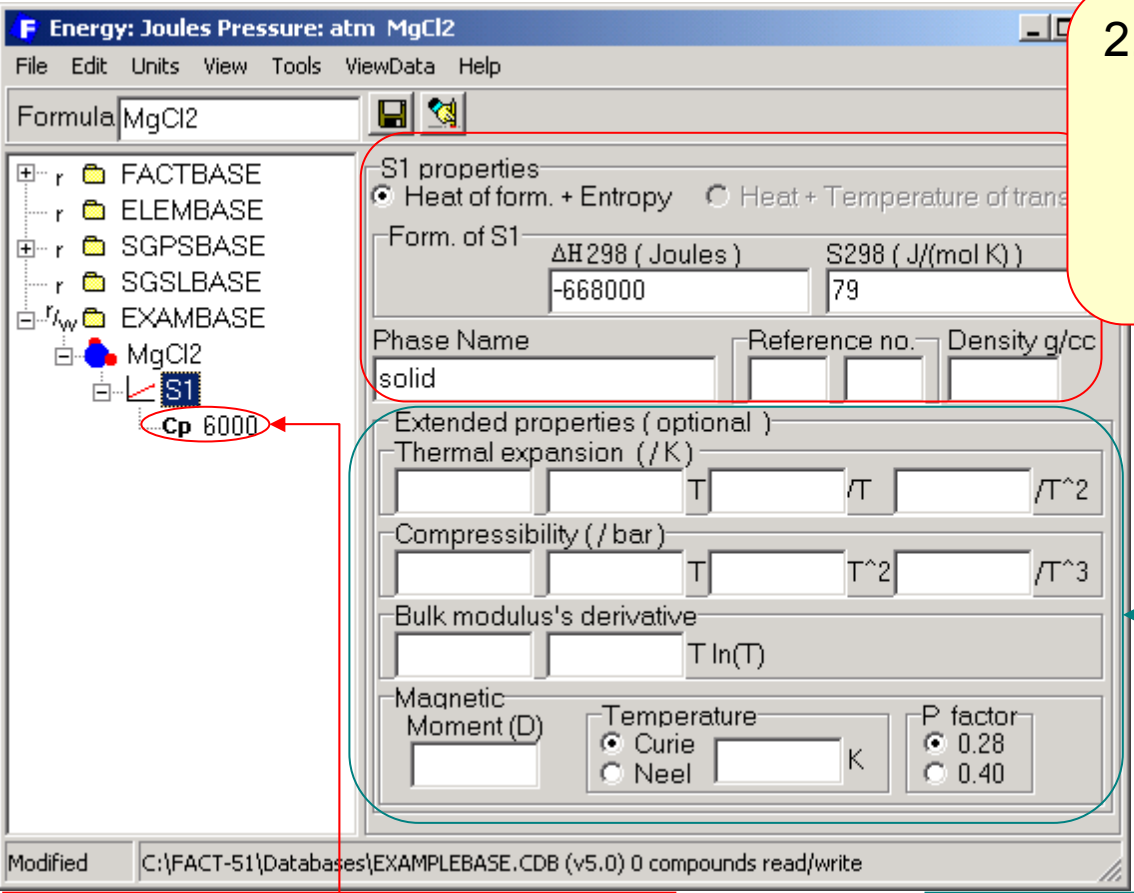
Data for **$MgCl_2$** are taken from this graph and entered into a **private database.**



Add a compound to the database: H_{298} and S_{298} for 1st phase, IV

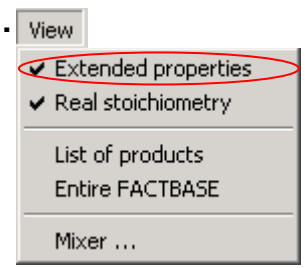


1. In the pop-up menu, point the arrow to «**Add phase…**» and select «**Solid**» from the sub menu with a left click.



2. Enter the values for the **enthalpy of formation** ($\Delta H°_{s,298.15}$) and **entropy** ($S°_{s,298.15}$). ***Compound*** only takes these values when entering data for the **first** phase.

The **Extended properties** input box appears if you have checked «Extended properties» in the menu **View**. This feature applies to a **phase exclusively**.

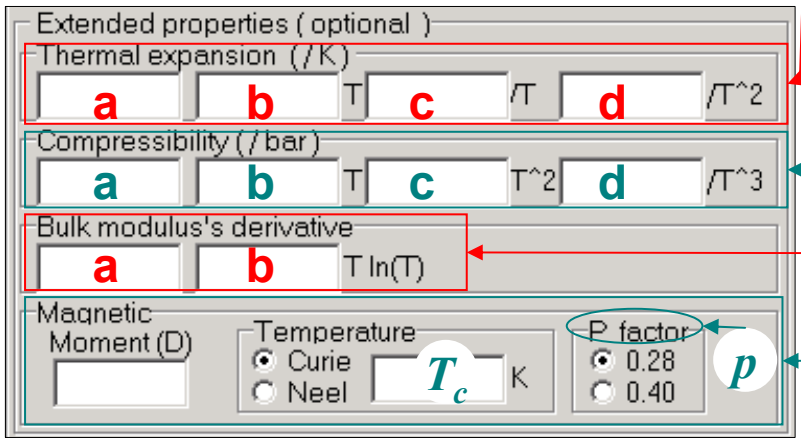


3. Left click on **Cp** 6000 to open the input box for C_p.

Values of $\Delta H°_{s,298.15}$ and $S°_{s,298.15}$ were obtained from the graph (see previous slide)

Add a **compound** to the database: **extended properties**, V

Thermal expansion expression: $a + bT + \frac{c}{T} + \frac{d}{T^2}\left[K^{-1}\right]$



Compressibility expression:

$a + bT + cT^2 + \frac{d}{T^3}\left[bar^{-1}\right]$

Bulk modulus derivative expression: $a + bT\ln T$

Magnetic contribution expression to the **Gibbs free energy** G_{mag}:

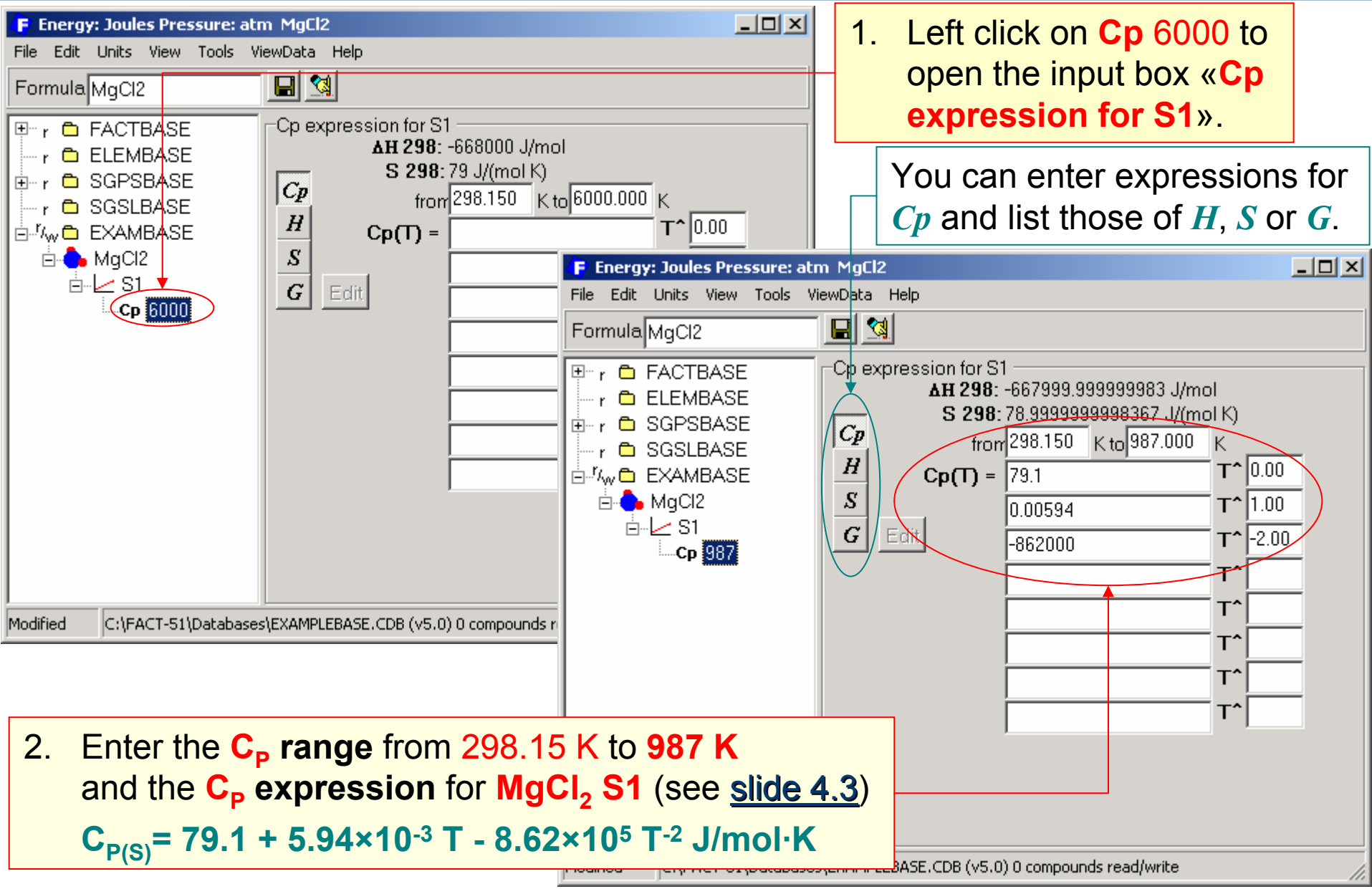
$G_{mag} = RT\ln(\beta+1)g(\tau)$ where $\tau = \frac{T}{T_c}$ and ß is the magnetic moment.

$$g(\tau) = \frac{1}{D}\left\{1 - \left[\frac{79\tau^{-1}}{140p} + \frac{474}{497}\left(p^{-1}-1\right)\left(\frac{\tau^3}{6} + \frac{\tau^9}{135} + \frac{\tau^{15}}{600}\right)\right]\right\} \quad \text{when} \quad \tau \le 1$$

$$g(\tau) = \frac{1}{D}\left[\frac{\tau^{-5}}{10} + \frac{\tau^{-15}}{315} + \frac{\tau^{-25}}{1500}\right] \quad \text{when} \quad \tau > 1$$

where $D = \frac{518}{1125} + \frac{11692}{15975}\left(p^{-1}-1\right)$, p is a phase (structure) dependent factor.

Add a **compound** to the database: C_p values for the 1st phase, VI

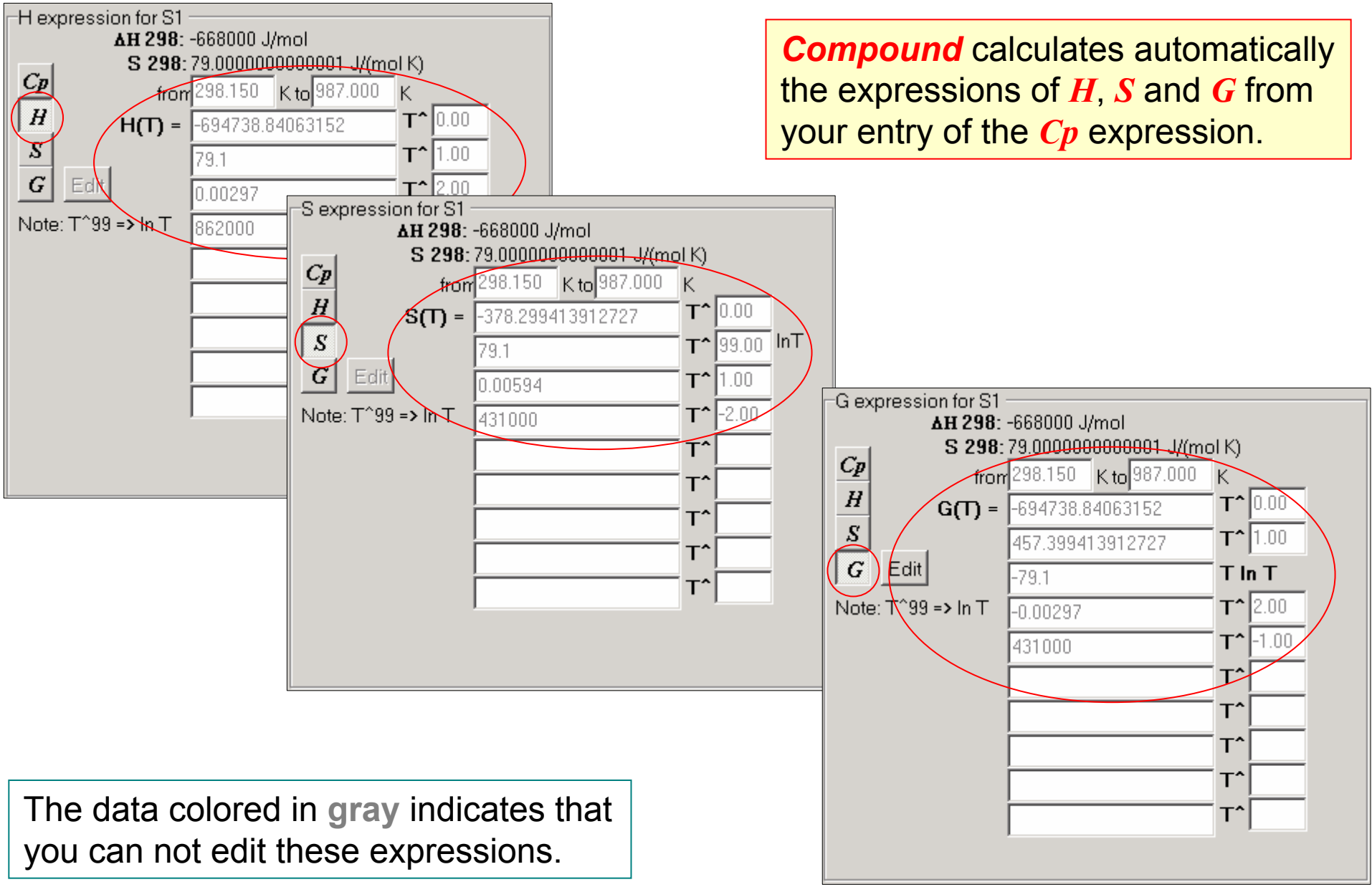


Show data as H, S and G functions

Compound permits the conversion of H_{298}, S_{298} and C_p input data into enthalpy, entropy and Gibbs energy functions.

The coefficients of these H, S and G functions can be viewed directly.

Show data as H, S and G functions



Compound calculates automatically the expressions of ***H***, ***S*** and ***G*** from your entry of the ***Cp*** expression.

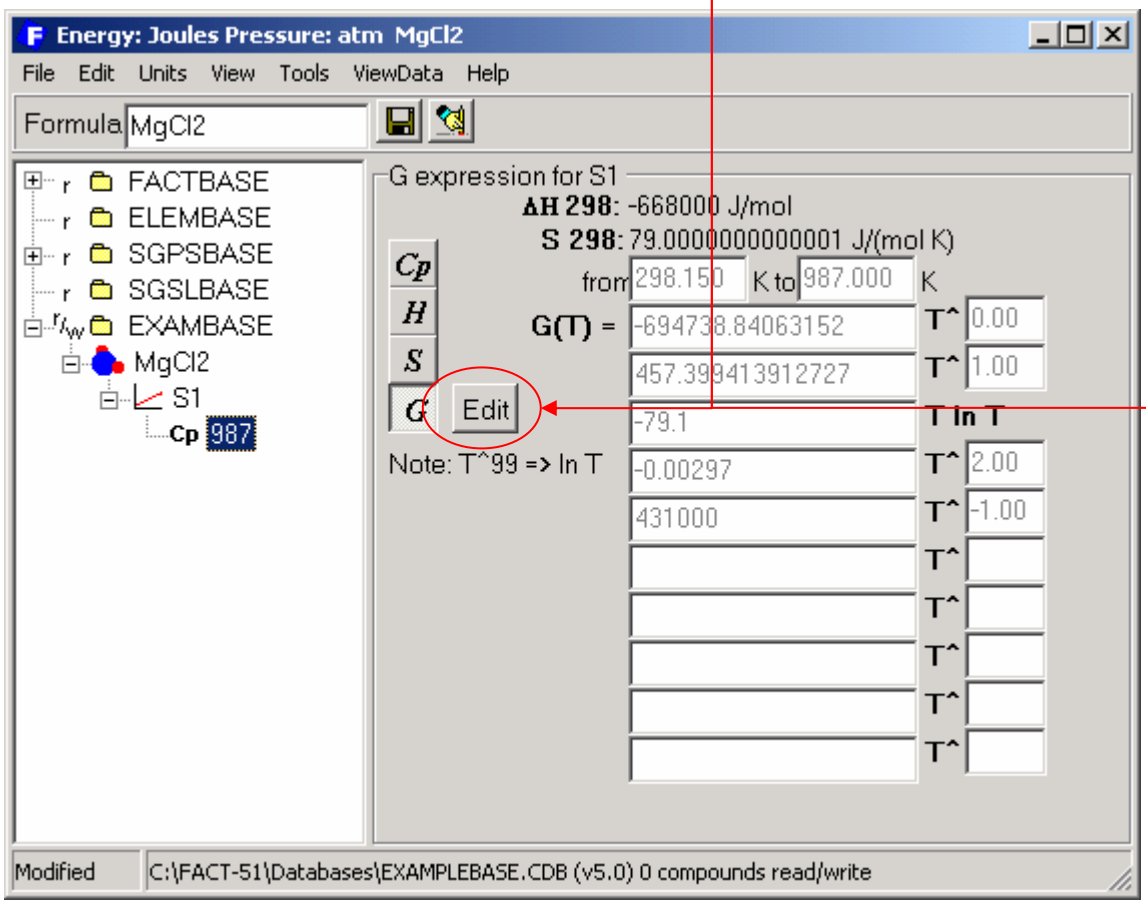
The data colored in **gray** indicates that you can not edit these expressions.

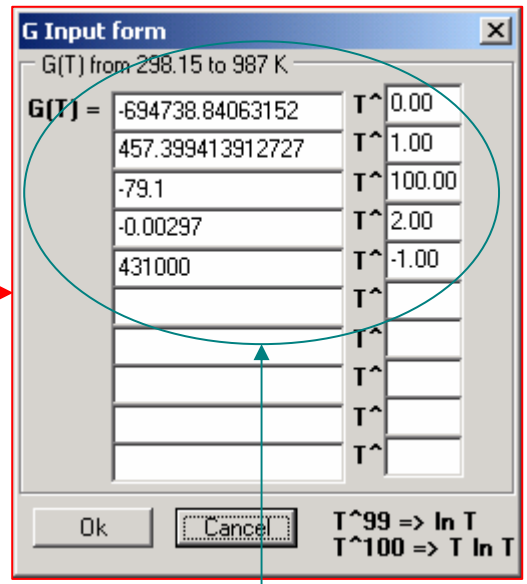
Edit the Gibbs Energy function

The following slide shows how to edit the data of a compound phase when using the Gibbs energy coefficients instead of H, S and C_p data.

Edit the Gibbs Energy function

Compound gives you the **possibility to edit** the Gibbs energy function by **pressing** the **Edit** button to open a **G Input form**.





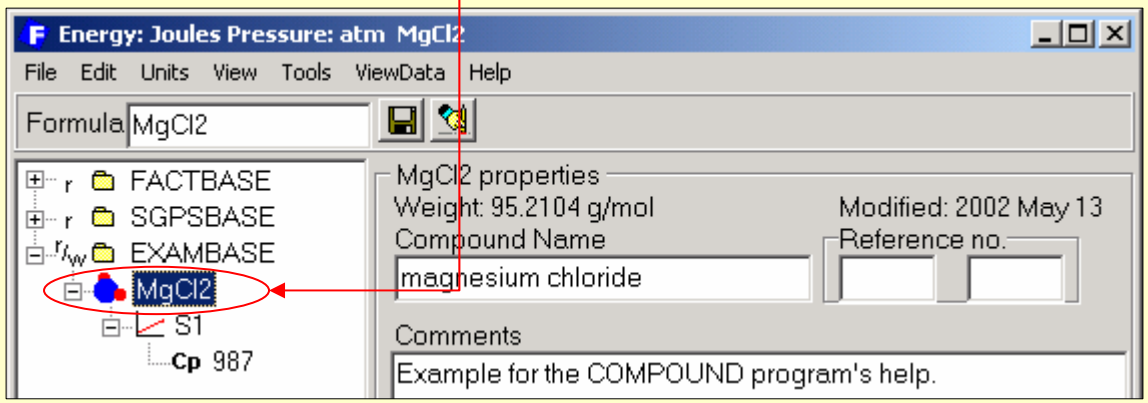
The data colored in **black** indicates that **you can edit** these expressions.

Entering phase transition data: the **liquid** phase

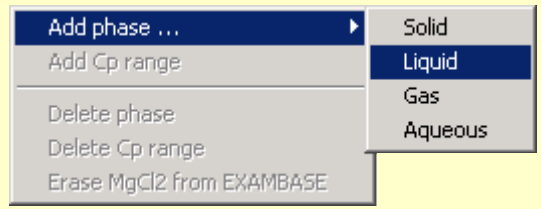
- The next three slides illustrate how to enter a new phase (here the liquid) if the data for the phase transition between the previous phase (here the solid) and the new phase, i.e. ΔH and T_{trans}, as well as the C_p data of the new phase are available.

Entering phase transition data: the **liquid** phase, I

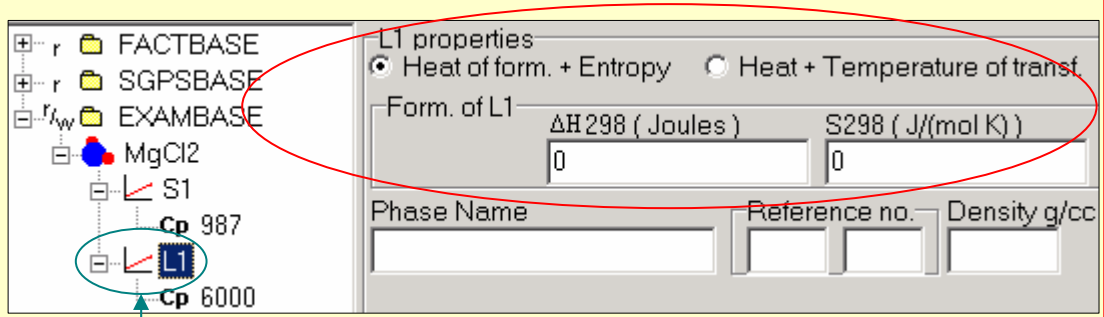
1. Right click on « MgCl2 » to open a **pop-up menu**.

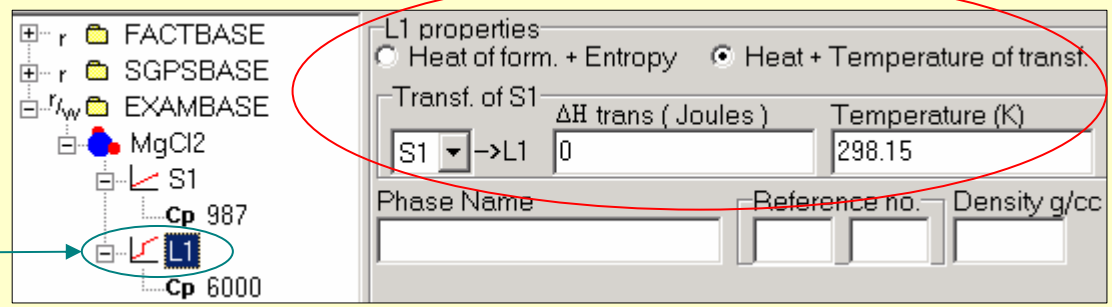


2. Point the arrow to «**Add phase…**» and select «**Liquid**» from the sub menu with a click.



3. ***Compound*** proposes two ways to enter the data:
   - either you enter the **enthalpy of formation** ($\Delta H°_{L,\,298.15}$) and **entropy** ($S°_{L,\,298.15}$) and the entry is flagged by the **icon** L1
   - or you enter the **enthalpy** and **temperature of transformation** and the entry is flagged by the **icon** L1

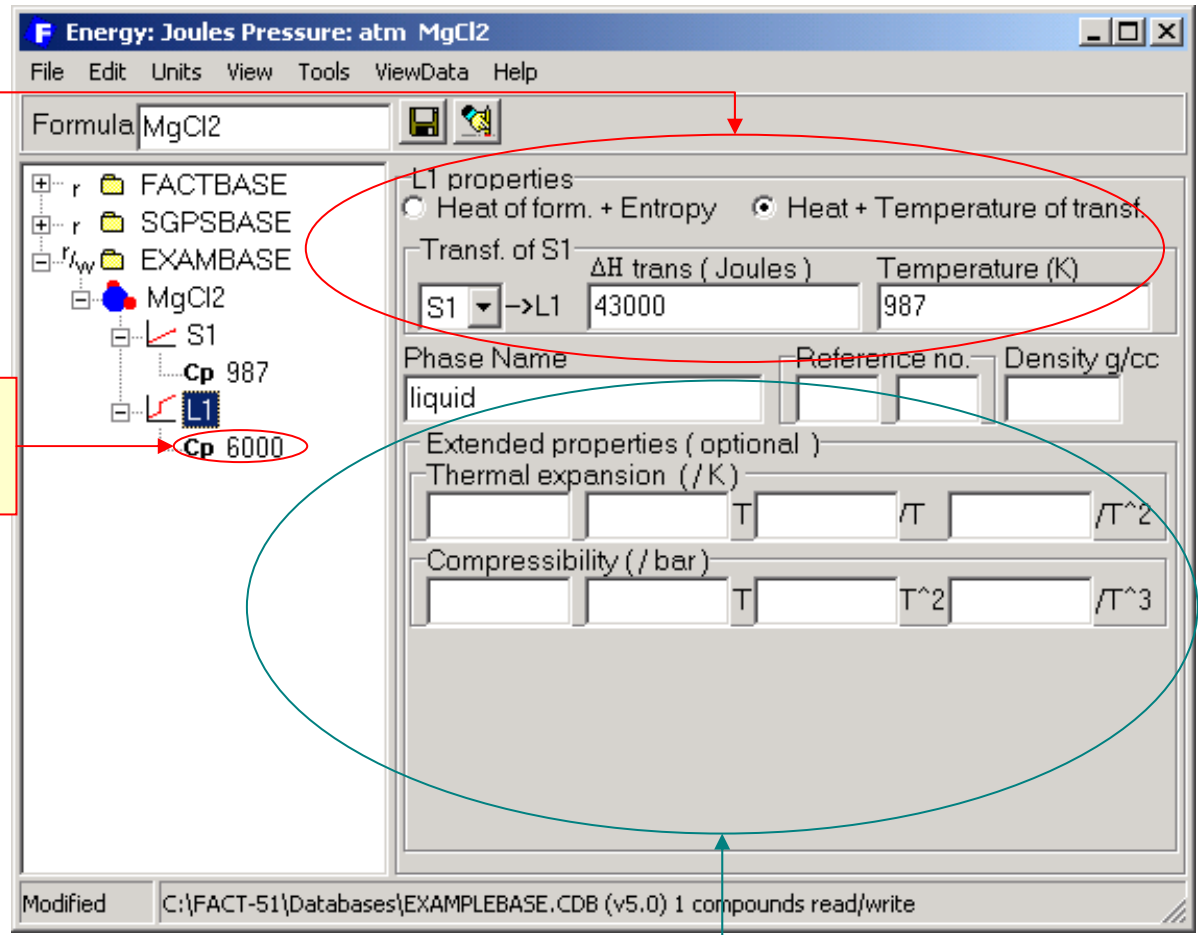


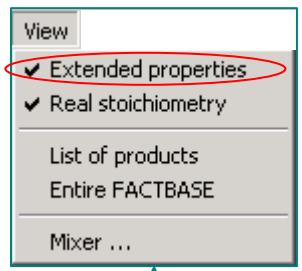


Entering phase transition data: the **liquid** phase, II

3.(continued)
Entering the **enthalpy** and **temperature** of **transformation**.

4. Click on **C_p 6000** to open the box «**Cp expression for L1**»

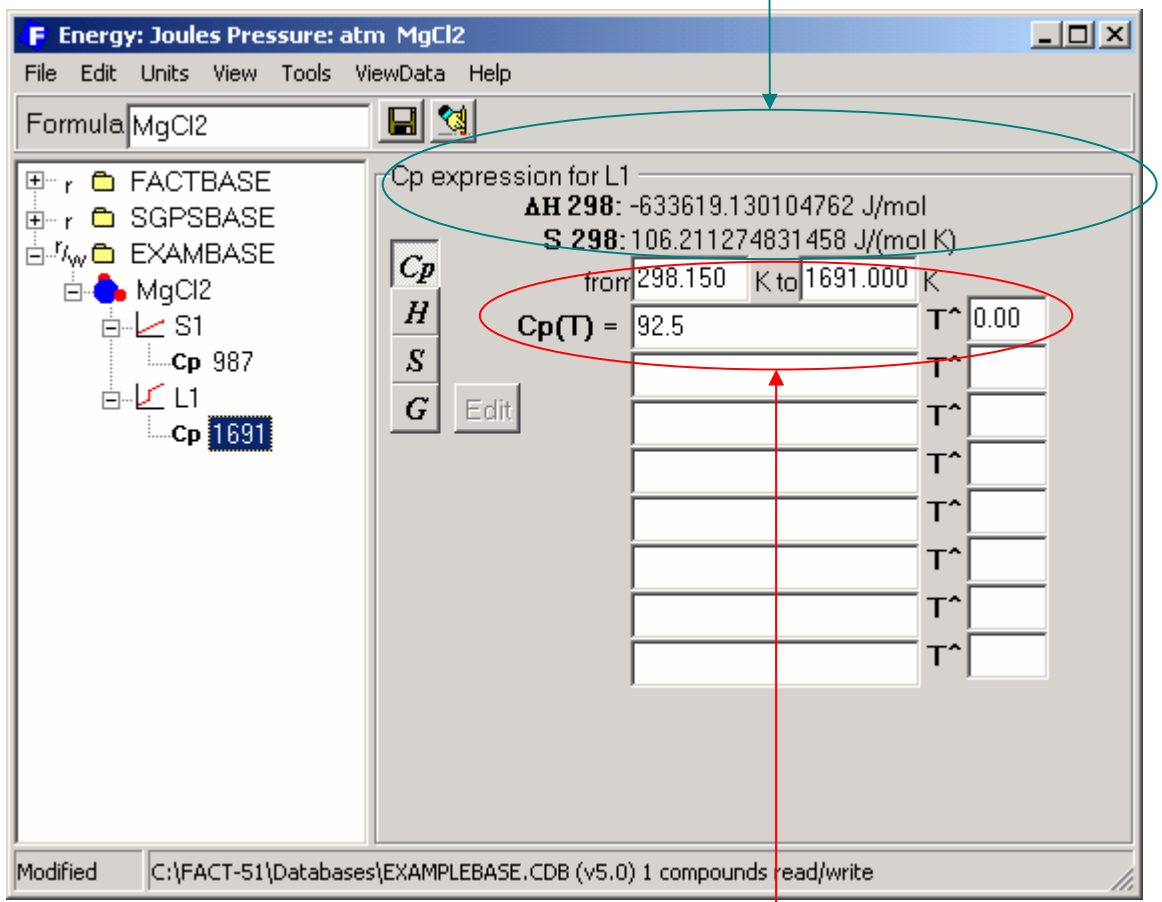




The **Extended properties** input box appears if you have checked «Extended properties» in the menu **View**. This feature applies to a **phase exclusively**.

Entering phase transition data: C_p coefficients of the liquid phase, III

Compound calculates **automatically** the values of $\Delta H°_{L,\,298.15}$ and $S°_{L,\,298.15}$ (these values are the same as those in slide 4.3).



5. **Enter** the C_P **range** from 298.15 K to **1691 K** and the C_P **expression** for **$MgCl_2$ liquid** (slide #6): $C_{P(L)} = 92.5 J/mol·K$

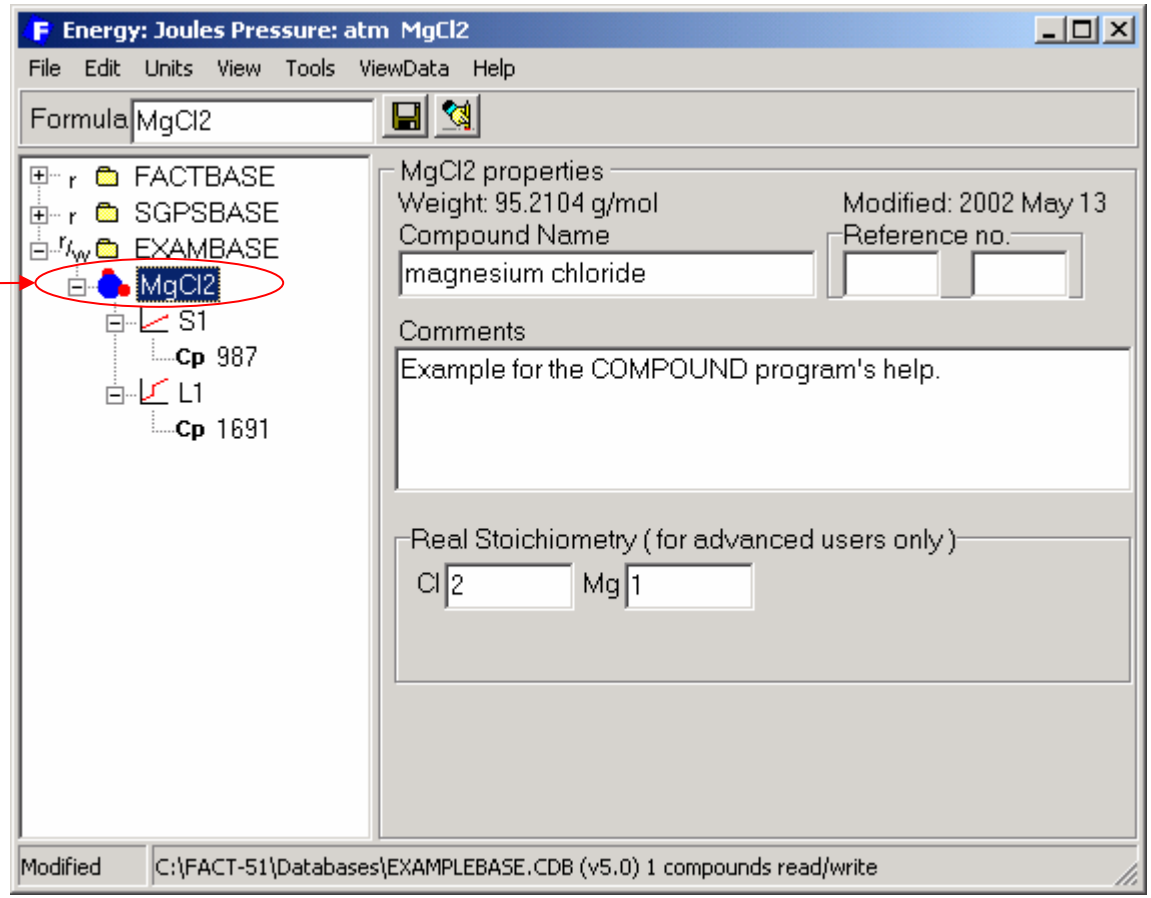
Entering a new phase with H_{298}, S_{298} and C_p: the **gaseous** phase

The following three slides show how an additional phase (here the gas) is entered for which H_{298}, S_{298} and C_p are known.

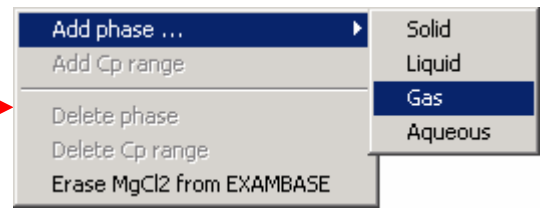
The entry of extended data for the non-ideal behaviour of the gas according to the Tsonopoulos method is also shown.

Entering a new phase with H_{298}, S_{298} and C_p: the **gaseous** phase, I

1. Right click on « MgCl2 » to open a **pop-up menu**.



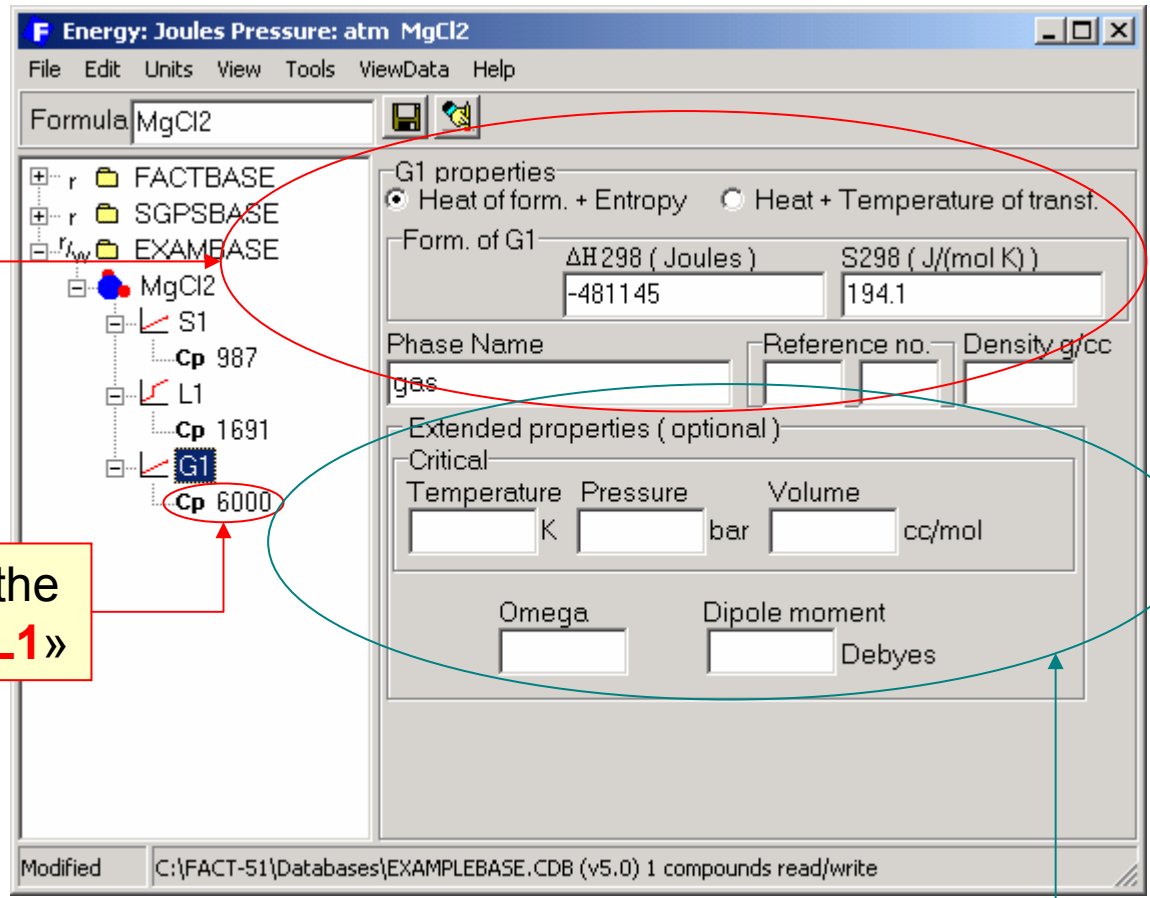
2. Point the arrow to «**Add phase…**» and select «**Gas**» from the sub menu with a click.

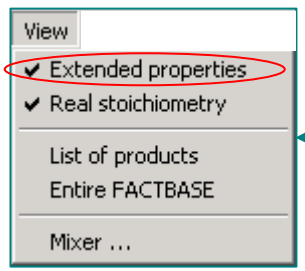


Entering a new phase with H_{298}, S_{298} and C_p: the **gaseous** phase, II

3. Enter the values for the **enthalpy of formation** ($\Delta H°_{G,298.15}$) and the **entropy** ($S°_{G,298.15}$). (See slide 4.3)

4. Click on **C_p 6000** to open the box «**Cp expression for L1**»



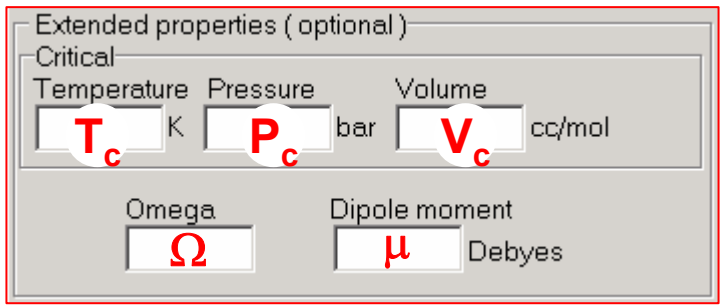


The **Extended properties** input box appears if you have checked «Extended properties» in the menu **View**. This feature applies to a **phase exclusively**.

The truncated virial equation of state is employed to treat real gases:

$$\frac{PV}{RT} = 1 + \frac{BP}{RT}$$

B is estimated for pure gases and mixtures by the Tsonopoulos* method from P_c, T_c, and Ω (omega, the acentric factor) for the pure gases. Gases are treated as non-polar. For **ideal gases**, the value of B is **zero**.



* «*An Empirical Correlation of Second Virial Coefficients*» by C. Tsonopoulos, AIChE Journal, vol. 20, No 2, pp. 263-271, 1974.

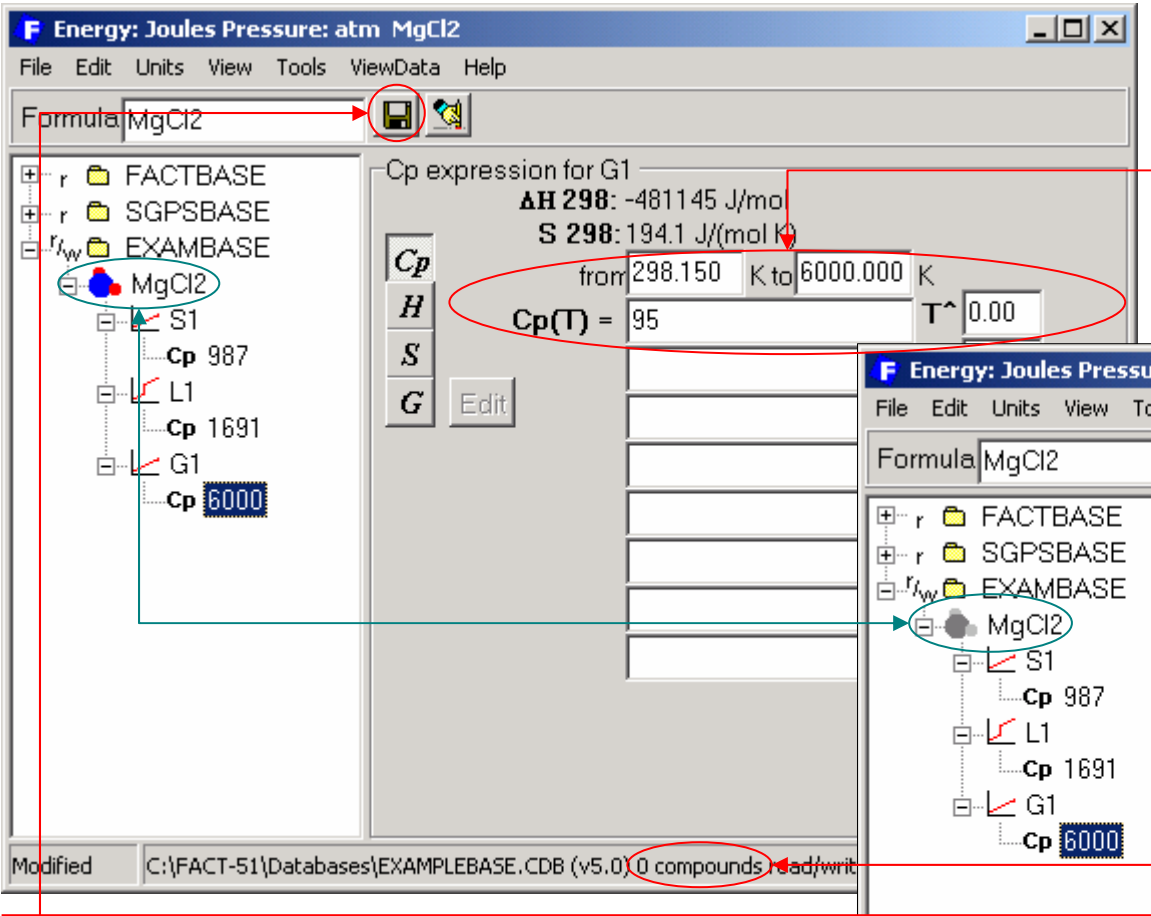
Finishing and saving the entry

The next slide shows how the last data item for $MgCl_2$, the C_p coefficient of the gas phase, is entered

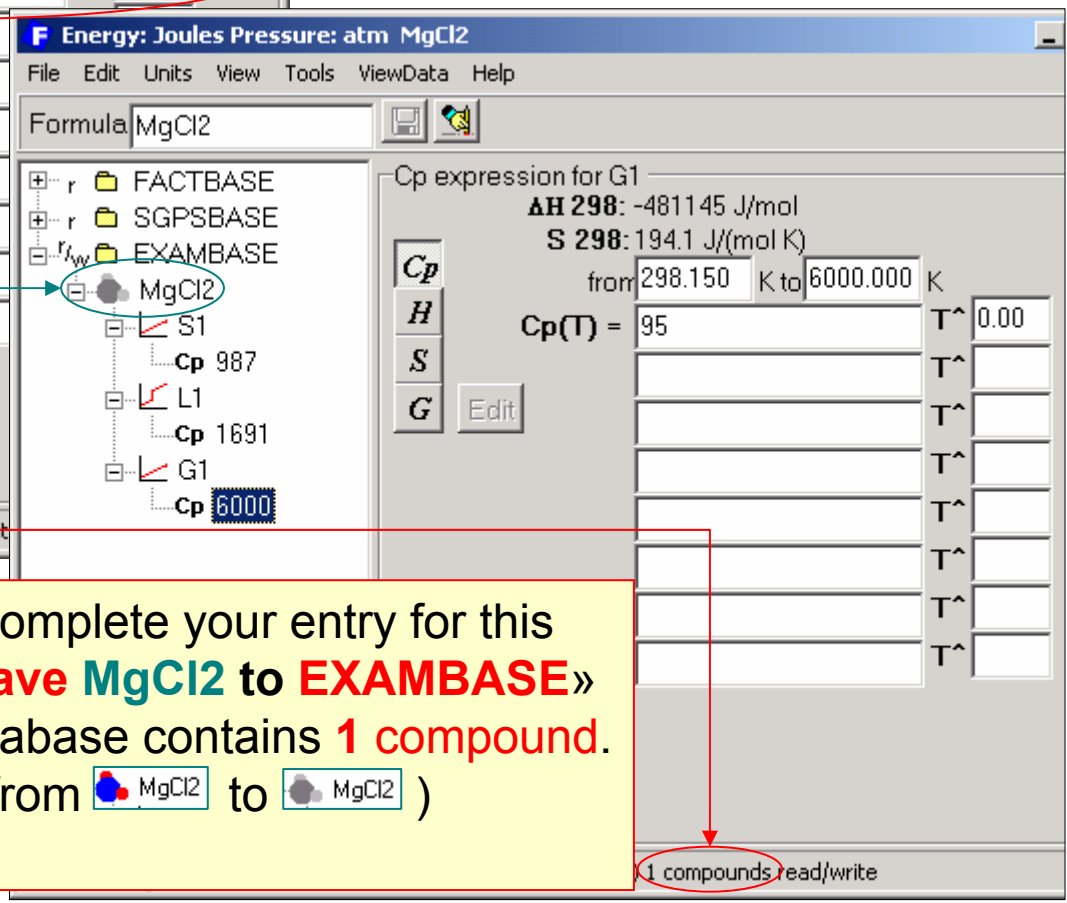
and

the complete dataset is saved in the private database.

Finishing and saving the entry, I



5. **Enter** the C_P range from 298.15 K to **6000 K** and the **C_P expression** for **$MgCl_2$ gas** (slide 4.3): $C_{P(G)}$ = 95 J/mol·K



6. **Press** on the **Save** button () to complete your entry for this compound (You can also select «**Save MgCl2 to EXAMBASE**» from the menu **Edit**). Now your database contains **1** compound. The fading of the compound **icon** (from to) indicates that your data are saved.

Viewing data and finding species

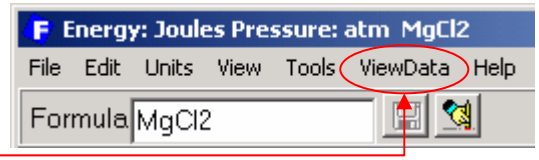
If you wish to inspect data for a compound in the format used by the ***View Data*** module you may do so from within the ***Compound*** module.

You may also inspect lists of chemical systems as generated by the ***View Data*** module from within the ***Compound*** module.

The following three view graphs show how to perform these tasks.

Viewing data and finding species, I

1. Click on «ViewData» in the menu bar to open the ***ViewData*** application at the compound (**$MgCl_2$**) and the database (**EXAMBASE**) you have selected (or the last you just worked in).



2. **Click** on the **Cp(T)** and **Phases** tabs to see the **data** you have just entered or the **values** calculated by ***Compound*** from your data entry.

MgCl2 Units: P(atm) Energy(J)

File Edit Units Summary Databases Table Graph Help

3 Phases | EXAM - EXAM compound database

Phases | **Cp(T)** | H(T) | G(T) | S(T) | Volume | Magnetic | Refs.

Name: magnesium chloride

$$C_P = \sum_{i=1}^{8} C_{(i)} T^{P(i)}$$

Cp range: T(min) - T(max).
When T < T(min), Cp(T) is extrapolated.
When T > T(max), Cp(T) at T(max) is used.

	DH(298.15) (J)	S(298.15) (J/K)	C(i)	P(i)	C(i)	P(i)	Cp (K)
S	-668000.00	79.000000	79.100000	0	5.94000000E-03	1	298 - 987
			-862000.00	-2			
L	-633619.13	106.211275	92.500000	0			298 - 1691
G	-481145.00	194.100000	95.000000	0			298 - 6000

FactSage 5.1 | C:\FACT-51\DATABASES\EXAMPLEBASE.CDB (v

Phases | Cp(T) | H(T) | G(T) | S(T) | Volume | Magnetic | Refs.

Name: magnesium chloride

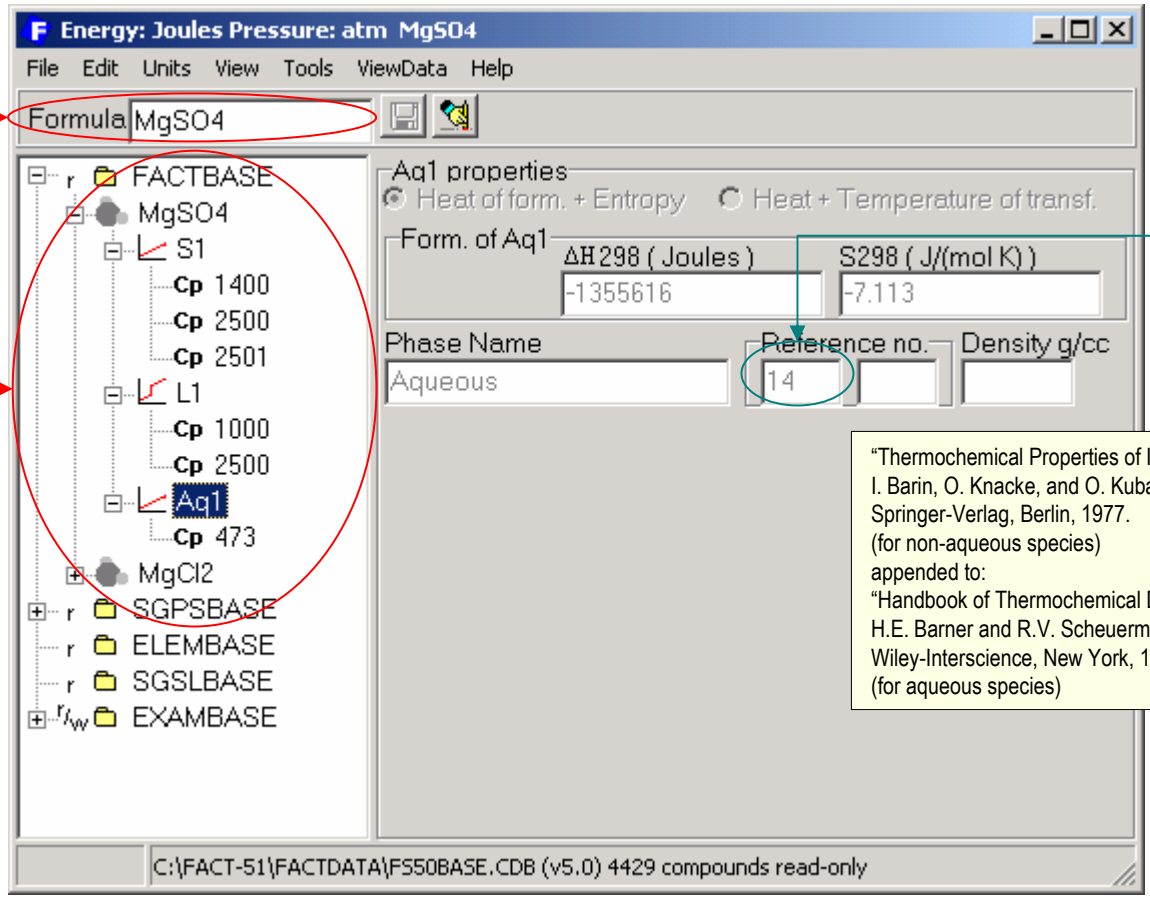
Formula Weight: 95.2104

Stoichiometric Compound: MgCl2

	Phase	Cp Range, K	Density, g/ml	Ref.
S	solid	298.15 - 987.00		
L	liquid	298.15 - 1691.00		
G	gas	298.15 - 6000.00	ideal	

Viewing data and finding species, II

1. To look at the data of a **compound** found in a **database**, for example **$MgSO_4$** in **FACTBASE**: **enter MgSO4** in the Formula input box.



Move the pointer over the reference text box to view the **detailed bibliography**

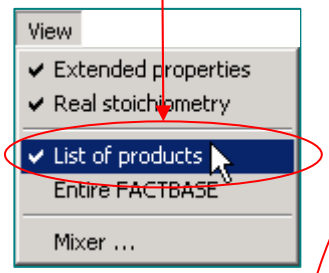
"Thermochemical Properties of Inorganic Substances",
I. Barin, O. Knacke, and O. Kubaschewski,
Springer-Verlag, Berlin, 1977.
(for non-aqueous species)
appended to:
"Handbook of Thermochemical Data for Compounds and Aqueous Species",
H.E. Barner and R.V. Scheuerman,
Wiley-Interscience, New York, 1978.
(for aqueous species)

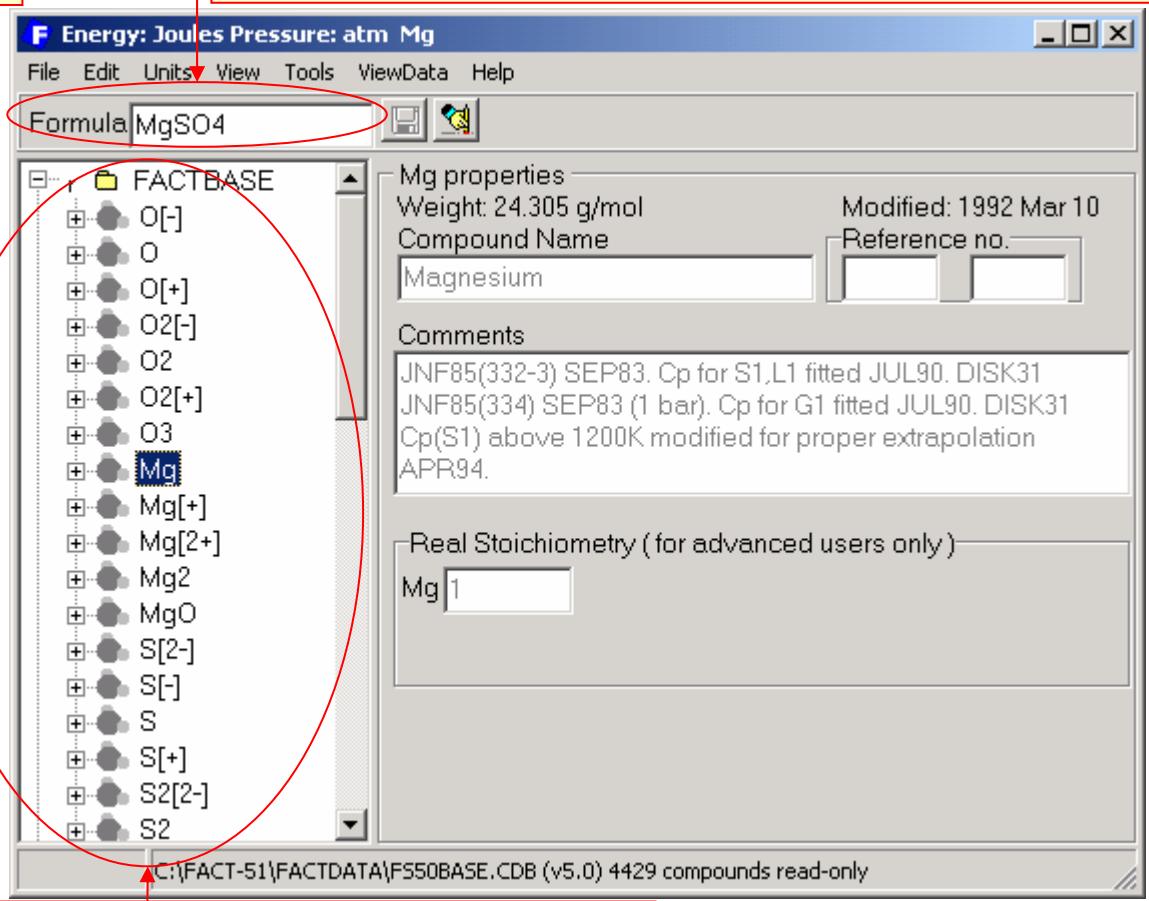
2. Expand the tree structure for **FACTBASE** and search through the **MgSO4** branches to list its data. Note that data for **$MgCl_2$** is also shown.

Viewing data and finding species, III

1. Select «**List of products**» in the **View** menu.

2. Enter a chemical formula of a compound (Formula MgSO4) or the elements (Formula OSMg) of interest in the Formula input box. For example **O**, **S** and **Mg**.





3. Expand the tree structure to see the list of compounds containing **O**, **S** and/or **Mg**.

Transferring data between databases

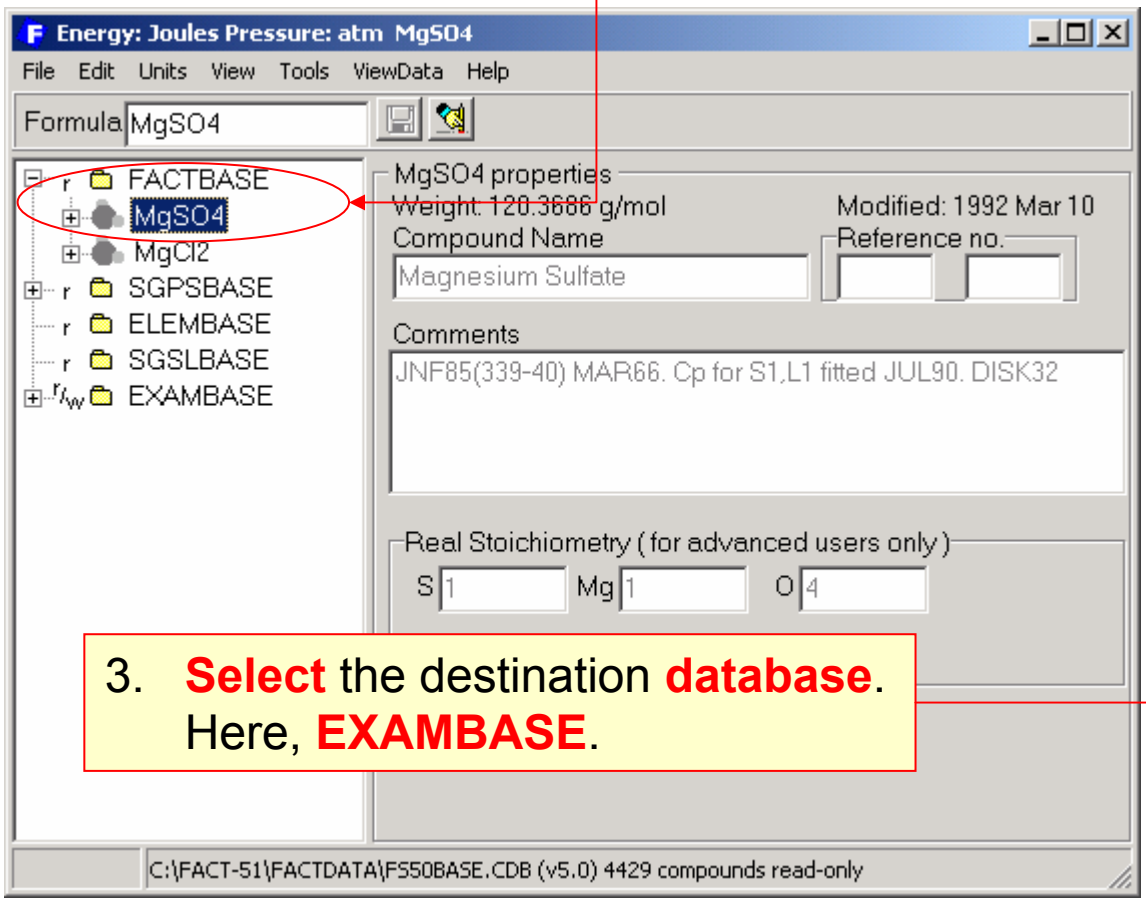
Data for single compounds can easily be transferred between databases.

This is particularly useful if you want to investigate how data changes for a compound in a read only database affect results in calculations. Simply generate your own private read and write database and copy the desired compound(s) from the read only database over to your private database.

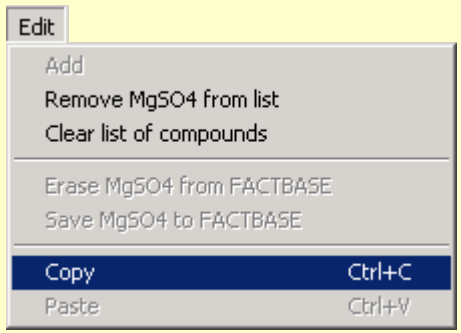
There are two ways how to do that which will are described in the following to view graphs.

Transferring data between databases, I

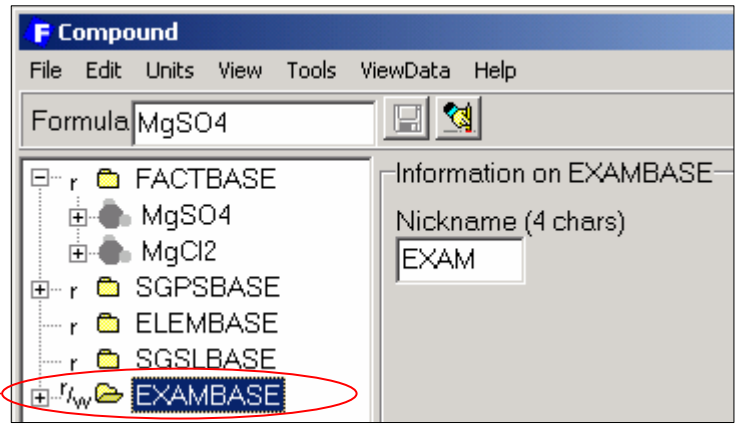
1. **Select** the **compound** of interest in its **database**. For example, **click** on **$MgSO_4$** in **FACTBASE**.



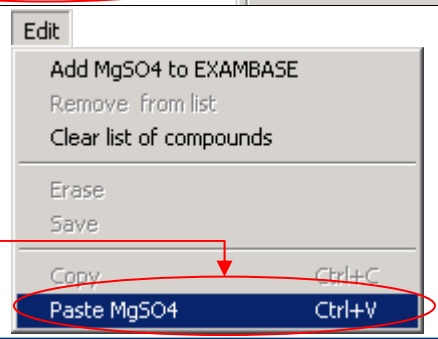
2. Select «**Copy**» from the **Edit** menu.



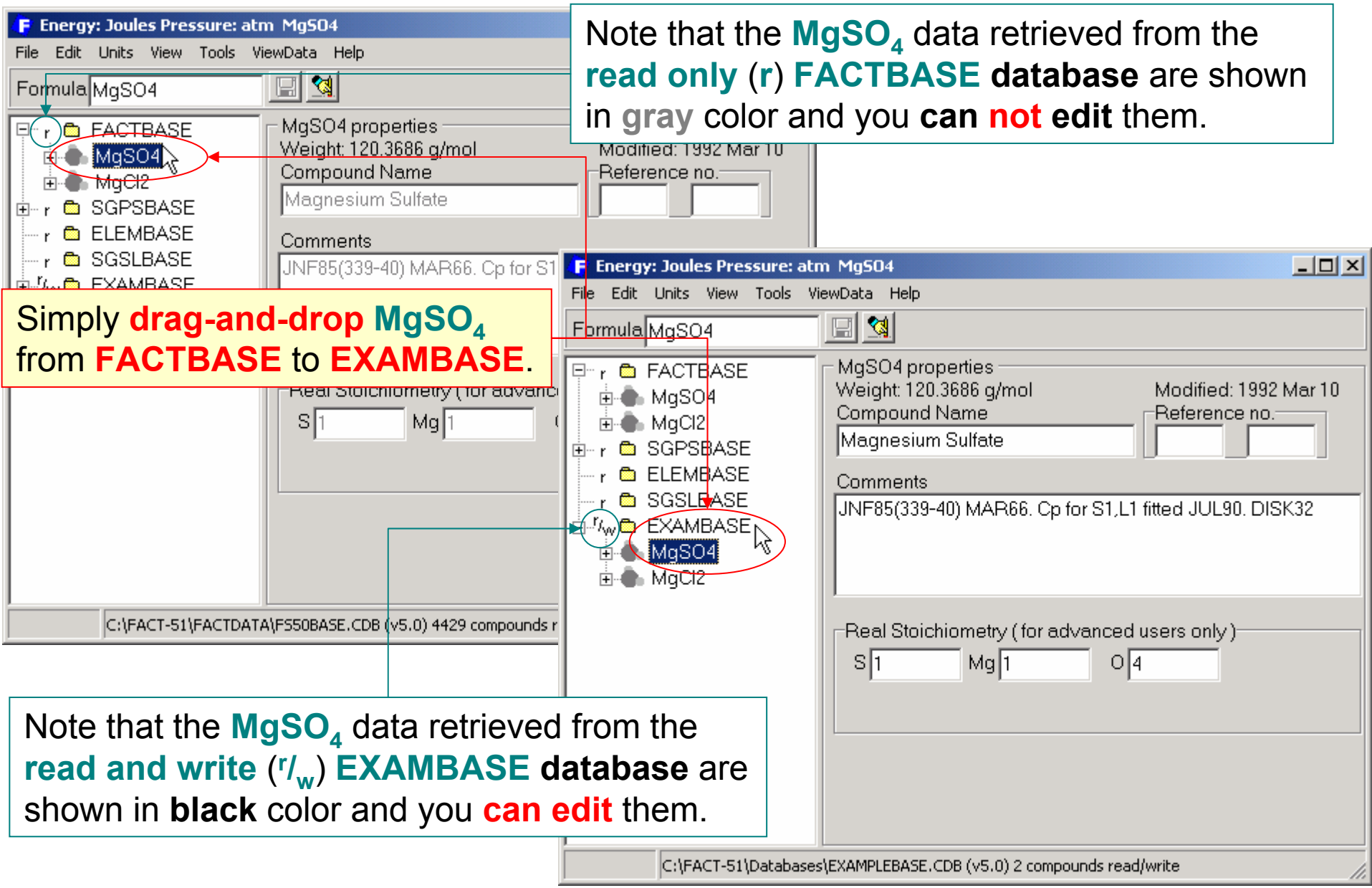
3. **Select** the destination **database**. Here, **EXAMBASE**.



4. Select «**Paste MgSO4**» from the **Edit** menu.



Transferring data between databases, II



Note that the $MgSO_4$ data retrieved from the **read only** (r) **FACTBASE database** are shown in **gray** color and you **can not edit** them.

Simply **drag-and-drop** $MgSO_4$ from **FACTBASE** to **EXAMBASE**.

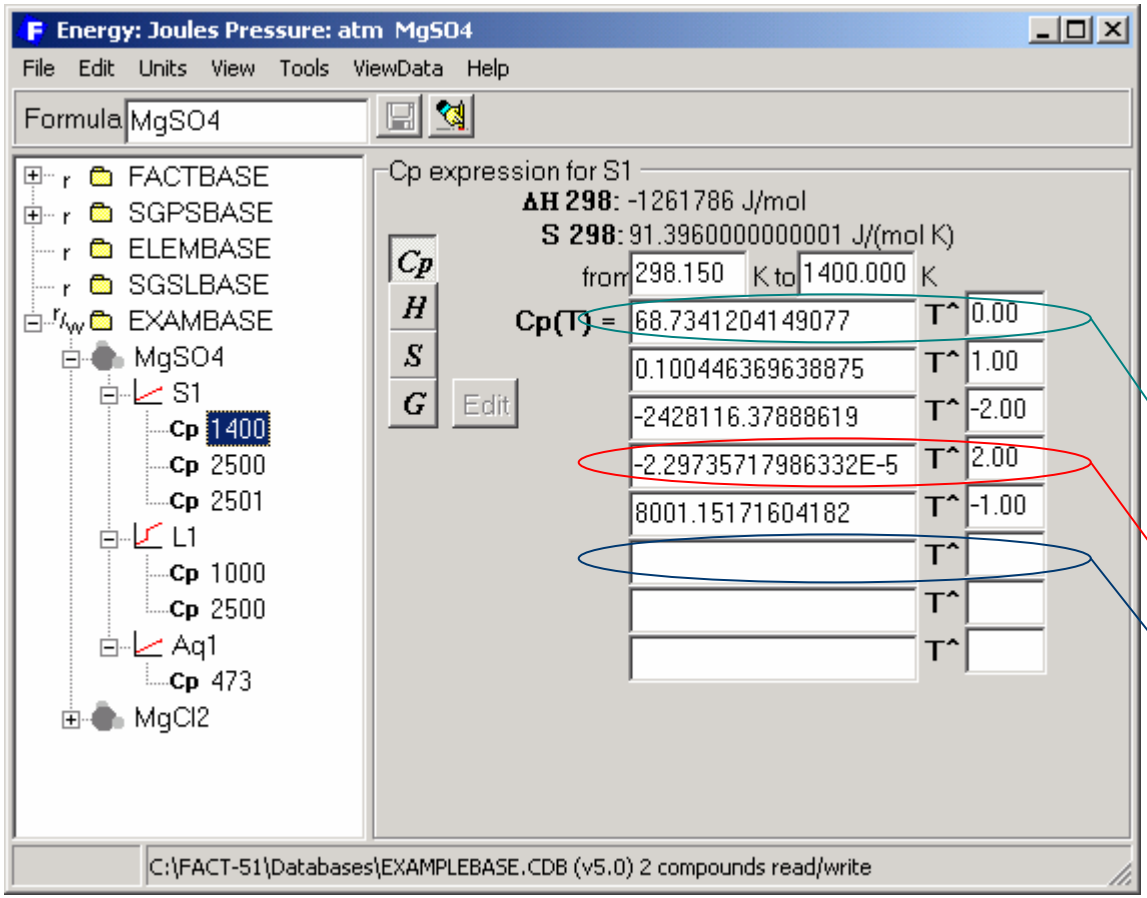
Note that the $MgSO_4$ data retrieved from the **read and write** ($^r/_w$) **EXAMBASE database** are shown in **black** color and you **can edit** them.

Editing a read and write ($^{r}/_{w}$) database

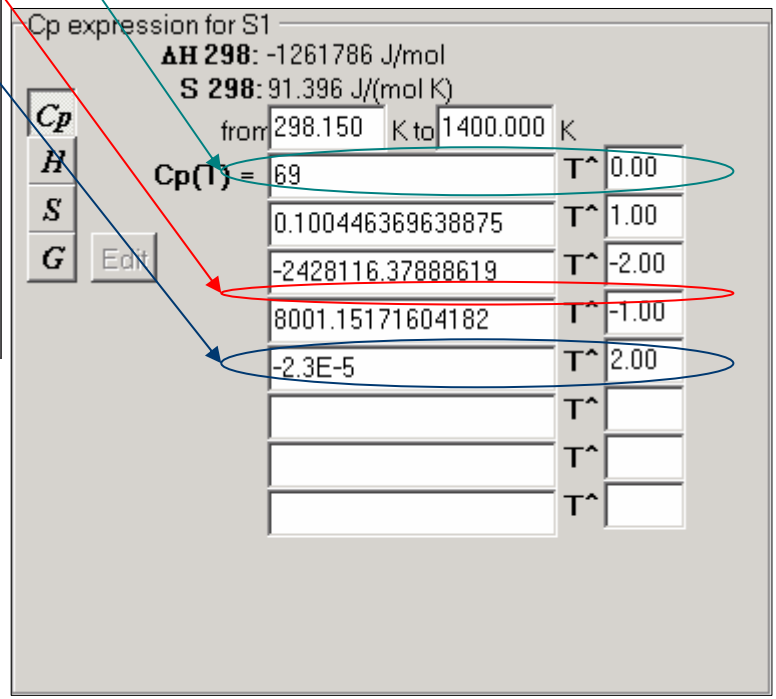
Data in a read and write database may be **added**, **removed** or **modified**.

In the example the **C_p** range for the solid (S1) phase of **$MgSO_4$** in the $^{r}/_{w}$ **EXAMBASE database** is **edited**.

Editing a read and write ($^{r}/_{w}$) database.



You can expand and reduce the extent of the tree structure of the **databases** by left clicking on the box at the right of an icon.



The Erase, Remove and Clear commands

The Erase, Remove and Clear commands permit

- to erase (delete) single compounds from a particular database,
- to remove single compounds from an edit list

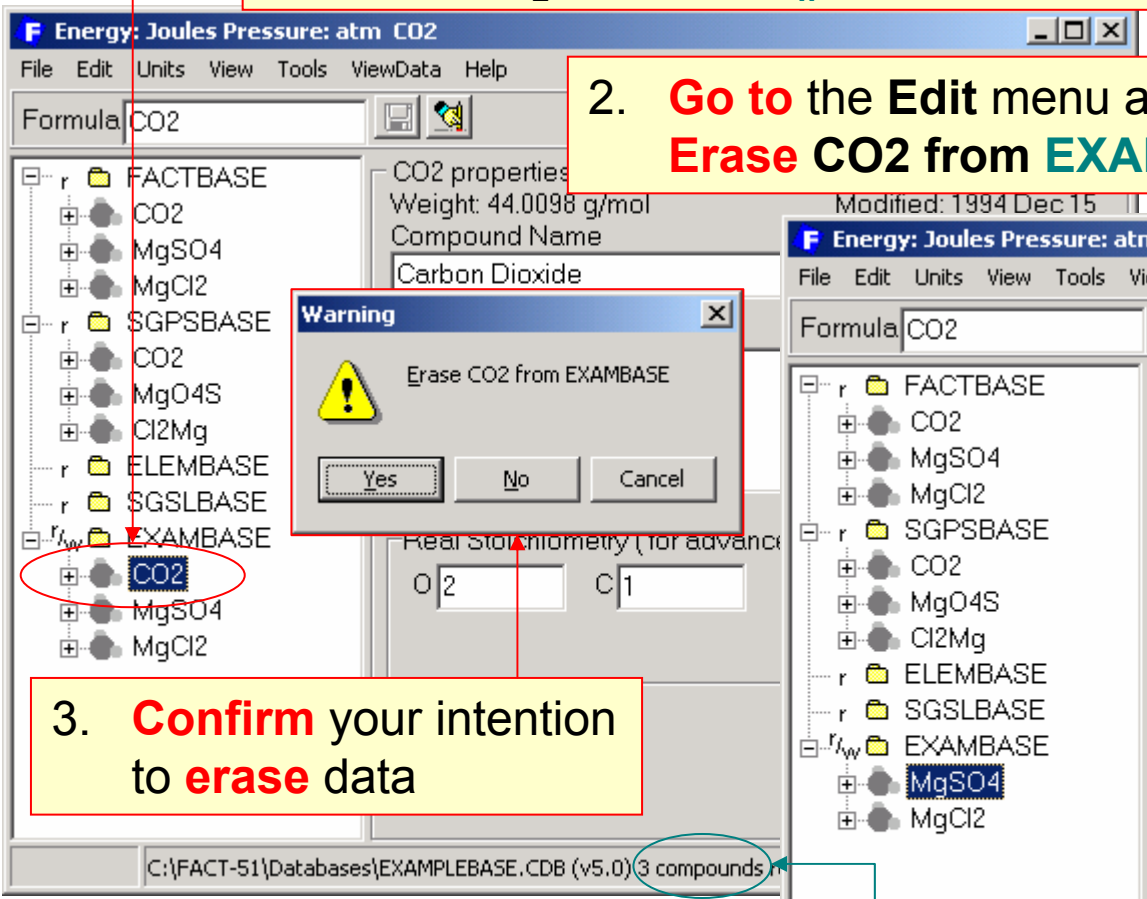
  and

- to clear complete edit lists.

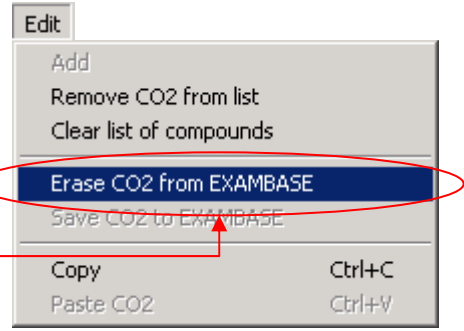
NOTE: The latter two commands do NOT interfer with the contents of databases. They are therefore applicable with all types of databases.
The Erase command only works for read/write databases.

The Erase, Remove and Clear commands, I

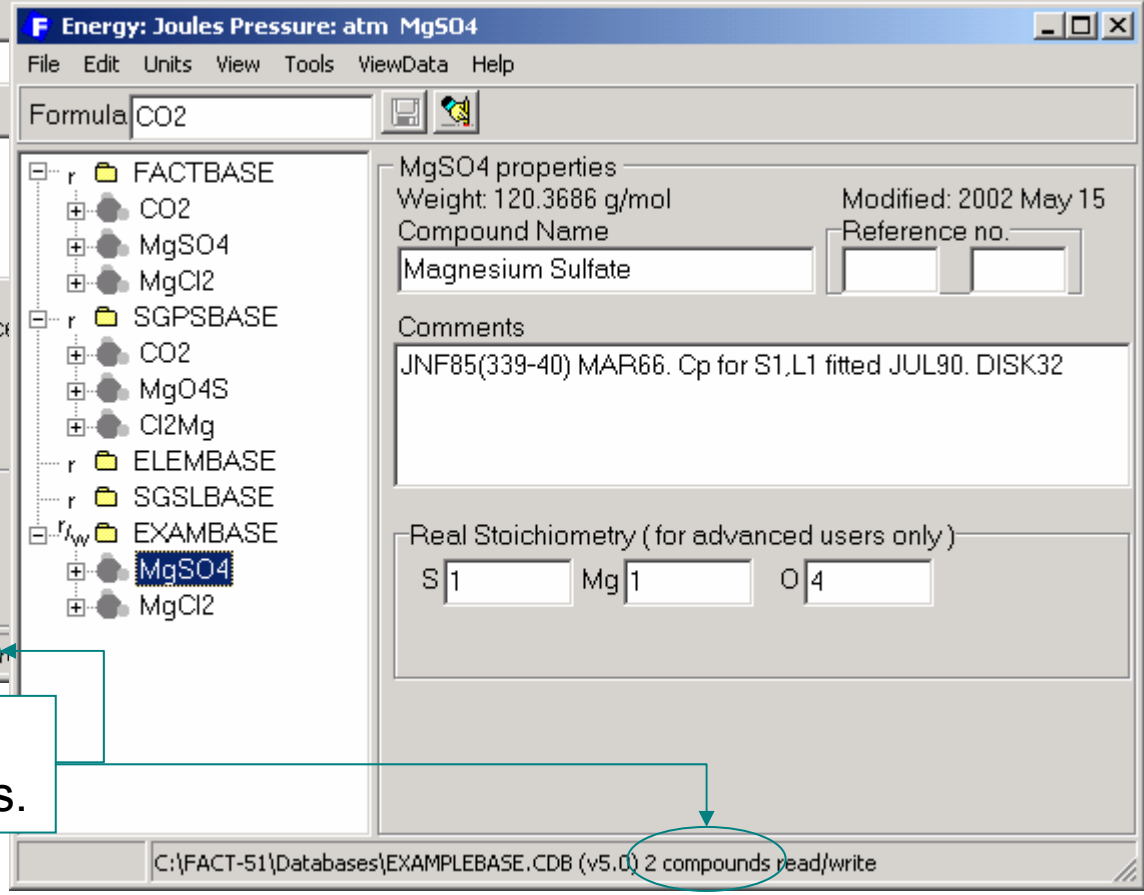
1. **Select** the compound you want to **delete** (say, CO_2) from the **$^r/_w$ database**.



2. **Go to** the **Edit** menu and select **Erase CO2 from EXAMBASE**.



3. **Confirm** your intention to **erase** data

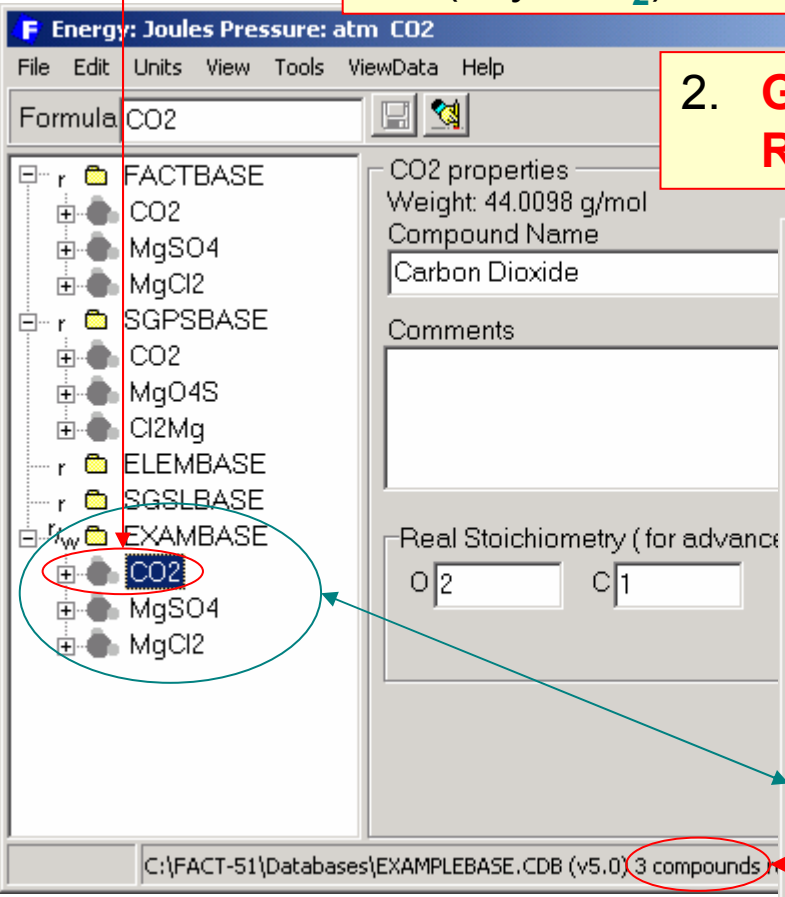


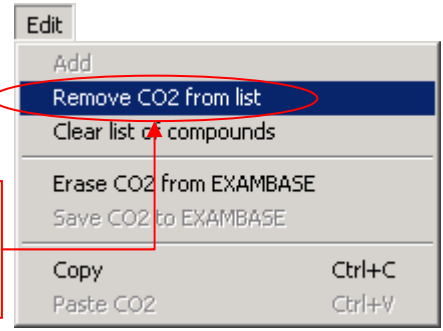
Now the database **EXAMBASE** contains only **2** (= **3** - **1**) compounds.

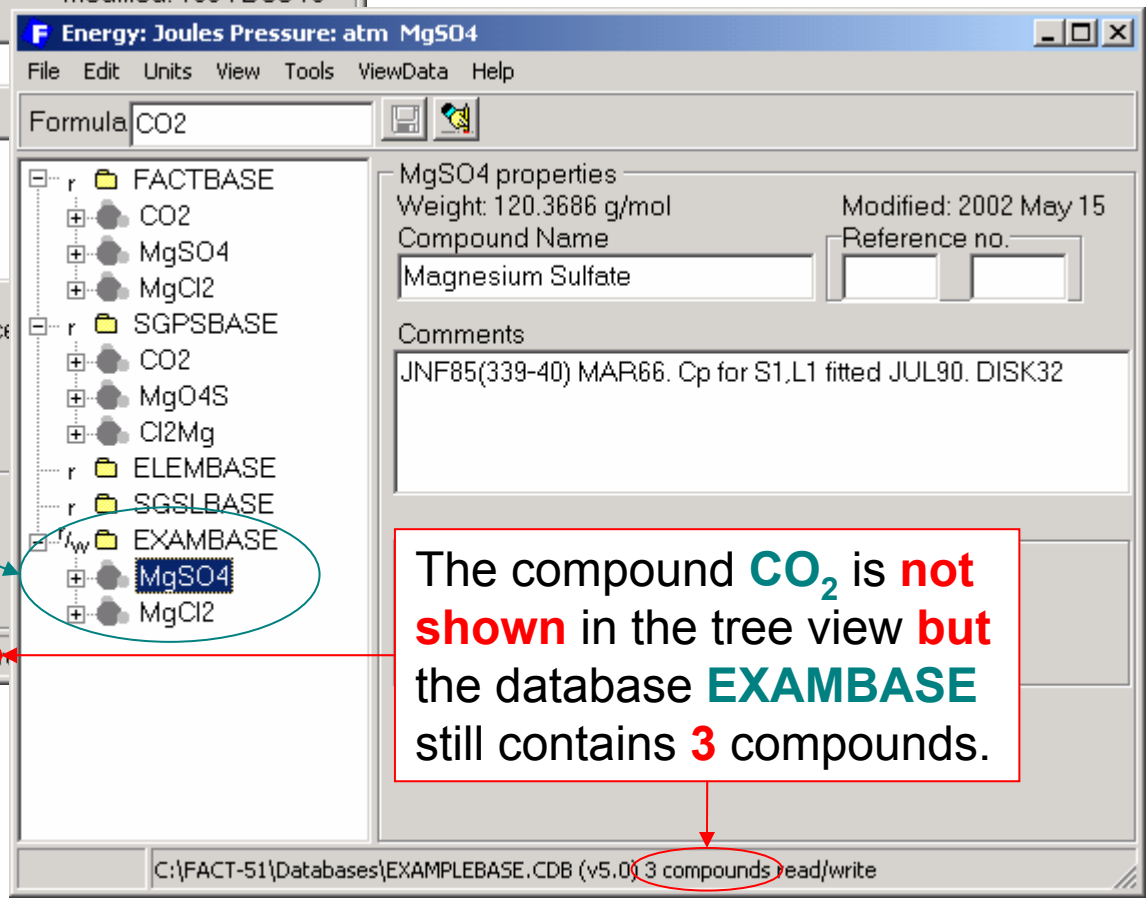
The Erase, Remove and Clear commands, II

1. **Select** the compound you want to **remove** (say, CO_2) from the tree view list.

2. **Go to** the **Edit** menu and **select Remove CO2 from list**.





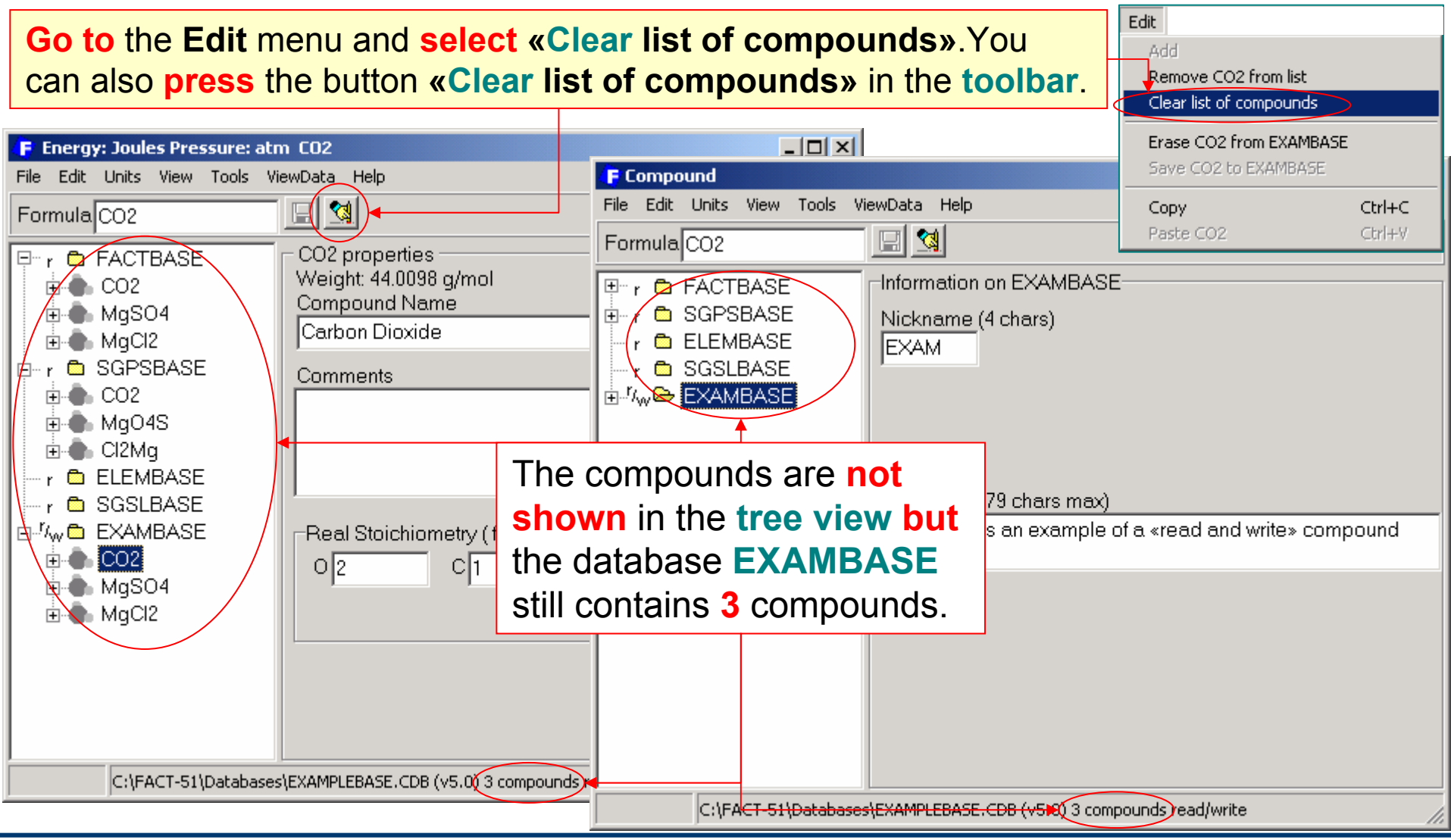


The compound CO_2 is **not shown** in the tree view **but** the database **EXAMBASE** still contains **3** compounds.

The Erase, Remove and Clear commands, III

To **remove** **all** the compounds from **all** the **lists** (you are **not** removing the compounds from the **databases**) in the **treeview** (i.e. to **clear** the **treeview**):

Go to the **Edit** menu and **select** **«Clear list of compounds»**.You can also **press** the button **«Clear list of compounds»** in the **toolbar**.



The compounds are **not shown** in the **tree view but** the database **EXAMBASE** still contains **3** compounds.

The «Mixer» feature

The «Mixer » feature permits the generation of new compound data using «simple algebra» on the data of already stored compounds.

The first example shows how the known data for Na_2O and Al_2O_3 are used in a Neumann-Kopp type sum to generate data for the unknown compound $NaAlO_4$. The scale down command is used to come to the desired formula.

Alternatively, the use of the scale up command is shown for the formula $Na_3Al_3O_6$.

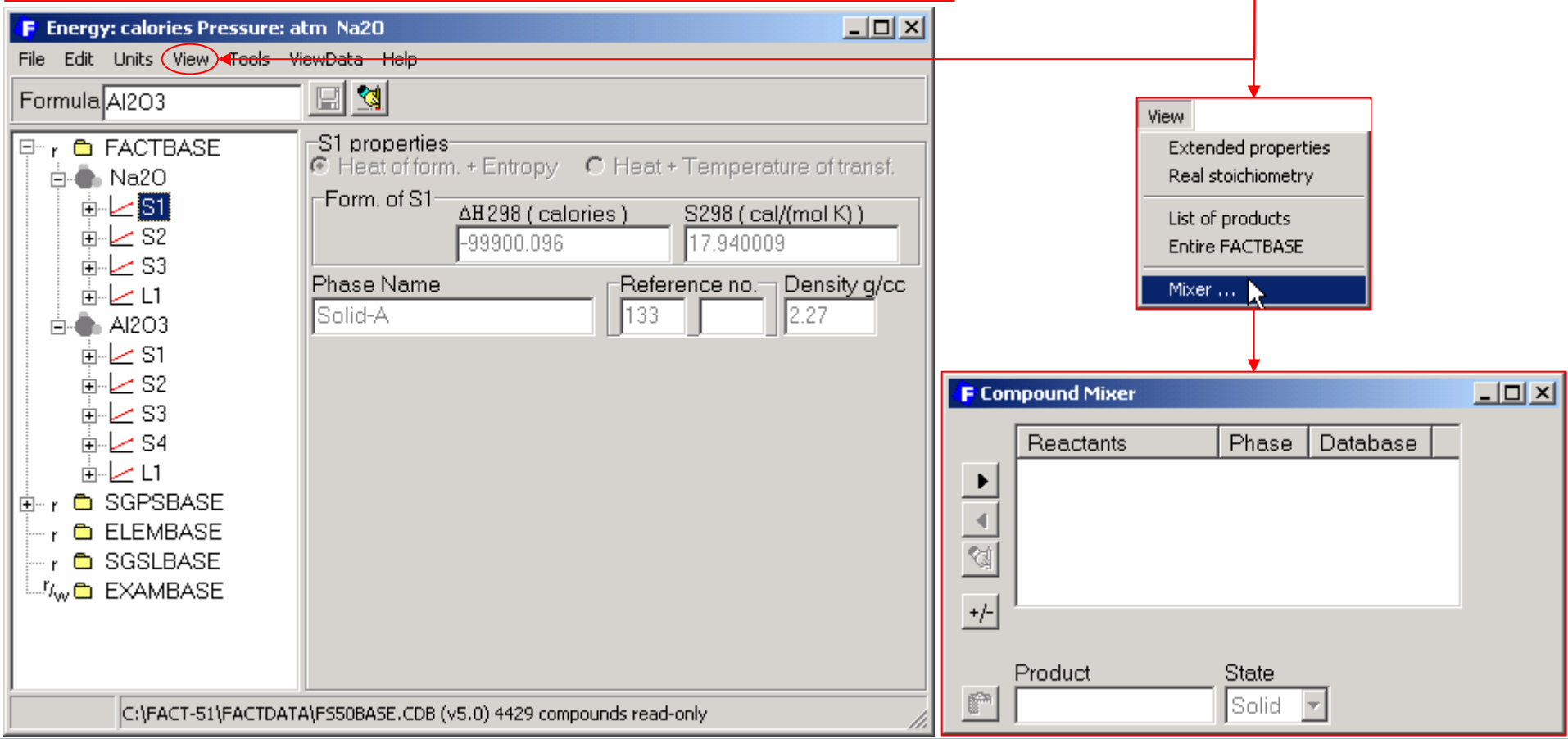
The second example shows how the known data for Li_3N, Li and Na are used to generate data for the unknown compound Na_3N using $Li_3N + 3Na - 3Li = Na_3N$.

The «Mixer» feature: Example 1, I

The «**Mixer**» option enables you to create and store compound data on a new (possibly hypothetical) species by mixing data of existing species. For example, new data on $NaAlO_2$ via the reaction: ½ Na_2O(s1) + ½ Al_2O_3(s1)→ $NaAlO_2$(s1).

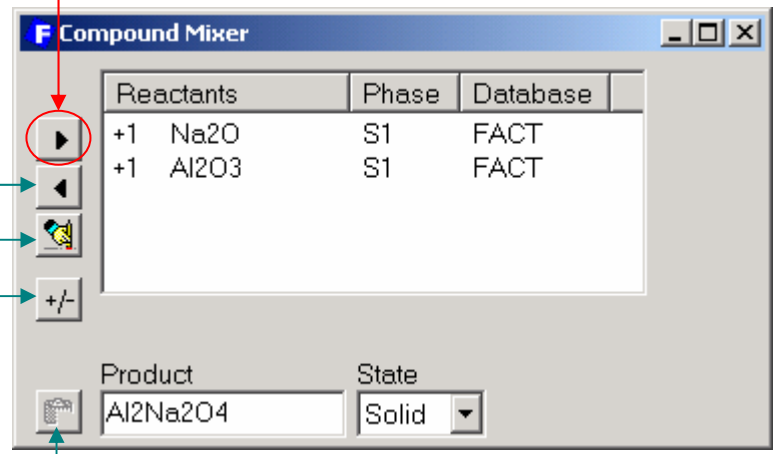
1. Open the database containing the data on Na_2O and Al_2O_3 and expand the treeview to list phases.

2. Click on View > Mixer…



The «Mixer» feature: Example 1, II

3. Drag and drop the phases to the **Compound Mixer** window or use the **Add Phase** button.



Remove the selected phase

Remove all phases

Add or substract the selected phase

Paste the new compound to a read and write database.

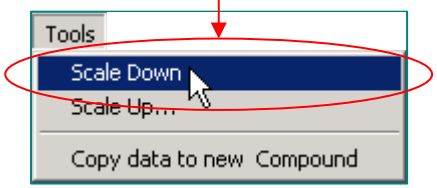
This stores the new compound $Al_2Na_2O_4$ in the database. To store $NaAlO_2$ you need to use the «**Scale Down**» command in the **Tools** menu.

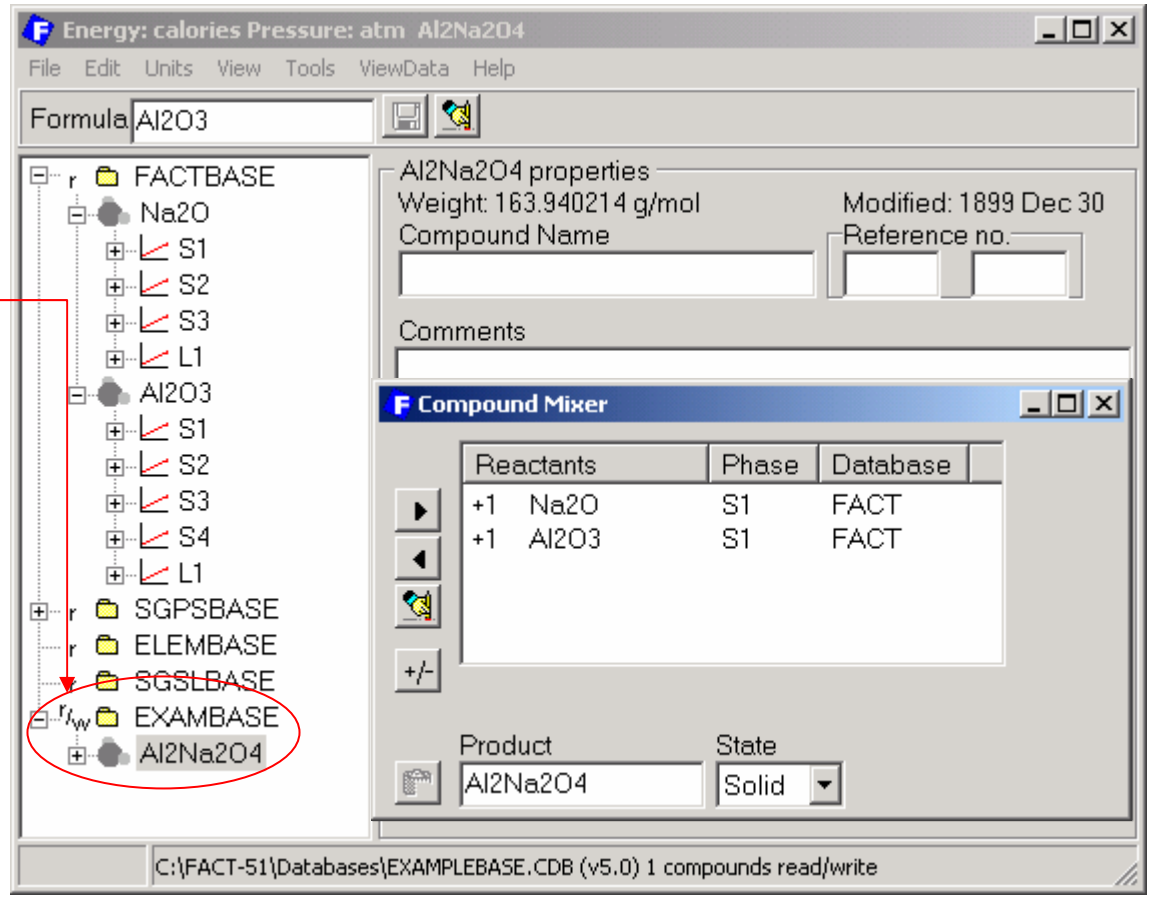
The «Mixer» feature: Example 1, III

To **scale down** a compound:

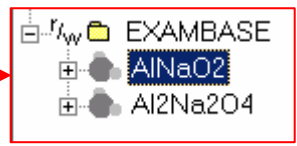
1. Save your compound in a $^{r}/_{w}$ database:
   A. Select a $^{r}/_{w}$ database.
   B. Paste your compound.

2. Go to the **Tools** menu and select **«Scale Down»**.





Now you have the **scaled down** compound **$AlNaO_2$** in your $^{r}/_{w}$ database.

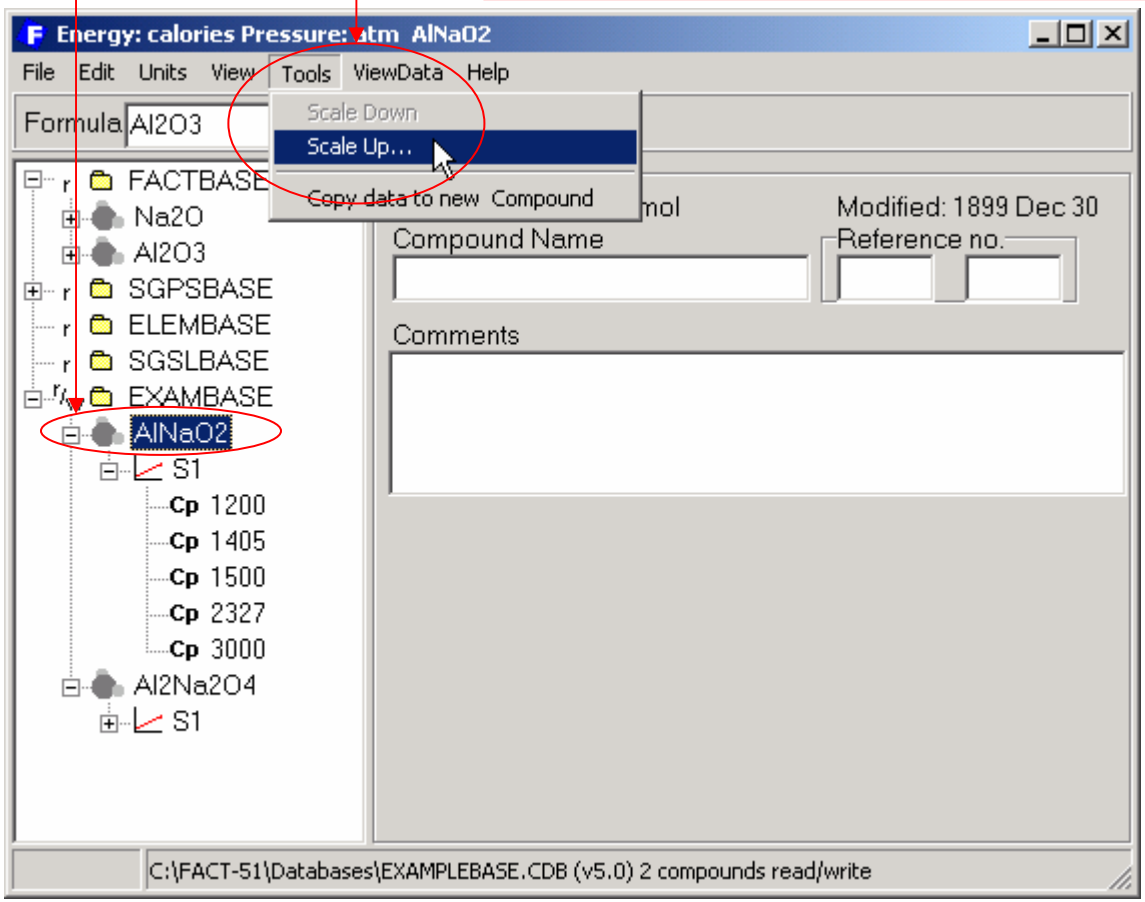


The «Mixer» feature: Example 1, IV

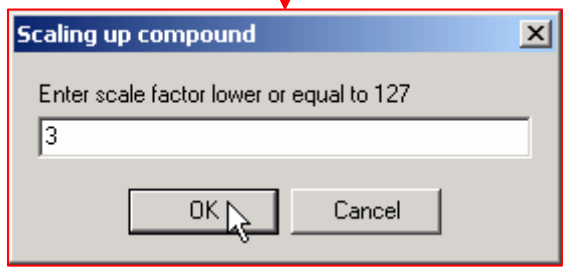
On the other hand, if you want the thermodynamic properties of $Na_3Al_3O_6$, which is 3 times $AlNaO_2$, use the **Scale Up** command.

1. **Select** the compound you want to **scale up**

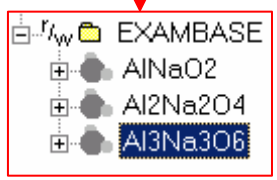
2. Go to the **Tools** menu and select **Scale Up…**



3. Enter the **scale factor** in the **Scaling up compound** dialog box and press «**OK**».



Now you have the compound $Al_3Na_3O_6$ in your $^r/_w$ database



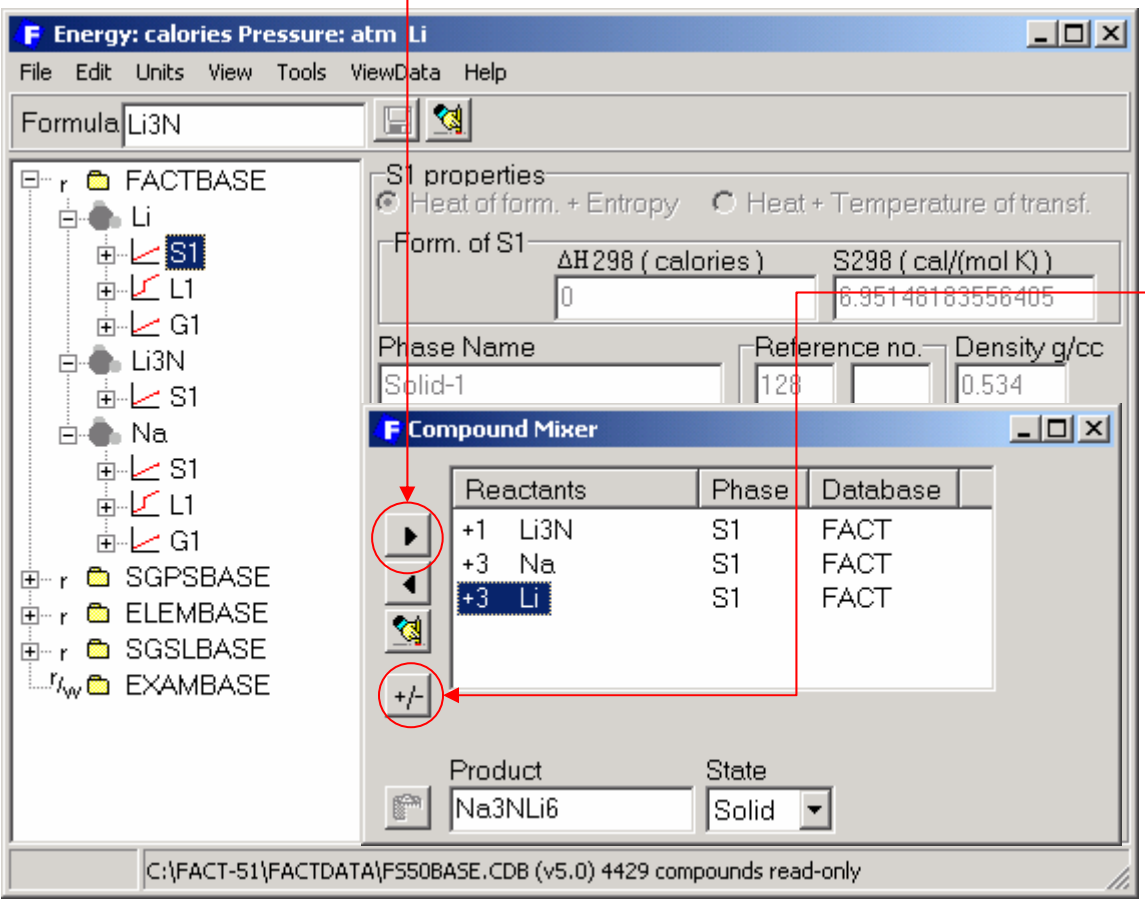
The «Mixer» feature: Example 2

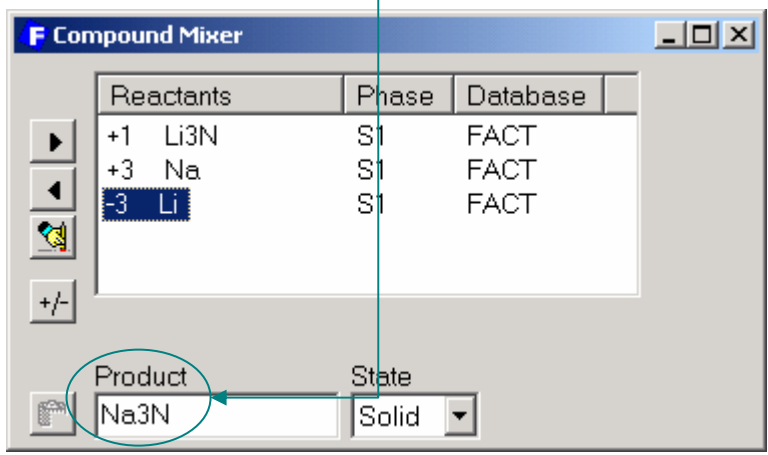
This example shows how to create new data on Li_3N via the synthesis of: $Li_3N + 3Na - 3Li$.

1. Drag and drop the Li_3N, Na and Li phases to **Compound Mixer**.

2. Click on the **Add Phase** button to add 3 Na and 3 Li.

3. Press the **Add and Substract** button to **substract 3 Li** from the reactants. This create **Na_3N** as product.





Using know data as template

In order to enter data for a new compound you may use the data of an already stored compound as a template.

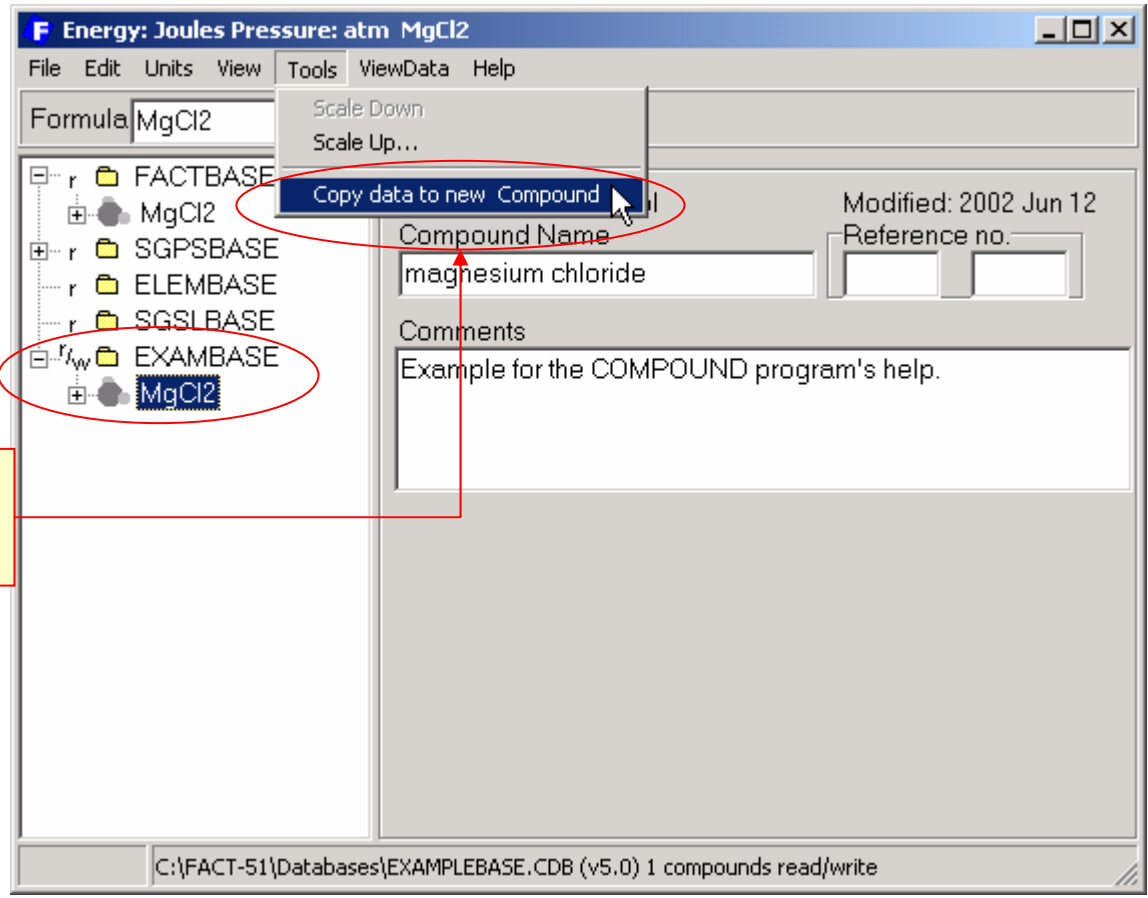
The following two view graphs give an example how to use the known data for $MgCl_2$ in order to generate new data for $CaCl_2$.

Using know data as template: «Copy data to new Compound» option, I

Suppose you do not want to enter the data of a new compound from scratch and that you already have the data of a similar compound in your $^{r}/_{w}$ database. You can use the latter compound's data as a template for the new one by using the **Copy data to new Compound** option in the Tools menu. For example, you have entered data on $MgCl_2$ in EXAMBASE previously and you want to enter data for $CaCl_2$ that is a similar compound:

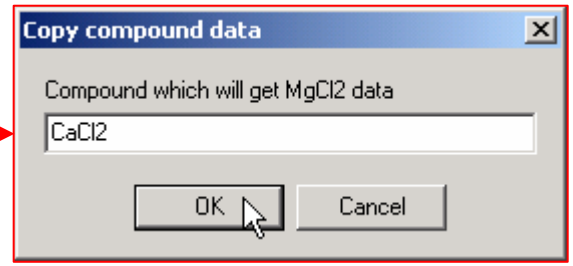
1. Select $MgCl_2$ in EXAMBASE.

2. In the Tools menu, select **Copy data to new Compound**

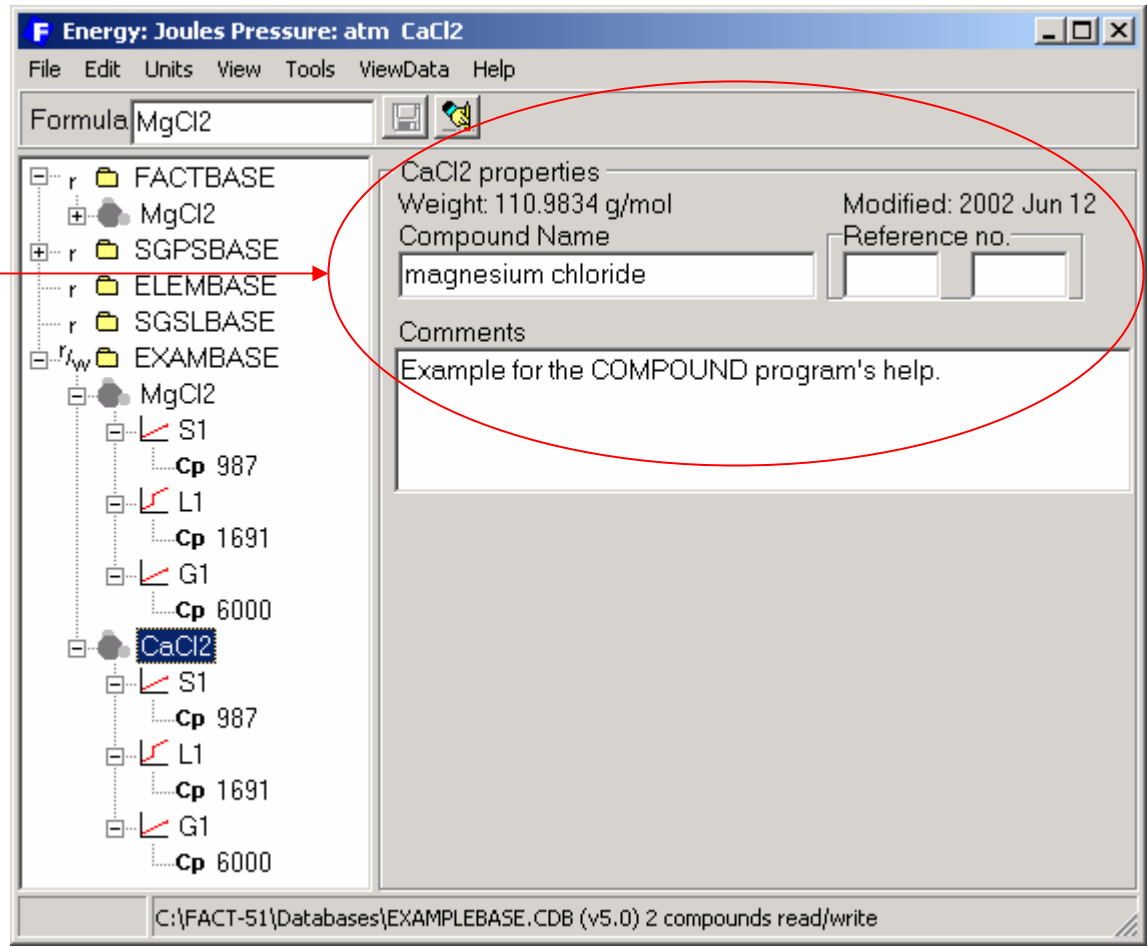


Using know data as template, II

3. In the dialog box, enter the new compound **$CaCl_2$** and press «**OK**».



4. You now have the **$CaCl_2$** template.



Changing Units of Energy or Pressure

Compound permits the change of the units of energy and pressure both for input and output of the data of a compound.

NOTE: Changing the energy units will affect H, S and C_p as well as H, S and G functions.

Changing the pressure units will ONLY influence the value of S_{298} of gas species, the first coefficient of the S function, and the second coefficient of the G function.

Changing Units of Energy or Pressure

Select the new **unit** from the cascade menu **Units**.