The *Compound* module

Use ***Compound*** to administer a private compound database, i.e. enter, edit or delete pure substance data in the database.

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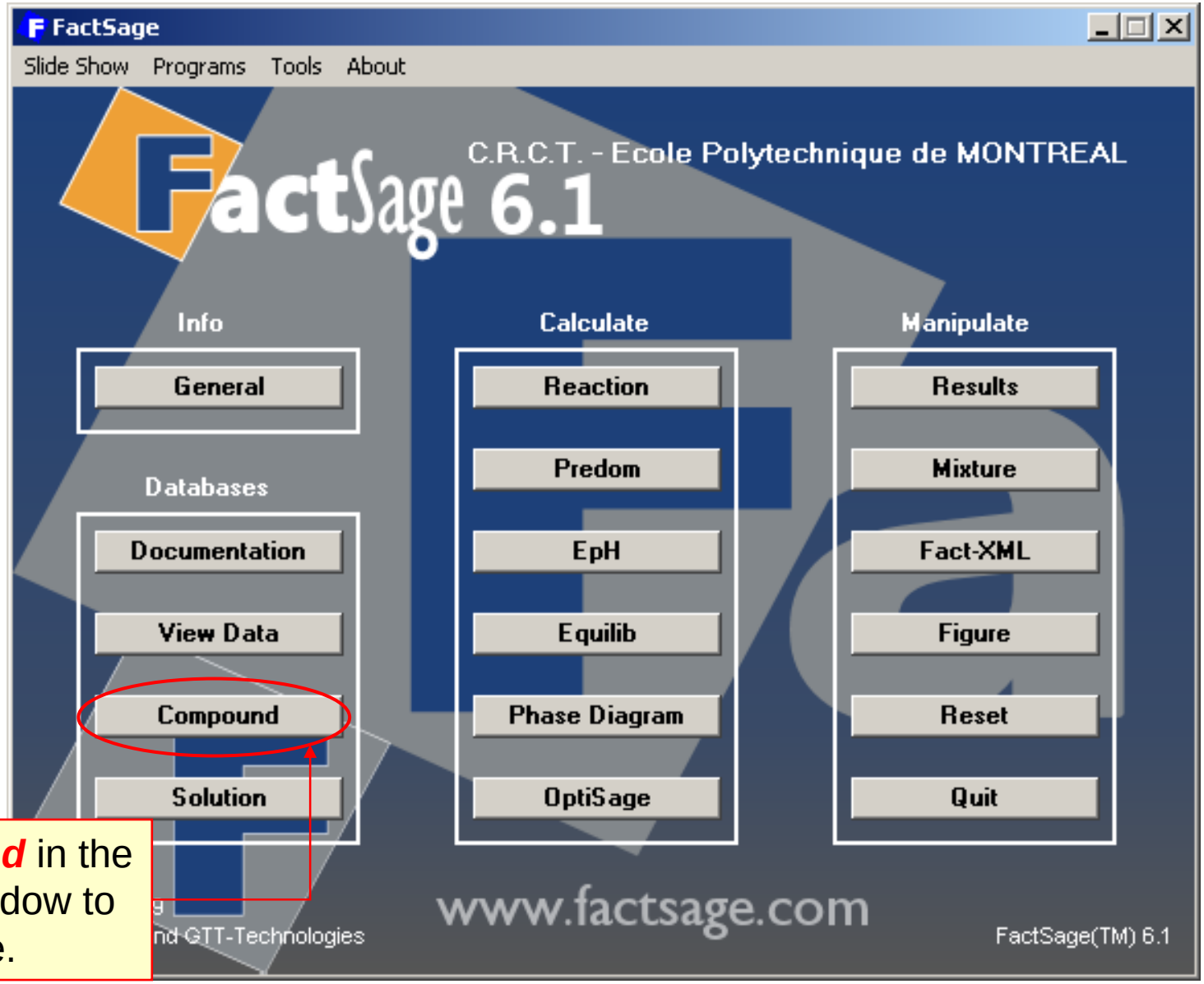
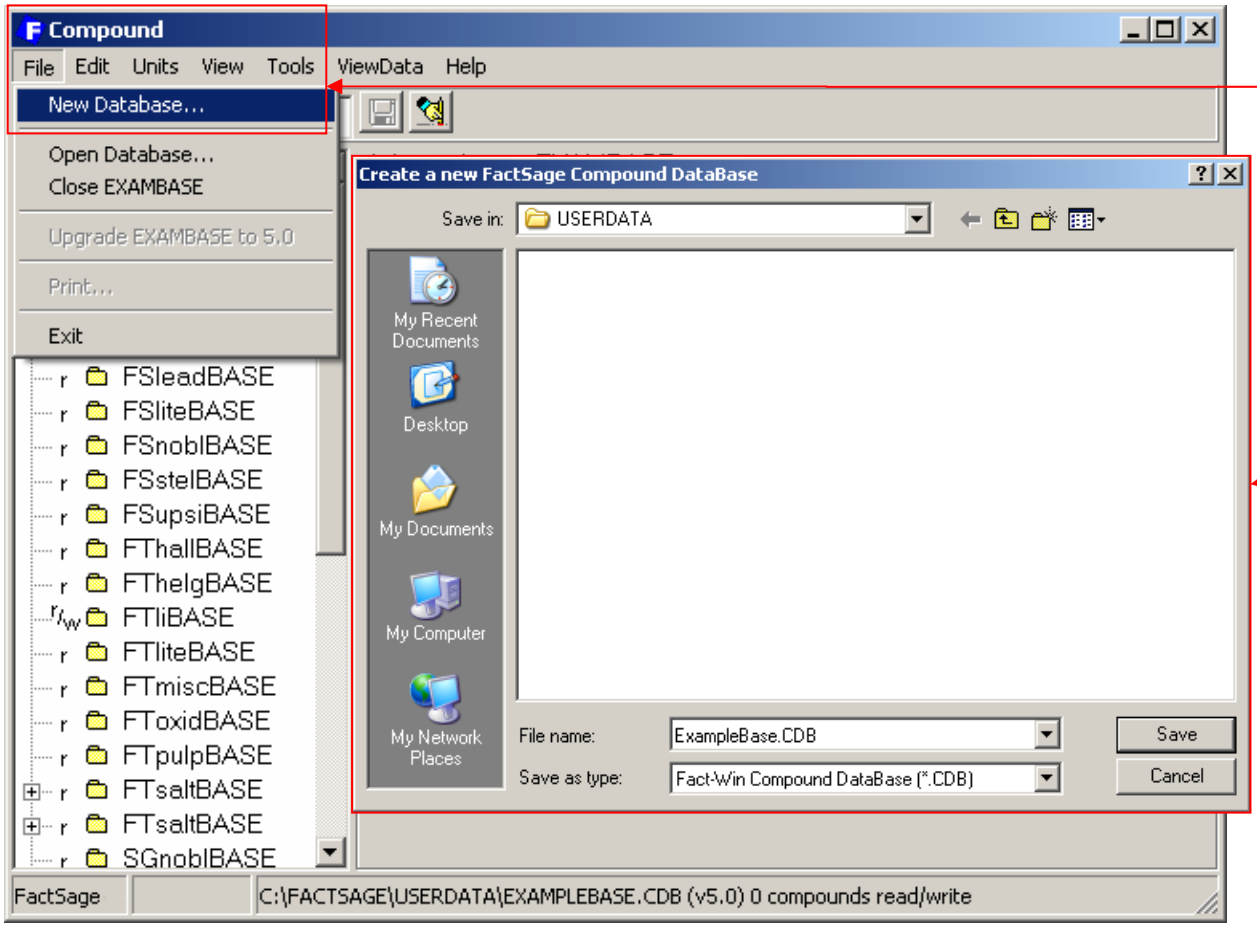
The ***Compound*** module



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

Create a private *Compound* database, I

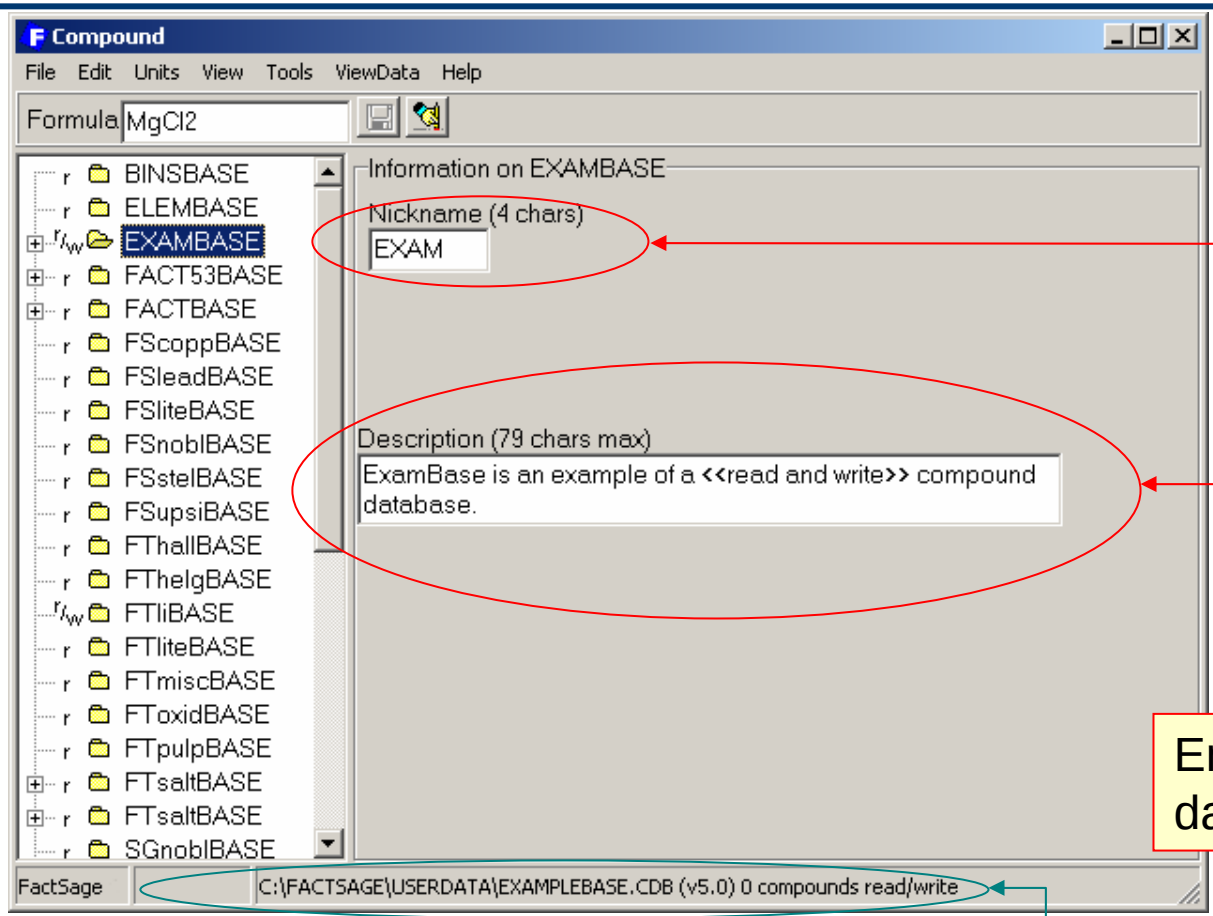
To create a read and write ($^{r}/_{w}$) database:



1. Click on «**File**» > «**New Database…**»

2. Select a **directory** and enter a **filename**

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



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

Enter a short description of the database.

The status bar provides information on the database:

- location: **C:\FACTSAGE\USERDATA\EXAMPLEBASE.CDB**;
- compounds: **0 compound(s)** (for now);
- version: **5.0**;
- access: **read/write**.

Add a **compound** to the database

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

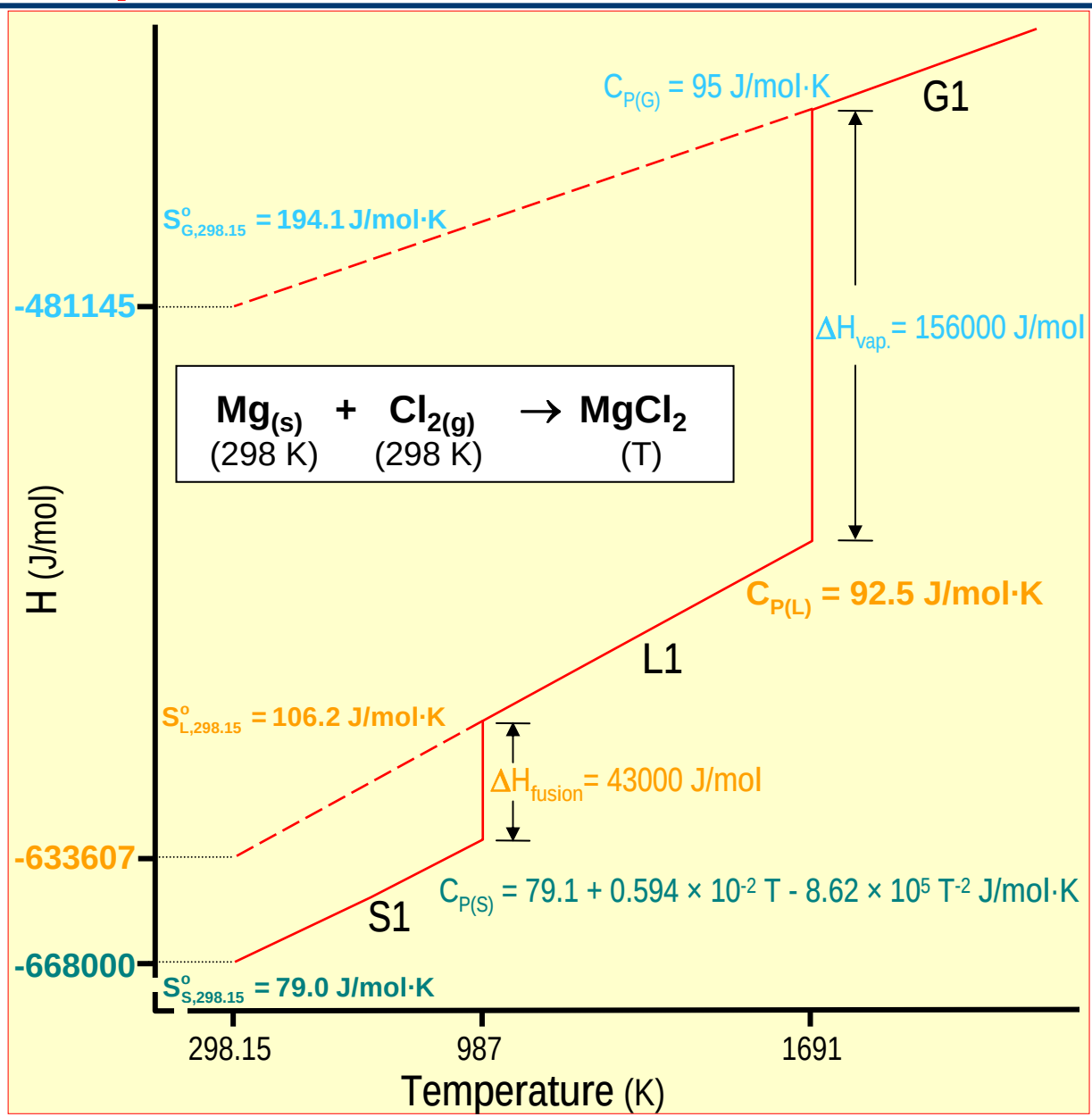
$MgCl_2$ is taken as the example. The data for this compound are summarized in the next slide. All entries are made using the values in this figure.

Two different methods 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).

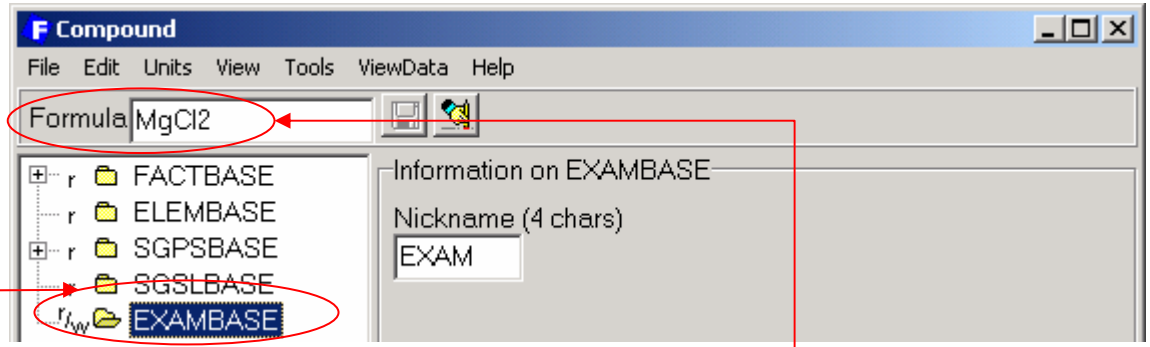
Add a **compound** to the database, III

Compound data for **$MgCl_2$** are taken from this graph.

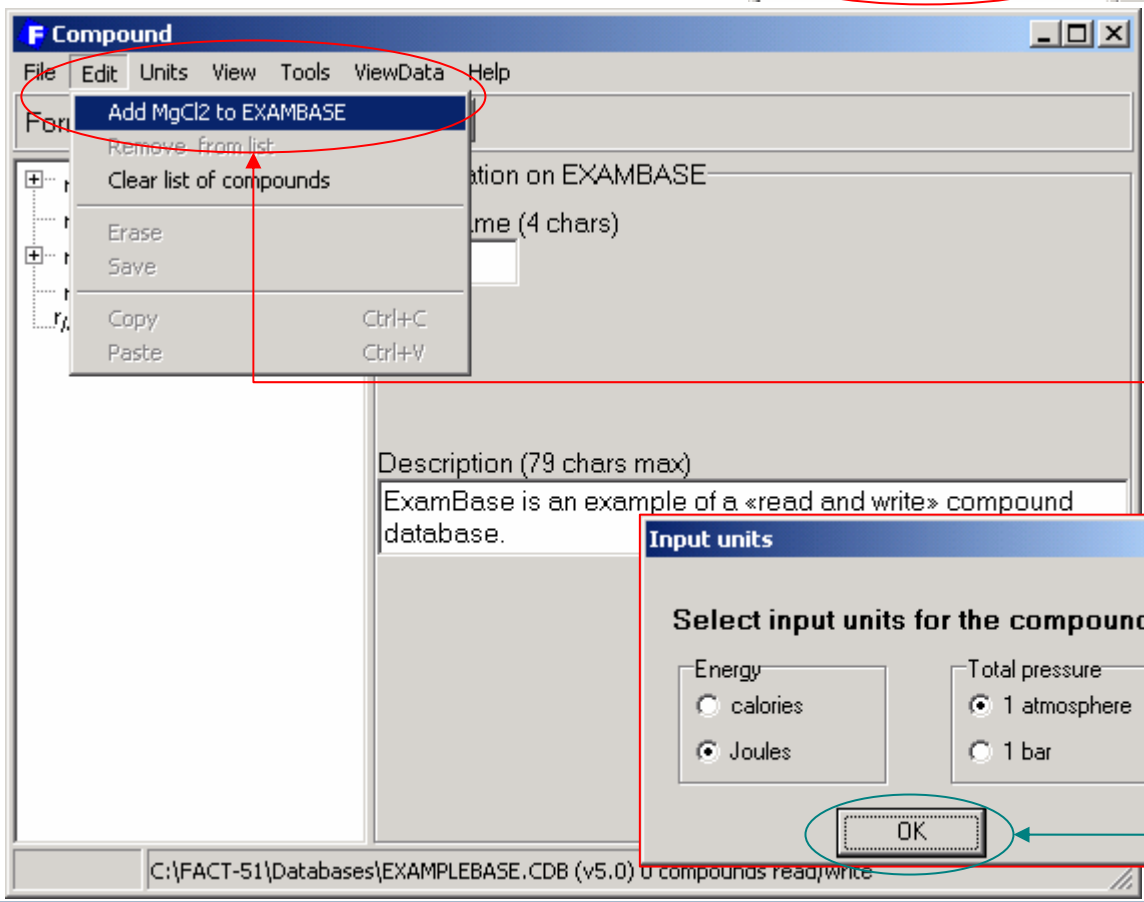


Add a **compound** to the database, I

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



1. Select **EXAMBASE** database



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

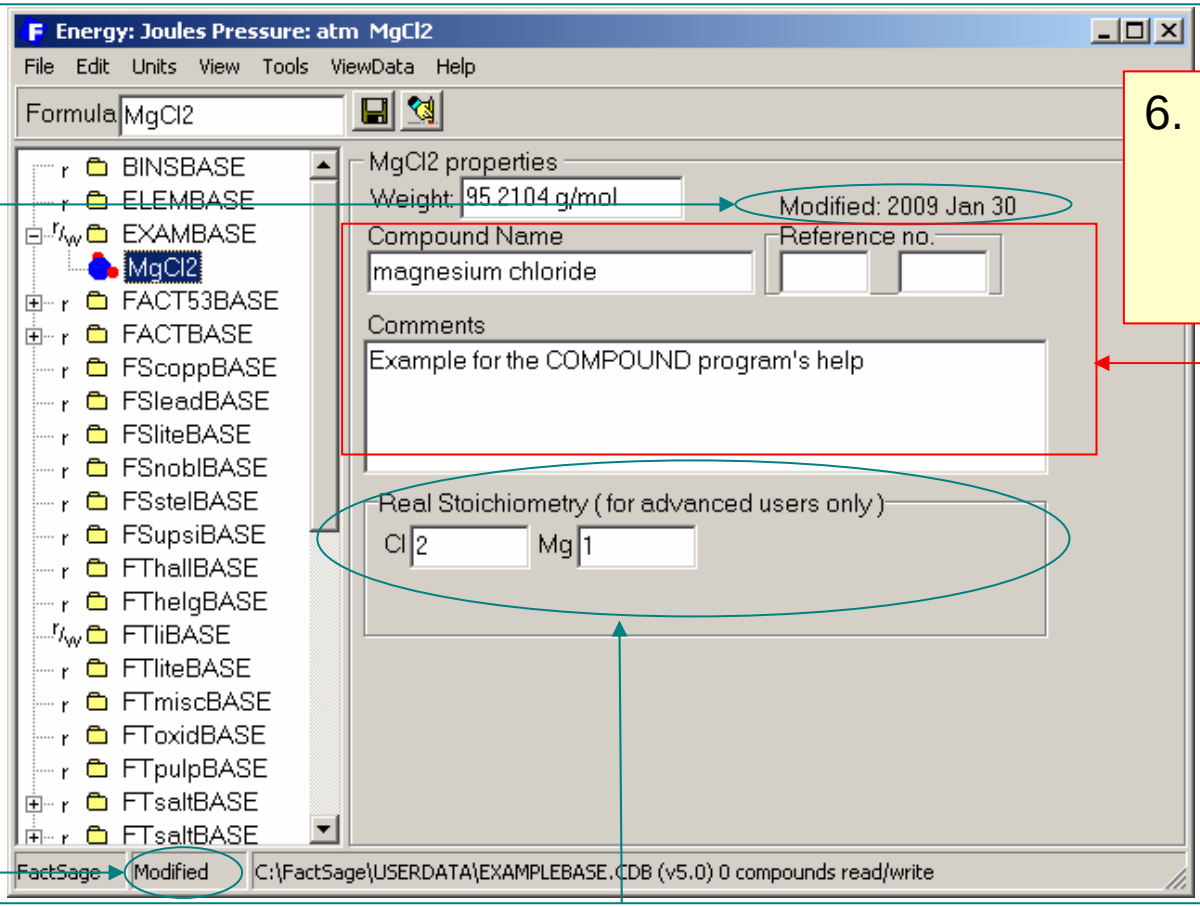
3. Select the function «**Add $MgCl_2$ to EXAMBASE**» from the **Edit** Menu.

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

5. Press «**OK**»

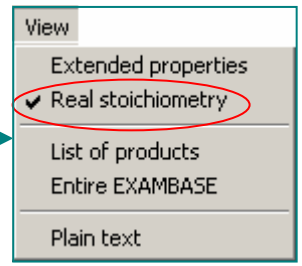
Add a **compound** to the database, II

The database is now ready for new entries and modification of existing data.

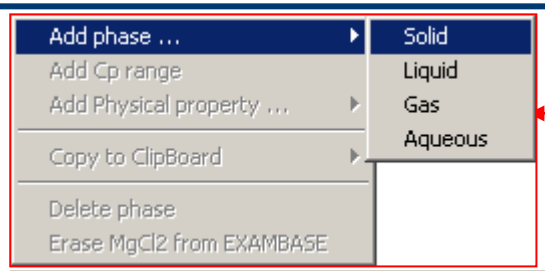


6. Enter:
   - **compound name**;
   - **reference number(s)**;
   - **comments**.

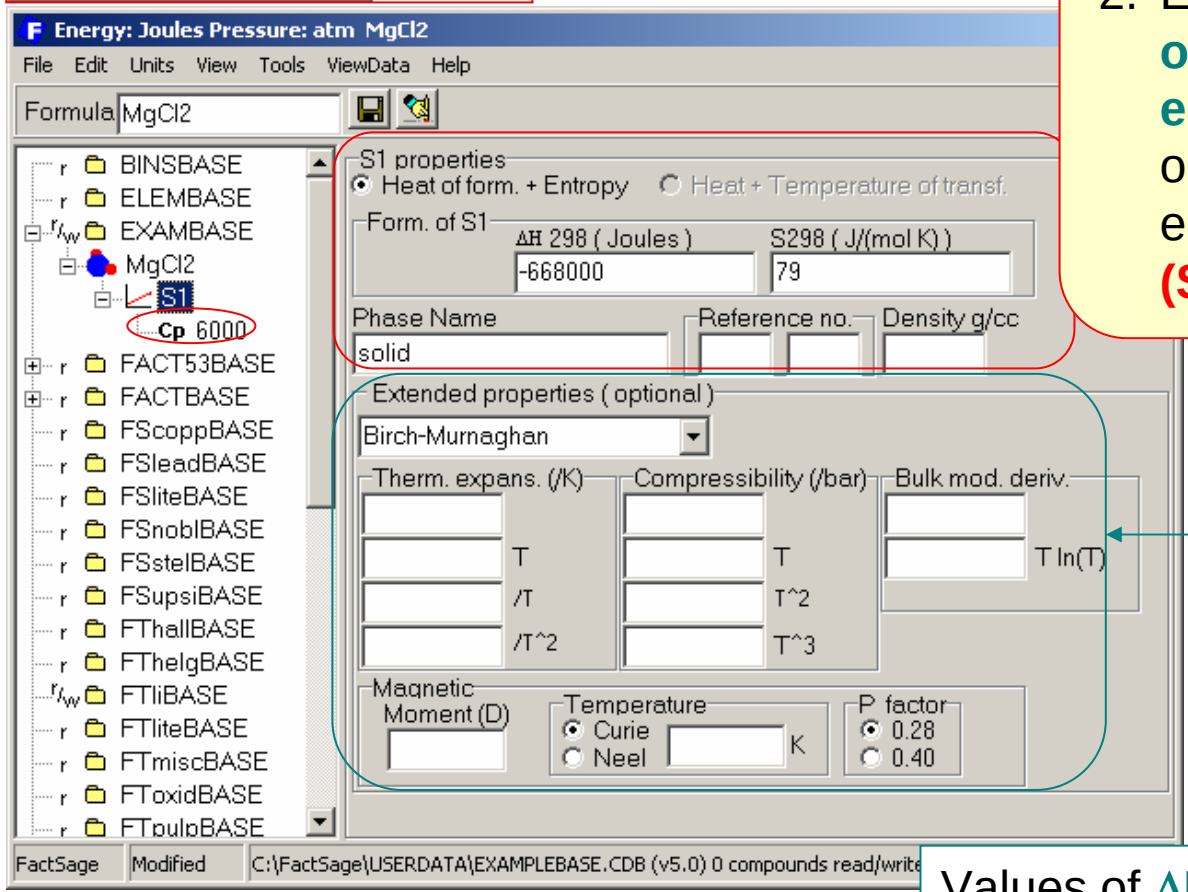
The **Real Stoichiometry** input box appears if you have checked «Real stoichiometry» in the menu **View**. This feature is for **advanced users** and applies to **all phases of the compound** (it does not apply to elements).



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

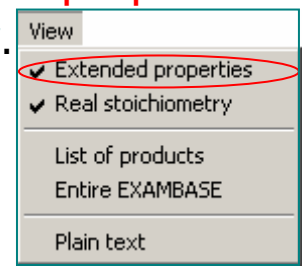


1. Right click on $MgCl_2$ and select «**Add phase…**» > «**Solid**».



2. Enter the values for the **enthalpy of formation ΔH°(298.15)** and **entropy S°(298.15)**. ***Compound*** only takes these values when entering data for the **first** phase **(S1).**

The **Extended properties** input box appears if you have checked «Extended properties» in the menu **View**. This feature only applies to a given **phase (S1)**.



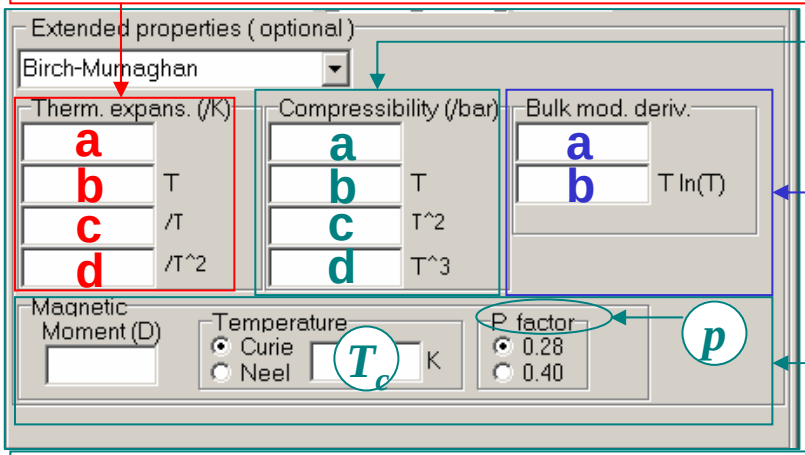
Values of **ΔH°(298.15)** and **S°(298.15)** for **S1** were obtained from the graph.

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}:

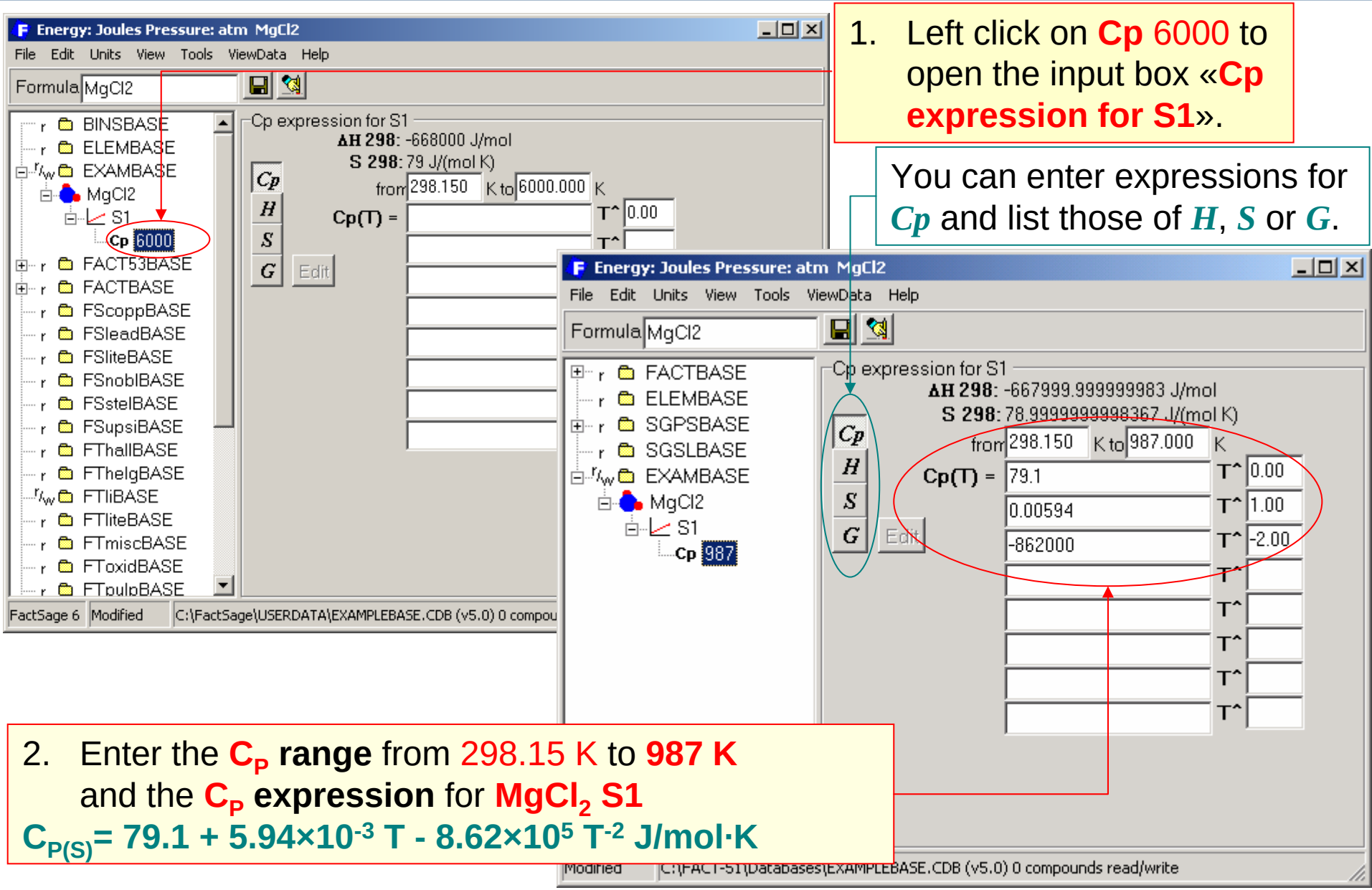
$G_{mag} = RT\ln(\beta+1)g(\tau)$ where $\tau = \frac{T}{T_c}$ and ß is the magnetic moment.

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

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

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



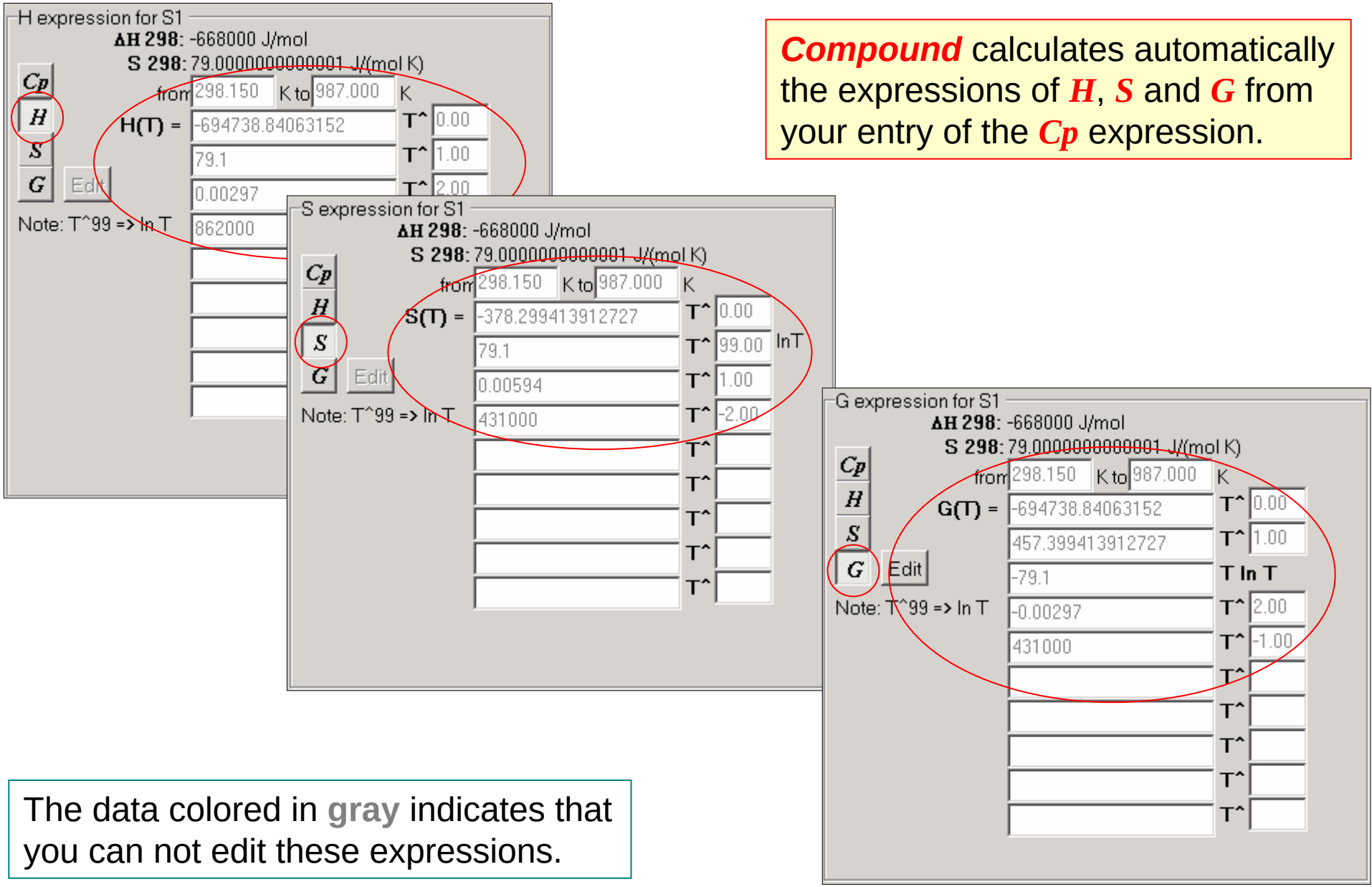
1. Left click on **Cp** 6000 to open the input box «**Cp expression for S1**».

You can enter expressions for ***Cp*** and list those of ***H***, ***S*** or ***G***.

2. Enter the **C_P range** from 298.15 K to **987 K** and the **C_P expression** for **$MgCl_2$ S1**

$C_{P(S)} = 79.1 + 5.94\times10^{-3}\,T - 8.62\times10^{5}\,T^{-2}$ J/mol·K

Show data as H, S and G functions

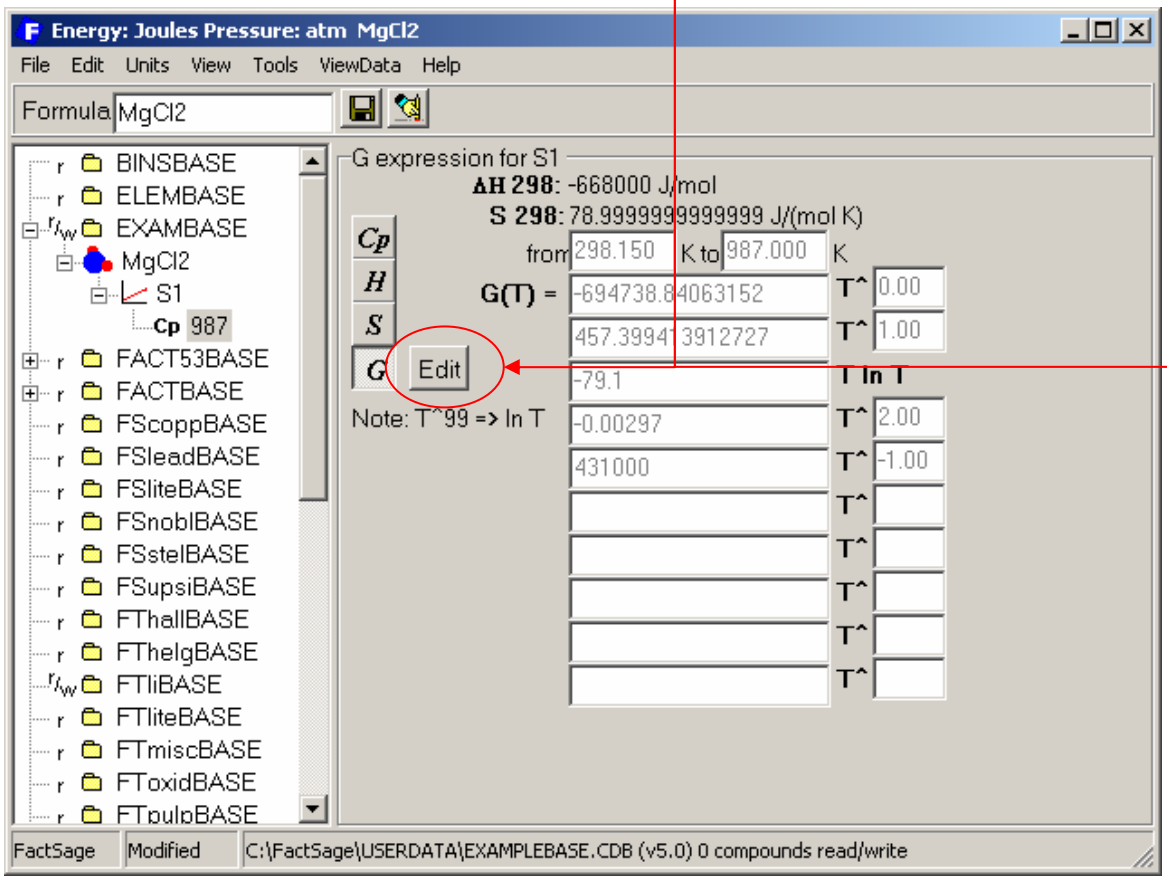


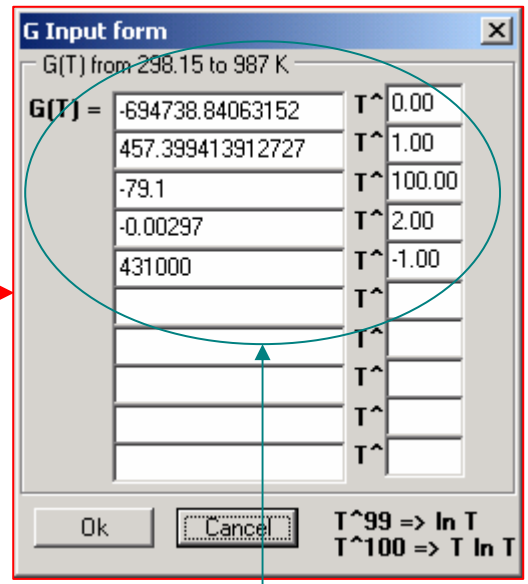
Compound calculates automatically the expressions of ***H***, ***S*** and ***G*** from your entry of the ***Cp*** expression.

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

Edit the Gibbs Energy function

Compound lets you edit the Gibbs energy function by **clicking** the **Edit** button to open the **G Input form**.





Here the Gibbs energy coefficients are used instead of H, S and C_p data.

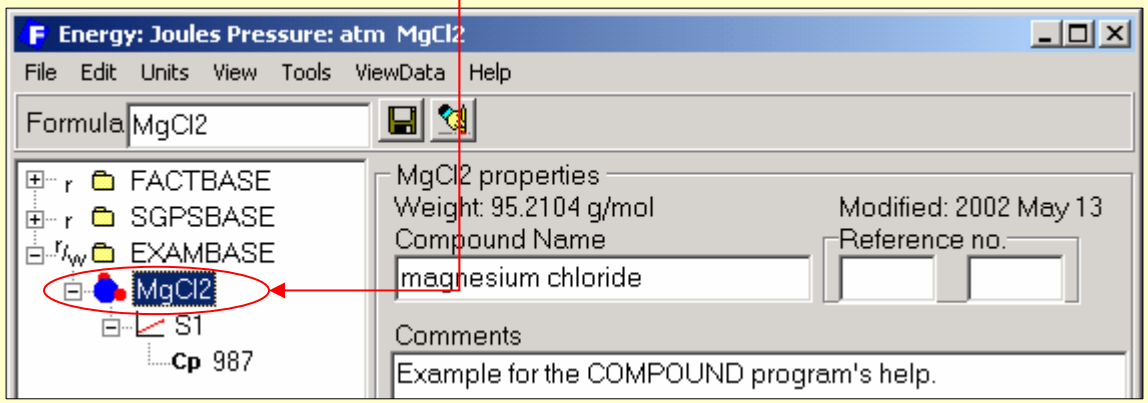
The data colored in **black** indicates that **you can edit** these expressions.

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

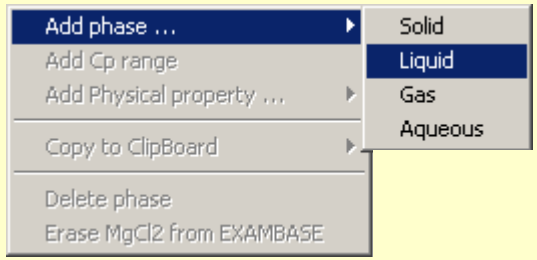
The next three slides illustrate how to enter a new phase (here the liquid) if the data for the phase transition between the previous phase (here the solid) and the new phase, i.e. ΔH and T_{trans}, as well as the C_p data of the new phase are available.

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

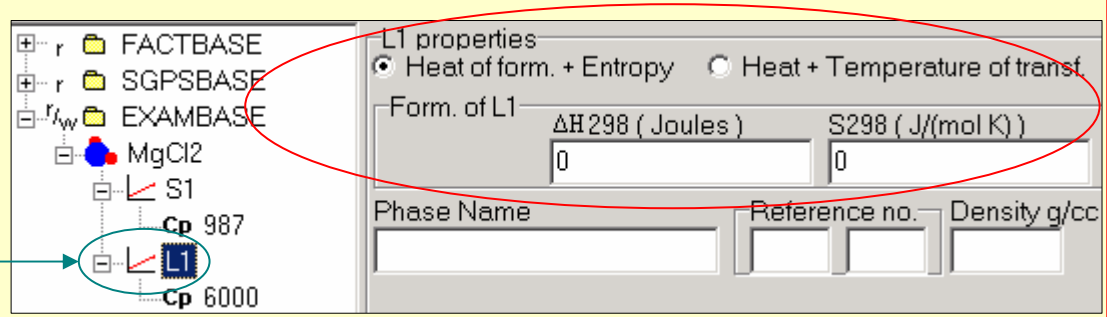
1. Right click on « MgCl2 » to open a **pop-up menu**.



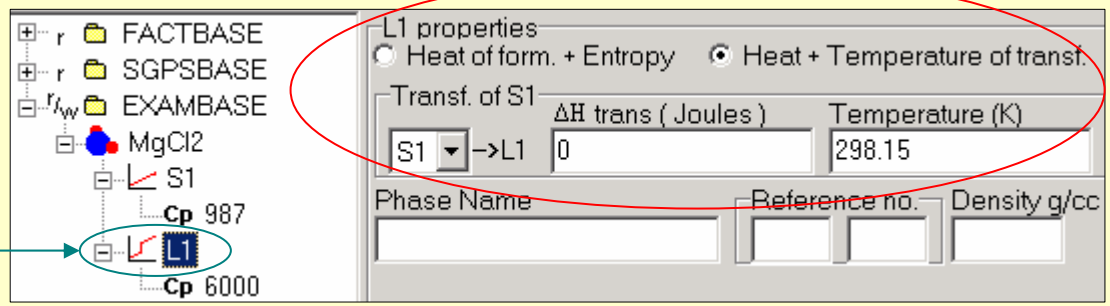
2. Point the arrow to «**Add phase…**» and select «**Liquid**» from the sub menu with a click.



3. ***Compound*** proposes two ways to enter the data:
   - either you enter the **enthalpy of formation ΔH°(298.15)** and **entropy S°(298.15)** for phase **L1** 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

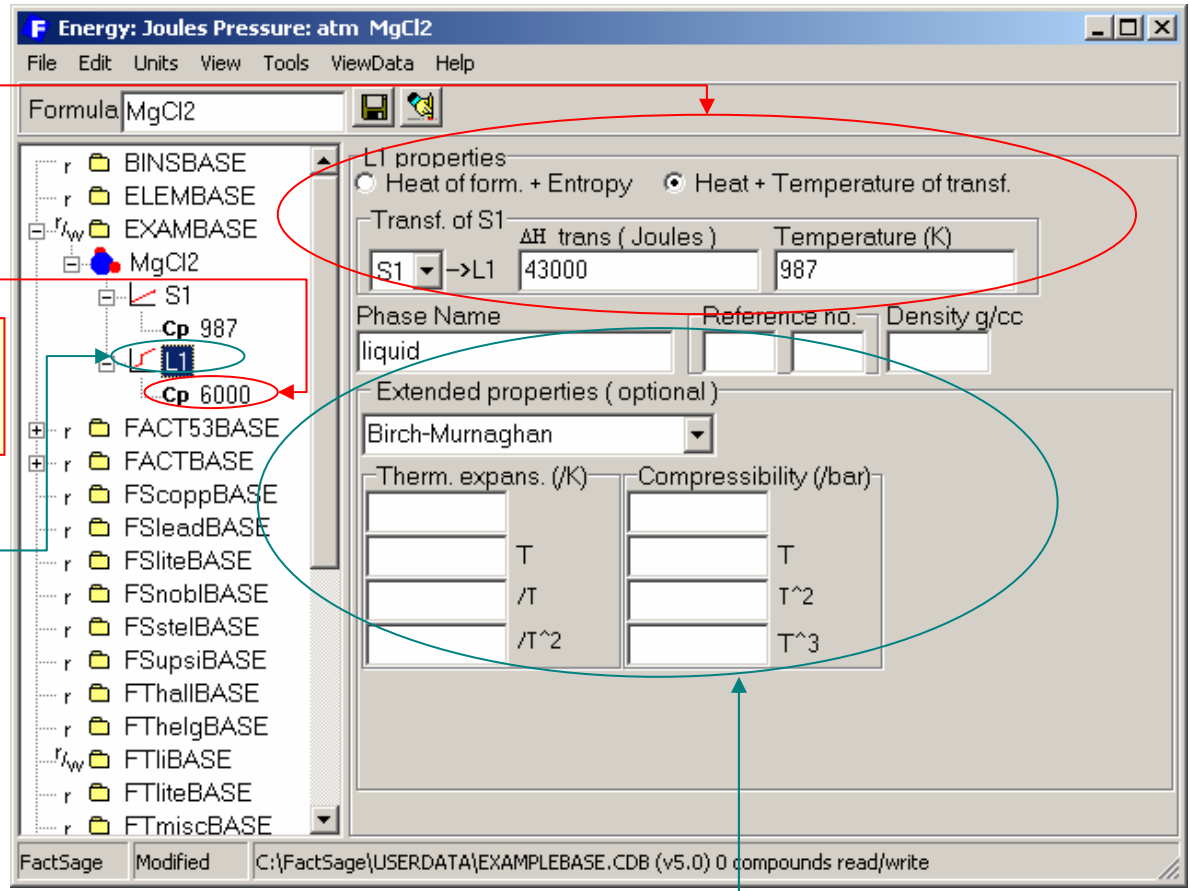


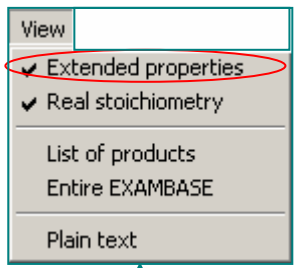
Entering phase transition data: the **liquid** phase, II

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

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

5. Click on **L1** to open the box of Extended properties

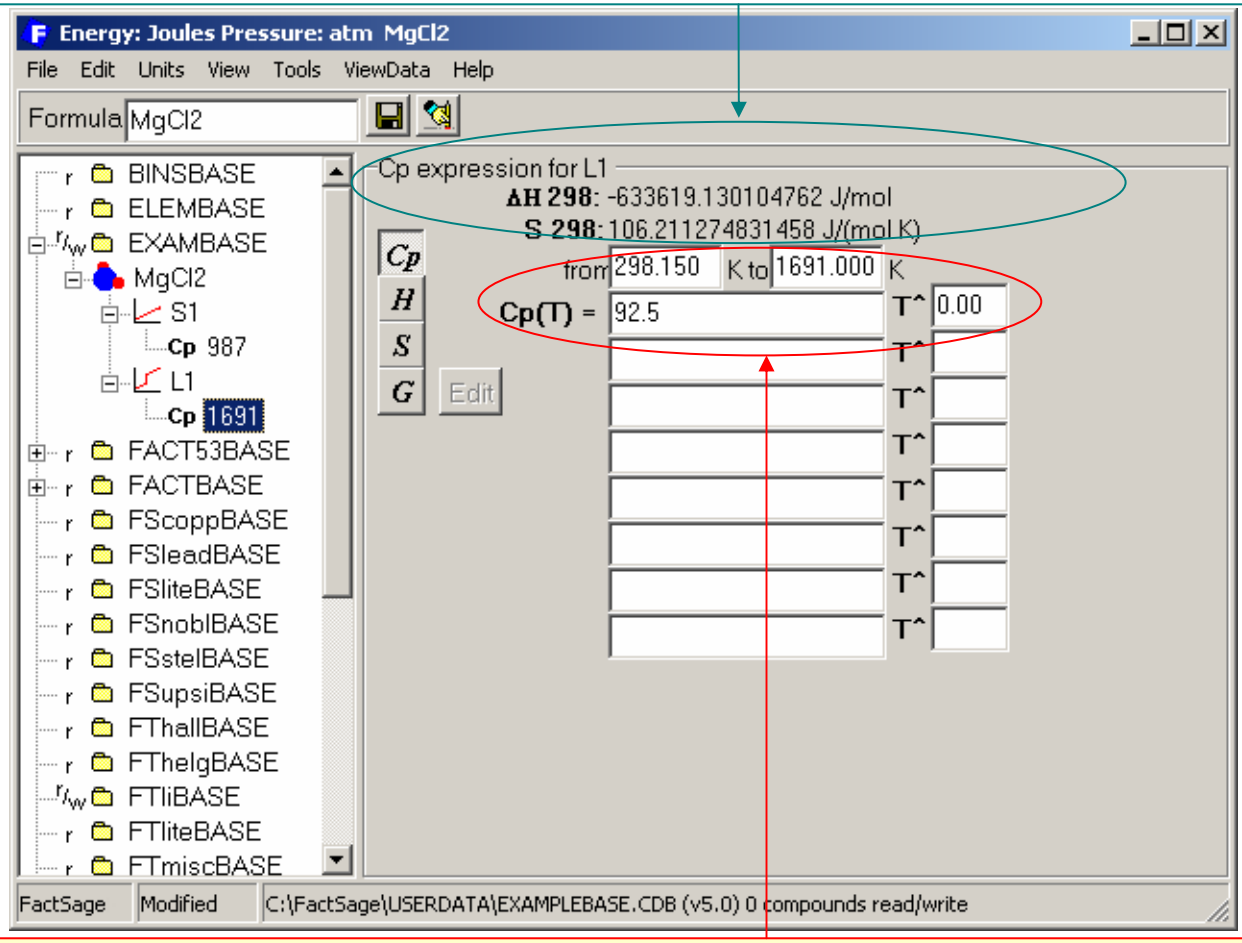




The **Extended properties** input box appears if you have checked «Extended properties» in the menu **View**. This feature applies to a **phase exclusively**.

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 the graph).



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

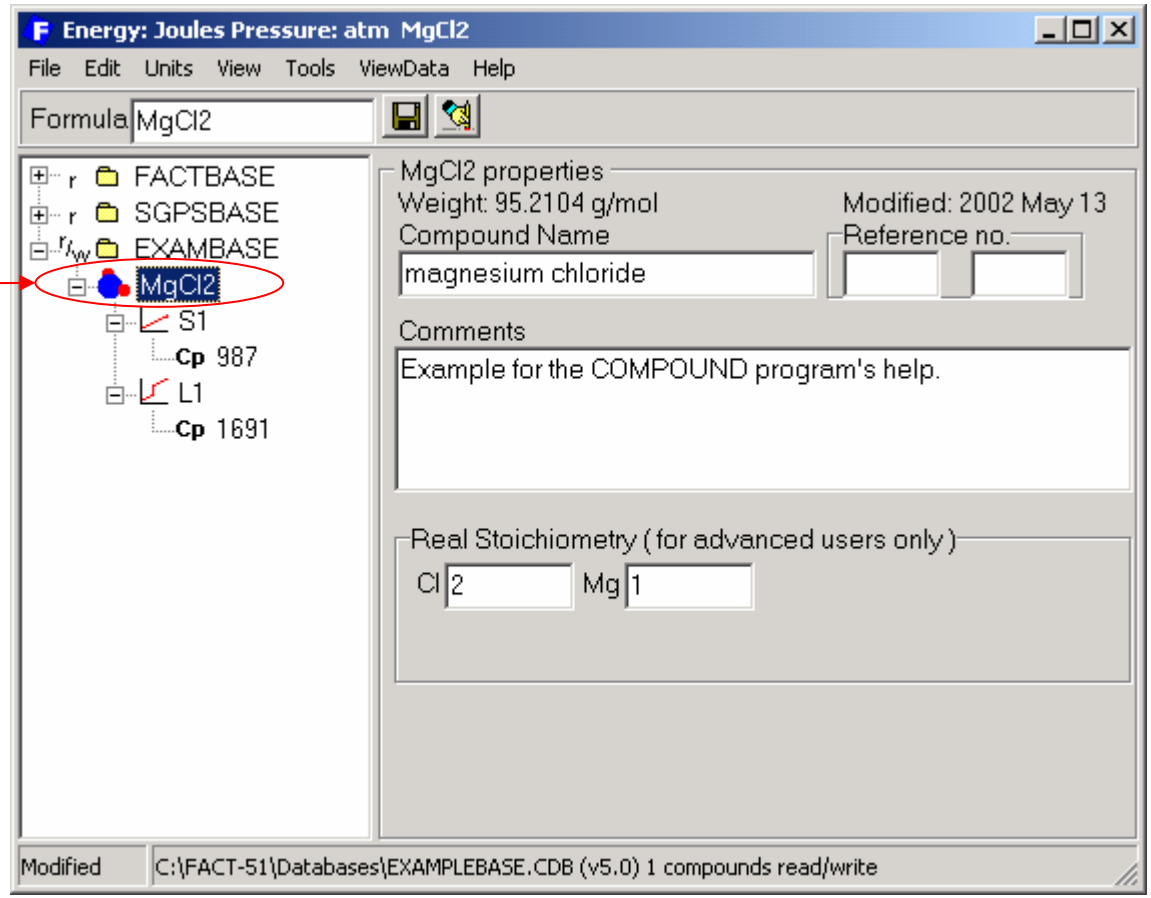
Entering a new phase with H_{298}, S_{298} and C_p: the **gaseous** phase

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.

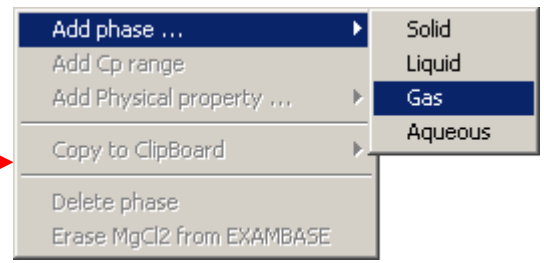
The entry of extended data for the non-ideal behaviour of the gas according to the Tsonopoulos method is also shown.

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**.



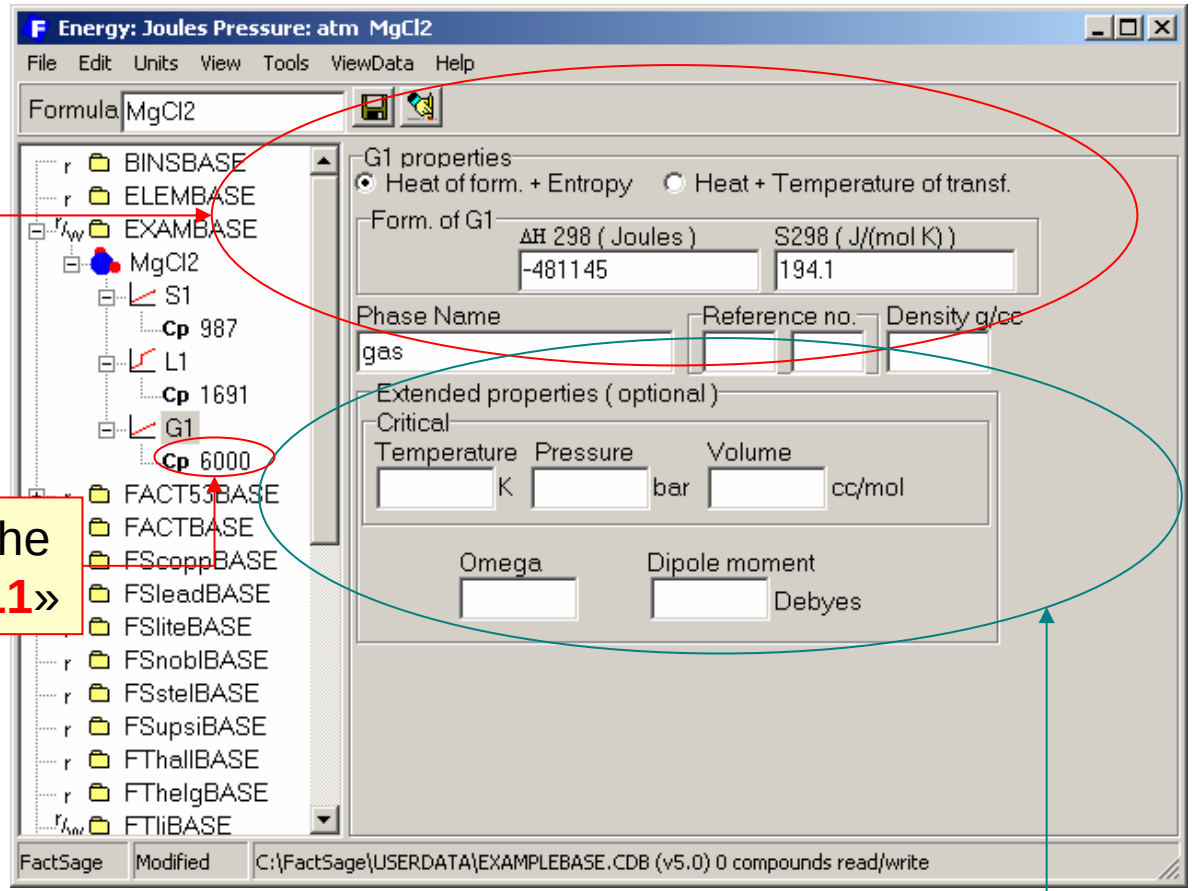
2. Point the arrow to «**Add phase…**» and select «**Gas**» from the sub menu with a click.

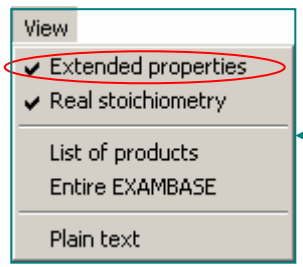


Entering a new phase with H_{298}, S_{298} and C_p: the **gaseous** phase, II

3. Enter the values for the **enthalpy of formation ΔH°(298.15) gas** and the **entropy S°(298.15) gas**. (See slide 4.3)

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



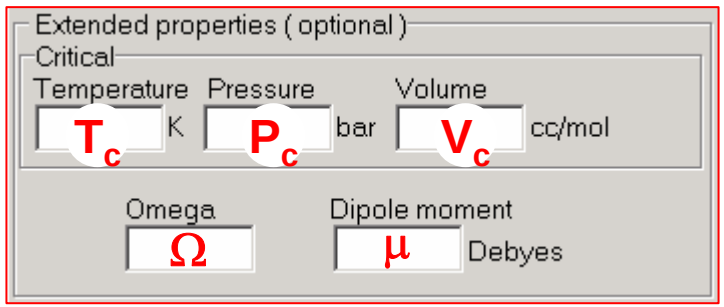


The **Extended properties** input box appears if you have checked «Extended properties» in the menu **View**. This feature applies to a **phase exclusively**.

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.

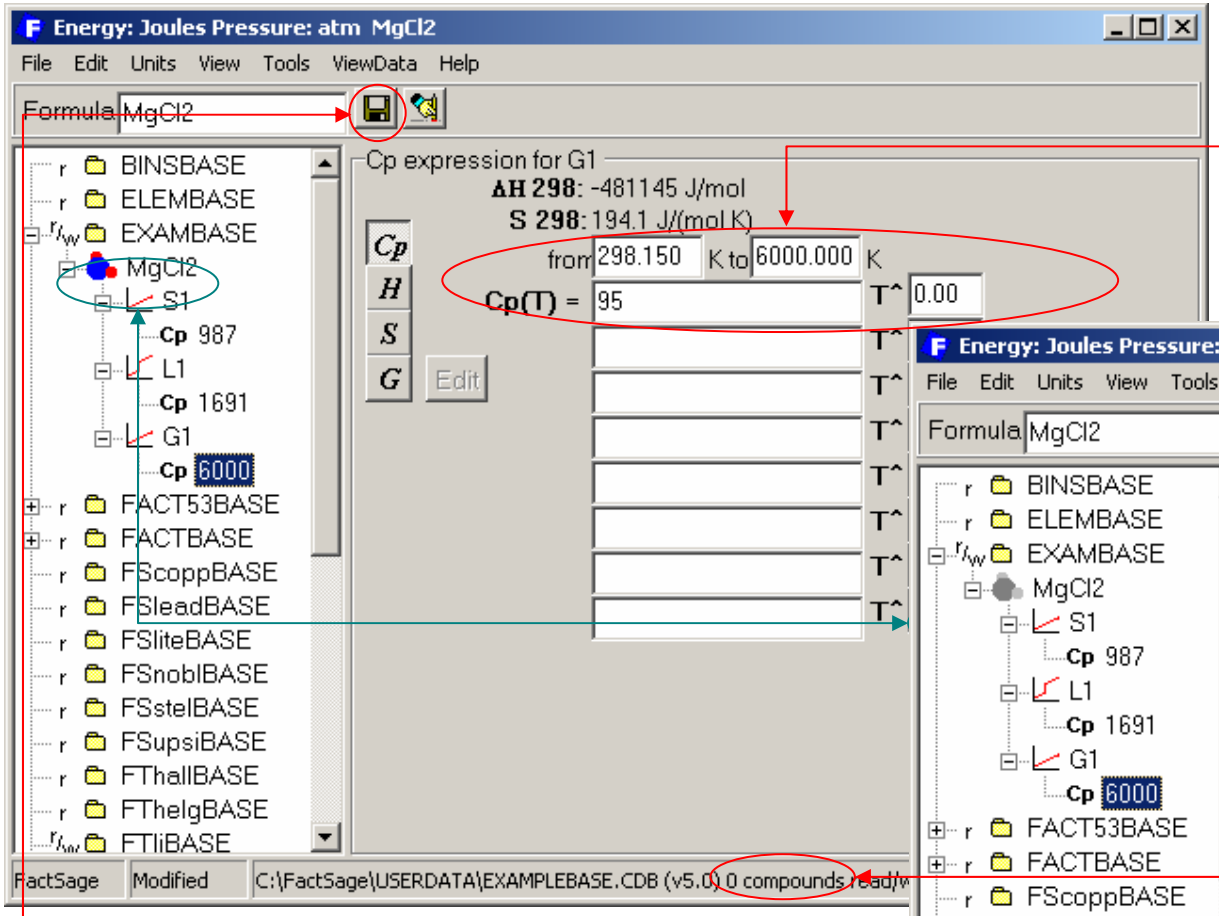
Finishing and saving the entry

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

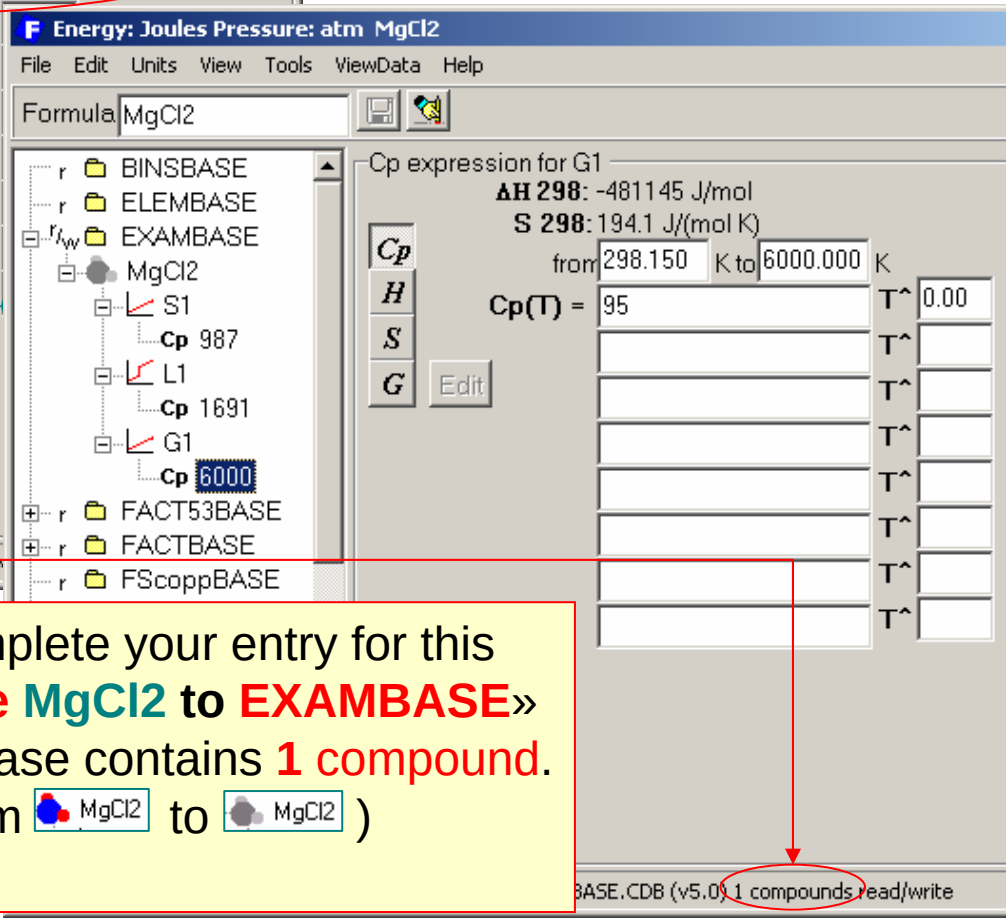
and

the complete dataset is saved in the private database.

Finishing and saving the entry, I



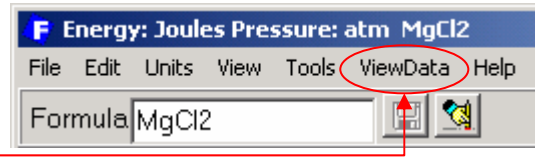
5. **Enter** the C_P range from 298.15 K to **6000 K** and the **C_P expression** for **$MgCl_2$ gas** (slide 4.3)**:** **$C_{P(G)}$= 95 J/mol·K**



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 MgCl2 to MgCl2) indicates that your data are saved.

Displaying data with ViewData, I

1. Click on «ViewData» in the menu bar to open the ***ViewData*** application.



2. **Click** on the **Cp(T)** and **Phases** tabs to display the **compound data**.

MgCl2 Units: T(K) P(atm) Energy(J) Mass(mol)

File Edit Units Summary Databases Table Graph Help

3 Phases | EXAM - EXAM database

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

Name: MgCl2

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

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/mol)	S(298.15) (J/mol-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 | C:\FACTSAGE\USERDATA\EXAMPLEBASE.CDB

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

Name: MgCl2

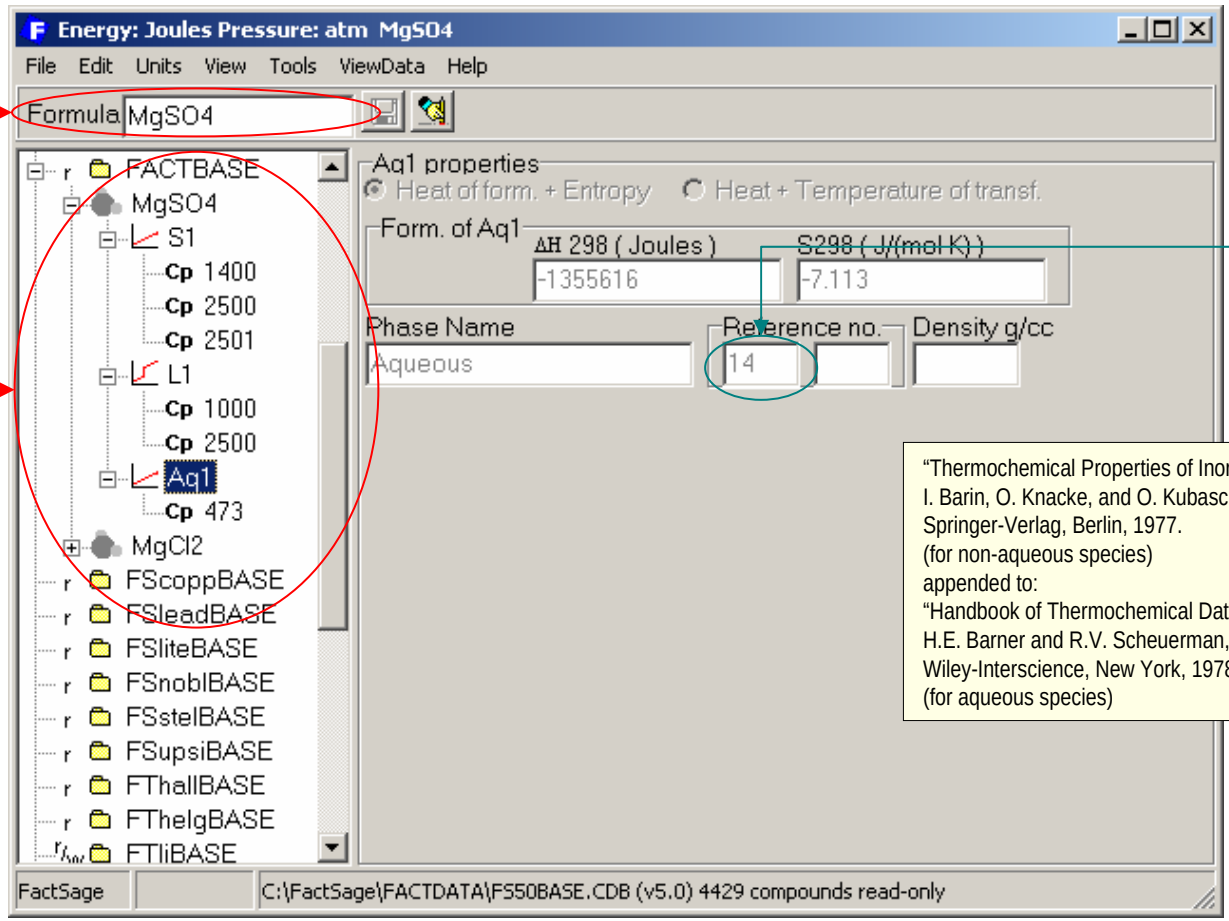
Formula Weight: 95.2104

Stoichiometric Compound: MgCl2

	Phase	Cp Range, K	Density, g/ml	Ref.
S	s1	298.15 - 987.00		
L	l1	298.15 - 1691.00		
G	gas	298.15 - 6000.00	ideal	

Displaying data with Compound, II

1. To display **compound data**, for example **$MgSO_4$** in **FACTBASE**, **enter MgSO4** in the Formula input box.



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

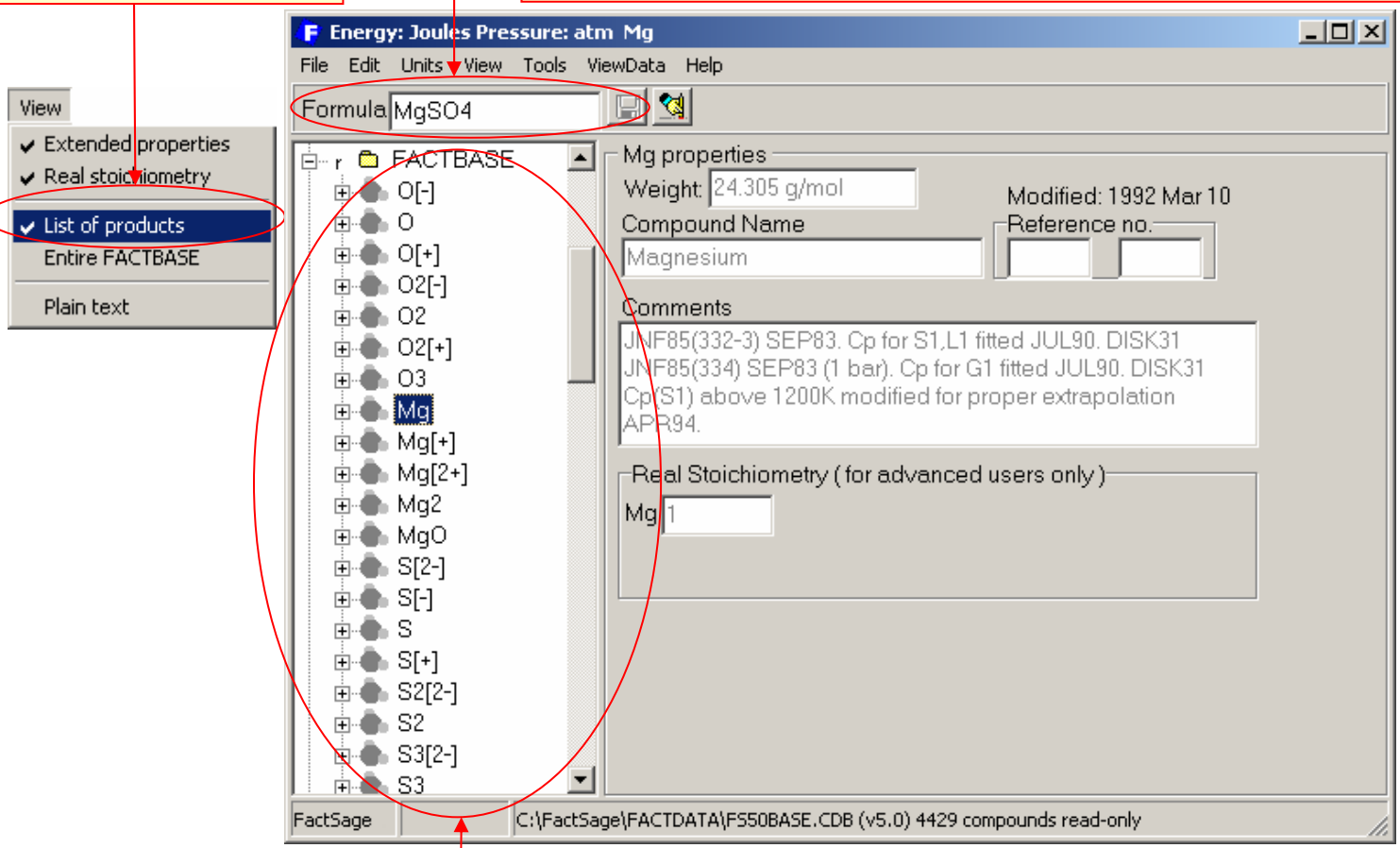
"Thermochemical Properties of Inorganic Substances",
I. Barin, O. Knacke, and O. Kubaschewski,
Springer-Verlag, Berlin, 1977.
(for non-aqueous species)
appended to:
"Handbook of Thermochemical Data for Compounds and Aqueous Species",
H.E. Barner and R.V. Scheuerman,
Wiley-Interscience, New York, 1978.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

2. Expand the tree structure for **FACTBASE** and search through the **MgSO4** branches to list its data.

Displaying data for a list of products, 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

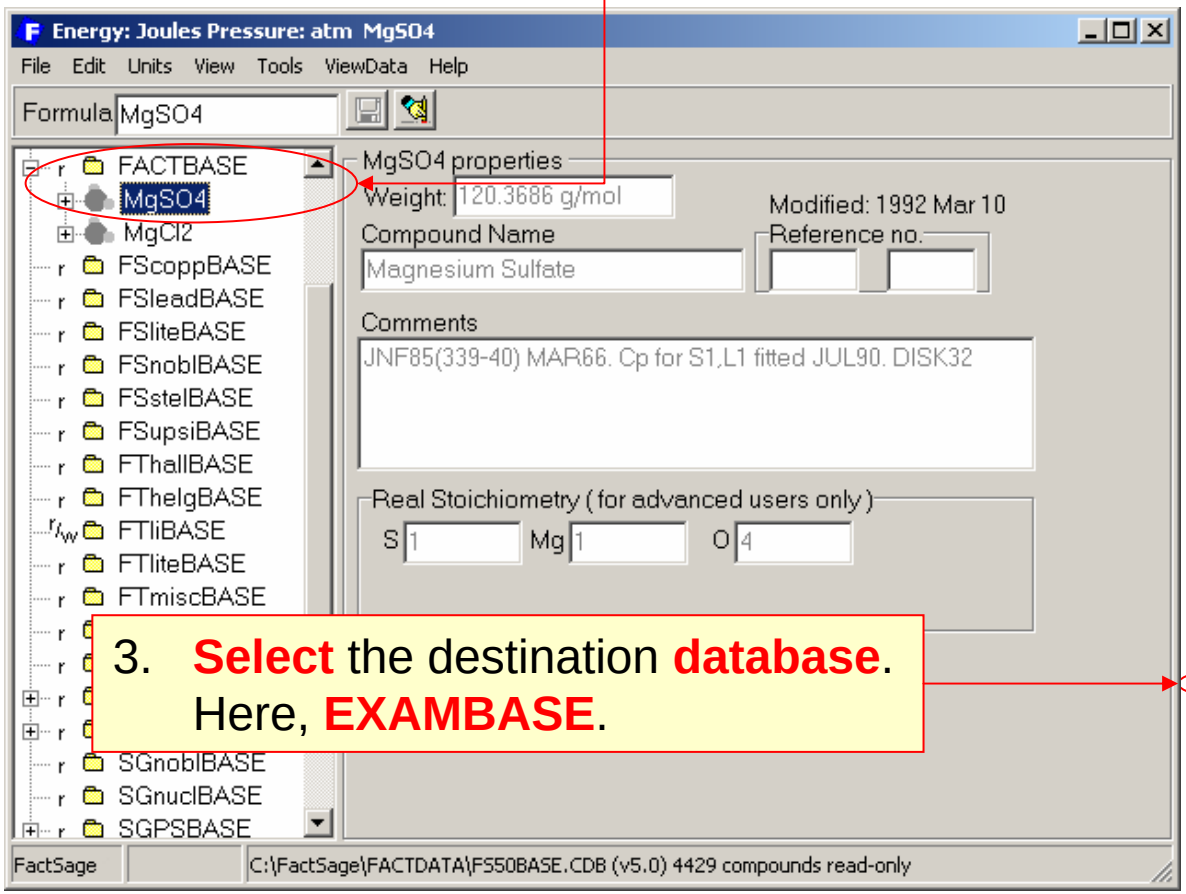
Data for single compounds can be easily transferred between databases.

This is 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 database and copy the desired compound(s) from the read-only database over to your private database.

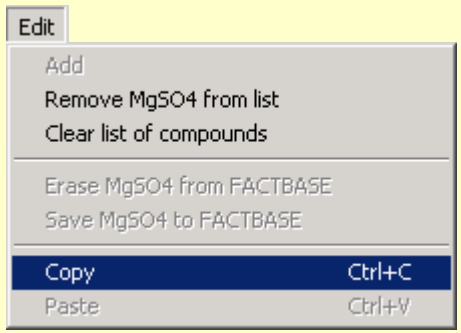
There are two ways to do this as shown in the following slides.

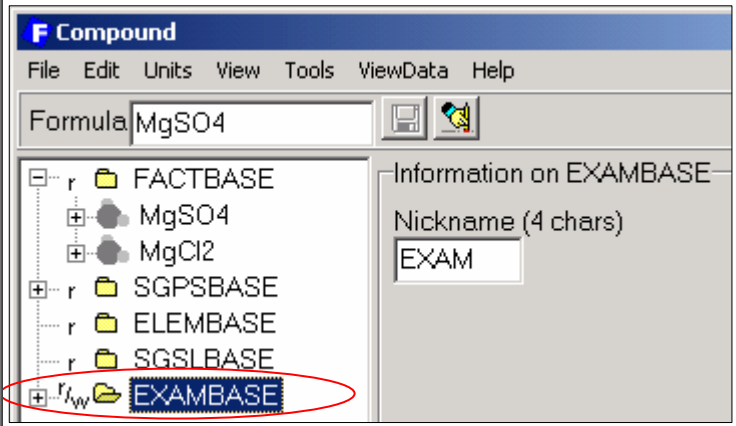
Transferring data between databases, I

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

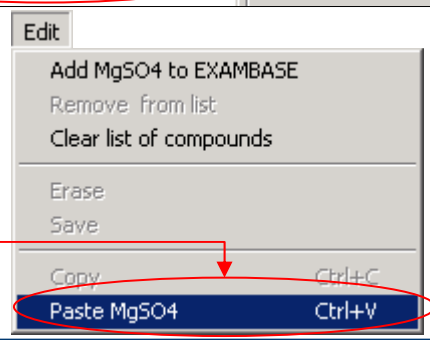


2. Select «**Copy**» from the **Edit** menu.



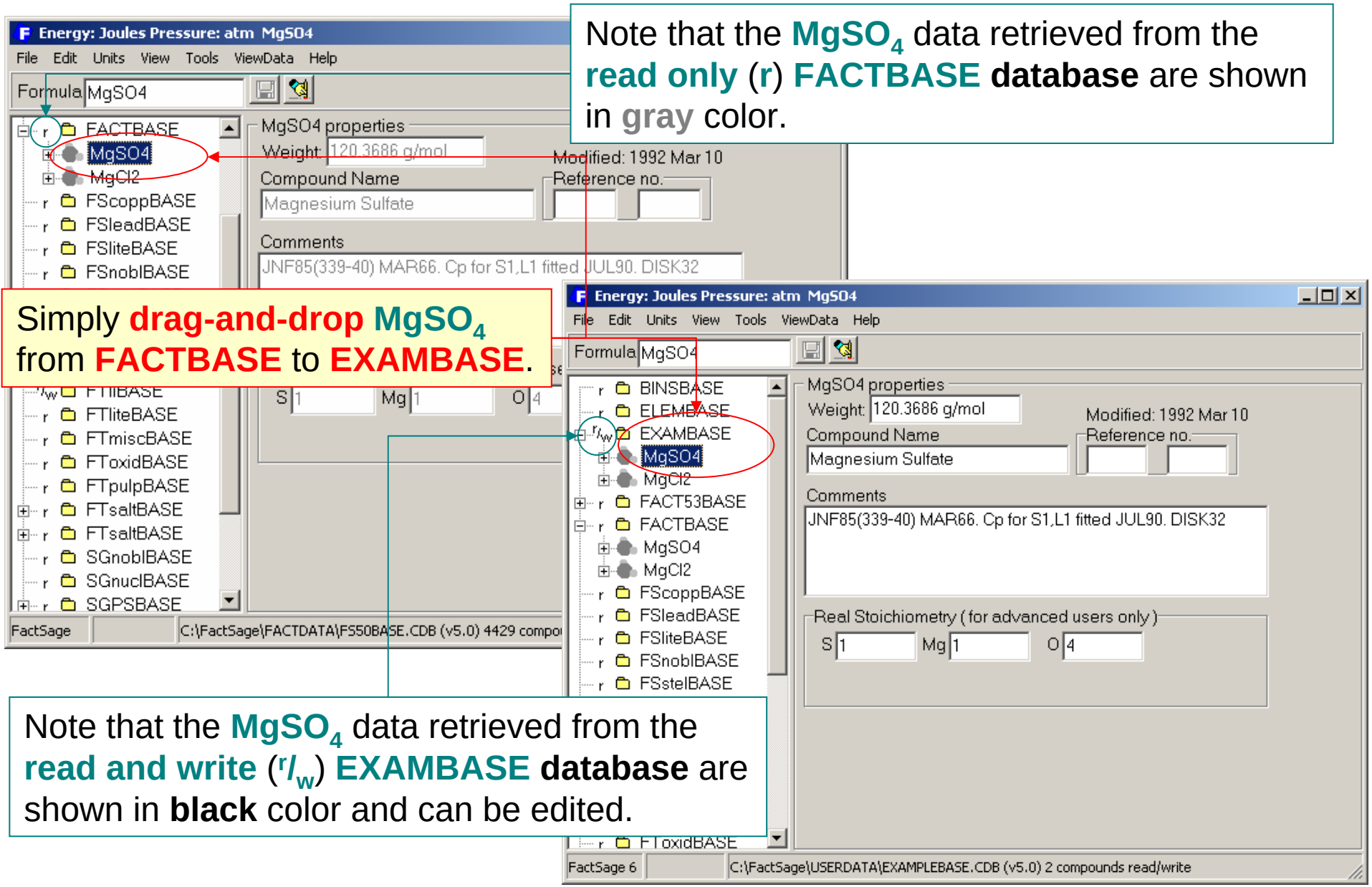


3. **Select** the destination **database**. Here, **EXAMBASE**.



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

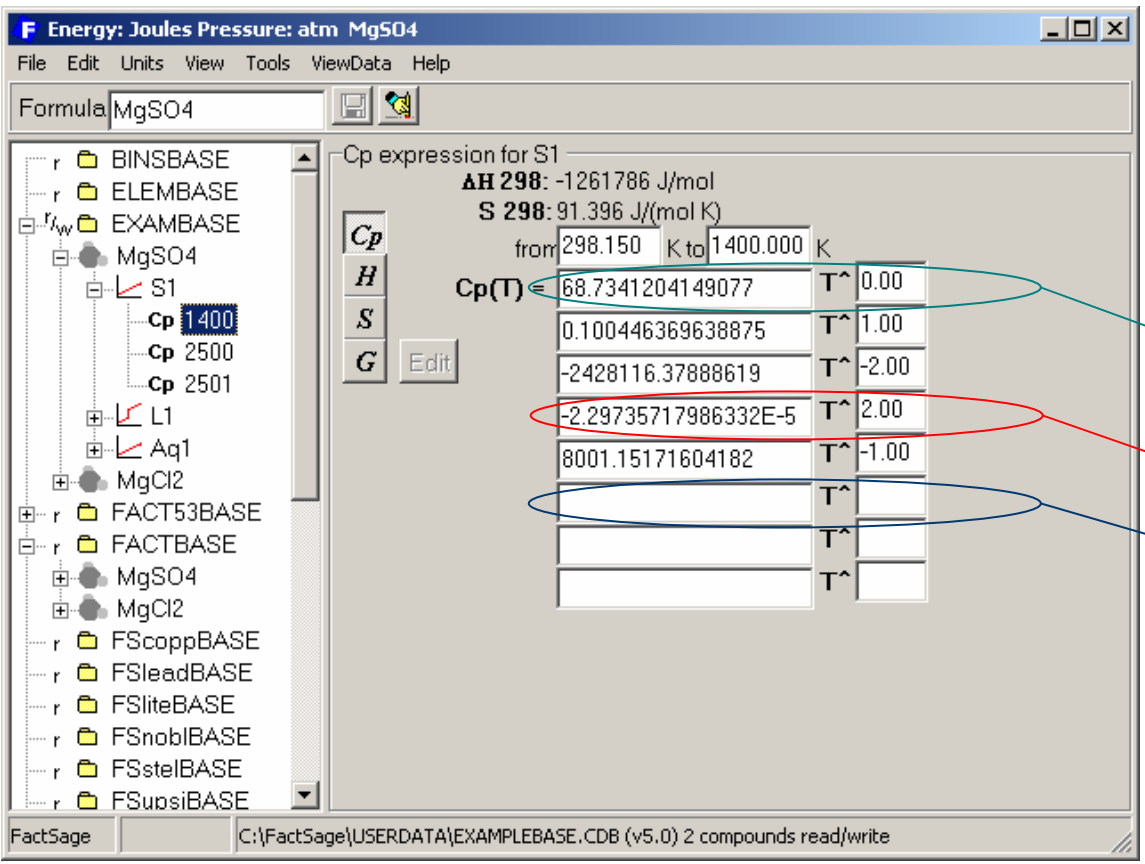
Transferring data between databases, II

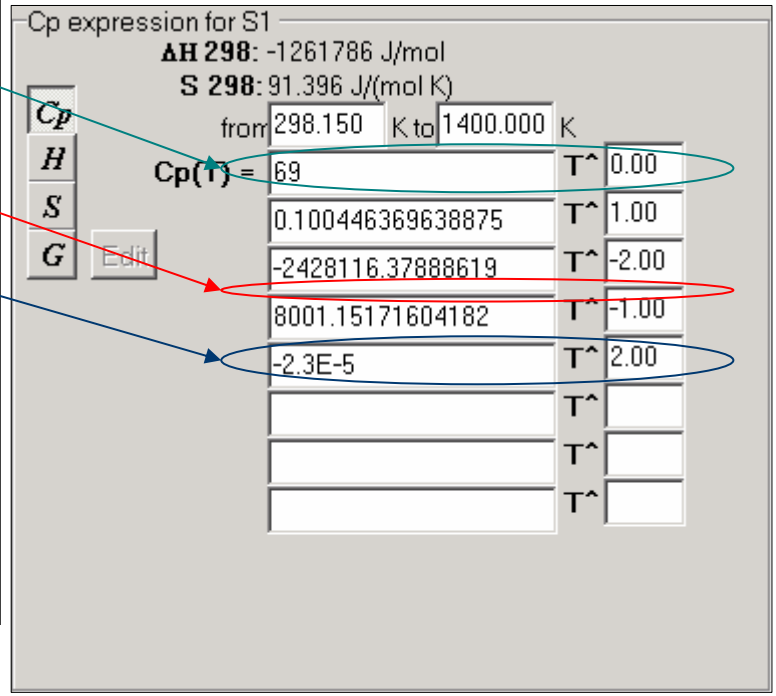


Editing a read and write ($^{r}/_{w}$) database.

Data in a read/write database may be **added**, **removed** or **modified**. Here the C_p range for the solid (S1) phase of $MgSO_4$ in the $^{r}/_{w}$ **EXAMBASE database** is **edited**.

You 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

- erase (delete) single compounds from a particular database
- remove single compounds from an edit list
- clear complete edit lists.

NOTE: The Remove and Clear commands do not interfer with the contents of databases and can be applied to all databases.
The Erase command only works for read/write databases.

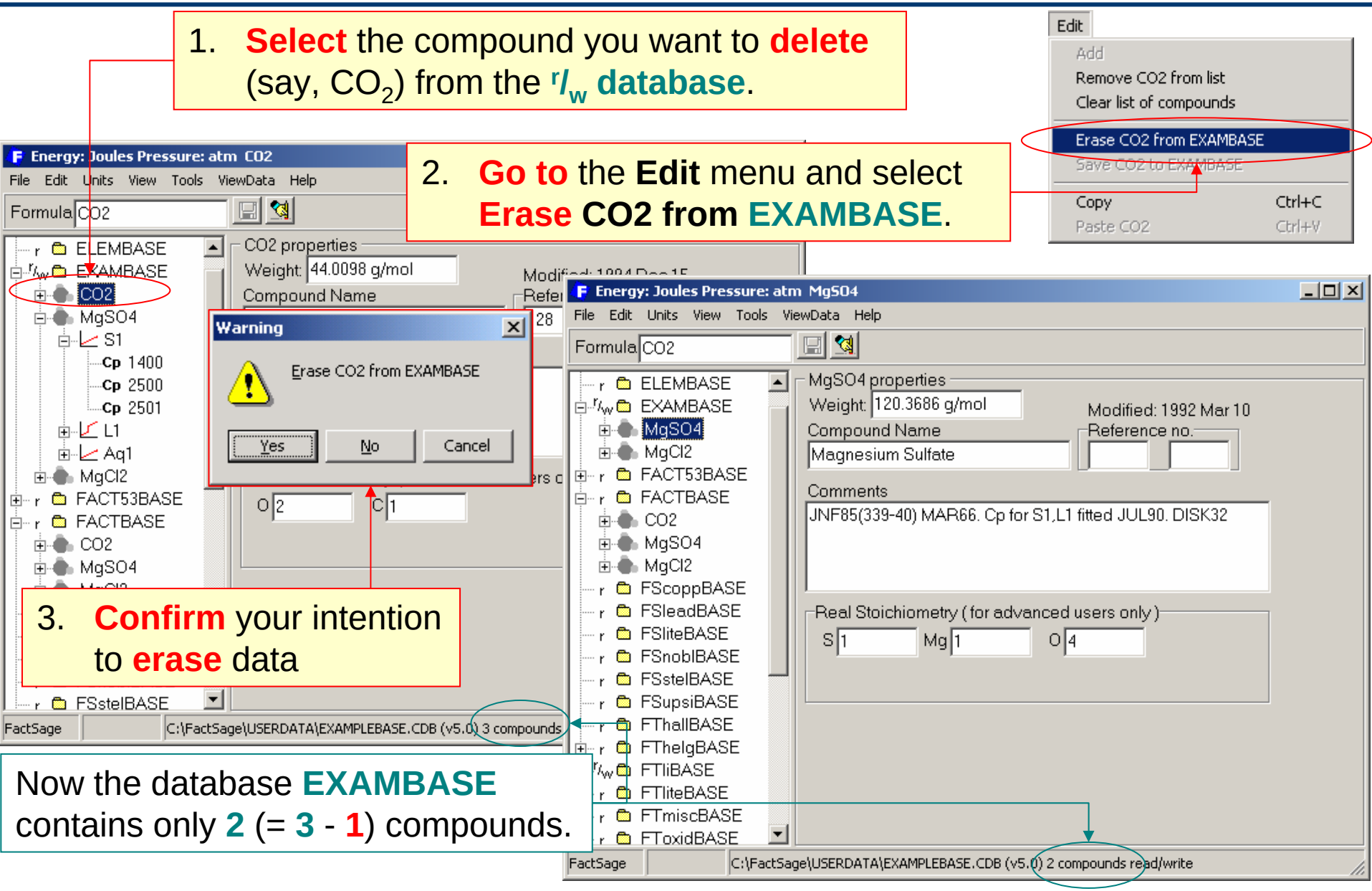
The Erase, Remove and Clear commands, I

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

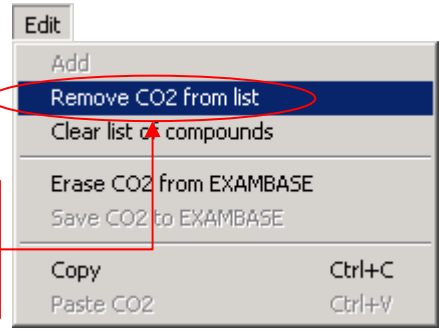
Now the database **EXAMBASE** contains only **2** (= **3** - **1**) compounds.

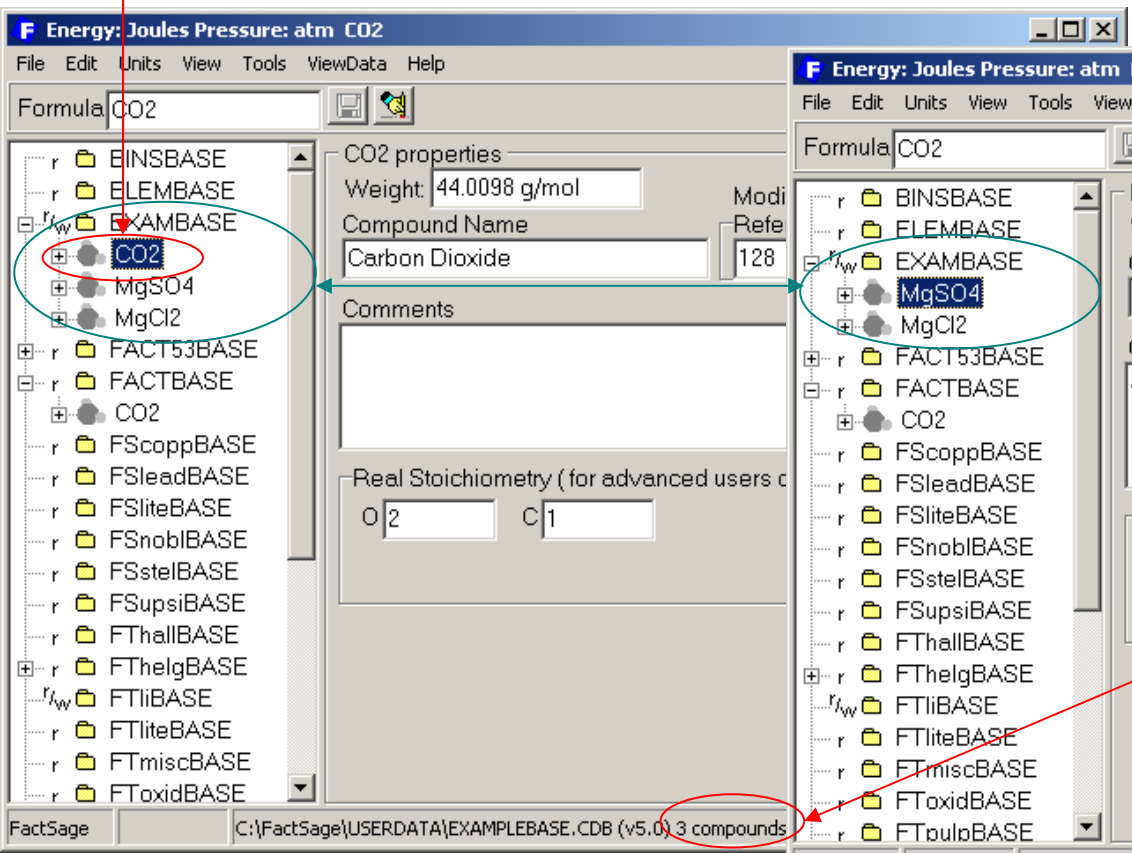


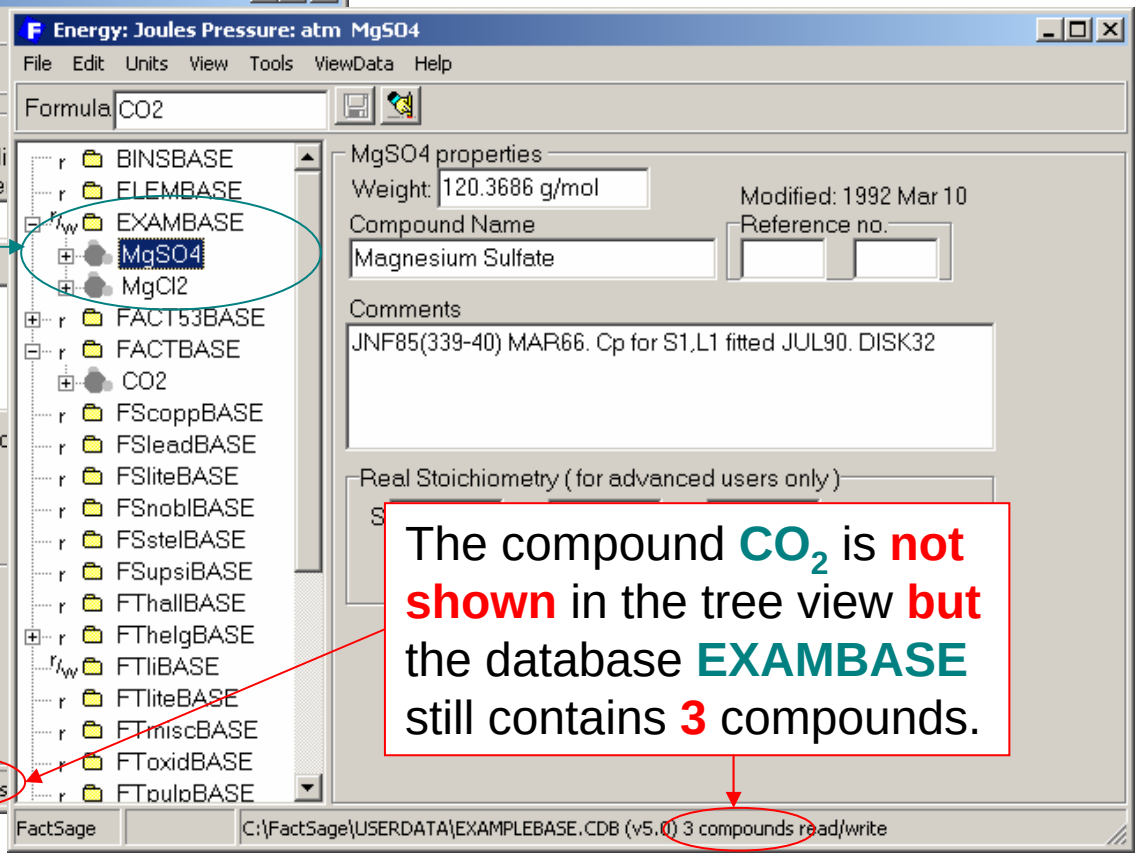
The Erase, Remove and Clear commands, II

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**.





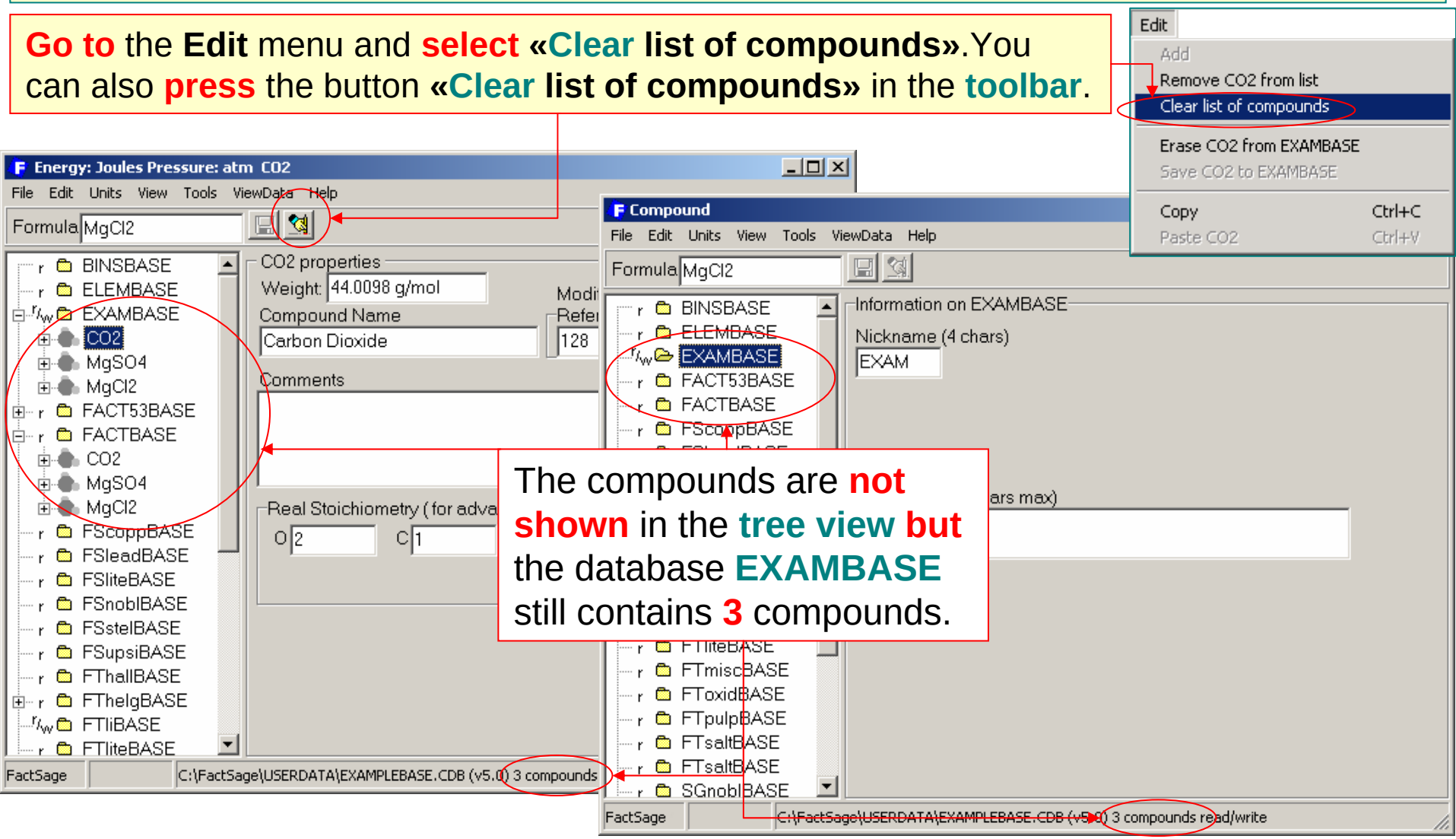


The compound CO_2 is **not shown** in the tree view **but** the database **EXAMBASE** still contains **3** compounds.

The Erase, Remove and Clear commands, III

To **remove** **all** the compounds from **all** the **lists** (you are **not** deleting 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 $Na_3Al_3O_6$.

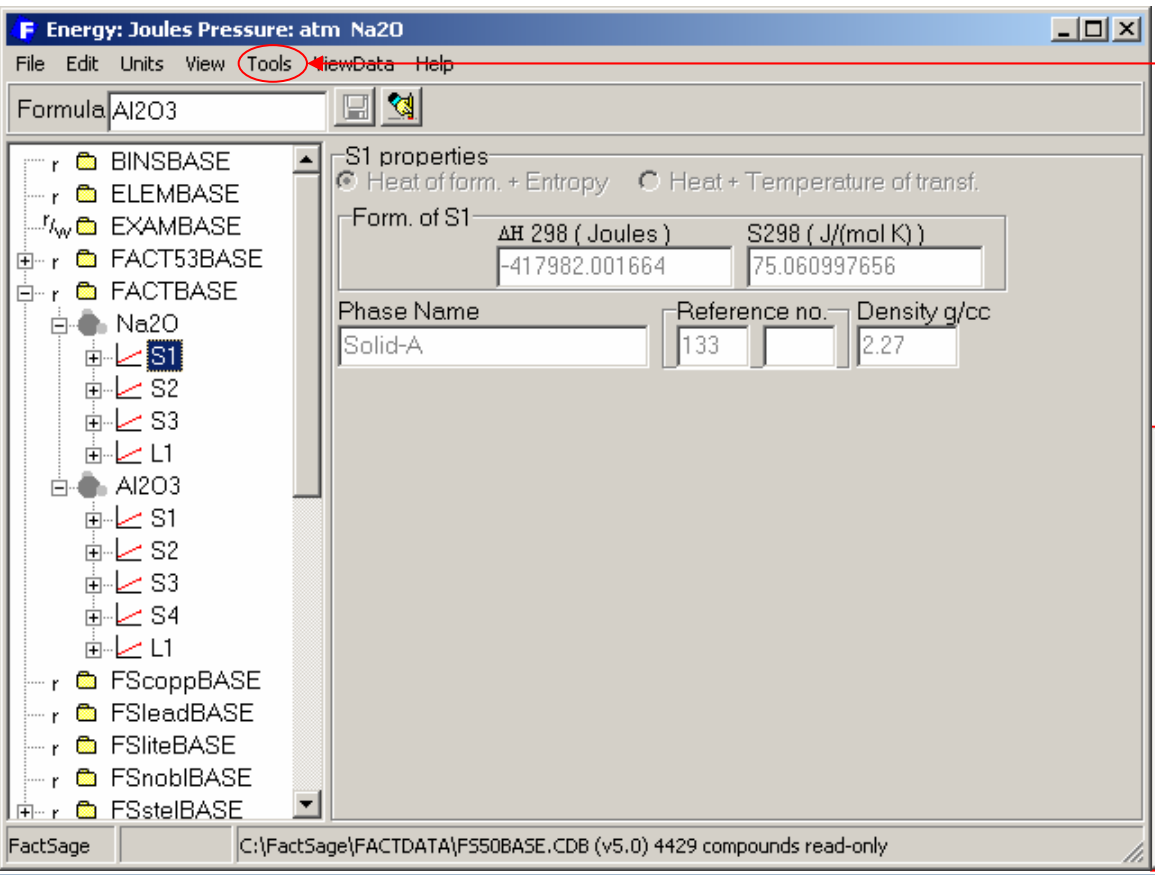
The second example shows how the known data for Li_3N, Li and Na are used to generate data for the unknown compound Na_3N using $Li_3N + 3Na - 3Li = Na_3N$.

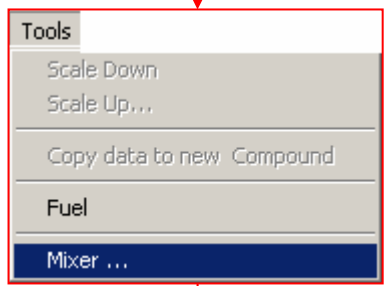
The «Mixer» feature: Example 1, I

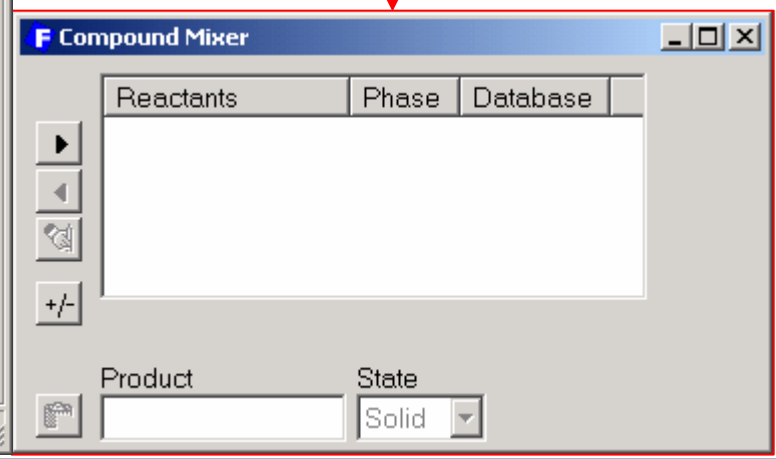
The «**Mixer**» option enables you to create and store compound data on a new (possibly hypothetical) species by mixing data of existing species. For example, new data on $NaAlO_2$ via the reaction: ½ Na_2O(s1) + ½ Al_2O_3(s1)→ $NaAlO_2$(s1).

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

2. Click on Tools > Mixer…

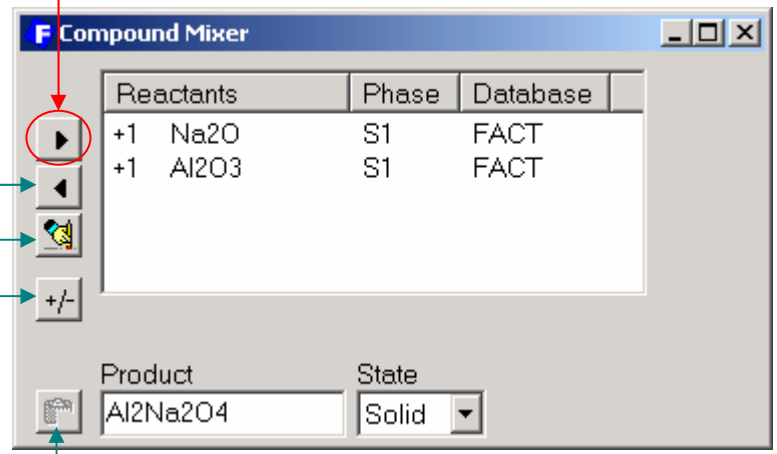






The «Mixer» feature: Example 1, II

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.

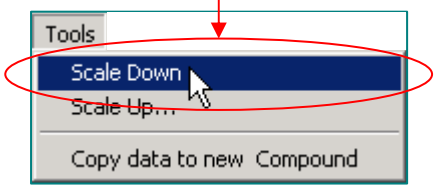
This stores the new compound $Al_2Na_2O_4$ in the database. To store $NaAlO_2$ you need to use the **«Scale Down»** command in the **Tools** menu.

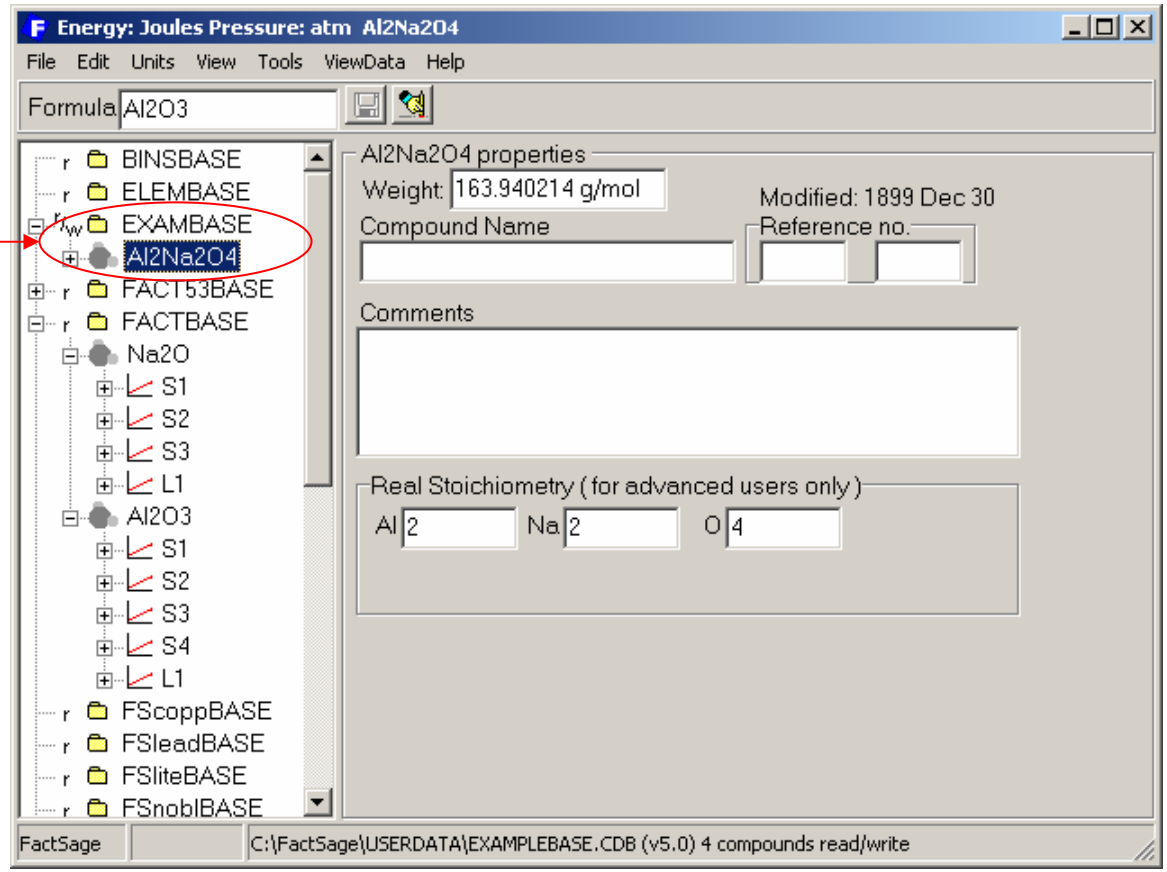
The «Mixer» feature: Example 1, III

To **scale down** a compound:

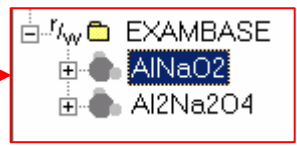
1. Save your compound in a $^{r}/_{w}$ database:
   A. Select a $^{r}/_{w}$ database.
   B. Paste your compound.

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





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

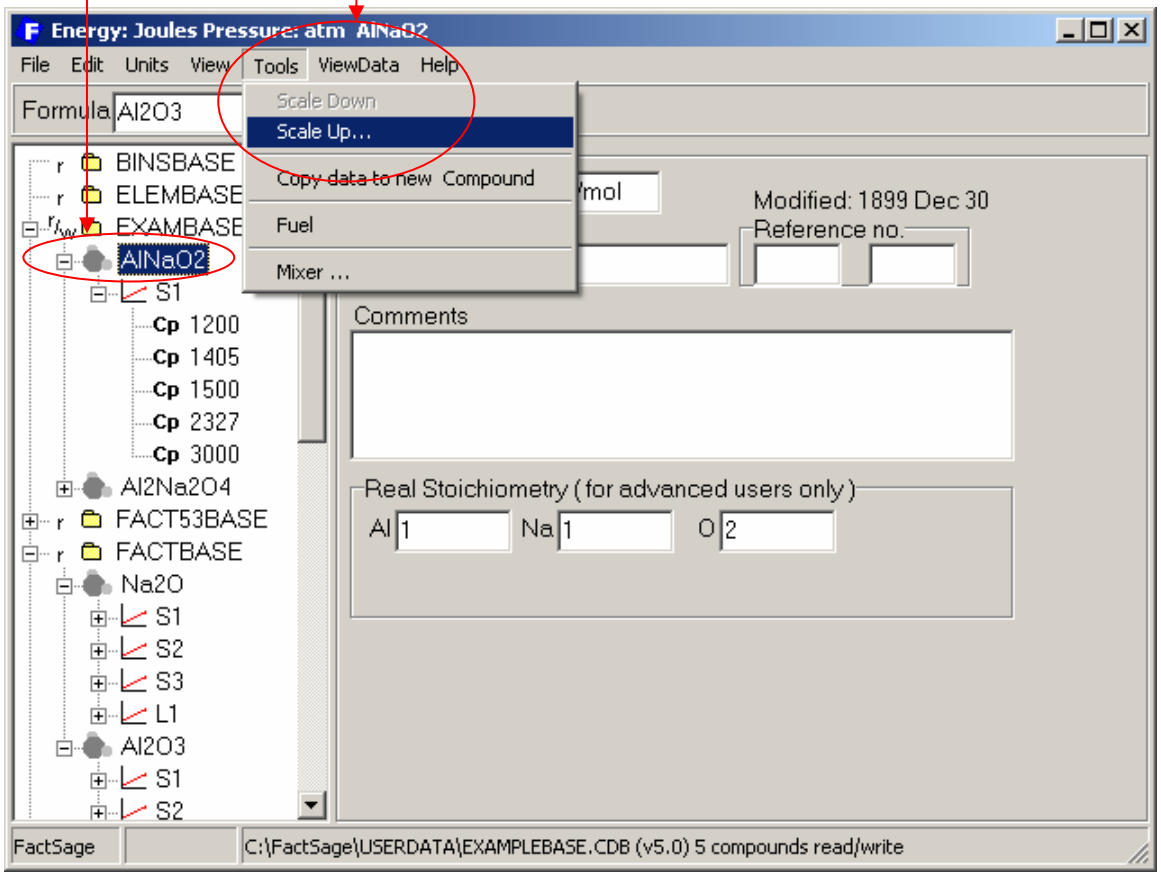


The «Mixer» feature: Example 1, IV

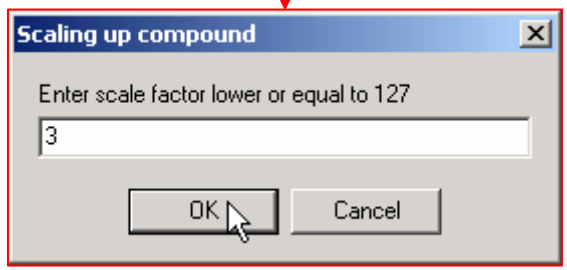
On the other hand, if you want the thermodynamic properties of $Na_3Al_3O_6$, which is 3 times $AlNaO_2$, use the **Scale Up** command.

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

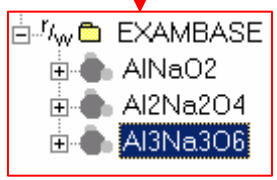
2. Go to the **Tools** menu and select **Scale Up…**



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



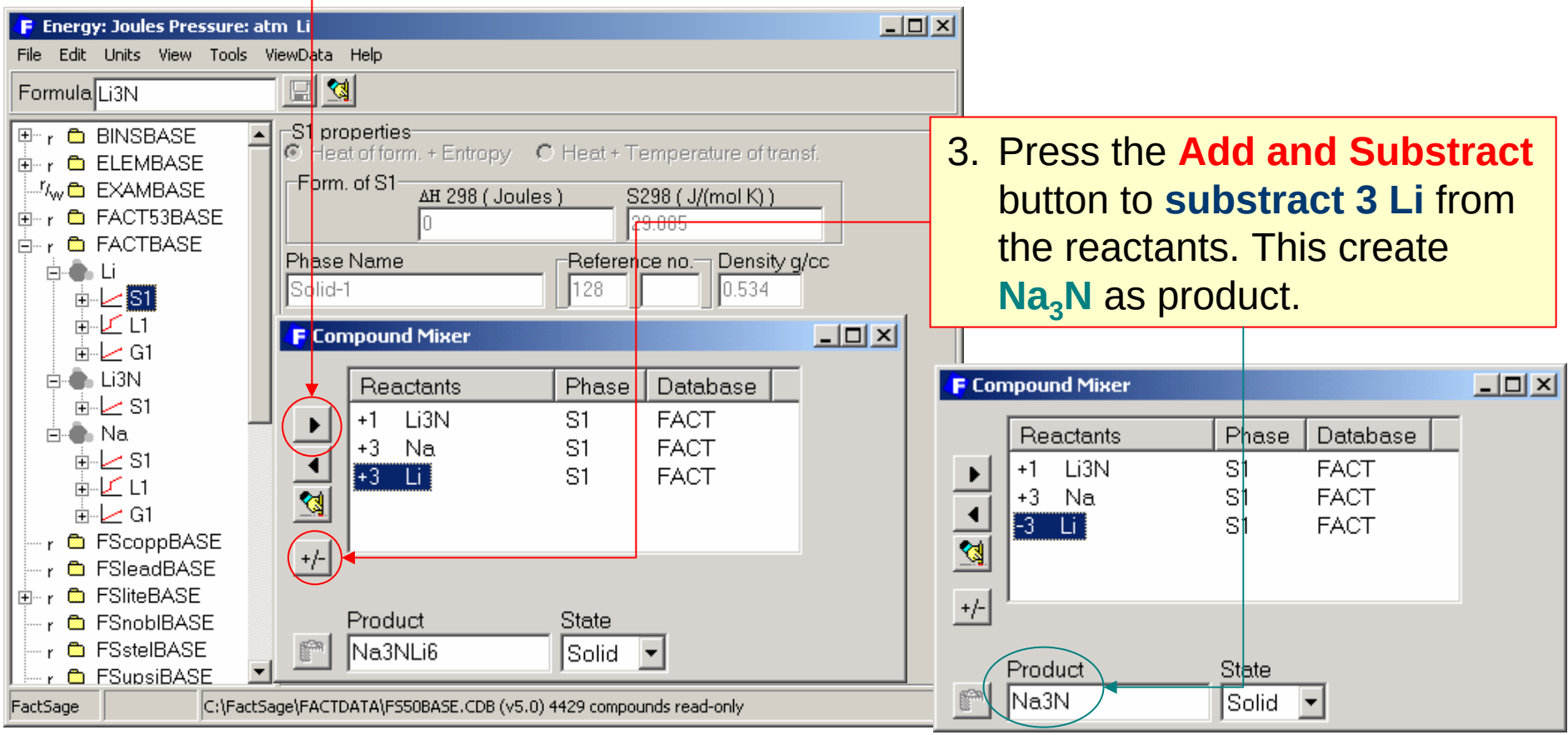
The «Mixer» feature: Example 2

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.

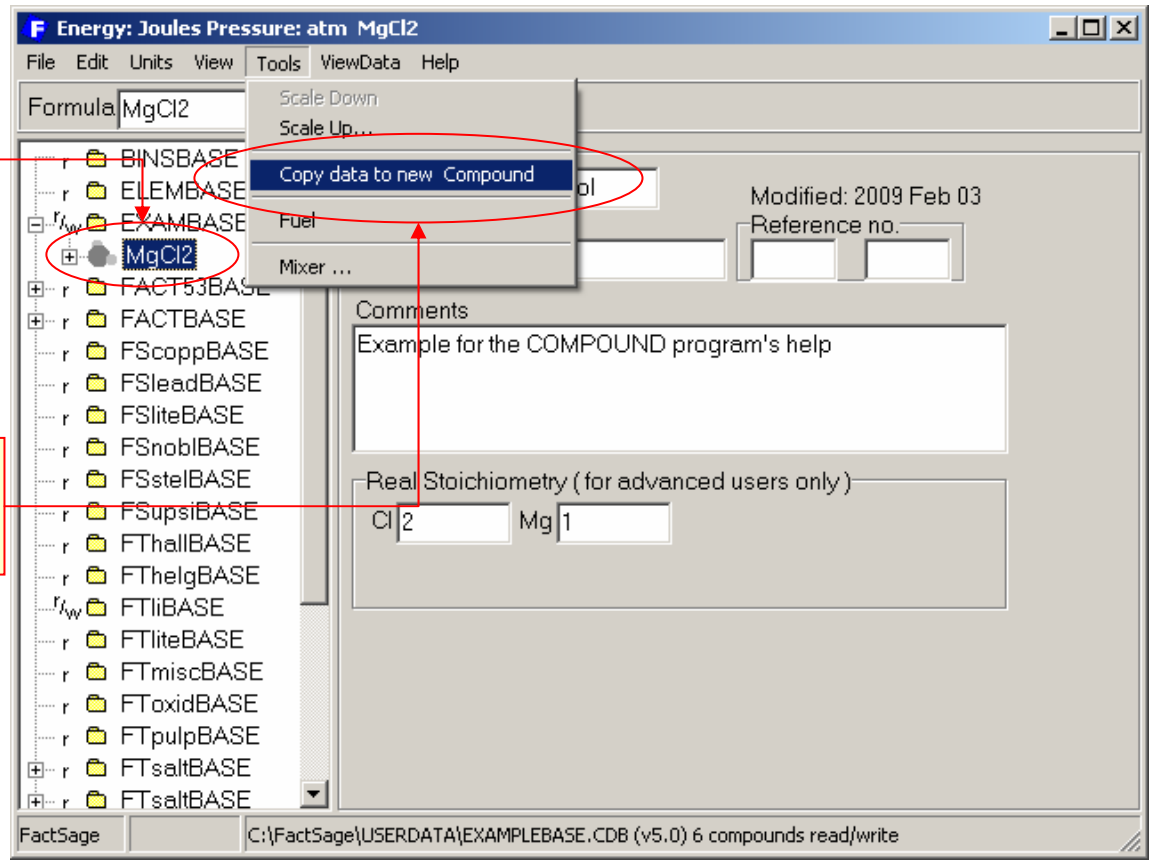


Using known data as template: «Copy data to new Compound», I

You may use data of an already stored compound as a template to enter data for a new compound. Here known data for $MgCl_2$ is used to generate new data for $CaCl_2$ by using the **Copy data to new Compound** option in the Tools menu.

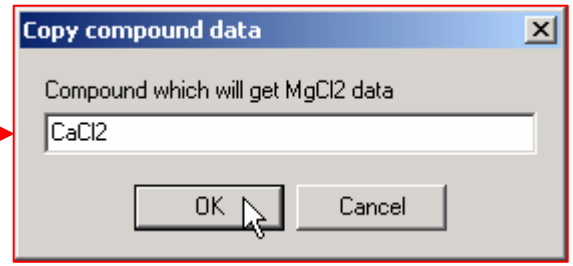
1. Select $MgCl_2$ in EXAMBASE.

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

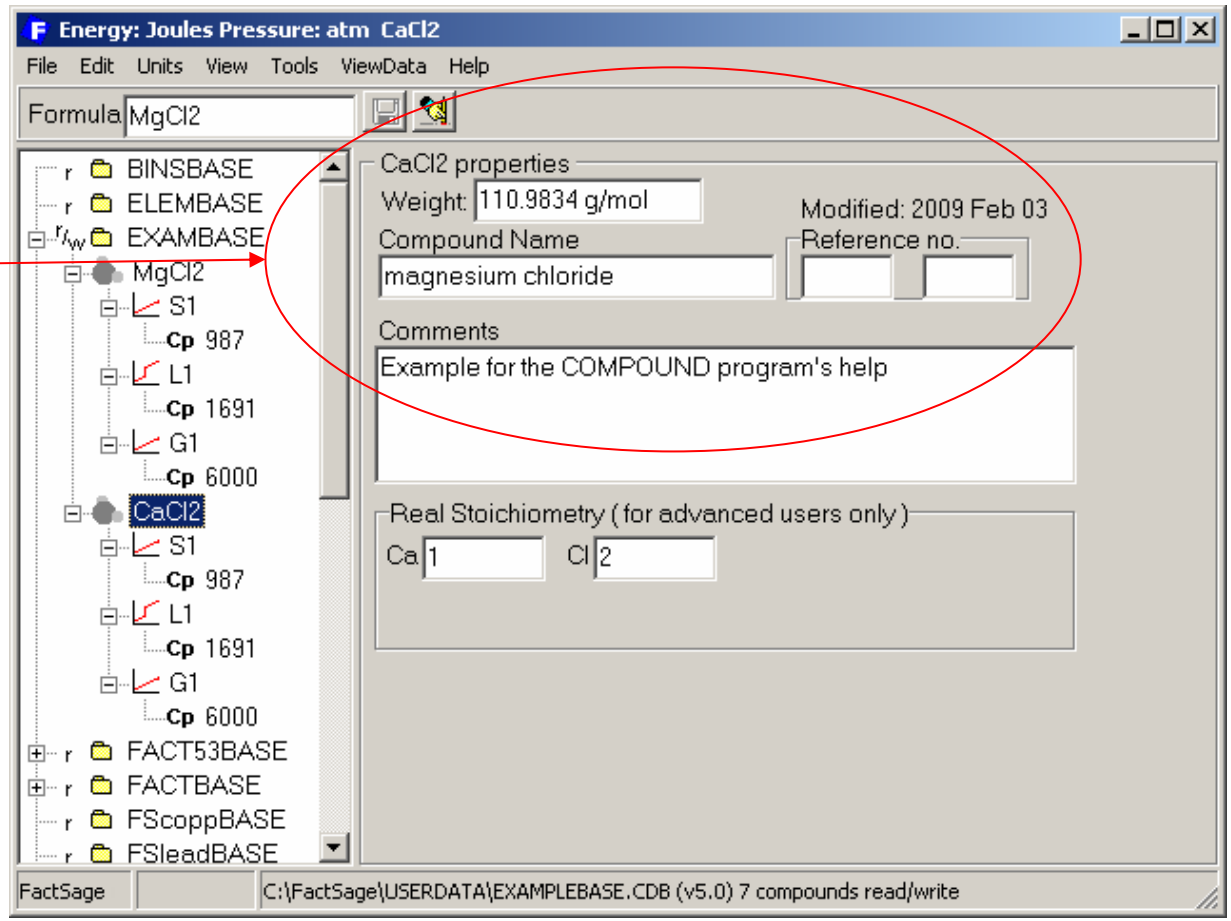


Using known data as template, II

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

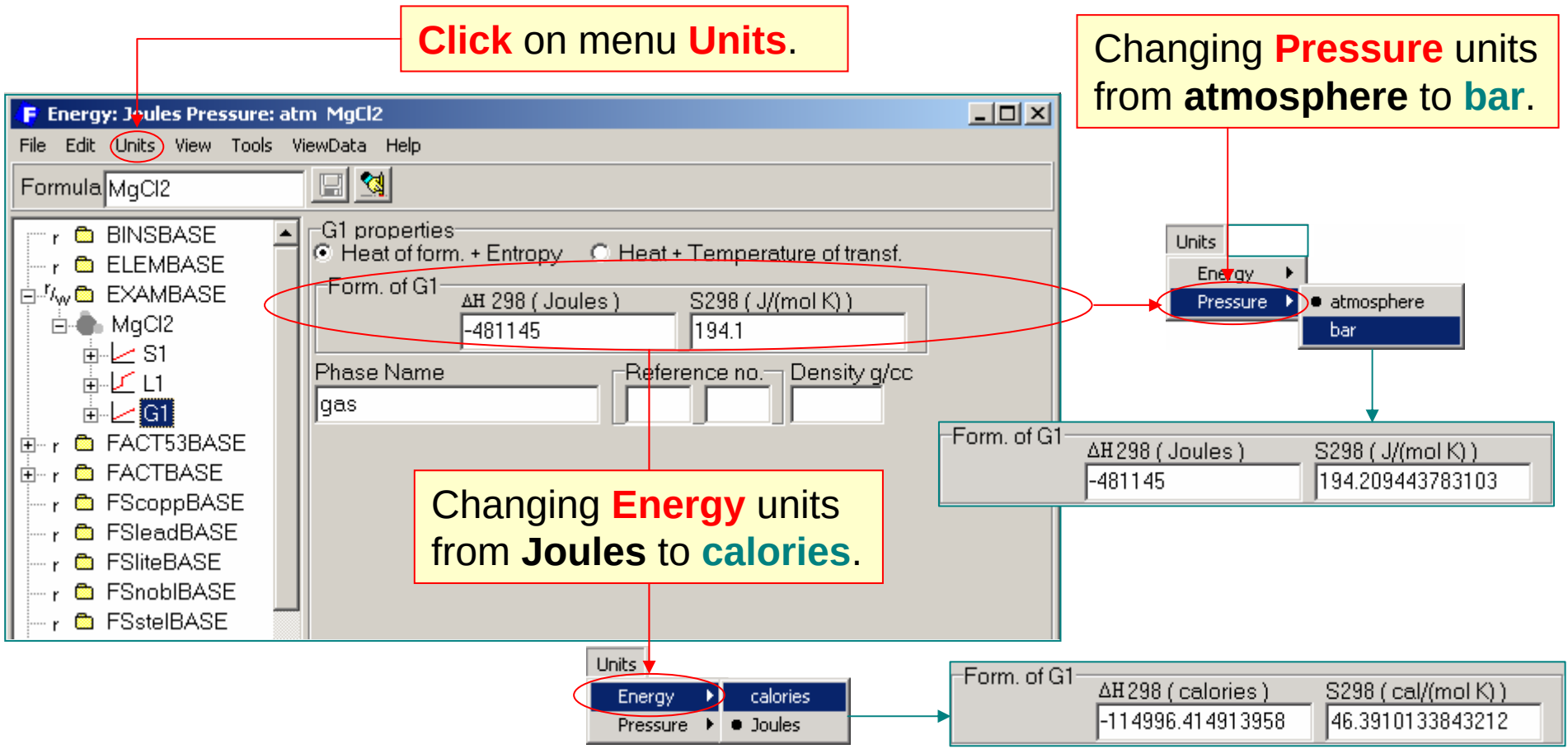


4. You now have the **$CaCl_2$** template.

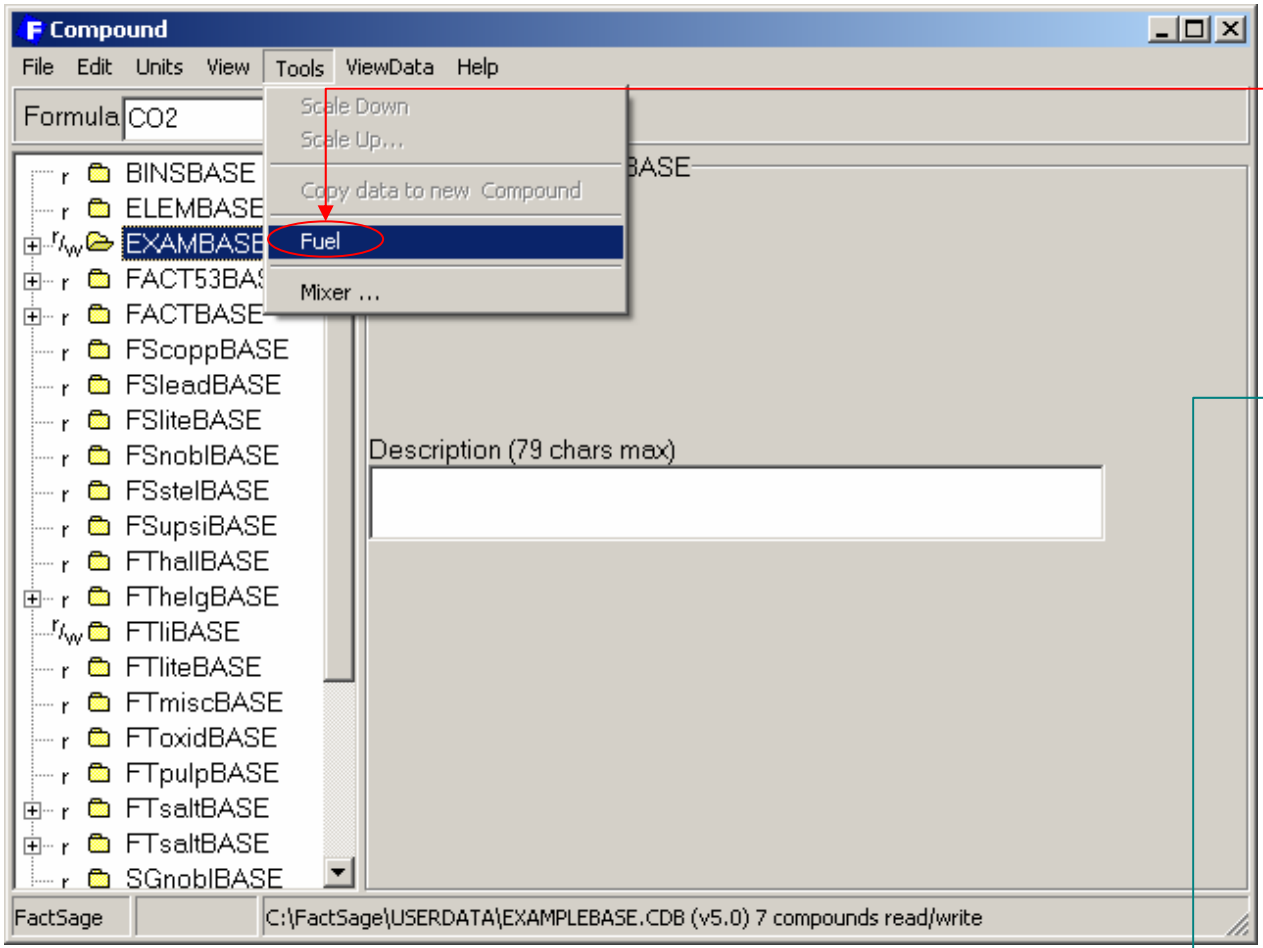


Changing Units of Energy and Pressure

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.

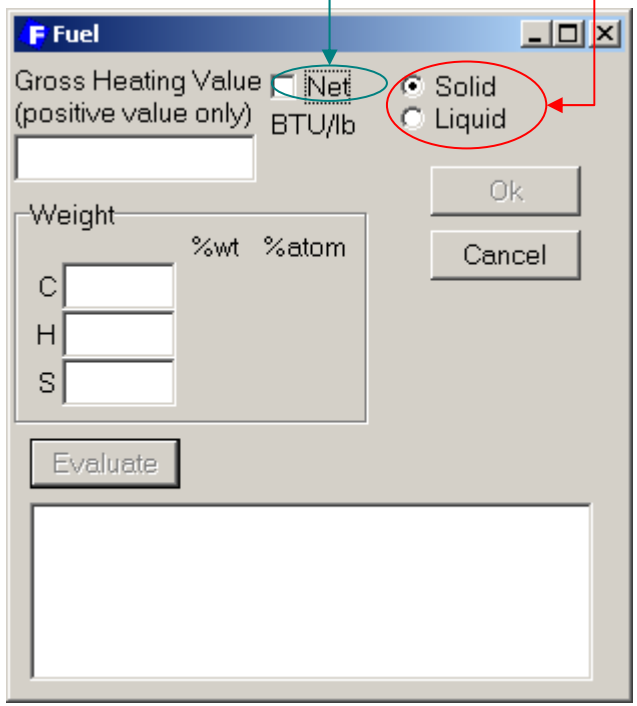


Entering **Fuel** consisting of **hydrocarbons** and **sulfur**, I



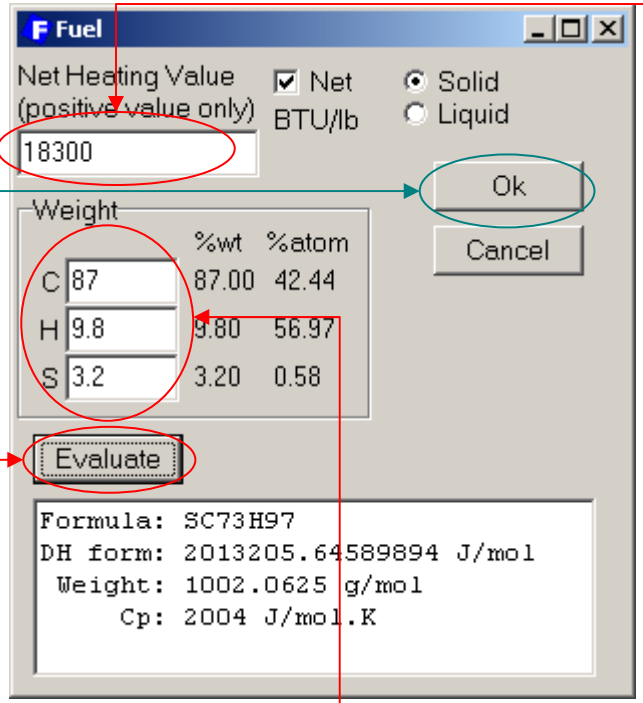
1. Click on «**Tools**» > «**Fuel**»

2. Select **Solid** or **Liquid** fuel

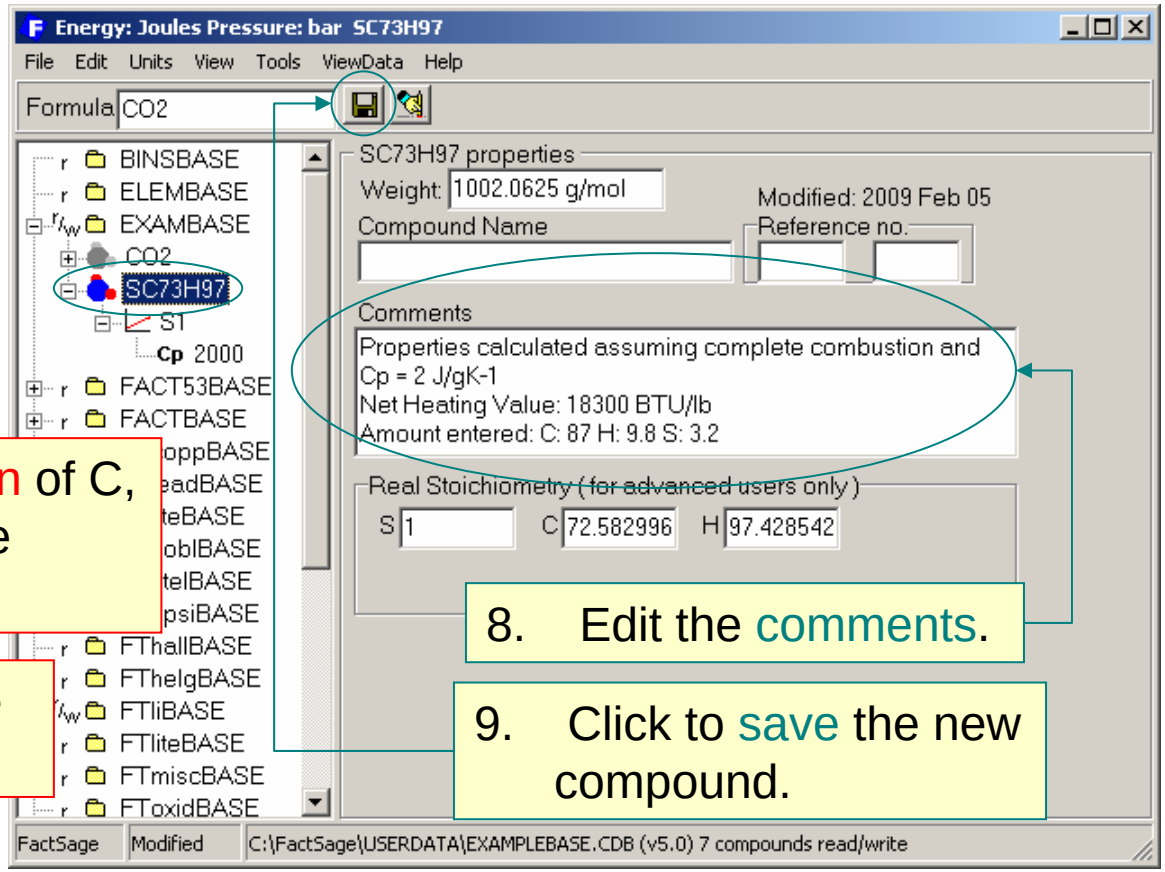


3. Select checkbox **Net** (Net Heating Value) if water in products is gaseous, or unselect checkbox **Net** (Gross Heating Value) if water in products is liquid.

Entering Fuel consisting of hydrocarbons and sulfur, II



4. Enter the Heating Value in BTU/lb – this assumes perfect combustion where products are solely CO_2, H_2O and SO_2.



5. Enter the weight composition of C, H and S of the fuel. Note the calculated %wt and %atom.

6. Click evaluate to display the properties of the fuel.

7. Press OK when finished.

8. Edit the comments.

9. Click to save the new compound.