

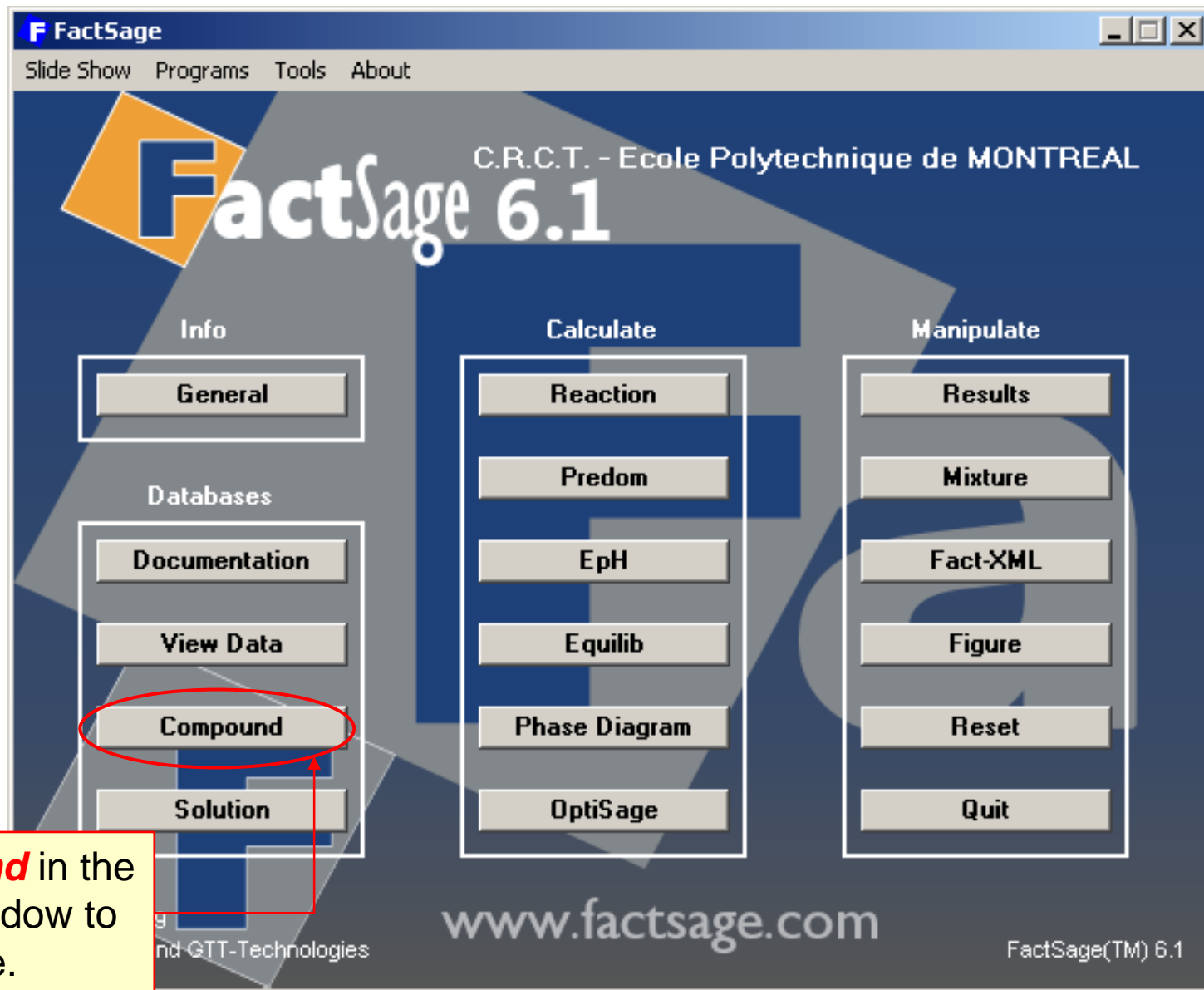
# The **Compound** module

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

## Table of Contents

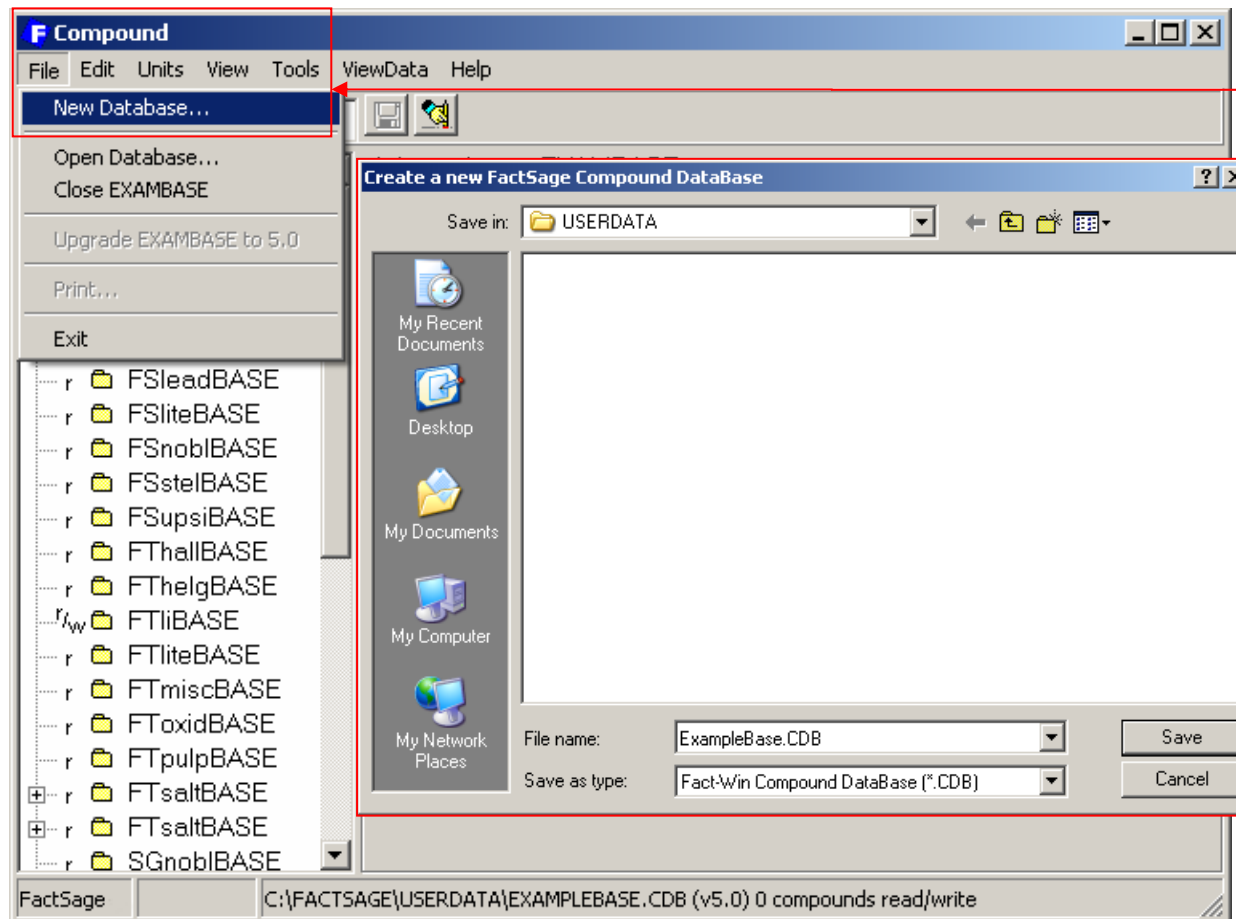
Section 1	<u>Table of Contents</u>
Section 2	<u>Activate COMPOUND</u>
Section 3	<u>Create a private compound database</u>
Section 4	<u>Add a compound to the database</u>
Section 5	<u>Show data as H, S and G functions</u>
Section 6	<u>Edit a G function</u>
Section 7	<u>Entering phase transition data</u>
Section 8	<u>Entering a new phase with <math>H_{298}</math>, <math>S_{298}</math> and <math>C_p</math> data</u>
Section 9	<u>Finishing and saving the entry</u>
Section 10	<u>Displaying data</u>
Section 11	<u>Transferring data between databases</u>
Section 12	<u>Editing data in a read/write database</u>
Section 13	<u>Erase, Remove and Clear commands</u>
Section 14	<u>The Mixer feature</u>
Section 15	<u>Using known data as template</u>
Section 16	<u>Changing units of Energy and Pressure</u>
Section 17	<u>Entering Fuel consisting of hydrocarbons and sulfur</u>

# The *Compound* module



# Create a private *Compound* database, I

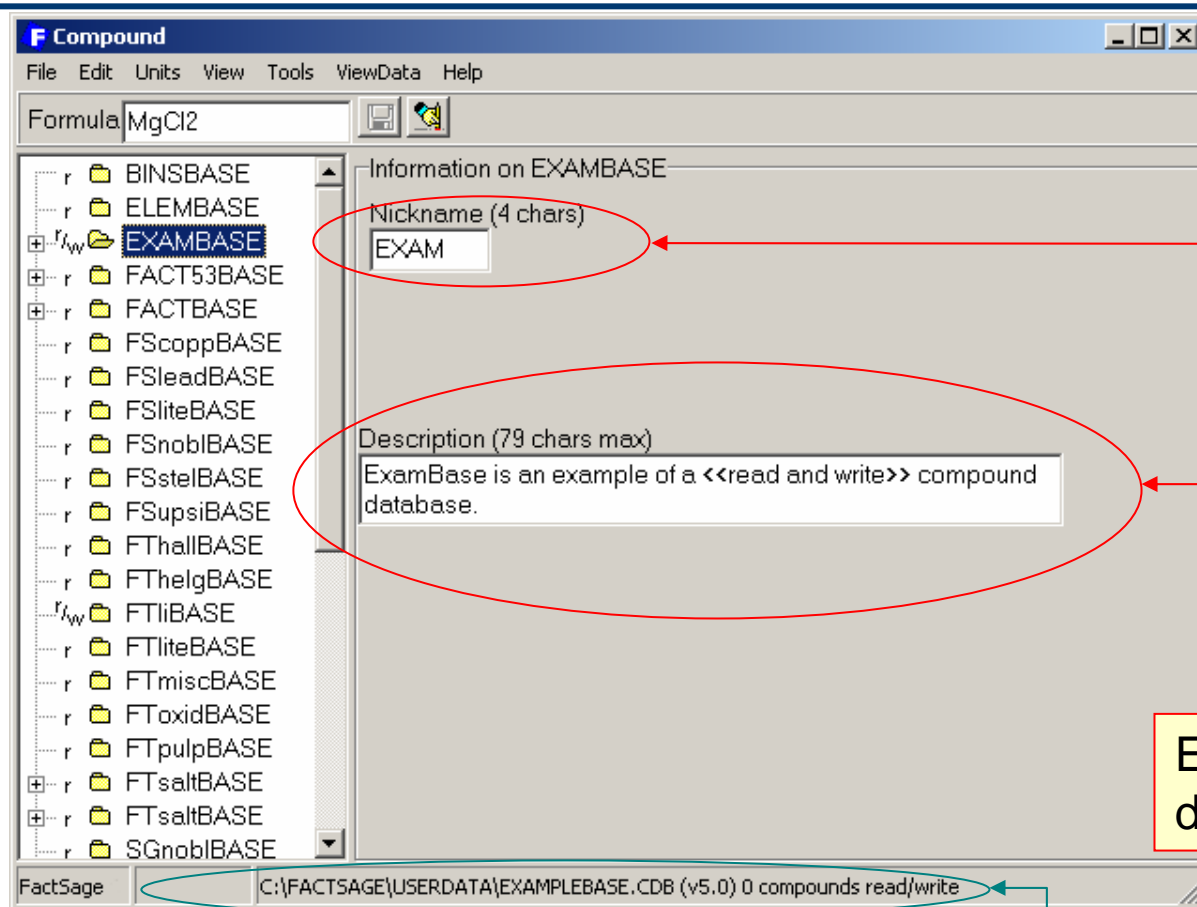
To create a read and write (r/w) database:



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.

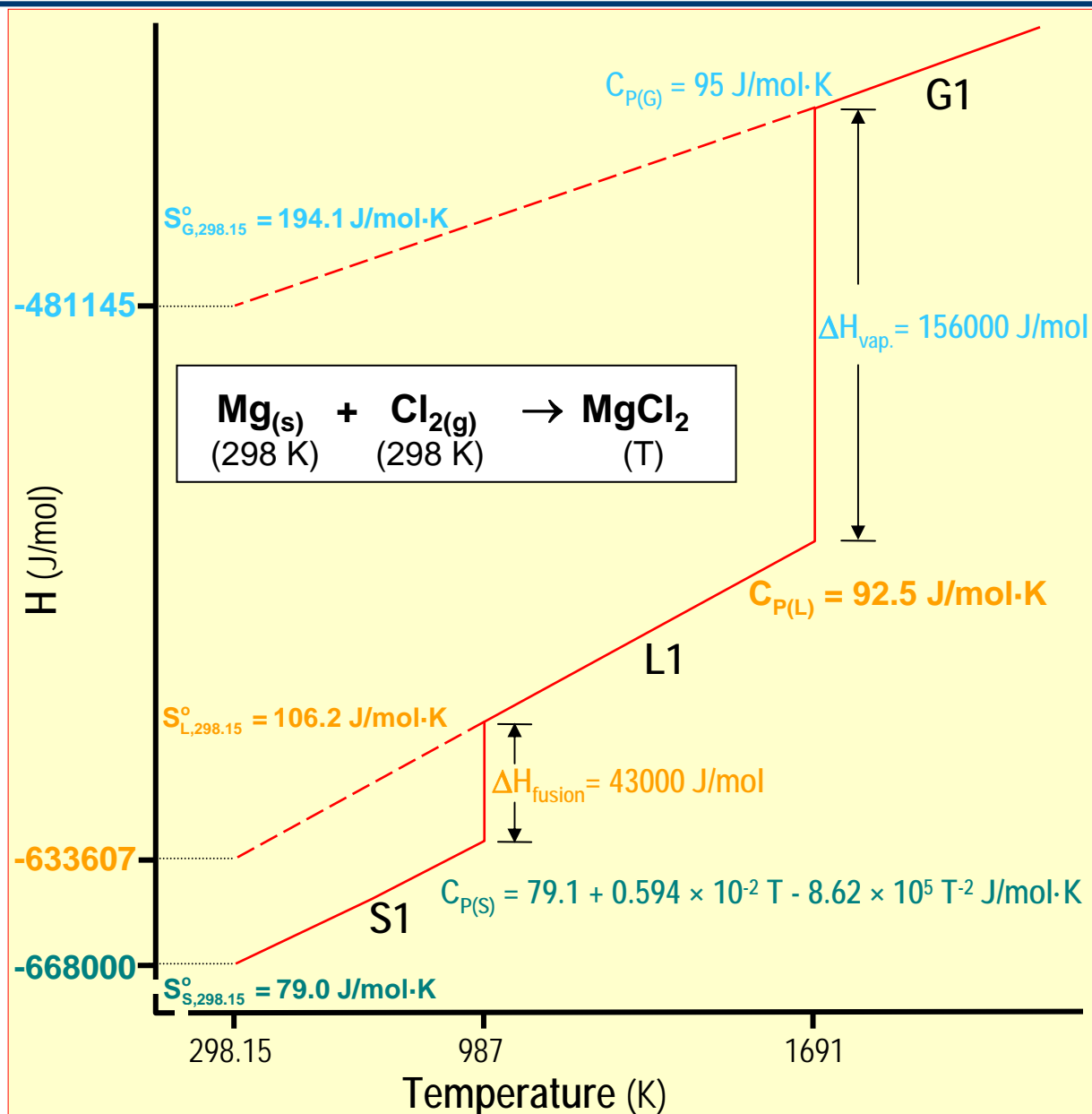
$\text{MgCl}_2$  is taken as the example. The data for this compound are summarized in the next slide. All entries are made using the values in this figure.

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  $\text{MgCl}_2$ )
- 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

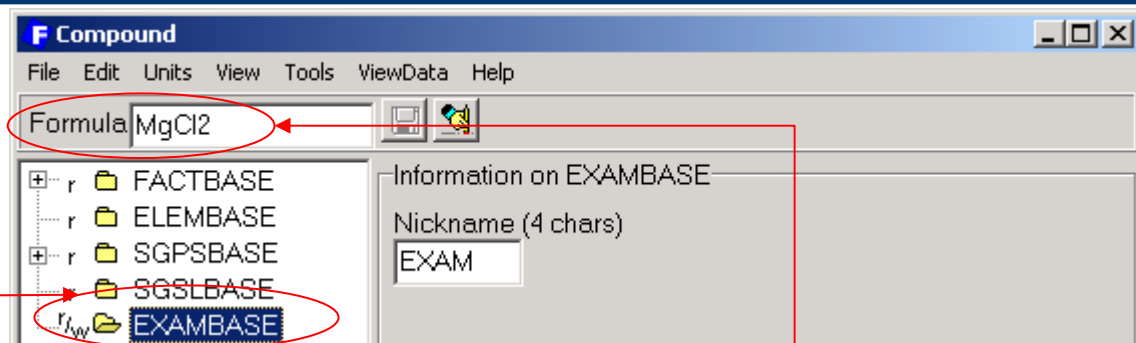
Compound data for **MgCl<sub>2</sub>** are taken from this graph.



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

To enter a new compound, for example **MgCl<sub>2</sub>**, in **EXAMBASE**:

1. Select **EXAMBASE** database

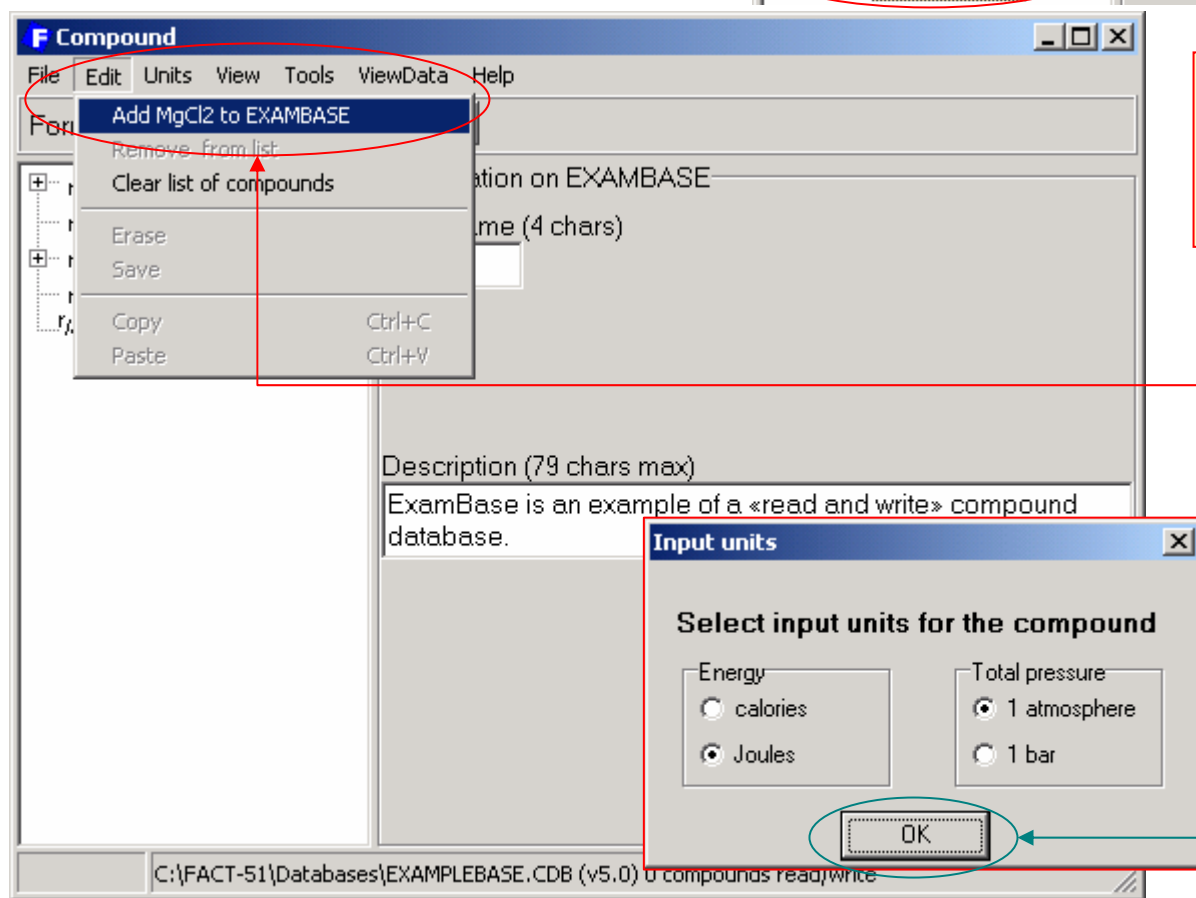


2. Type the chemical formula of the compound: **MgCl<sub>2</sub>**, in the **Formula** input box

3. Select the function «**Add MgCl<sub>2</sub> to EXAMBASE**» from the **Edit** Menu.

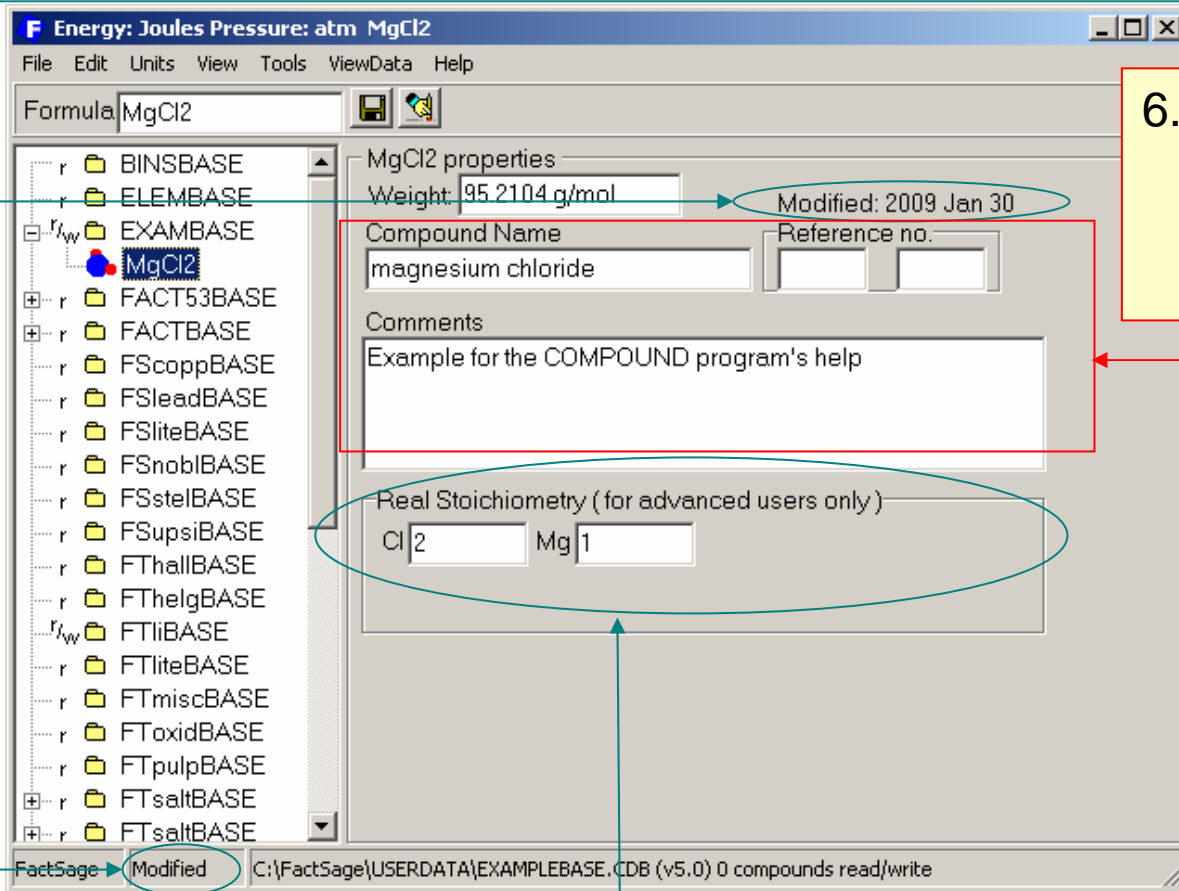
4. Select **Input units** for the compound.

5. Press «**OK**»



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

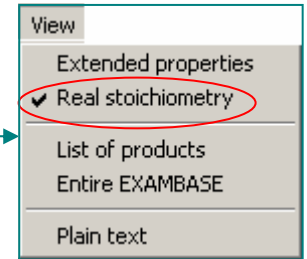
The database is now ready for new entries and modification of existing data.



6. Enter:

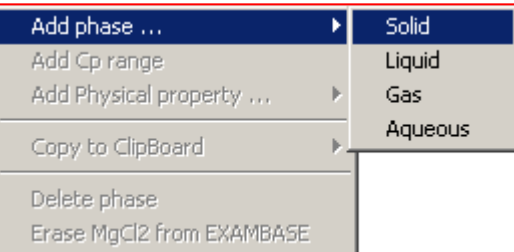
- **compound name**;
- **reference number(s)**;
- **comments**.

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).



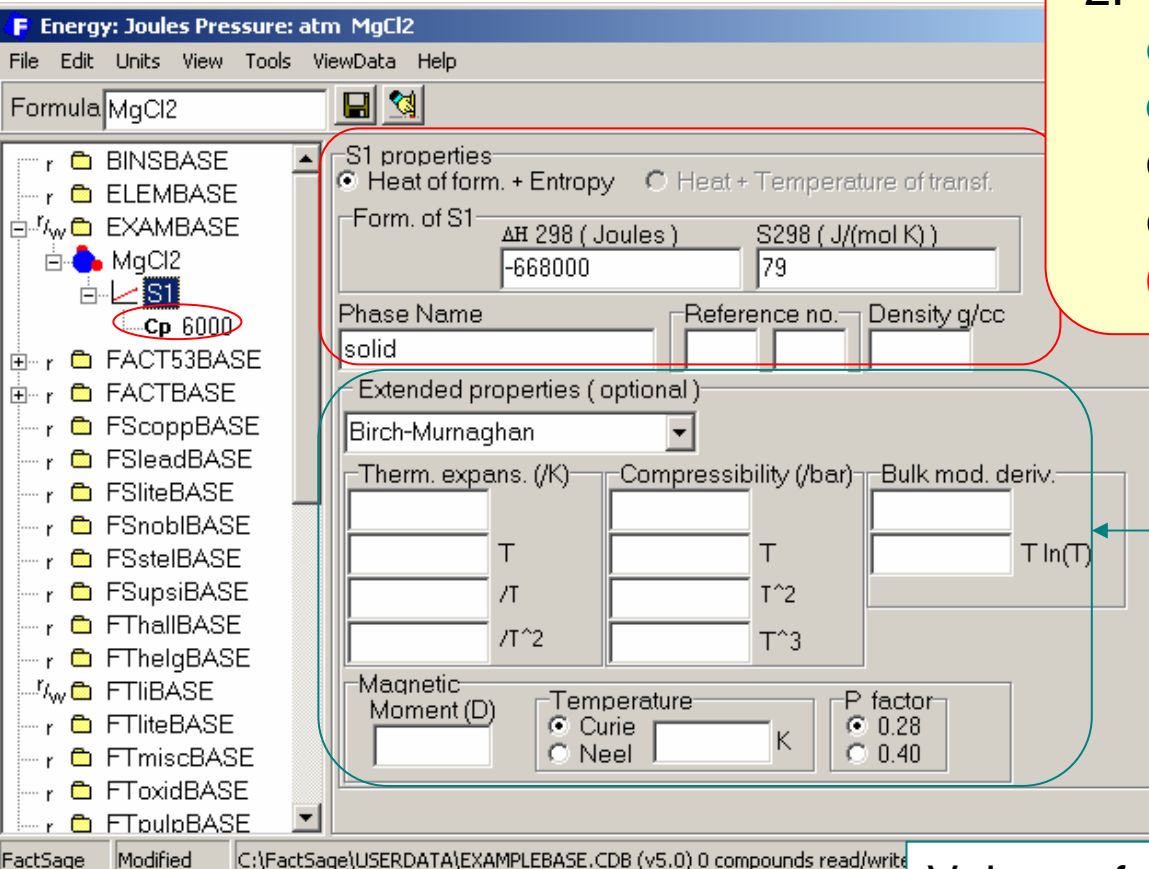


# Add a **compound** to the database: $H_{298}$ and $S_{298}$ for **1<sup>st</sup>** phase, IV



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

2. Enter the values for the **enthalpy of formation  $\Delta H^\circ(298.15)$**  and **entropy  $S^\circ(298.15)$** . **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  $\Delta H^\circ(298.15)$  and  $S^\circ(298.15)$  for **S1** were obtained from the graph.

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

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

Compressibility expression:

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

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

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

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

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

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

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

# Add a **compound** to the database: $C_p$ values for the **1<sup>st</sup>** phase, VI

Energy: Joules Pressure: atm MgCl2

Formula MgCl2

Cp expression for S1

$\Delta H_{298}$ : -668000 J/mol

$S_{298}$ : 79 J/(mol K)

from 298.150 K to 6000.000 K

$C_p(T) =$

T^ 0.00

T^

T^

T^

T^

T^

T^

T^

T^

T^

T^

FactSage 6 Modified C:\FactSage\USERDATA\EXAMPLEBASE.CDB (v5.0) 0 compou

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

You can enter expressions for  $C_p$  and list those of  $H$ ,  $S$  or  $G$ .

Energy: Joules Pressure: atm MgCl2

Formula MgCl2

Cp expression for S1

$\Delta H_{298}$ : -667999.9999999983 J/mol

$S_{298}$ : 78.9999999998367 J/(mol K)

from 298.150 K to 987.000 K

$C_p(T) =$

79.1 T^ 0.00

0.00594 T^ 1.00

-862000 T^ -2.00

T^

T^

T^

T^

T^

T^

T^

T^

T^

FactSage 6 Modified C:\FACT-S1\Databases\EXAMPLEBASE.CDB (v5.0) 0 compounds read/write

2. Enter the  $C_p$  range from **298.15 K** to **987 K** and the  $C_p$  expression for **MgCl<sub>2</sub> S1**

$C_{P(S)} = 79.1 + 5.94 \times 10^{-3} T - 8.62 \times 10^5 T^{-2} \text{ J/mol}\cdot\text{K}$

# Show data as H, S and G functions

**Compound** calculates automatically the expressions of **H**, **S** and **G** from your entry of the **C<sub>p</sub>** expression.

H expression for S1

$\Delta H_{298}$ : -668000 J/mol  
 $S_{298}$ : 79.00000000000001 J/(mol K)

from 298.150 K to 987.000 K

**H(T) =**

-694738.84063152	T <sup>0.00</sup>
79.1	T <sup>1.00</sup>
0.00297	T <sup>2.00</sup>

Note: T<sup>99</sup> => ln T

862000

**C<sub>p</sub>**  
**H**  
**S**  
**G** Edit

S expression for S1

$\Delta H_{298}$ : -668000 J/mol  
 $S_{298}$ : 79.00000000000001 J/(mol K)

from 298.150 K to 987.000 K

**S(T) =**

-378.299413912727	T <sup>0.00</sup>	
79.1	T <sup>99.00</sup>	ln T
0.00594	T <sup>1.00</sup>	
431000	T <sup>-2.00</sup>	

Note: T<sup>99</sup> => ln T

**C<sub>p</sub>**  
**H**  
**S**  
**G** Edit

G expression for S1

$\Delta H_{298}$ : -668000 J/mol  
 $S_{298}$ : 79.00000000000001 J/(mol K)

from 298.150 K to 987.000 K

**G(T) =**

-694738.84063152	T <sup>0.00</sup>
457.399413912727	T <sup>1.00</sup>
-79.1	T ln T
-0.00297	T <sup>2.00</sup>
431000	T <sup>-1.00</sup>

Note: T<sup>99</sup> => ln T

**C<sub>p</sub>**  
**H**  
**S**  
**G** Edit

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**.

Energy: Joules Pressure: atm MgCl2

Formula: MgCl2

G expression for S1

$\Delta H$  298: -668000 J/mol

S 298: 78.99999999999999 J/(mol K)

from 298.150 K to 987.000 K

G(T) =

-694738.84063152	T <sup>0.00</sup>
457.399413912727	T <sup>1.00</sup>
-79.1	T <sup>100.00</sup>
-0.00297	T <sup>2.00</sup>
431000	T <sup>-1.00</sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>

Note: T<sup>99</sup> => ln T

FactSage Modified C:\FactSage\USERDATA\EXAMPLEBASE.CDB (v5.0) 0 compounds read/write

G(T) from 298.15 to 987 K

G(T) =

-694738.84063152	T <sup>0.00</sup>
457.399413912727	T <sup>1.00</sup>
-79.1	T <sup>100.00</sup>
-0.00297	T <sup>2.00</sup>
431000	T <sup>-1.00</sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>
	T <sup></sup>

Ok Cancel T<sup>99</sup> => ln T T<sup>100</sup> => T ln T


Here the **Gibbs energy** coefficients are used instead of H, S and C<sub>p</sub> data.

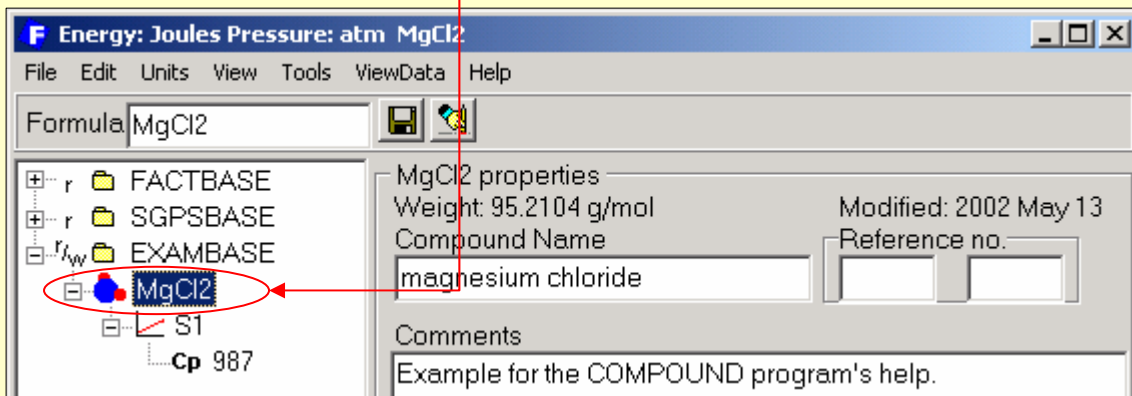
The data colored in **black** indicates that **you can edit** these expressions.

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

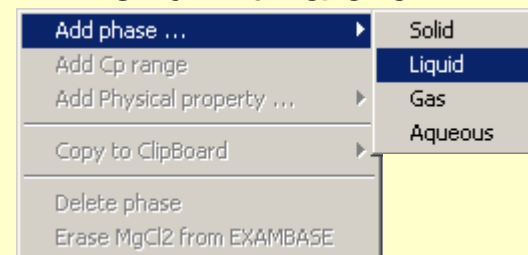
The next three slides illustrate how to enter a new phase (here the **liquid**) if the data for the **phase transition** between the previous phase (here the **solid**) and the new phase, i.e.  $\Delta H$  and  $T_{\text{trans}}$ , as well as the  $C_p$  data of the new phase are available.

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


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

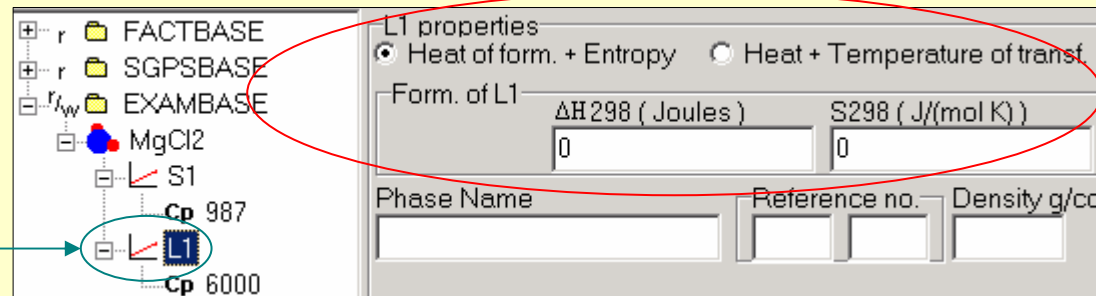



2. Point the arrow to « **Add phase...** » and select « **Liquid** » from the sub menu with a click.

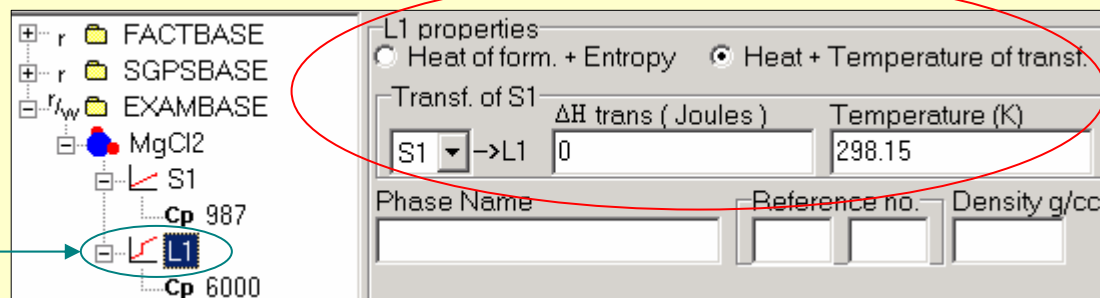


3. **Compound** proposes two ways to enter the data:

- either you enter the **enthalpy of formation  $\Delta H^\circ(298.15)$**  and **entropy  $S^\circ(298.15)$**  for phase **L1** and the entry is flagged by the **icon** 



- or you enter the **enthalpy and temperature of transformation** and the entry is flagged by the **icon** 



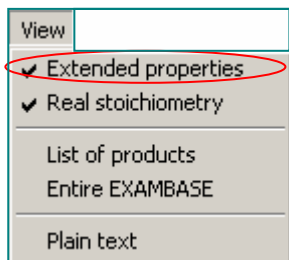
# Entering phase transition data: the **liquid** phase, II

3.(continued)

Entering the **enthalpy** and **temperature** of **transformation**.

4. Click on **C<sub>p</sub> 6000** to open the box «**C<sub>p</sub> 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**.

The screenshot shows the 'Energy: Joules Pressure: atm MgCl2' window. The 'Formula' is MgCl2. The 'L1 properties' section is active, with 'Heat + Temperature of transf.' selected. The 'Transf. of S1' section shows a transition from S1 to L1 with  $\Delta H$  trans (Joules) = 43000 and Temperature (K) = 987. The 'Cp 6000' option is selected in the tree view. The 'Extended properties (optional)' section is visible, showing the 'Birch-Murnaghan' model and a table for 'Therm. expans. (/K)' and 'Compressibility (/bar)'. The table has columns for T, T^2, and T^3.

Therm. expans. (/K)		Compressibility (/bar)	
	T		T
	/T		T <sup>2</sup>
	/T <sup>2</sup>		T <sup>3</sup>



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

**Compound** calculates automatically the values of  $\Delta H^\circ_{L, 298.15}$  and  $S^\circ_{L, 298.15}$  (these values are the same as those in the graph).

The screenshot shows the FactSage software interface for MgCl2. The left sidebar lists various databases, with MgCl2 selected. The main window displays the Cp expression for L1, with the following values:

- $\Delta H_{298}$ : -633619.130104762 J/mol
- $S_{298}$ : 106.211274831458 J/(mol K)

The Cp expression is defined for the temperature range from 298.150 K to 1691.000 K. The Cp(T) expression is entered as 92.5. The Cp coefficient is highlighted with a red oval, and the temperature range is also highlighted with a red oval. A red arrow points to the Cp coefficient input field.

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

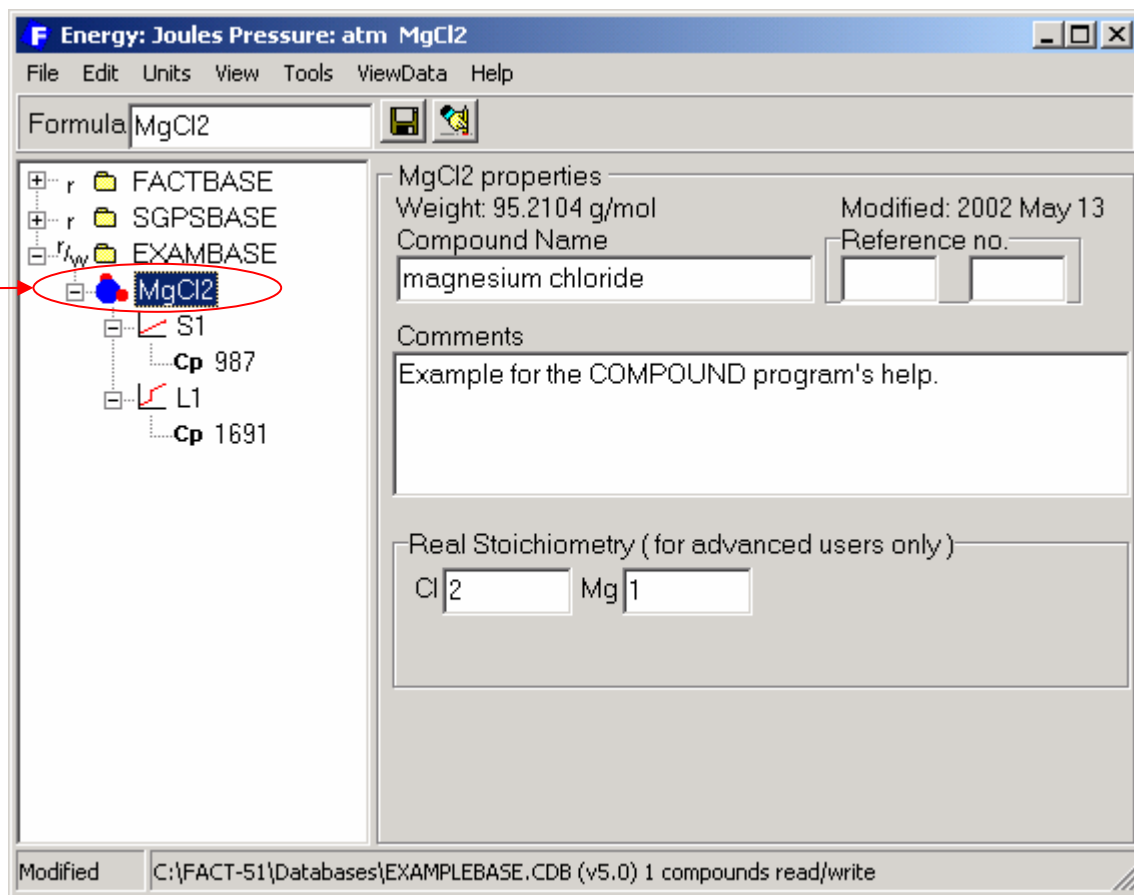
# Entering a new phase with $H_{298}$ , $S_{298}$ and $C_p$ : the **gaseous** phase

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 «  » to open a **pop-up menu**.



Energy: Joules Pressure: atm MgCl2

File Edit Units View Tools ViewData Help

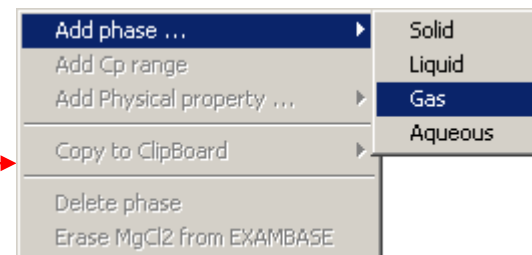
Formula MgCl2

FACTBASE  
SGPSBASE  
EXAMBASE  
MgCl2  
S1  
Cp 987  
L1  
Cp 1691

MgCl2 properties  
Weight: 95.2104 g/mol Modified: 2002 May 13  
Compound Name Reference no.  
magnesium chloride  
Comments  
Example for the COMPOUND program's help.  
Real Stoichiometry (for advanced users only)  
Cl 2 Mg 1

Modified C:\FACT-51\Databases\EXAMPLEBASE.CDB (v5.0) 1 compounds read/write

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



- Add phase ...
  - Solid
  - Liquid
  - Gas
  - Aqueous
- Add Cp range
- Add Physical property ...
- Copy to Clipboard
- Delete phase
- Erase MgCl2 from EXAMBASE

# 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  $\Delta H^\circ(298.15)$  gas** and the **entropy  $S^\circ(298.15)$  gas**. (See slide 4.3)

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

Energy: Joules Pressure: atm MgCl2

File Edit Units View Tools ViewData Help

Formula MgCl2

BINSBASE  
ELEMBASE  
EXAMBASE  
MgCl2  
S1  
Cp 987  
L1  
Cp 1691  
G1  
Cp 6000  
FACT53BASE  
FACTBASE  
FScompBASE  
FSleadBASE  
FSliteBASE  
FSnoblBASE  
FSstelBASE  
FSupsiBASE  
FThallBASE  
FThelgBASE  
FTliBASE

G1 properties  
 Heat of form. + Entropy  Heat + Temperature of transf.

Form. of G1  
 $\Delta H$  298 (Joules) -481145  
 $S_{298}$  (J/(mol K)) 194.1

Phase Name Reference no. Density g/cc  
gas

Extended properties (optional)  
Critical  
Temperature Pressure Volume  
K bar cc/mol  
Omega Dipole moment  
Debyes

FactSage Modified C:\FactSage\USERDATA\EXAMPLEBASE.CDB (v5.0) 0 compounds read/write

View

- Extended properties
- Real stoichiometry
- List of products
- Entire EXAMBASE
- Plain text

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  $\Omega$  (omega, the acentric factor) for the pure gases. Gases are treated as non-polar. For **ideal gases**, the value of  $B$  is **zero**.

Extended properties (optional)

Critical

Temperature	Pressure	Volume
<input type="text" value="T&lt;sub&gt;c&lt;/sub"/>	<input type="text" value="P&lt;sub&gt;c&lt;/sub"/>	<input type="text" value="V&lt;sub&gt;c&lt;/sub"/>
K	bar	cc/mol

Omega	Dipole moment
<input type="text" value="Ω"/>	<input type="text" value="μ"/>
	Debyes

\* «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  $\text{MgCl}_2$ , 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

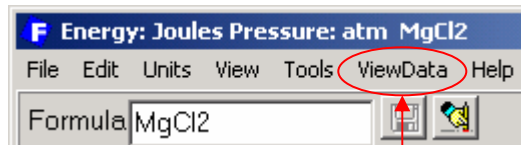
5. Enter the  $C_p$  range from 298.15 K to 6000 K and the  $C_p$  expression for  $MgCl_2$  gas (slide 4.3):  $C_{p(G)} = 95 \text{ J/mol}\cdot\text{K}$

The image displays two screenshots of the FactSage software interface. The top screenshot shows the 'Cp' tab for the compound  $MgCl_2$  in the 'EXAMBASE' database. The 'Cp(T) = 95' expression is entered, and the temperature range is set from 298.150 K to 6000.000 K. The 'Save' button is highlighted with a red circle. The bottom screenshot shows the same interface after saving, with the  $MgCl_2$  icon faded and the status bar indicating '1 compounds read/write'.

6. Press on the **Save** button (  ) to complete your entry for this compound (You can also select «**Save  $MgCl_2$  to EXAMBASE**» from the menu **Edit**). Now your database contains **1** compound. The fading of the compound **icon** (from   $MgCl_2$  to   $MgCl_2$  ) 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

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

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
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 **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	298.15 - 987.00		
L	298.15 - 1691.00		
G	298.15 - 6000.00	ideal	



# Displaying data with Compound, II

1. To display **compound data**, for example  $\text{MgSO}_4$  in **FACTBASE**, enter **MgSO4** in the Formula input box.

Energy: Joules Pressure: atm MgSO4

File Edit Units View Tools ViewData Help

Formula MgSO4

FACTBASE

- MgSO4
  - S1
    - Cp 1400
    - Cp 2500
    - Cp 2501
  - L1
    - Cp 1000
    - Cp 2500
  - Aq1
    - Cp 473
- MgCl2
- FScoppBASE
- FSleadBASE
- FSliteBASE
- FSnobIBASE
- FSstelBASE
- FSupsiBASE
- FThallBASE
- FThelgBASE
- FTliBASE

Aq1 properties

Heat of form. + Entropy Heat + Temperature of transf.

Form. of Aq1

ΔH 298 (Joules)	S298 (J/(mol·K))
-1355616	-7.113

Phase Name Reference no. Density g/cc

Aqueous 14

FactSage C:\FactSage\FACTDATA\F550BASE.CDB (v5.0) 4429 compounds read-only

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 (  ) or the elements (  ) of interest in the Formula input box. For example **O**, **S** and **Mg**.

The screenshot shows the FactSage software interface. The 'View' menu is open, with 'List of products' selected. The 'Formula' input box contains 'MgSO4'. The tree structure on the left is expanded to show a list of compounds containing O, S, and Mg. The right panel displays the properties for Mg, including weight (24.305 g/mol) and compound name (Magnesium). The status bar at the bottom indicates the database path and the number of compounds read-only.

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<sub>4</sub>** in **FACTBASE**.

Energy: Joules Pressure: atm MgSO<sub>4</sub>

File Edit Units View Tools ViewData Help

Formula MgSO<sub>4</sub>

FACTBASE

MgSO<sub>4</sub>

MgSO<sub>4</sub> properties

Weight: 120.3686 g/mol Modified: 1992 Mar 10

Compound Name Reference no.

Magnesium Sulfate

Comments

JNF85(339-40) MAR66. Cp for S1,L1 fitted JUL90. DISK32

Real Stoichiometry (for advanced users only)

S 1 Mg 1 O 4

FactSage C:\FactSage\FACTDATA\F550BASE.CDB (v5.0) 4429 compounds read-only

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

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

Edit

Add

Remove MgSO<sub>4</sub> from list

Clear list of compounds

Erase MgSO<sub>4</sub> from FACTBASE

Save MgSO<sub>4</sub> to FACTBASE

**Copy** Ctrl+C

Paste Ctrl+V

Compound

File Edit Units View Tools ViewData Help

Formula MgSO<sub>4</sub>

FACTBASE

MgSO<sub>4</sub>

MgCl<sub>2</sub>

SGPSBASE

ELEMBASE

SGSLBASE

EXAMBASE

Information on EXAMBASE

Nickname (4 chars)

EXAM

Edit

Add MgSO<sub>4</sub> to EXAMBASE

Remove from list

Clear list of compounds

Erase

Save

Copy Ctrl+C

**Paste MgSO<sub>4</sub>** Ctrl+V

4. Select «**Paste MgSO<sub>4</sub>**» from the **Edit** menu.

# Transferring data between databases, II

Note that the  $\text{MgSO}_4$  data retrieved from the **read only (r) FACTBASE** database are shown in gray color.

Simply **drag-and-drop**  $\text{MgSO}_4$  from **FACTBASE** to **EXAMBASE**.

Note that the  $\text{MgSO}_4$  data retrieved from the **read and write (r/w) EXAMBASE** database are shown in **black** color and can be edited.

# 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.

Energy: Joules Pressure: atm MgSO4

Formula: MgSO4

Tree structure:

- BINSBASE
- ELEMBASE
- EXAMBASE
  - MgSO4
    - S1
      - Cp 1400
      - Cp 2500
      - Cp 2501
    - L1
    - Aq1
    - MgCl2
  - FACT53BASE
  - FACTBASE
  - MgSO4
  - MgCl2
  - FScoppBASE
  - FSleadBASE
  - FSliteBASE
  - FSnobIBASE
  - FSstelIBASE
  - FSubsiBASE

Cp expression for S1

$\Delta H_{298}$ : -1261786 J/mol  
 $S_{298}$ : 91.396 J/(mol K)

from 298.150 K to 1400.000 K

$C_p(T)$	68.7341204149077	$T^{0.00}$
	0.100446369638875	$T^{1.00}$
	-2428116.37888619	$T^{-2.00}$
	-2.29735717986332E-5	$T^{2.00}$
	8001.15171604182	$T^{-1.00}$
		$T^{\quad}$
		$T^{\quad}$
		$T^{\quad}$

Cp expression for S1

$\Delta H_{298}$ : -1261786 J/mol  
 $S_{298}$ : 91.396 J/(mol K)

from 298.150 K to 1400.000 K

$C_p(T)$	69	$T^{0.00}$
	0.100446369638875	$T^{1.00}$
	-2428116.37888619	$T^{-2.00}$
	8001.15171604182	$T^{-1.00}$
	-2.3E-5	$T^{2.00}$
		$T^{\quad}$
		$T^{\quad}$
		$T^{\quad}$

Annotations: Red circles highlight the  $C_p(T)$  value (69), the  $T^{-2.00}$  coefficient (-2428116.37888619), and the  $T^{2.00}$  coefficient (-2.3E-5). Blue circles highlight the  $T^{0.00}$  term and the  $T^{-1.00}$  term. A red arrow points from the  $T^{-2.00}$  term in the left screenshot to the right screenshot. A blue arrow points from the  $T^{2.00}$  term in the left screenshot to the right screenshot.

# 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 interfere with the contents of databases and can be applied to all databases.

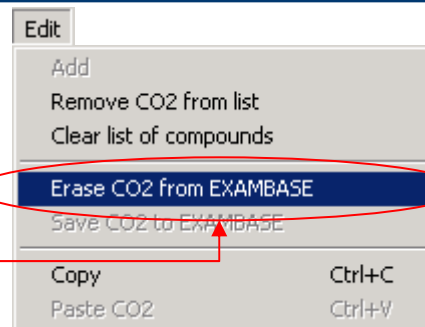
The **Erase** command only works for read/write databases.

# The Erase, Remove and Clear commands, I

1. **Select** the compound you want to **delete** (say, CO<sub>2</sub>) from the **r/w database**.

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

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



The screenshot displays the FactSage software interface. On the left, a tree view shows the database structure with 'EXAMBASE' expanded and 'CO2' selected. A 'Warning' dialog box is open, asking 'Erase CO2 from EXAMBASE' with 'Yes', 'No', and 'Cancel' buttons. The 'Yes' button is highlighted. In the background, the 'Energy: Joules Pressure: atm CO2' window shows the 'CO2 properties' and the 'Formula' field containing 'CO2'. The 'Energy: Joules Pressure: atm MgSO4' window shows the 'MgSO4 properties' and the 'Formula' field containing 'CO2'. The 'FactSage' status bar at the bottom indicates '3 compounds' in the database. A red arrow points from the 'Yes' button to the 'FactSage' status bar.

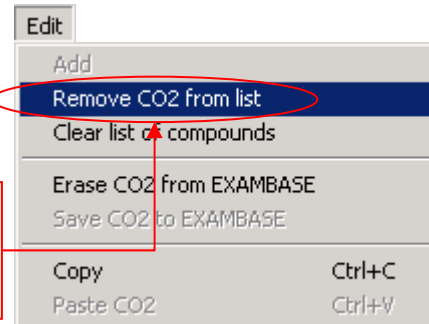
Now the database **EXAMBASE** contains only **2** (= **3** - **1**) compounds.



# The Erase, Remove and Clear commands, II

1. **Select** the compound you want to **remove** (say,  $\text{CO}_2$ ) from the tree view list.

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



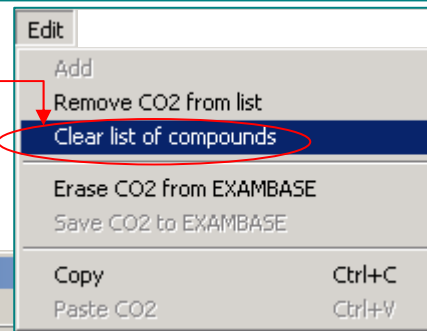
The image displays two screenshots of the FactSage software interface. The left screenshot shows the 'Energy: Joules Pressure: atm CO2' window. The tree view on the left has 'EXAMBASE' selected, and 'CO2' is highlighted with a red oval. The 'CO2 properties' panel shows 'Weight: 44.0098 g/mol' and 'Compound Name: Carbon Dioxide'. The 'Real Stoichiometry' section shows 'O2' and 'C1'. The status bar at the bottom indicates '3 compounds'. The right screenshot shows the 'Energy: Joules Pressure: atm MgSO4' window. The tree view has 'EXAMBASE' selected, and 'MgSO4' is highlighted with a red oval. The 'MgSO4 properties' panel shows 'Weight: 120.3686 g/mol' and 'Compound Name: Magnesium Sulfate'. The 'Real Stoichiometry' section is empty. The status bar at the bottom indicates '3 compounds read/write'. A red box with text is overlaid on the right screenshot, pointing to the tree view.

The compound  $\text{CO}_2$  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 screenshot displays the FactSage Compound 13.3 interface. The main window is titled 'Energy: Joules Pressure: atm CO2'. The 'Formula' field contains 'MgCl2'. The left sidebar shows a tree view of databases, with 'EXAMBASE' selected and 'CO2' highlighted. The right sidebar shows the 'Compound' window for 'MgCl2', with 'EXAMBASE' selected in the tree view. A red box highlights the 'EXAMBASE' entry in the tree view. A red box highlights the 'CO2' entry in the tree view. A red box highlights the '3 compounds' status at the bottom of the window. A red box highlights the '3 compounds' status at the bottom of the window. A red box highlights the '3 compounds' status at the bottom of the window.

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  $\text{Na}_2\text{O}$  and  $\text{Al}_2\text{O}_3$  are used in a Neumann-Kopp type sum to generate data for the unknown compound  $\text{NaAlO}_4$ . 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  $\text{Na}_3\text{Al}_3\text{O}_6$ .

The second example shows how the known data for  $\text{Li}_3\text{N}$ ,  $\text{Li}$  and  $\text{Na}$  are used to generate data for the unknown compound  $\text{Na}_3\text{N}$  using  $\text{Li}_3\text{N} + 3\text{Na} - 3\text{Li} = \text{Na}_3\text{N}$ .

# 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  $\text{NaAlO}_2$  via the reaction:  $\frac{1}{2} \text{Na}_2\text{O}(\text{s1}) + \frac{1}{2} \text{Al}_2\text{O}_3(\text{s1}) \rightarrow \text{NaAlO}_2(\text{s1})$ .

1. Open the database containing the data on  $\text{Na}_2\text{O}$  and  $\text{Al}_2\text{O}_3$  and expand the treeview to list phases.

2. Click on Tools > Mixer...

The screenshot shows the FactSage software interface. The main window title is "Energy: Joules Pressure: atm Na2O". The menu bar includes "File", "Edit", "Units", "View", "Tools", "ViewData", and "Help". The "Tools" menu is highlighted. The formula input field contains "Al2O3". The treeview on the left shows a hierarchy of databases: BINSBASE, ELEMBASE, EXAMBASE, FACT53BASE, FACTBASE, Na2O, Al2O3, FScoppBASE, FSleadBASE, FSliteBASE, FSnoblBASE, and FSstelBASE. The "S1" phase for both Na2O and Al2O3 is selected. The "S1 properties" section shows "Heat of form. + Entropy" selected, with "Form. of S1" set to "Solid-A". The "Reference no." is 133, and the "Density g/cc" is 2.27. The "ΔH 298 (Joules)" is -417982.001664 and the "S298 (J/(mol K))" is 75.060997656.

The screenshot shows the "Tools" menu with the following options: "Scale Down", "Scale Up...", "Copy data to new Compound", "Fuel", and "Mixer ...". The "Mixer ..." option is highlighted in blue.

The screenshot shows the "Compound Mixer" dialog box. It has a title bar "Compound Mixer" and a table with columns "Reactants", "Phase", and "Database". Below the table are navigation buttons: a right arrow, a left arrow, a hand icon, and a "+/-" button. At the bottom, there are fields for "Product" and "State" (set to "Solid").

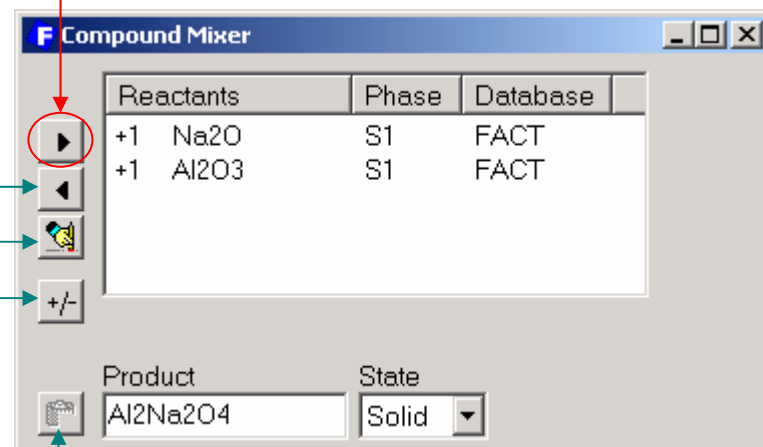
# The «Mixer» feature: Example 1, II

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 subtract the selected phase



Paste the new compound to a read and write database.

This stores the new compound  $\text{Al}_2\text{Na}_2\text{O}_4$  in the database. To store  $\text{NaAlO}_2$  you need to use the «**Scale Down**» command in the **Tools** menu.

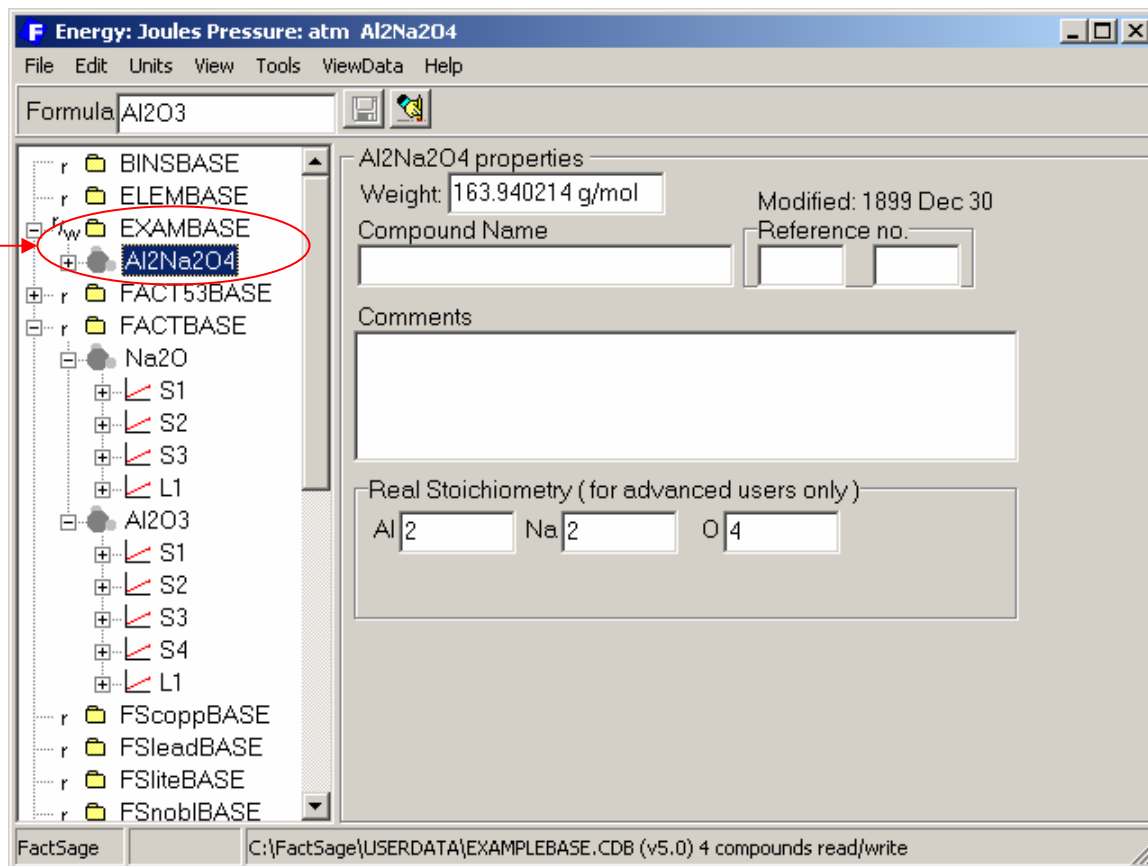
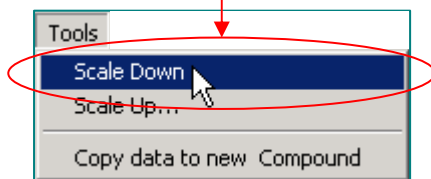
# The «Mixer» feature: Example 1, III

To **scale down** a compound:

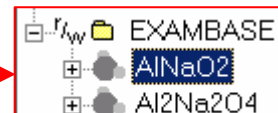
1. Save your compound in a  $r/w$  database:

- Select a  $r/w$  database.
- Paste your compound.

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



Now you have the **scaled down** compound  $\text{AlNaO}_2$  in your  $r/w$  database.



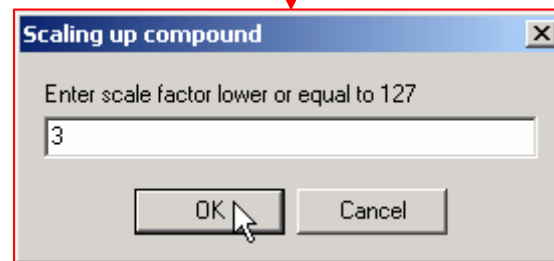
# The «Mixer» feature: Example 1, IV

On the other hand, if you want the thermodynamic properties of  $\text{Na}_3\text{Al}_3\text{O}_6$ , which is 3 times  $\text{AlNaO}_2$ , use the **Scale Up** command.

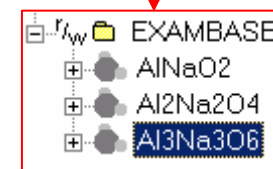
1. Select the compound you want to **scale up**

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  $\text{Al}_3\text{Na}_3\text{O}_6$  in your  $r/w$  database



# The «Mixer» feature: Example 2

This example shows how to create new data on  $\text{Li}_3\text{N}$  via the synthesis of:  
 $\text{Li}_3\text{N} + 3\text{Na} - 3\text{Li}$ .

1. Drag and drop the  $\text{Li}_3\text{N}$ , 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 Subtract** button to **subtract 3 Li** from the reactants. This create  **$\text{Na}_3\text{N}$**  as product.

The screenshot shows the FactSage interface. The main window is titled "Energy: Joules Pressure: atm Li". The "Formula" field contains "Li3N". The "S1 properties" section shows "Form. of S1" with "ΔH 298 (Joules)" set to 0 and "S298 (J/(mol K))" set to 29.005. The "Phase Name" is "Solid-1", "Reference no." is "128", and "Density g/cc" is "0.534". The "Compound Mixer" window is open, showing a table of reactants:

Reactants	Phase	Database
+1 Li3N	S1	FACT
+3 Na	S1	FACT
+3 Li	S1	FACT

The "Product" field is set to "Na3NLI6" and the "State" is "Solid". The "Add and Subtract" button (+/-) is circled in red, and a red arrow points to it from the text box above.

The screenshot shows the "Compound Mixer" window after adjustments. The table of reactants is:

Reactants	Phase	Database
+1 Li3N	S1	FACT
+3 Na	S1	FACT
-3 Li	S1	FACT

The "Product" field is now set to "Na3N" and the "State" is "Solid". The "Add and Subtract" button (+/-) is circled in green, and a green arrow points to it from the text box above.

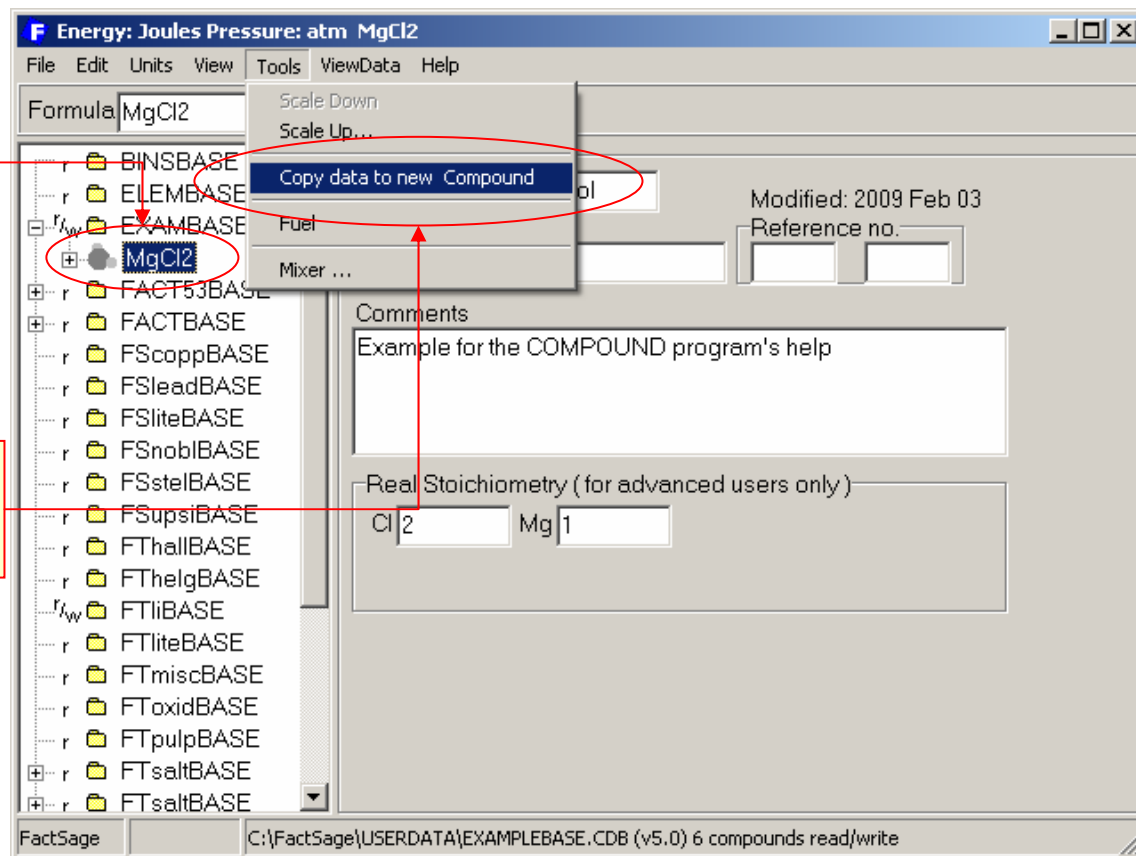


# Using known data as **template**: «**Copy data to new Compound**», I

You may use data of an **already stored** compound as a **template** to enter data for a new compound. Here **known data for  $\text{MgCl}_2$**  is used to generate **new data for  $\text{CaCl}_2$**  by using the **Copy data to new Compound** option in the Tools menu.

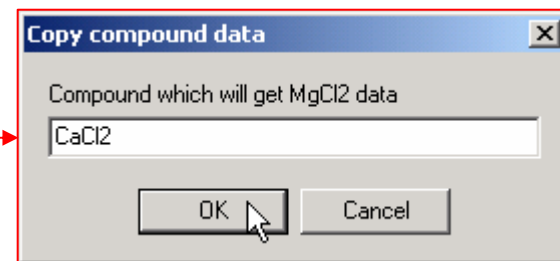
1. Select  $\text{MgCl}_2$  in EXAMBASE.

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

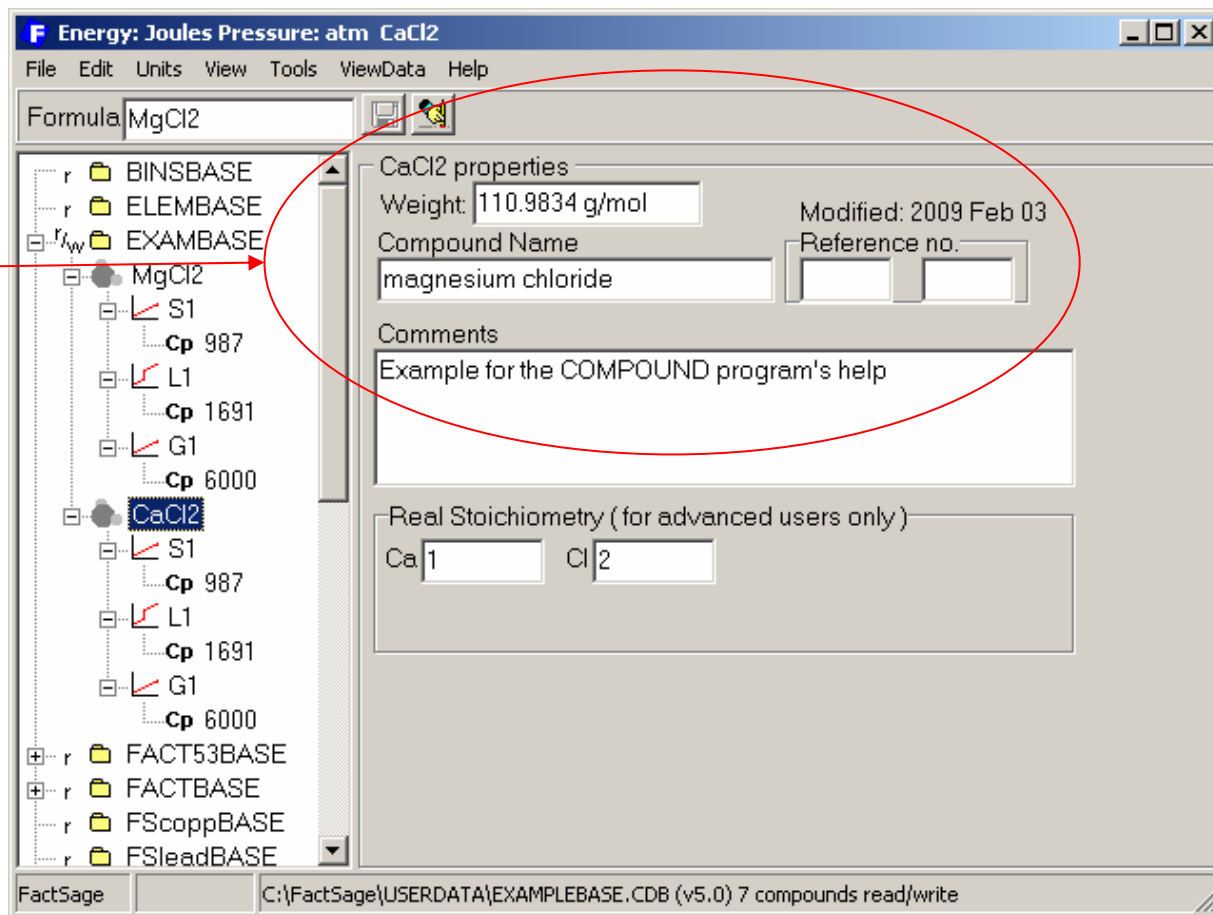


# Using known data as **template**, II

3. In the dialog box, enter the new compound **CaCl<sub>2</sub>** and press «OK».



4. You now have the **CaCl<sub>2</sub>** 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.

Click on menu **Units**.

Changing **Pressure** units from **atmosphere** to **bar**.

Changing **Energy** units from **Joules** to **calories**.

The screenshot shows the FactSage software interface for MgCl2. The 'Units' menu is highlighted in the top menu bar. The 'Form. of G1' table is shown with the following data:

Form. of G1	$\Delta H_{298}$ (Joules)	$S_{298}$ (J/(mol K))
	-481145	194.1

The 'G1 properties' section shows 'Heat of form. + Entropy' selected, 'Phase Name' as 'gas', and 'Density g/cc' as an empty field.

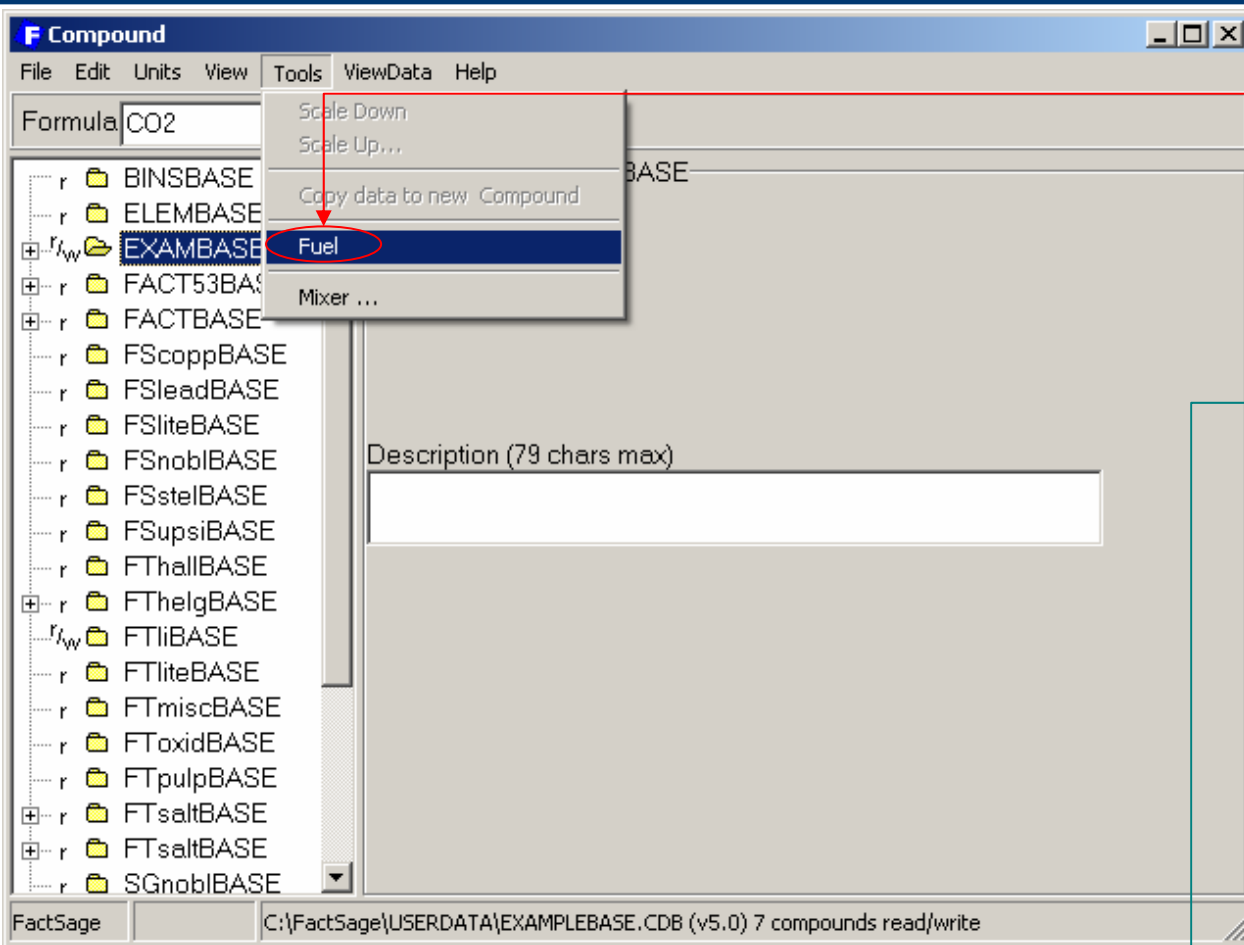
The 'Units' menu is open, showing 'Energy' and 'Pressure' options. The 'Pressure' option is selected, and the 'bar' option is chosen from the sub-menu.

Form. of G1	$\Delta H_{298}$ (Joules)	$S_{298}$ (J/(mol K))
	-481145	194.209443783103

The 'Units' menu is open, showing 'Energy' and 'Pressure' options. The 'Energy' option is selected, and the 'calories' option is chosen from the sub-menu.

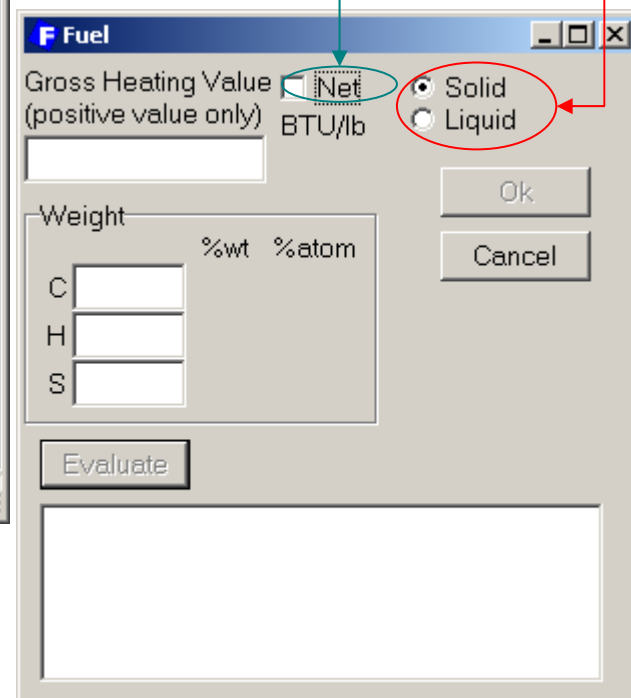
Form. of G1	$\Delta H_{298}$ (calories)	$S_{298}$ (cal/(mol K))
	-114996.414913958	46.3910133843212

# 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

**F Fuel**

Net Heating Value (positive value only)  Net  Solid  Liquid  
BTU/lb

18300

Weight

	%wt	%atom
C 87	87.00	42.44
H 9.8	9.80	56.97
S 3.2	3.20	0.58

Ok  
Cancel

Evaluate

Formula: SC73H97  
DH form: 2013205.64589894 J/mol  
Weight: 1002.0625 g/mol  
Cp: 2004 J/mol.K

4. Enter the **Heating Value** in BTU/lb – this assumes perfect combustion where products are solely CO<sub>2</sub>, H<sub>2</sub>O and SO<sub>2</sub>.

**F Energy: Joules Pressure: bar SC73H97**

File Edit Units View Tools ViewData Help

Formula CO2

SC73H97 properties

Weight: 1002.0625 g/mol Modified: 2009 Feb 05  
Compound Name Reference no.

Comments

Properties calculated assuming complete combustion and Cp = 2 J/gK-1  
Net Heating Value: 18300 BTU/lb  
Amount entered: C: 87 H: 9.8 S: 3.2

Real Stoichiometry (for advanced users only)

S 1 C 72.582996 H 97.428542

Save

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.