

The *Figure* module

Use *Figure* to manipulate, edit and plot figure and phase diagrams already calculated by *FactSage*.

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The *Figure* module



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

Figure Main Window

Figure menu bar

Normal edition mode toolbar

Figure toolbar

If you don't see the Figure edition toolbar, go to the menu **View** and check **Tool Bar**.

Pixel coordinates of the cursor

Graphic coordinates of the cursor

File name

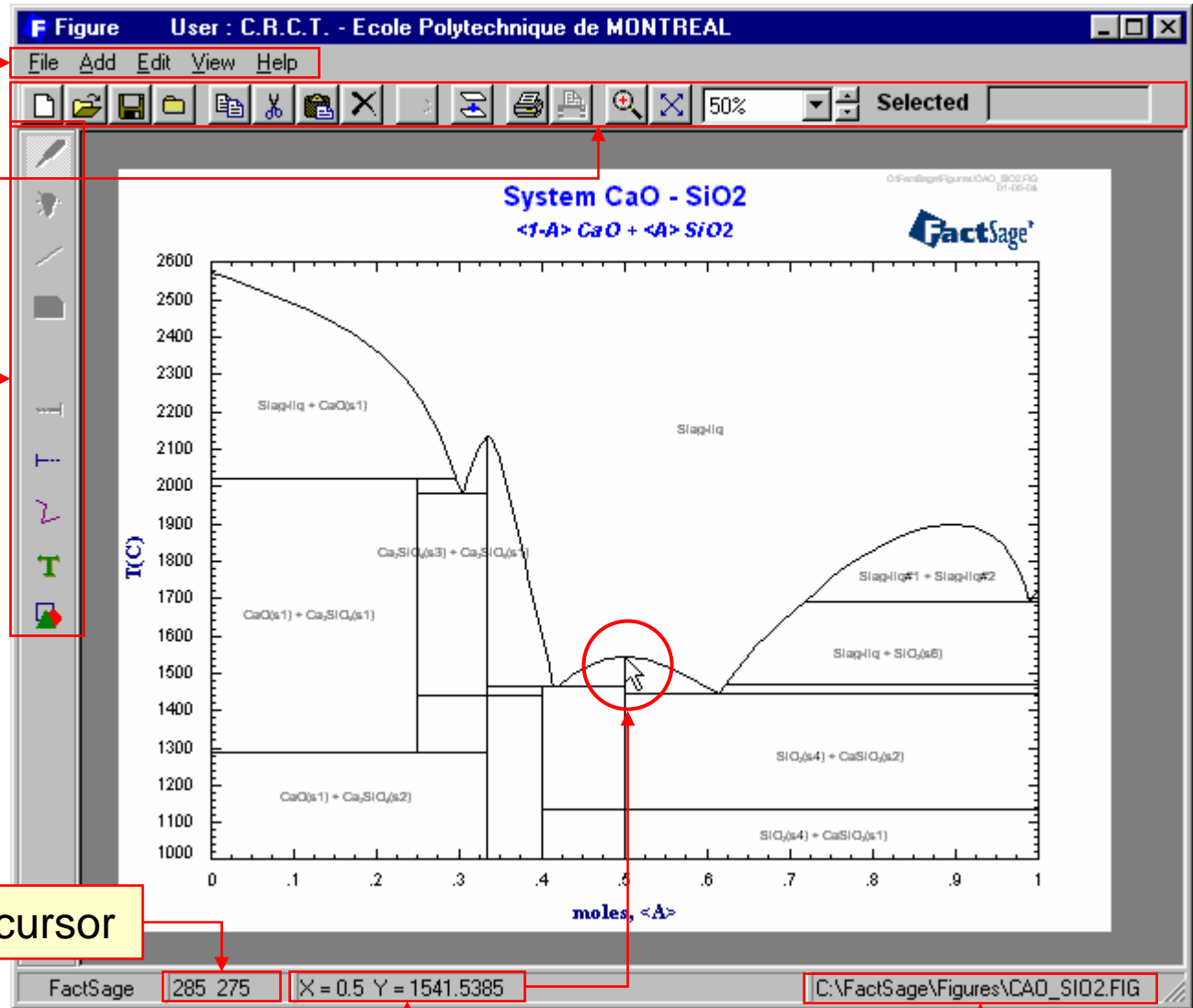


Figure Menu and Tool bars

The following three slides show the basic command environment of the *Figure* module.

A Menu bar and a Tool bar are available in order to perform the various tasks that are possible with *Figure*.

Figure Menu Bar

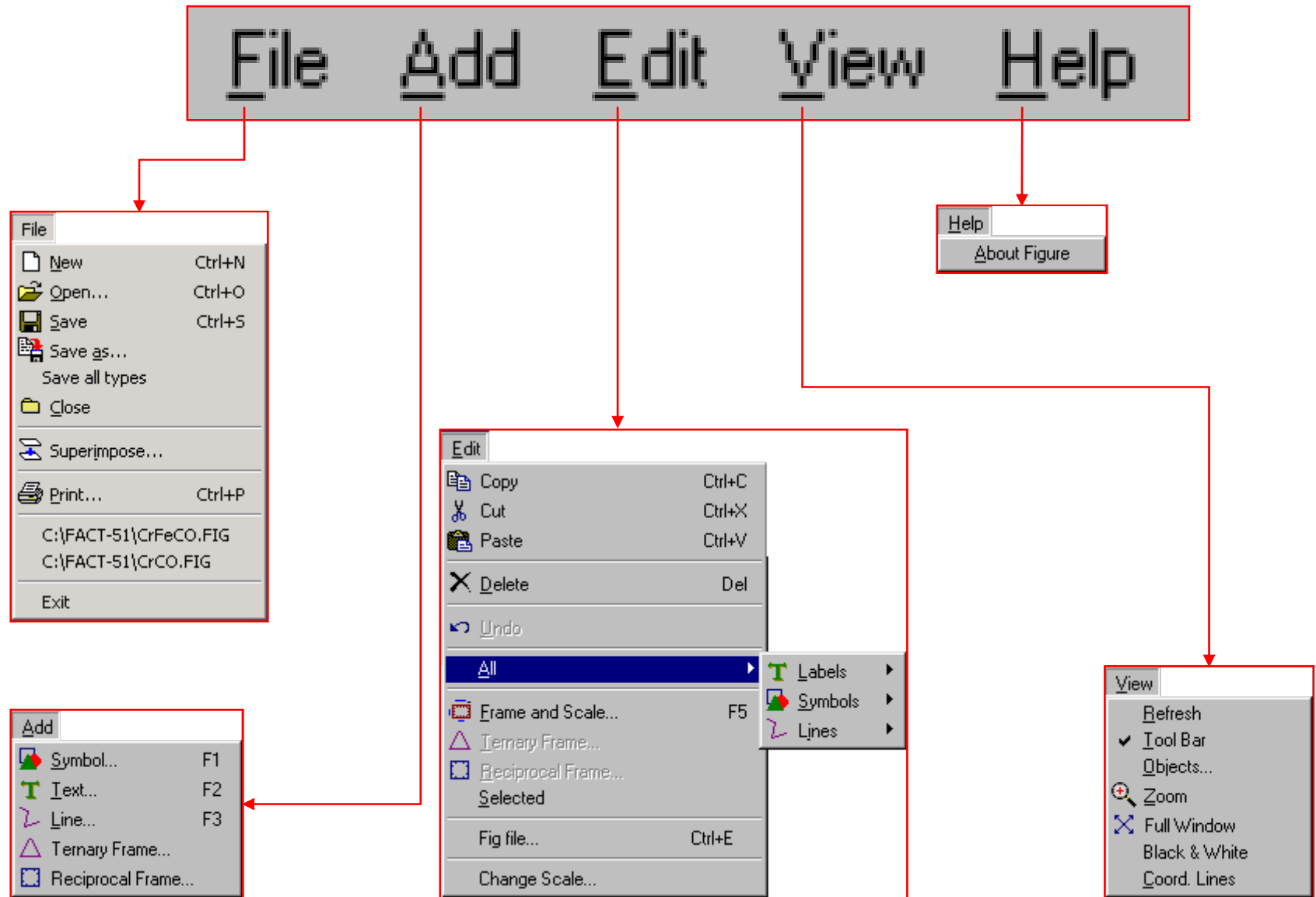


Figure Normal Edition Mode Toolbar

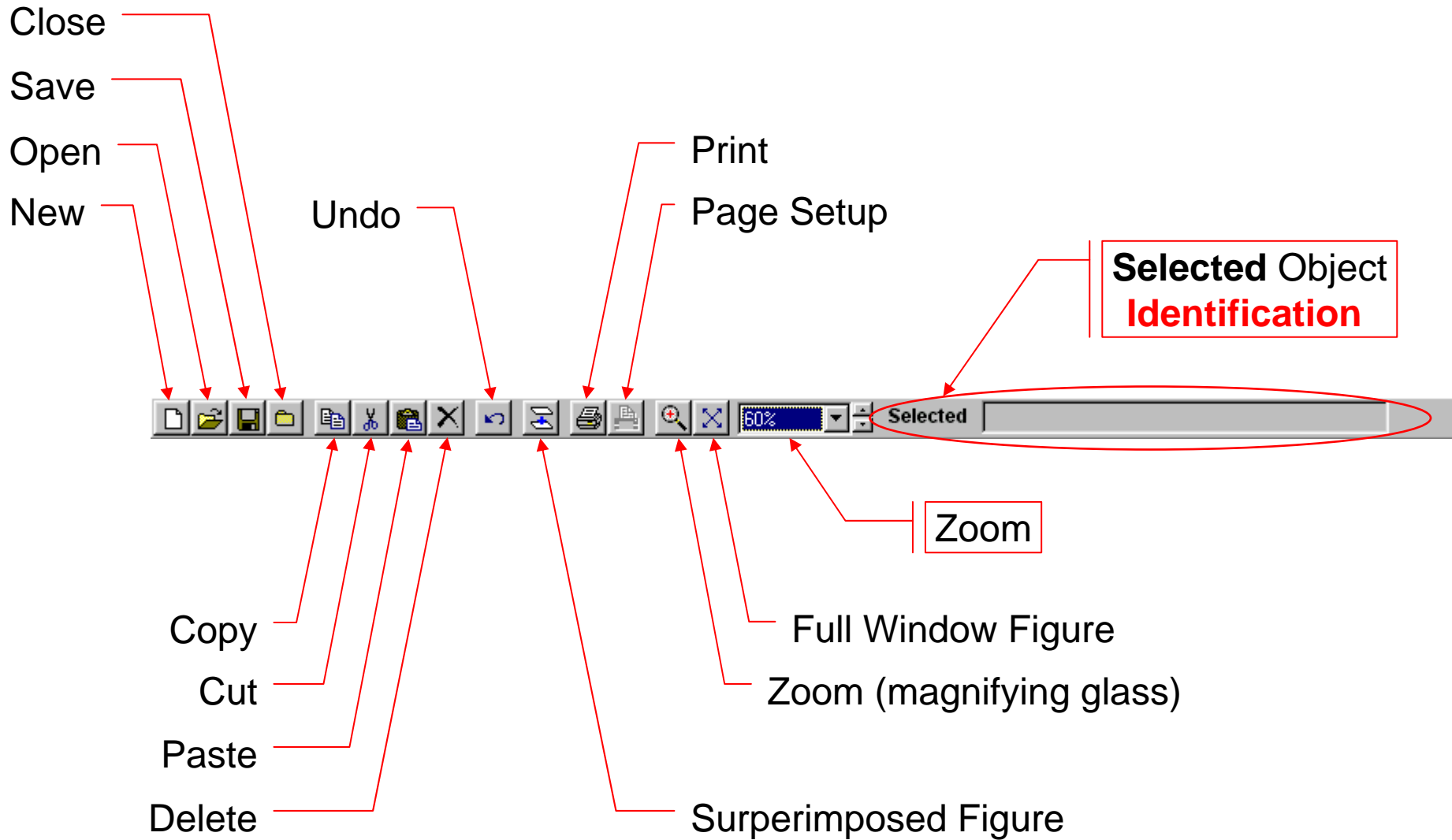


Figure Toolbar

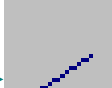
Phase diagram program

normal edition mode

phase equilibrium mode

2-phases tie-lines mode

stable phases label mode



Click to **enable** the **normal edition mode**

Click to **enable** the **Show results** window mode to see the output of the calculation of a phase diagram at the selected coordinates.

Select to **enable** the mouse activated drawing (with a click) of 2-phases tie-lines.

Select to **enable** the mouse activated labeling (with a click) of stable phases.

Close the new line

Open a new line

Add Line

Add Label

Add Symbol



Click to **disable** the mouse activated mode for the entry of points coordinates of a line.

Click to **enable** the mouse activated mode for the entry of points coordinates of a line.

Keyboard mode for the entry of points coordinates of a line (**opens** the **Add Line** window).

Opens the **Add Label** window.

Opens the **Add Symbol** window.

Opening and editing a **FIGure** file

Graphical output from calculational modules such as **Reaction**, **Predom**, **Equilib** or **Phase Diagram** can be post-viewed and edited using the **Figure** module.

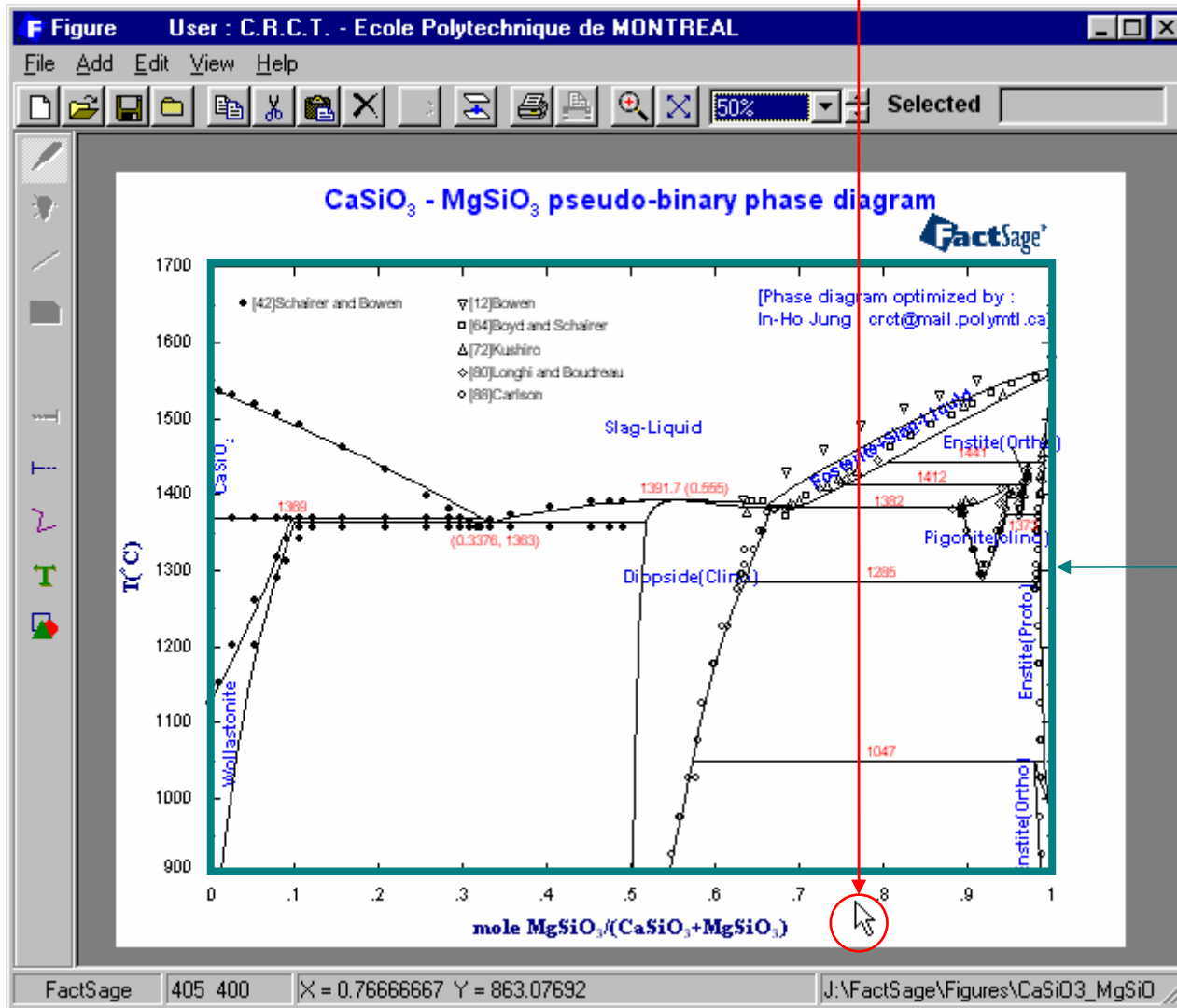
Such output is stored in files with the extension **FIG**. Use the Open File dialog box to select the desired file from the folder in which it is stored. The pre-view window helps you to select the file you want.

Once the file is opened the figure is displayed on the screen and ready for further operations.

The following two slides show how to select and open a figure file.

The CaSiO_3 - MgSiO_3 pseudo-binary phase diagram

Double-click in the area **outside** the **graph frame area**, **press «F5»** or **select Edit > Frame and Scale...** from the **Menu Bar** to **open** the **«Frame and Axis»** dialog box.



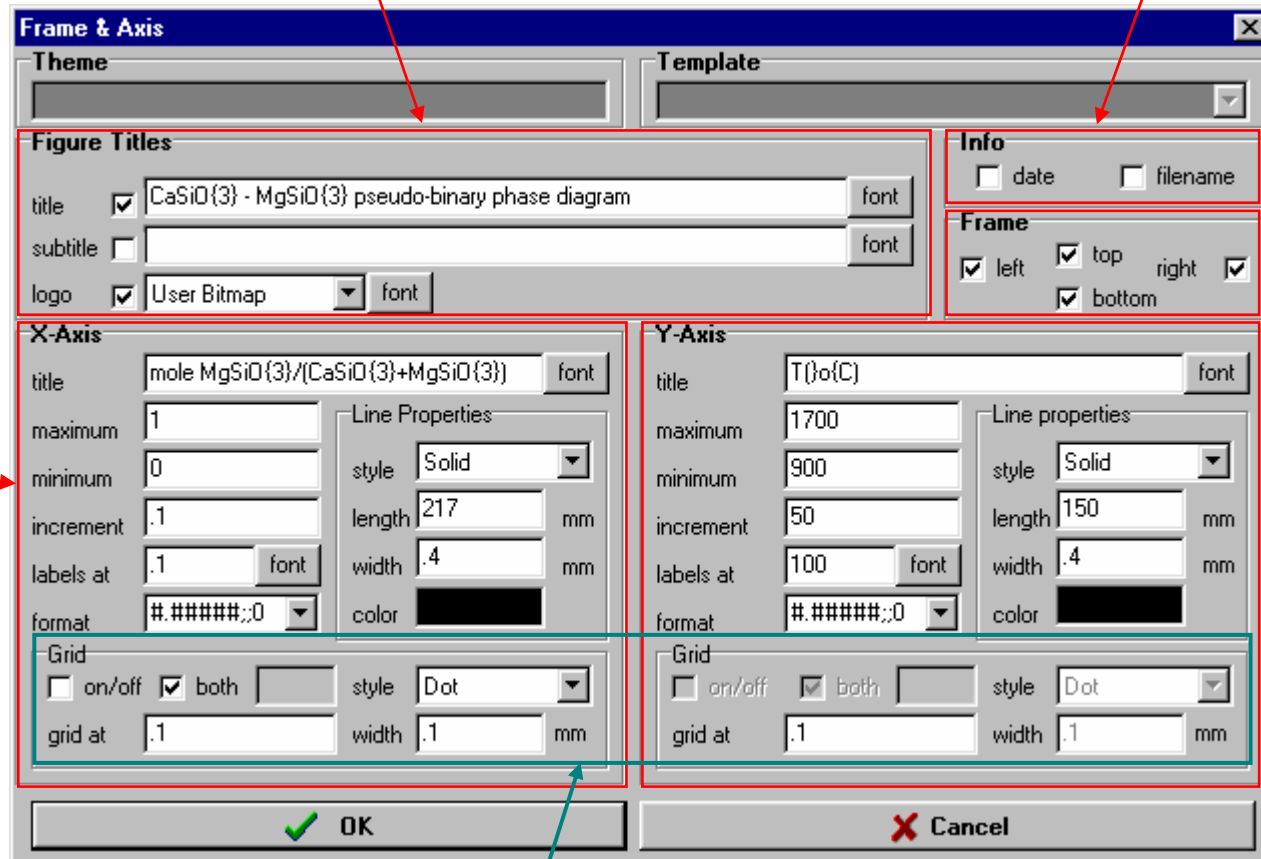
Graph frame area

Figure permits to manipulate the frame and the axes of a diagram.
The following two slides show how this is done.

The Frame and Axis Window

Figure title, subtitle and logo edition

Info selection (date and filename)



Frame borders selection

X-Axis edition

Y-Axis edition

Grid edition

Editing the frame and the axes

Making changes:

1. Modification of the figure title

3. Addition of a subtitle

4. Removal of a logo

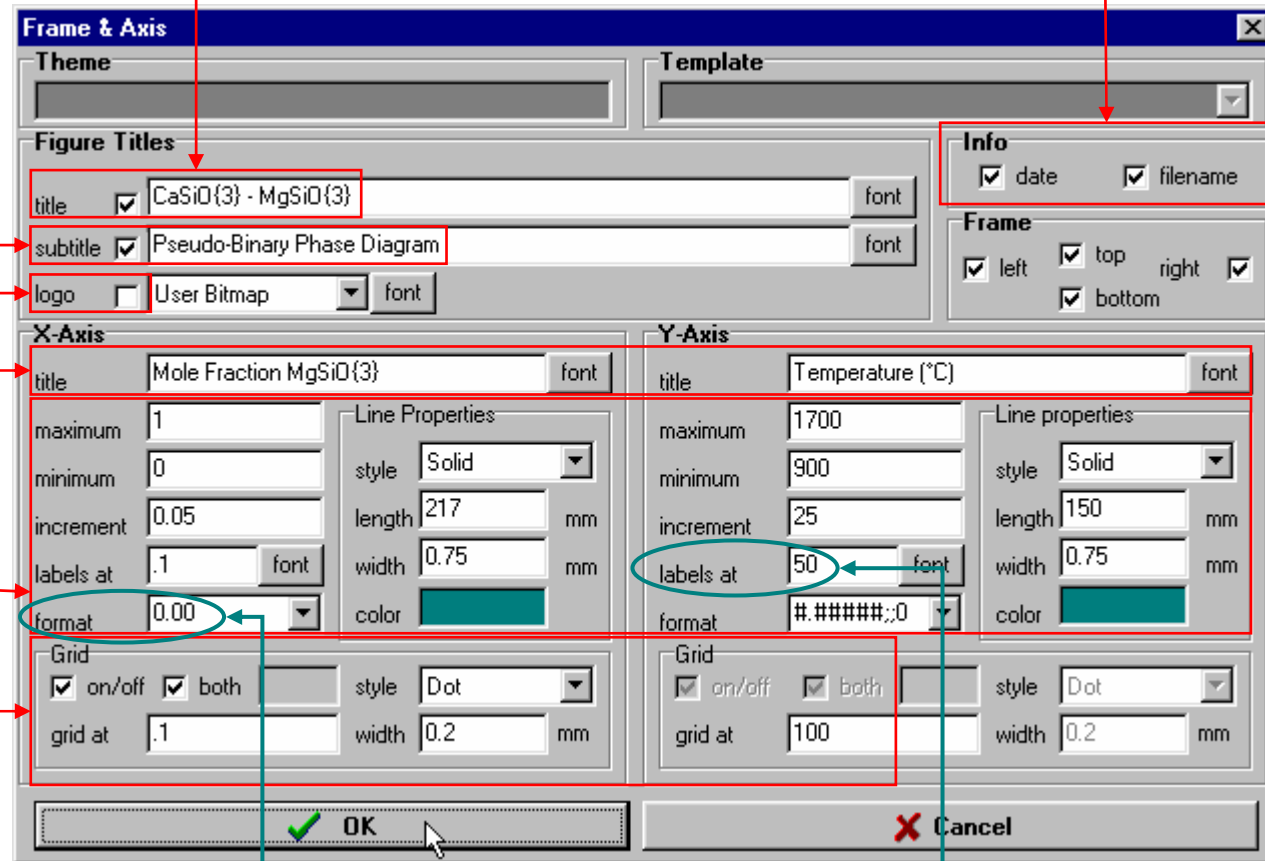
5. Modification of the axes titles

6. Change (on both axes):

- of the increments
- of the font of the labels
- of the width and the color of the lines

7. Addition of grid and specification of the separation and the width of the lines

2. Addition of the date and the filename at the top right corner



8. Modification of the format of the labels on the X-axis

9. Modification of the labeling increment on the Y-axis

Saving the edited diagram and viewing the result

Once all modifications of a diagram have been made it is possible to **store** this diagram **for further use**. Various output formats are available such that a diagram can be directly transferred to Windows based text editors for report writing or to PowerPoint for the generation of computer based presentations.

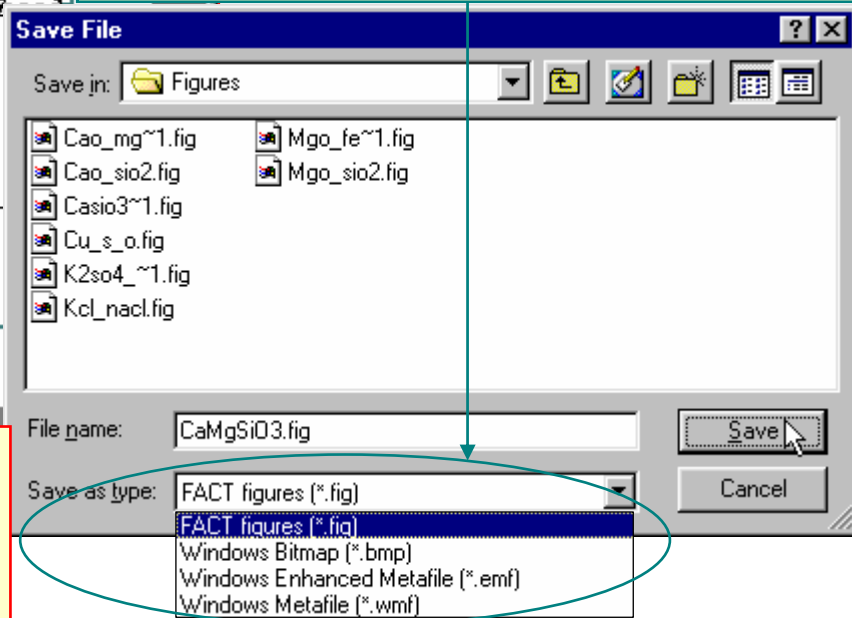
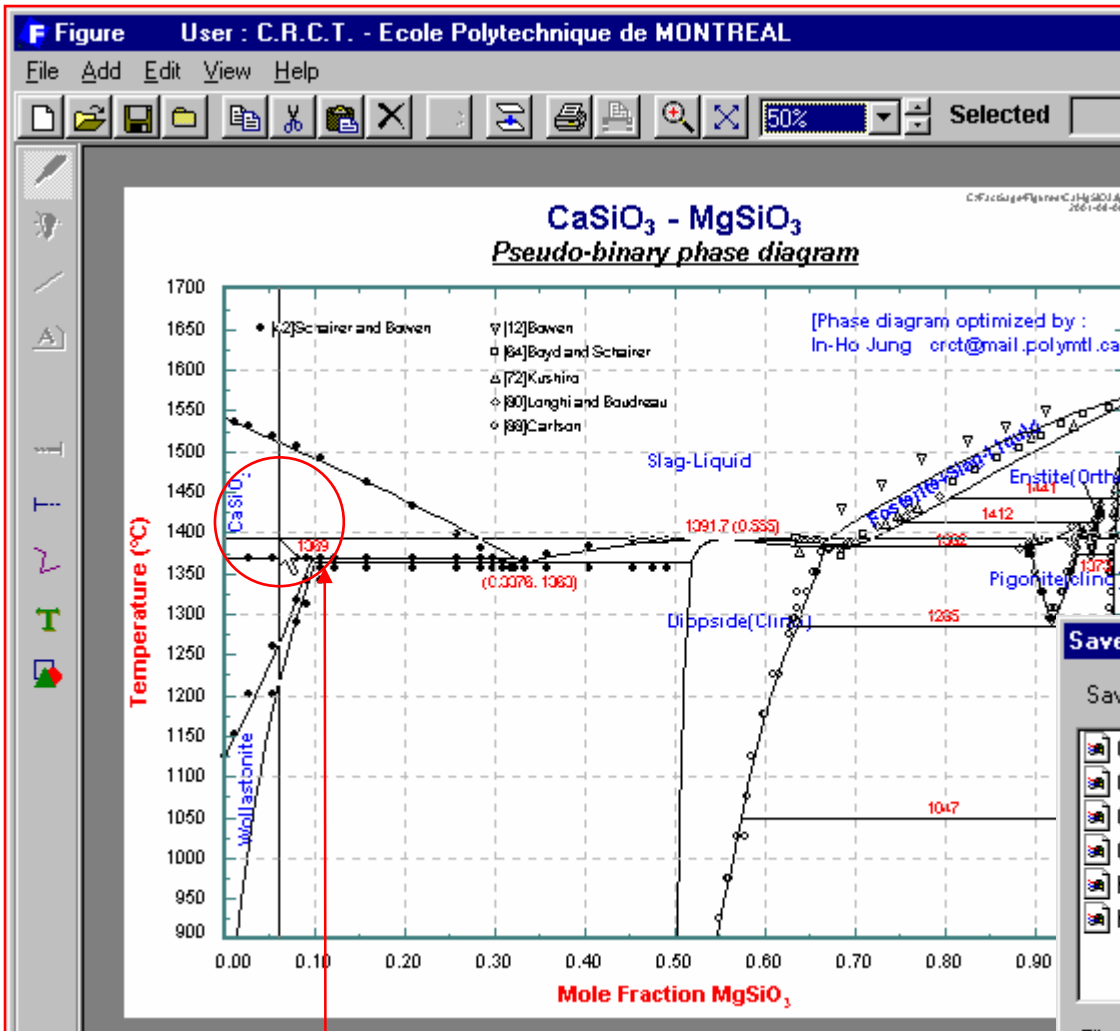
A further task that can be performed with the **Figure** module is the **numerical inspection** of a diagram. The cursor can be used for the purpose, and it is also possible to use a **zoom window** in order to have a better means for positioning of the cursor in the diagram.

Saving the **results** of the edition of the frame and the axes

Here, you have the choice between **two** kinds of file types:

- **FACT** figures (*.fig), ASCII files, which are **editable** with **Figure**;
- **Windows** (*.bmp, *.emf and *.wmf) which are **exportable** files.

It is **strongly** recommended to save the figure under **.fig** format before saving under any other format.

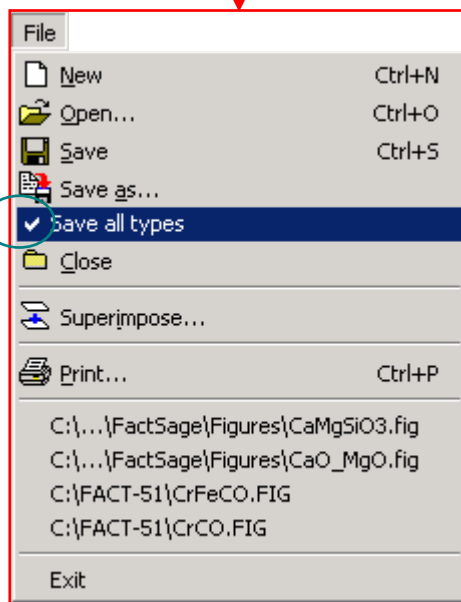


Crosshairs can be viewed when you **press** the mouse left button and **maintain** it (the option **Coord. Lines** (**V**iew menu) has to be checked).

« Save all types » option

You can now save your figure in all 4 formats (*.fig, *.bmp, *.emf and *.wmf) by enabling the «**Save all types**» option.

To **enable** this option, go in the **File** menu and click on **Save all types**.



A **checkmark** in front of the option's name indicates that the option is **enabled**.

The next time you select the « **Save** » or the « **Save as...** » command you save your file in 4 formats (*.fig, *.bmp, *.emf and *.wmf) in the directory of your choice.

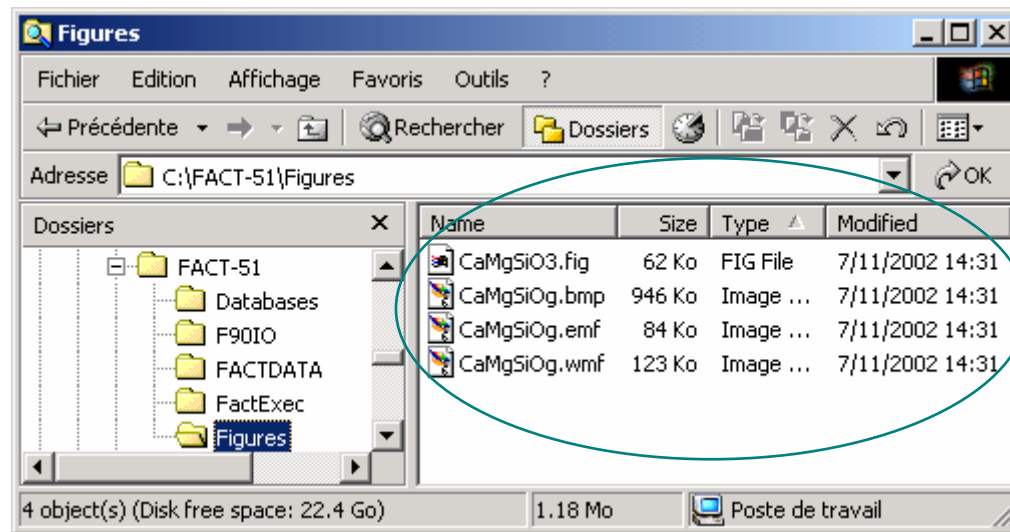


Figure 6.2

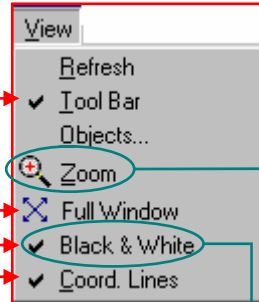
Viewing options

Show / hide the **Edition Tool Bar**

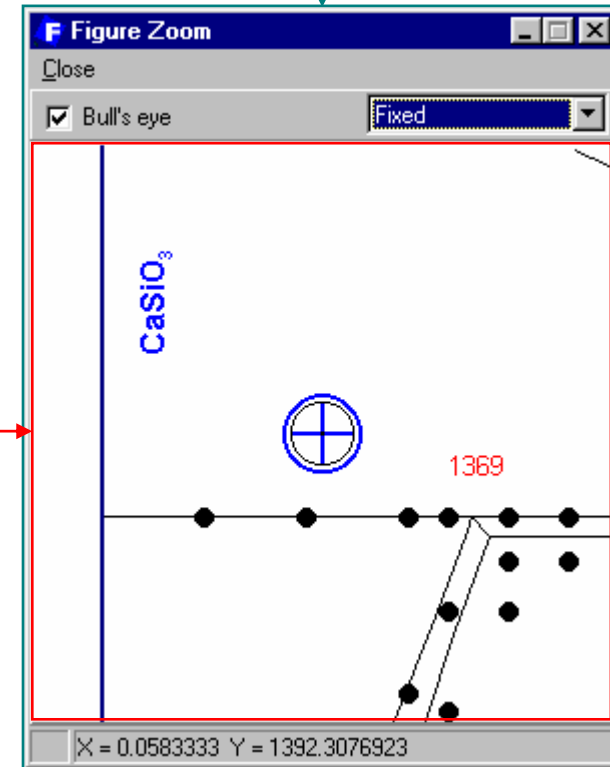
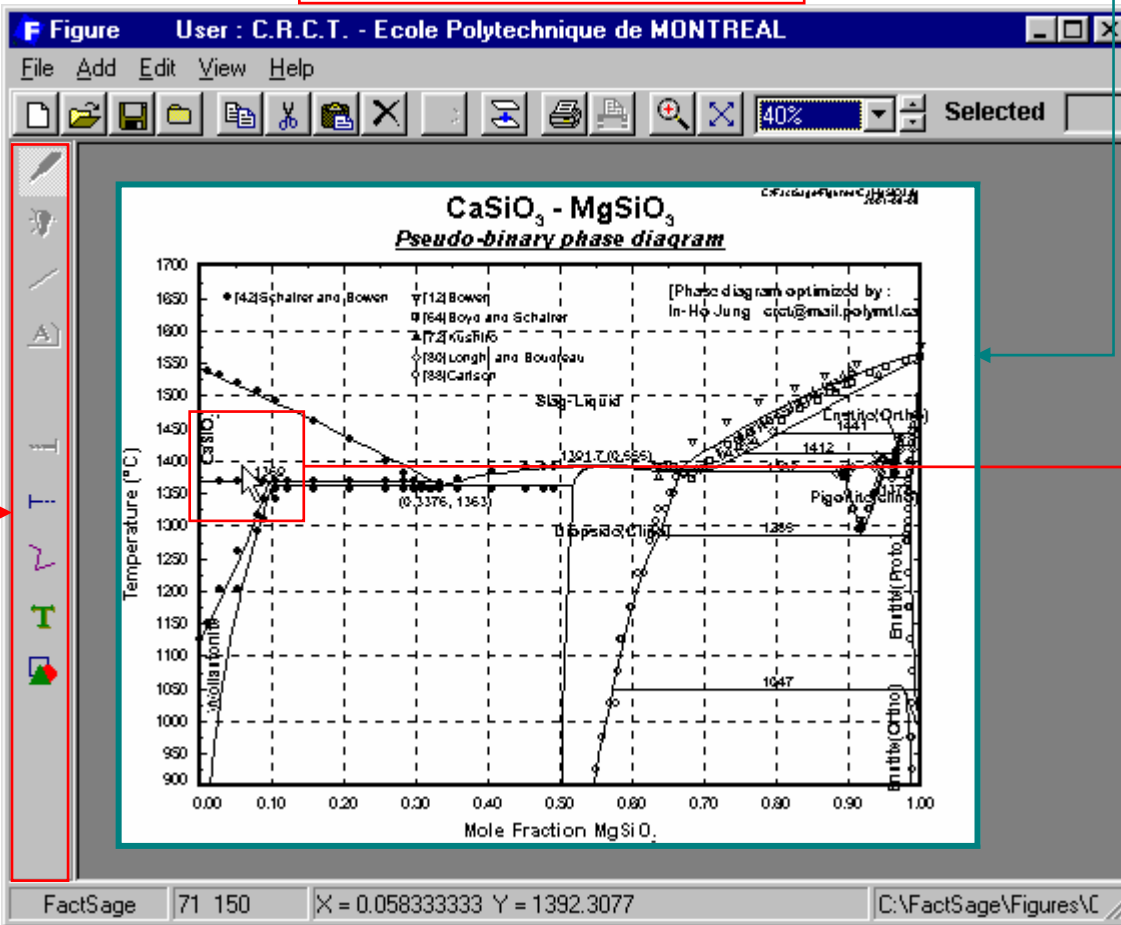
Maximise the figure in the window

Show in **black and white**

Show the **crosshairs**



Magnifying glass
(6X current zoom),
• **bull's eye** enabled,
• **fixed mode**
(instead of **proportional**)



Adding and editing **experimental data** points

The following four slides show how to use a diagram generated with the **Reaction** module as a basis into which experimental data are added.

Obtaining a *figure* file from the *Reaction* program

Heating of 1 mole NaF from 298.15 K to T = 300 K to 1800 K under P = 1atm (standard state)

Graph of the enthalpy ΔH in function of the temperature T

Table Reaction

File Units Output Figure Help

Reactants: NaF = NaF (298.15K) (T)

T(K)	Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)
-----	NaF(s-CRYO)	NaF(s-CRYO)	-----	
300.00	88.3	-95.0	0.0000E+00	0.295
500.00	10058.1	-13117.4	0.0000E+00	25.677
700.00	20658.1	-30360.1	0.0000E+00	43.484
900.00	31780.3	-50743.5	0.0000E+00	57.446
1100.00	43395.0	-73670.5	0.0000E+00	69.092
1269.00	53584.9	-94743.1	0.0000E+00	77.706
-----	NaF(s-CRYO)	NaF(l-CRYO)	-----	
NaF(1 mol):	DH = 33348.0	DG = 0	-----	DS = 26.27
1269.00	86930.9	-94743.1	0.0000E+00	103.983
1300.00	89118.5	-99580.6	0.0000E+00	105.686
1500.00	103231.9	-131994.2	0.0000E+00	115.785
1700.00	117345.4	-166295.2	0.0000E+00	124.617

Dialog box: Axes: Delta H(J) vs T(K)

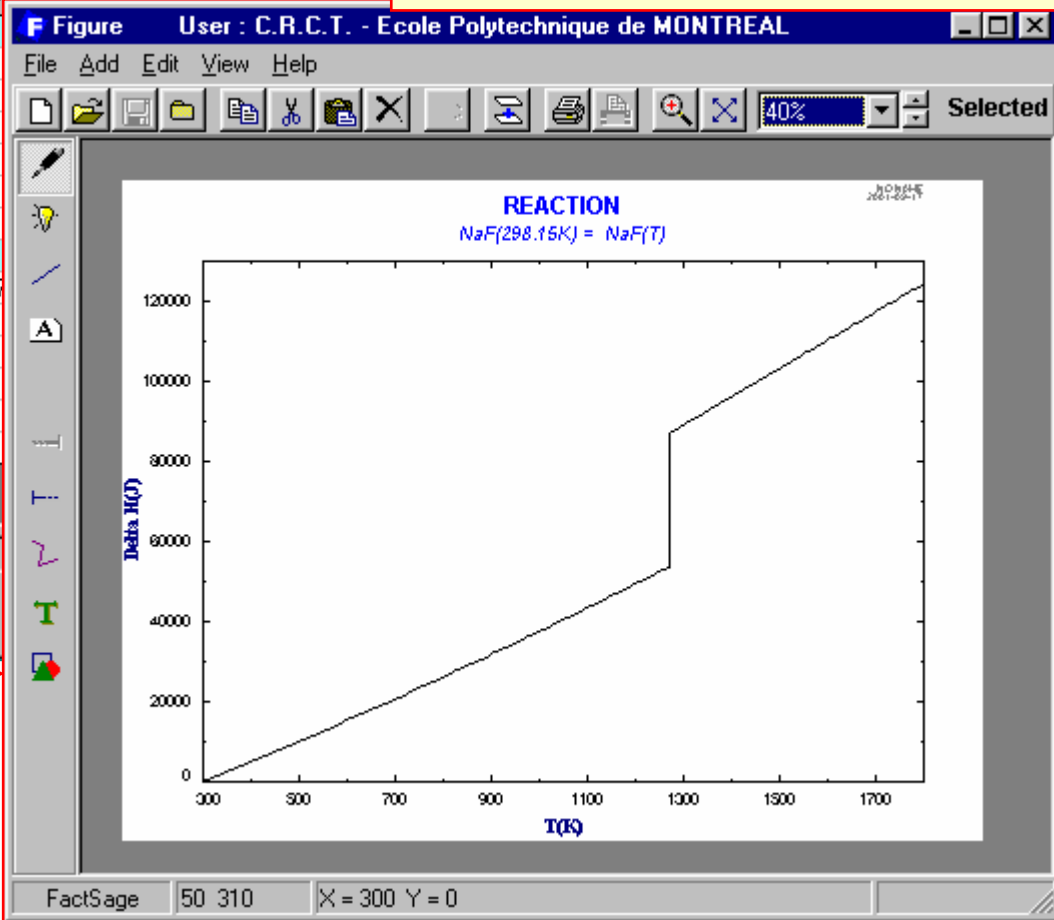
Y-axis: Delta H(J)

X-axis: T(K)

Y-axis settings: maximum 130000, minimum 0, tick every 10000

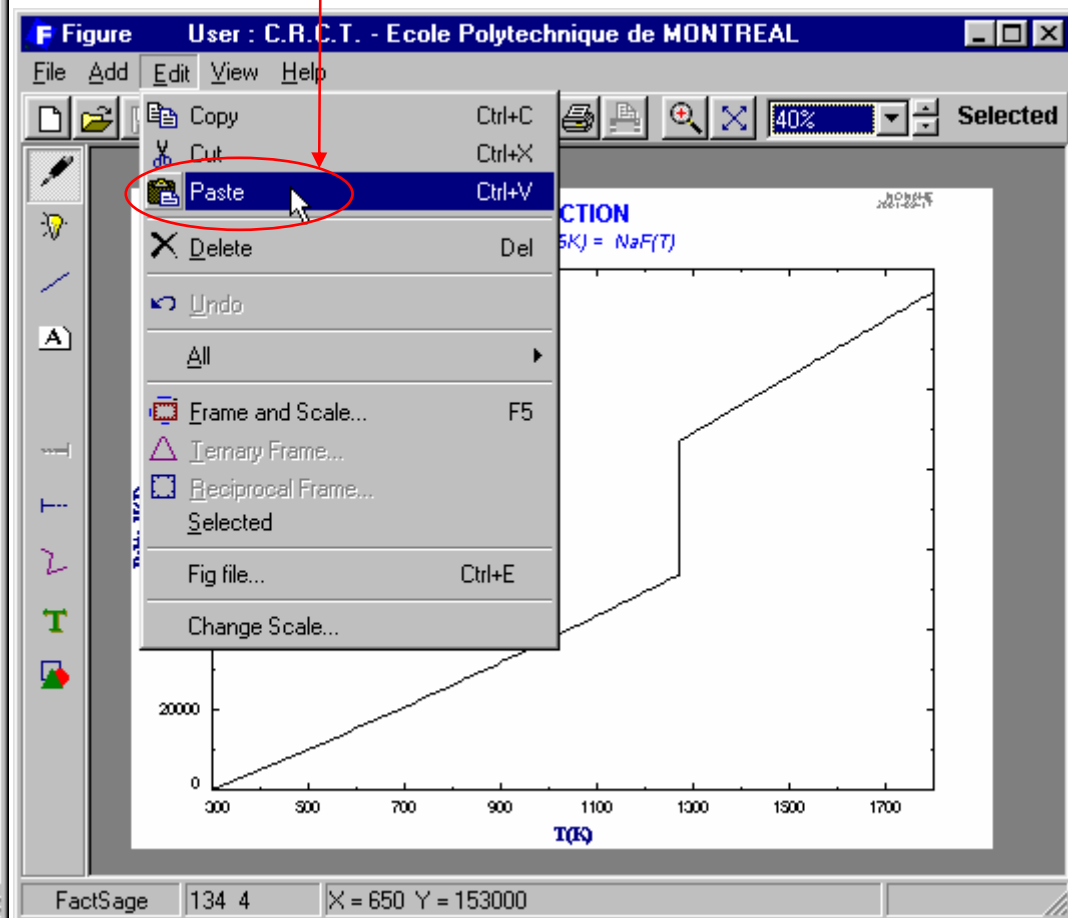
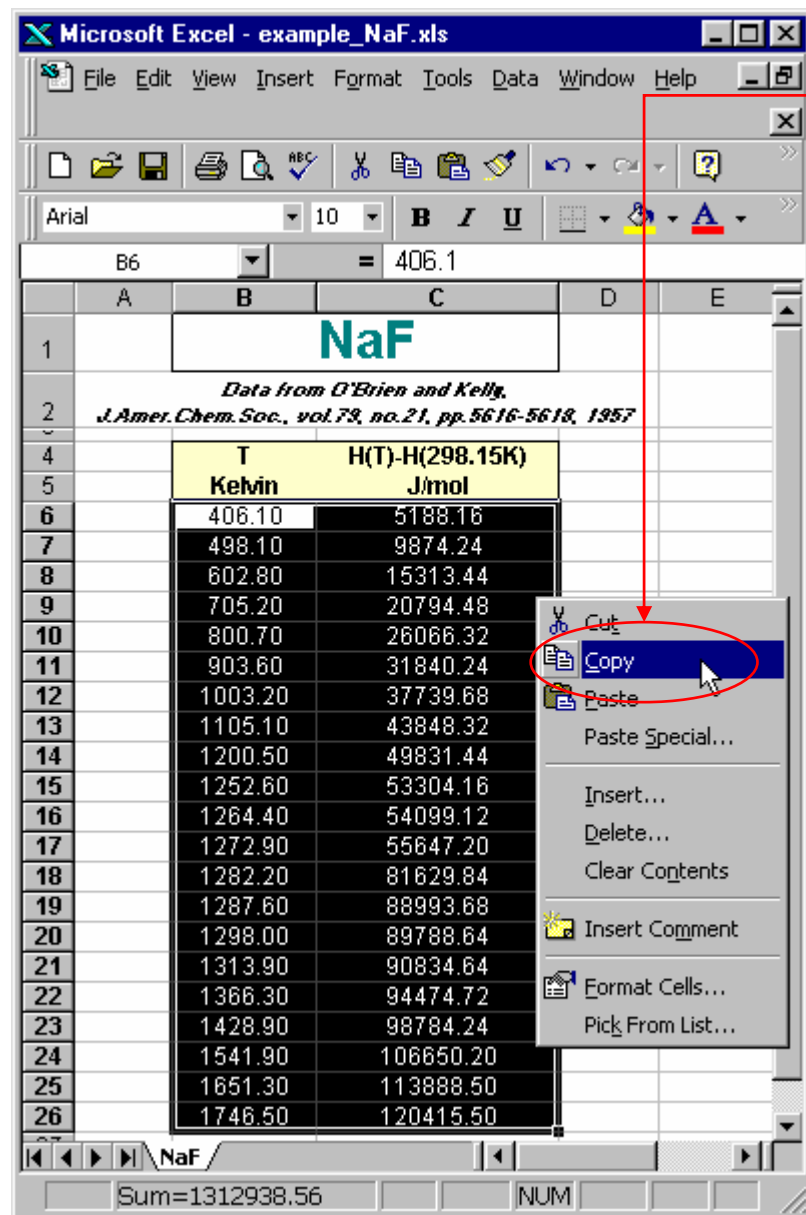
X-axis settings: maximum 1800, minimum 300, tick every 100

Buttons: Cancel, OK



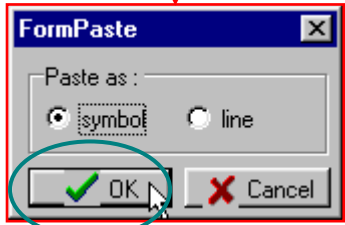
Adding experimental data from an Excel file to the *Figure* program

You **select** and **Copy** your data points from the Excel® file and you **Paste** it in the *Figure* program.



Editing the experimental data: Selection

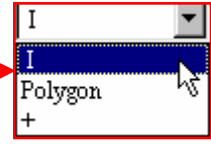
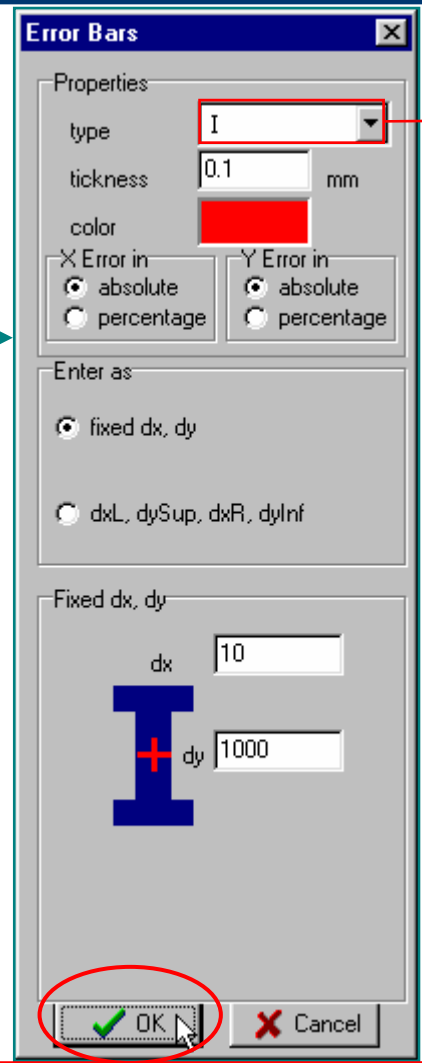
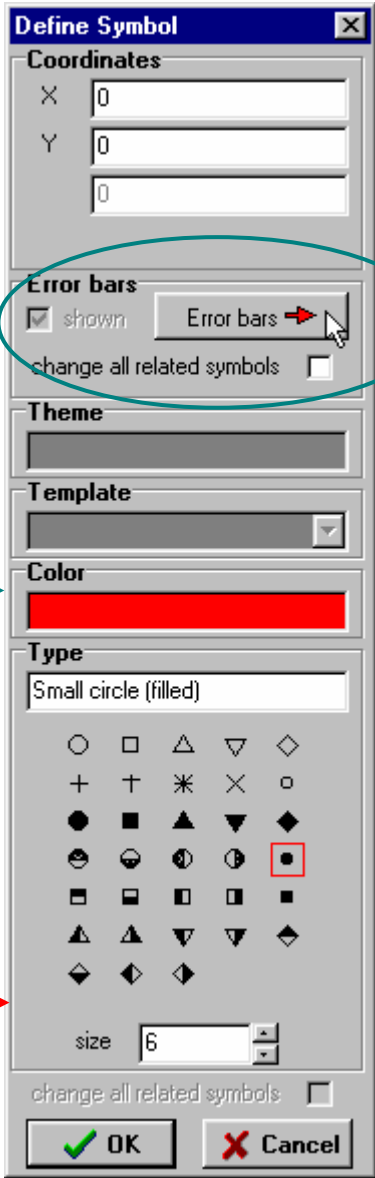
Choose your data representation: **symbol** or line. Press «**OK**».



Define your Symbol:

- Color: **Red**
- Type: **Small circles (filled)**
- Size: **6**

Press «**Error bars**→».



Make your choice of Error bars properties: type, thickness, color and dimensions. Press «**OK**».

Editing the experimental data: Output

The image shows two windows from the FactSage software interface. On the left is the 'Define Symbol' dialog box, which is used to define the appearance of symbols in a plot. It includes fields for 'Coordinates' (X, Y, Z), 'Error bars' (checked), 'Theme', 'Template', 'Color' (set to red), and 'Type' (set to 'Small circle (filled)'). The 'OK' button is highlighted with a red circle and a red arrow pointing to a yellow callout box. On the right is the 'Figure' window, titled 'User : C.R.C.T. - Ecole Polytechnique de MONTREAL'. It displays a plot of 'Delta H(J)' versus 'T(K)' for the reaction $\text{NaF}(298.15\text{K}) = \text{NaF}(T)$. The plot shows a series of red data points with error bars connected by a black line. A red circle with error bars is highlighted in the plot, and a red arrow points from the 'Define Symbol' dialog to this symbol. A yellow callout box contains the text: 'Press «OK» in the Define Symbol widow.'

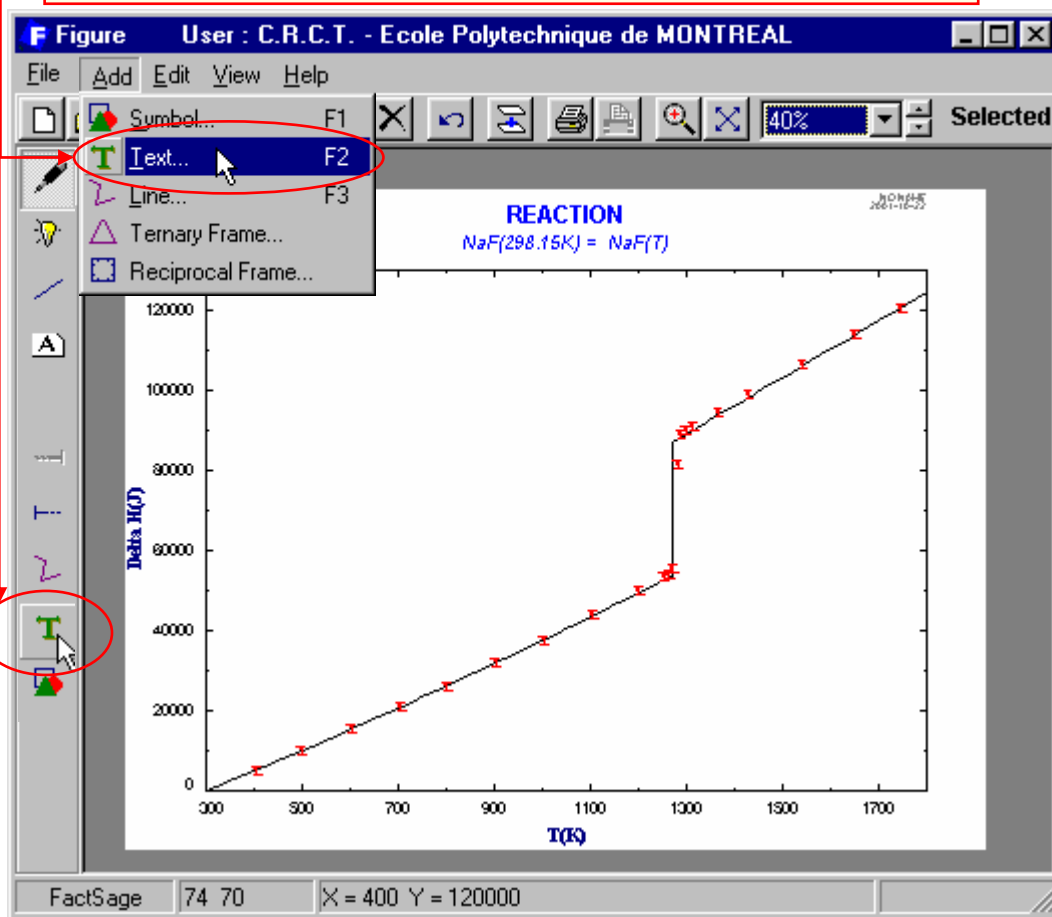
Adding a **legend** into a figure

Figure permits the addition of a legend into a diagram.
The following two slides show how to do that.

Adding a legend or text to your *Figure*

To **open** the **Add Label** window, you can:

- **click** on the **Add Label** icon on the edition tool bar,
- **select** **Text...** from the **Add** menu **or**
- **press** «**F2**» on the keyboard.



The 'Add Label' dialog box is shown with the following settings:

- Text:** Data from O'Brien and Kelly, J.Amer.Chem.Soc., Symbol
- Coordinates:** X=400, Y=120000
- Angle:** 0°
- Alignment:** Left Justify
- Font:** Arial, size 12, color black
- Theme:** (empty)
- Template:** (empty)
- Buttons:** OK (checked), Cancel

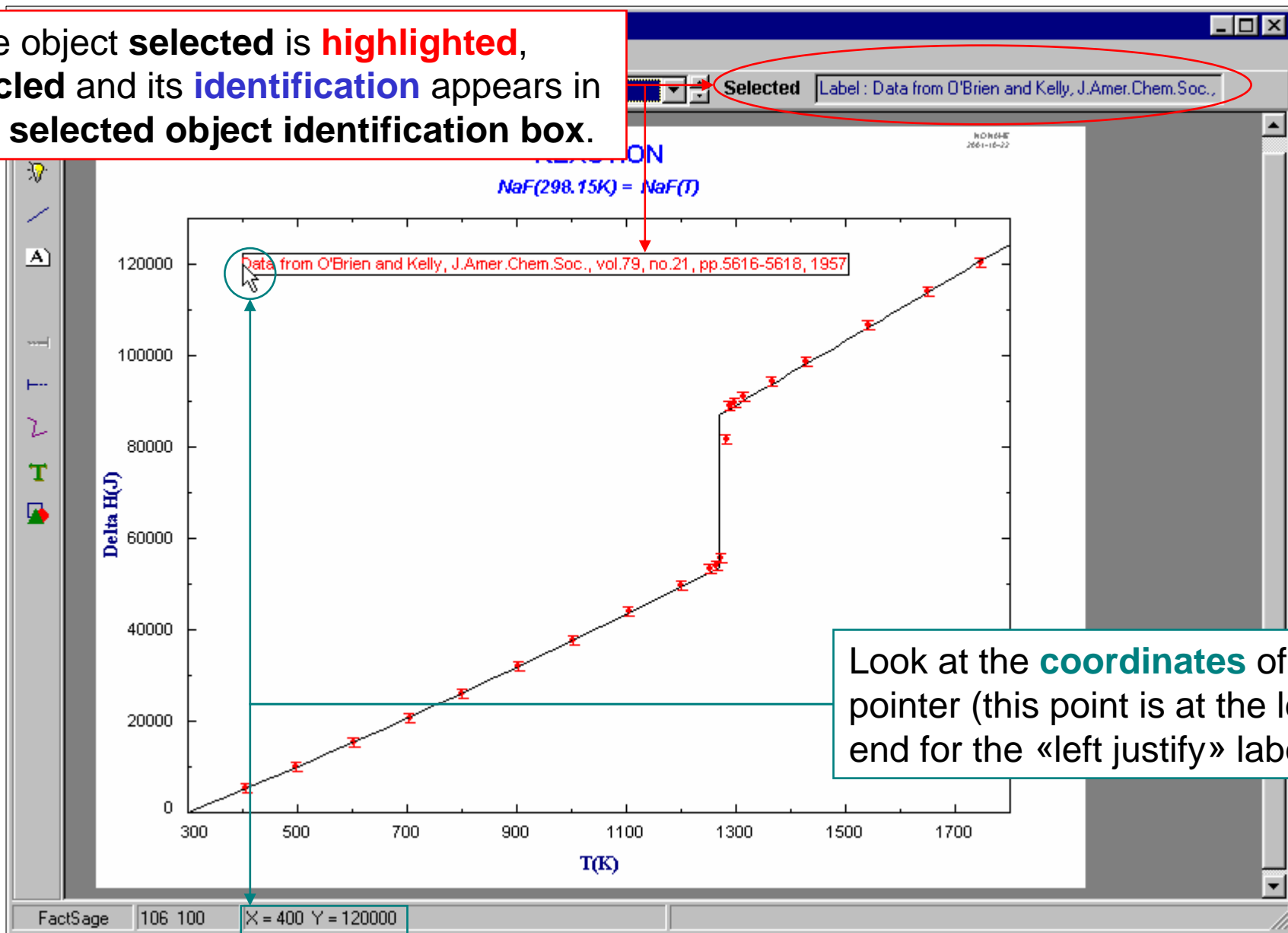
Type:

- your **Text**;
- the **Coordinates** of the anchor of the text box (here **X=400** and **Y=120000**);
- the **Angle** of the text box;
- the **Alignment** of the text box;
- the text **Font**, size and color.

Press «**OK**».

An Enthalpy ΔH vs temperature $T(K)$ graph

The object selected is **highlighted**, **circled** and its **identification** appears in the **selected object identification box**.



Look at the **coordinates** of the pointer (this point is at the left end for the «left justify» label).

Adding and editing **symbols** to a figure

Figure permits the addition of symbols into a diagram. Symbols that have been added may also be edited.

The following three slides show how to make use of the adding and editing of symbols.

Adding a symbol to your *Figure*

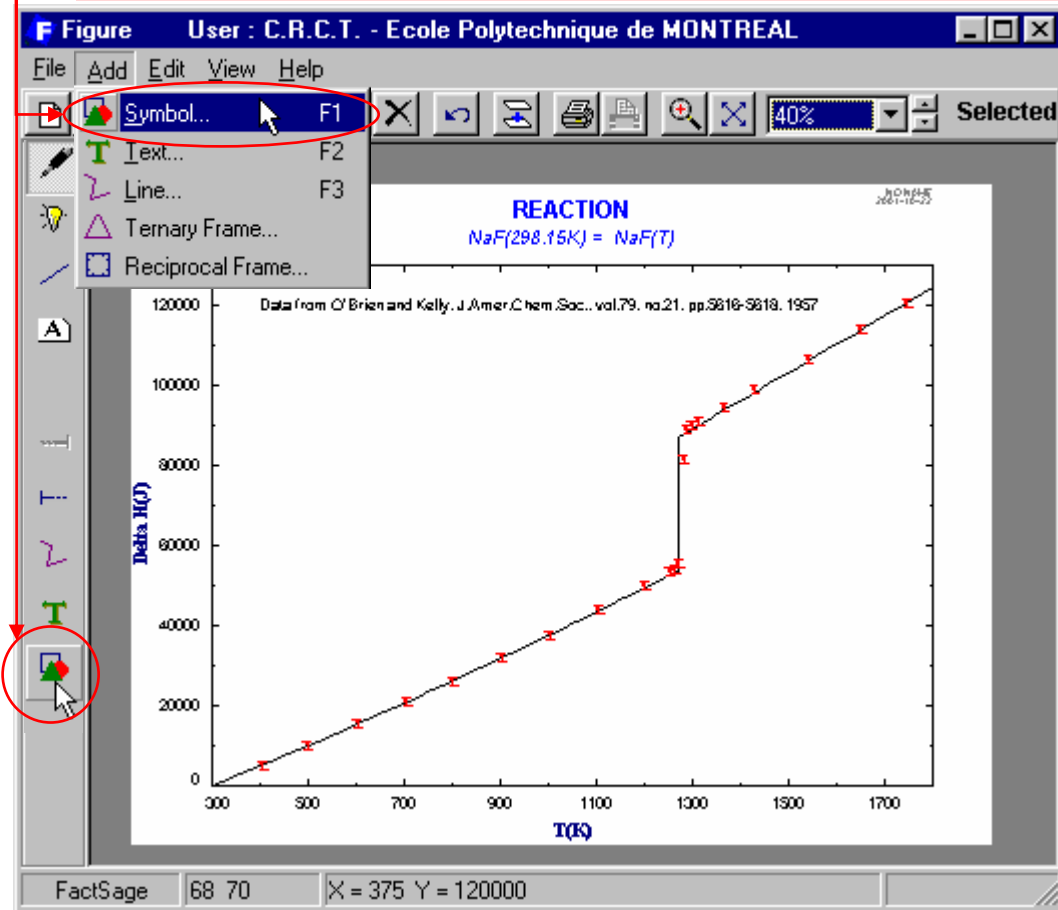
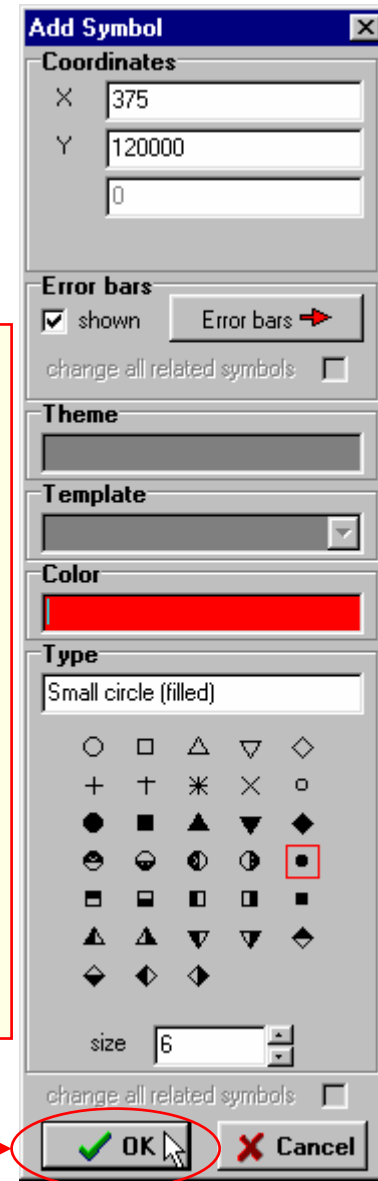
To **open** the **Add Symbol** window, you can:

- **click** on the **Add Symbol** icon on the edition tool bar,
- **select** **Symbol...** from the **Add** menu or
- **press** «F1» on the keyboard.

Select:

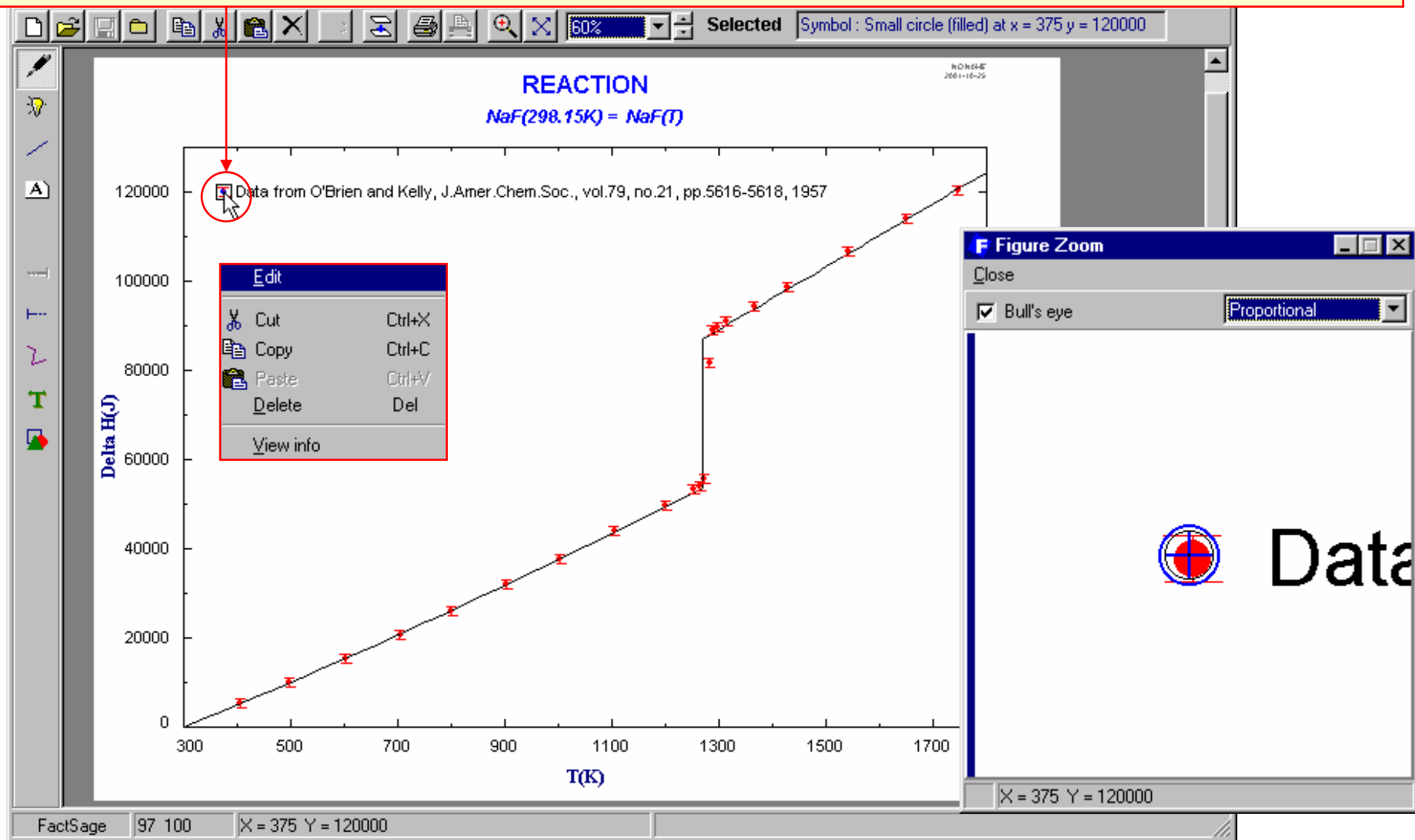
- the **Coordinates** of the symbol (here **X=375** and **Y=120000**);
- the **Color**, the **Type** and the size;
- and the **Error bars**.

Press «OK».

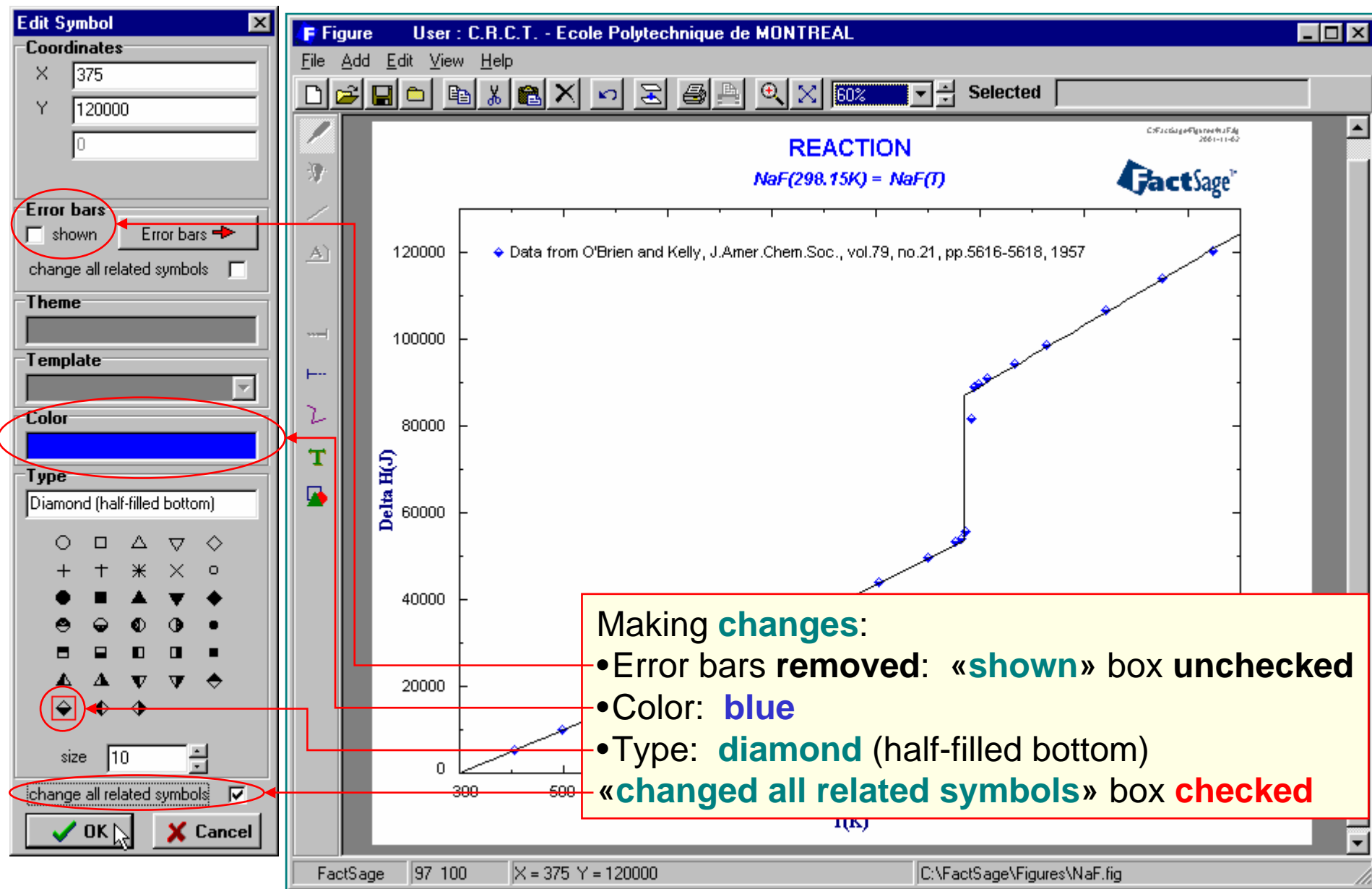


Editing all symbols together

Left click on a symbol to open a pop-up menu, then select **Edit**. The **Edit symbol** window will appear (shortcut: **double-click** on a symbol will do the same).



Editing all symbols together: Results



Making changes:

- Error bars removed: «shown» box unchecked
- Color: blue
- Type: diamond (half-filled bottom)
- «changed all related symbols» box checked

Adding and editing **lines**


The **Figure** module permits the addition of lines into an already existing diagram. Once the line has been added it is also possible to edit it, e.g. in terms of the line color, line thickness etc.


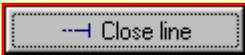
The following four slides show how to make use of the adding and editing of lines.

Adding lines to a figure using the mouse

The image shows two windows from the FactSage software. The left window is titled 'Figure' and shows a toolbar with the 'Open a new line' button highlighted. The right window is also titled 'Figure' and shows a plot of Delta H(J) vs. Temperature (T) for the reaction $\text{NaF}(298.15\text{K}) = \text{NaF}(T)$. A new line is being added to the plot, and the 'Close New Line' dialog box is open.

To add a line using the mouse:

- **Select** the «Open a new line» **button**  (the pointer is now a **cross**);
- **Move** the pointer to the location of the first point of the line and **click**;
- **Repeat** for the next points.

And **close** the line by pressing on the «Close the new line» **button**  in the **Edition toolbar** or the Close line **button**  in the **Close New Line** window. This will open the **Add Line** window.

The **Add Line (Edit Line)** window features

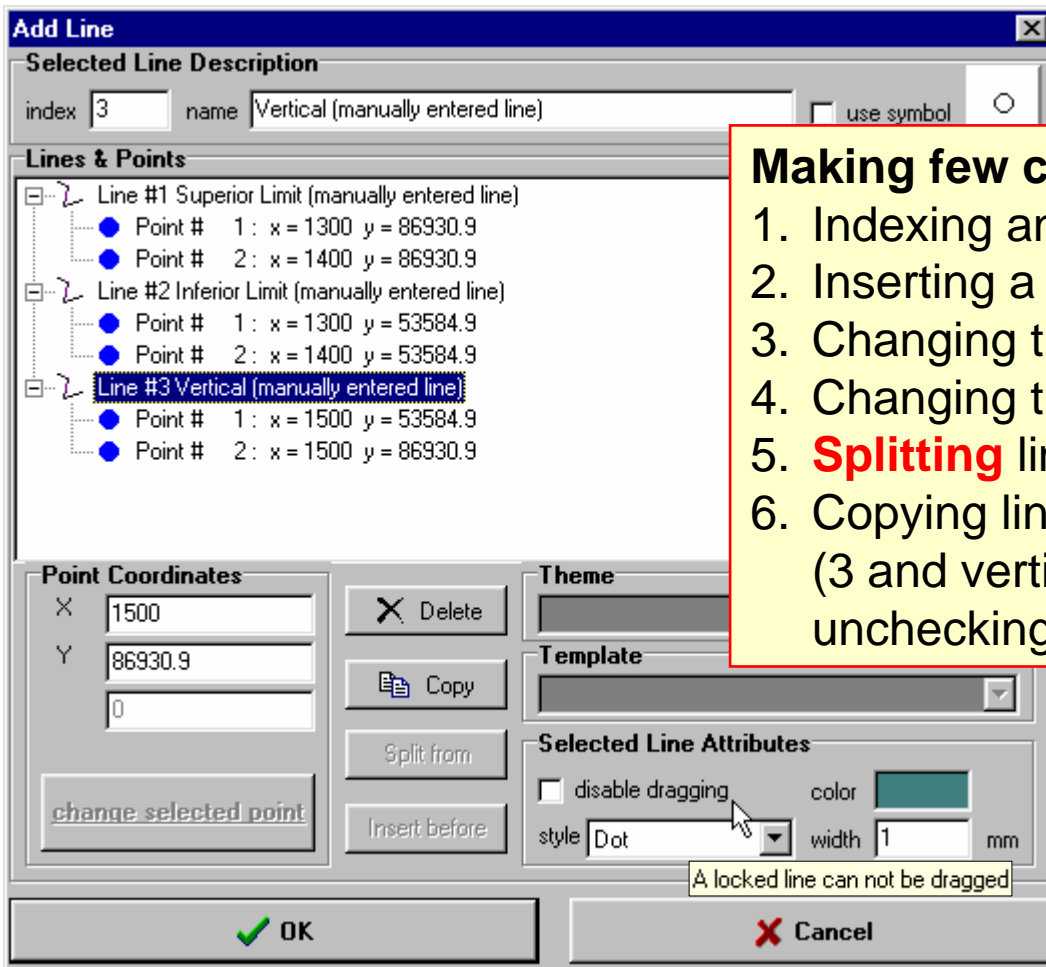
The screenshot shows the 'Add Line' dialog box with the following sections and callouts:

- Selected Line Description:**
 - index: 0
 - name: Manually entered line
 - use symbol
 - (Symbol type selector)
- Lines & Points:**
 - Line #1 Manually entered line
 - Point # 1: x = 1300 y = 87000
 - Point # 2: x = 1400 y = 87000
 - Point # 3: x = 1475 y = 82000
- Point Coordinates:**
 - X: 1475
 - Y: 82000
 - 0
- Buttons:** Delete, Copy, Split from, Insert before, change selected point
- Theme and Template:** Theme, Template
- Selected Line Attributes:**
 - disable dragging
 - color: [black swatch]
 - style: Solid
 - width: 0.35 mm
- Bottom Buttons:** OK, Cancel

Callouts and their corresponding features:

- Enter a line number (points to index field)
- Enter a line name (points to name field)
- Click to change symbol type (points to symbol type radio button)
- Check to put a symbol at every calculated point of the line (points to 'use symbol' checkbox)
- Delete the selected object (points to Delete button)
- Copy the selected object (points to Copy button)
- Split the line from the selected point (points to Split from button)
- Change the selected point by the new value (points to 'change selected point' button)
- Insert a new point before the selected point (points to Insert before button)
- Change the selected point by the new value (points to X and Y coordinate fields)
- Delete the selected object (points to Delete button)
- Copy the selected object (points to Copy button)
- Check to enable the drag-and-drop of the selected line (points to 'disable dragging' checkbox)
- Select the line appearance (points to style dropdown)
- Click to change the color of the selected line and symbol (points to color swatch)
- Enter the width of the selected line (points to width field)
- Clicking on the **Add Line** button or selecting **Add > Line...** also opens the Add Line window and you can enter the points coordinates of lines **using the keyboard.** (points to the dialog box)

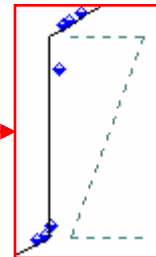
Editing in the **Add Line (Edit Line)** window



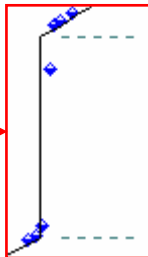
Making few changes:

1. Indexing and labeling the line;
2. Inserting a point before point #2;
3. Changing the coordinates of the four points;
4. Changing the color, style and width of the line;
5. **Splitting** line #1 at point #3;
6. Copying line #2, indexing and naming the new line (3 and vertical), changing coordinates and unchecking «disable dragging» of line #3

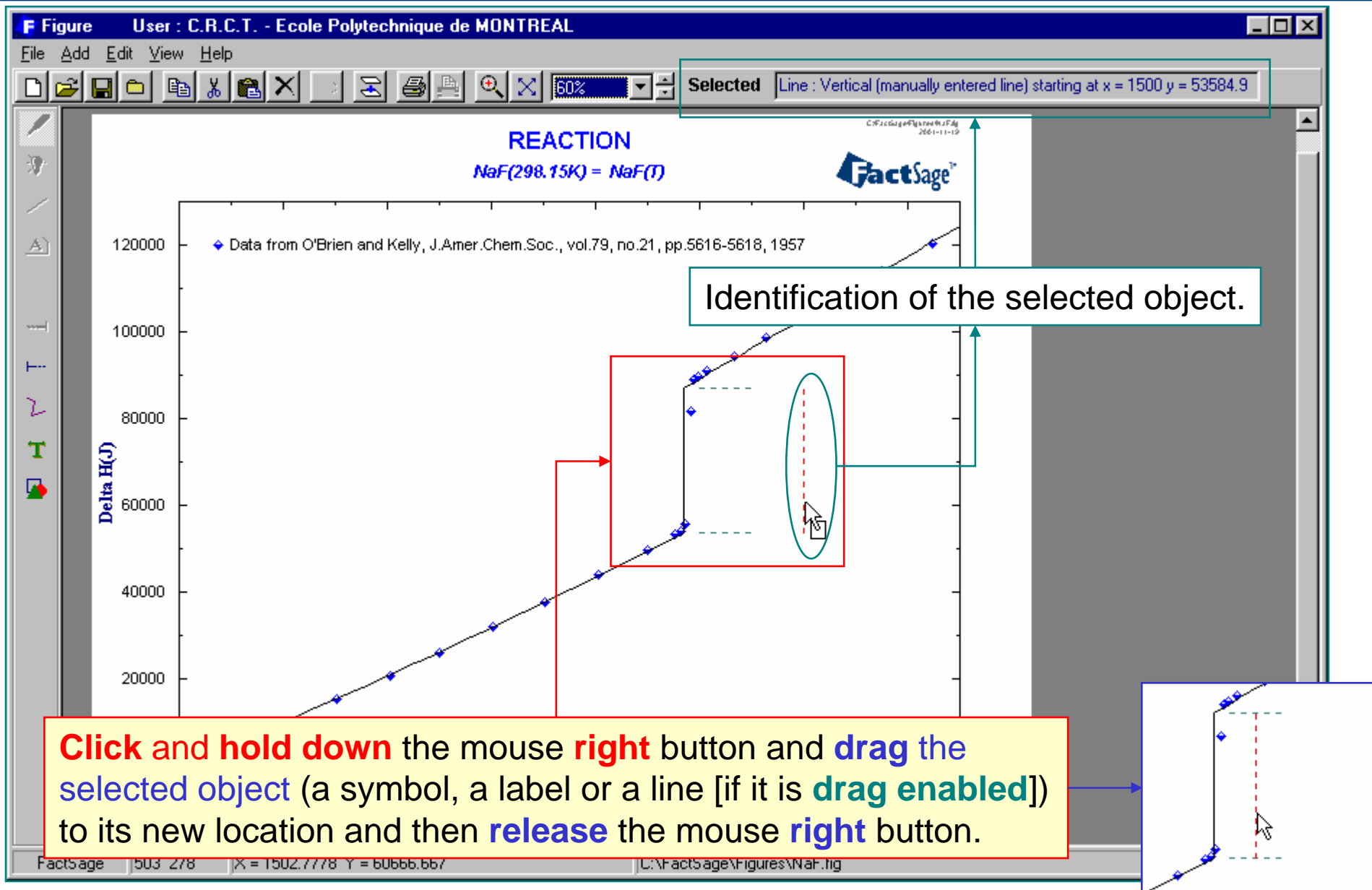
Step 5:
Before splitting



Step 5:
After splitting



Result of the lines' edition and **Drag-and-Drop** feature



Changing Scale

The following two slides show how the **Change Scale** option is called and applied in adjusting the axes variables of a diagram.

The **Change Scale** window

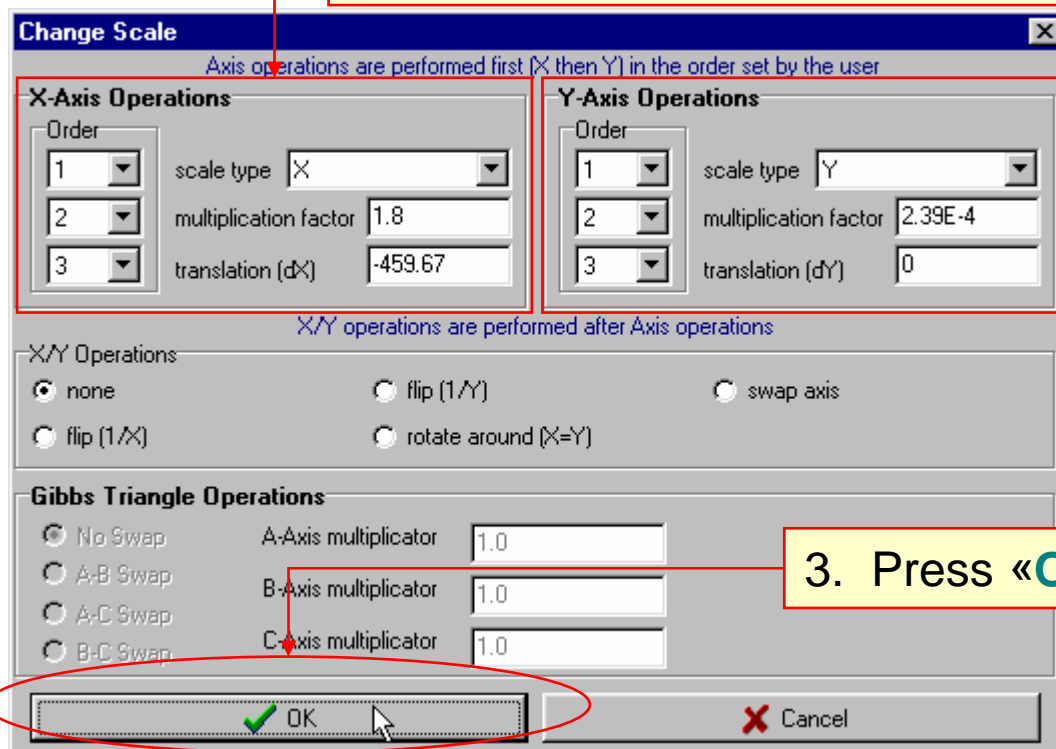
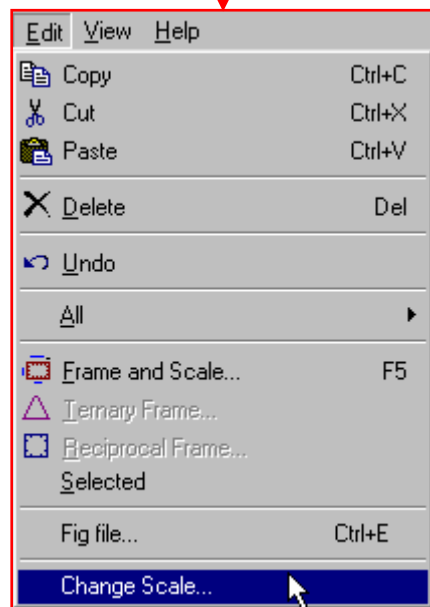
For example, you want to change **enthalpy** values from **joules** to **calories** and change **temperature** values from **Kelvins** to **Fahrenheit degrees**.

2. Enter the operation you want to perform.

For the X-axis, the **temperature**:
 $1.8 \times [T(K) - 273.15] + 32 = T(^{\circ}F)$
or $1.8 \times T(K) - 459.67 = T(^{\circ}F)$

For the y-axis, the **enthalpy**:
 $\Delta H(J) \times [1 \text{ Kcal} / 4184 \text{ J}] = \Delta H(\text{Kcal})$
or $\Delta H(J) \times [2.39 \times 10^{-4}] = \Delta H(\text{Kcal})$

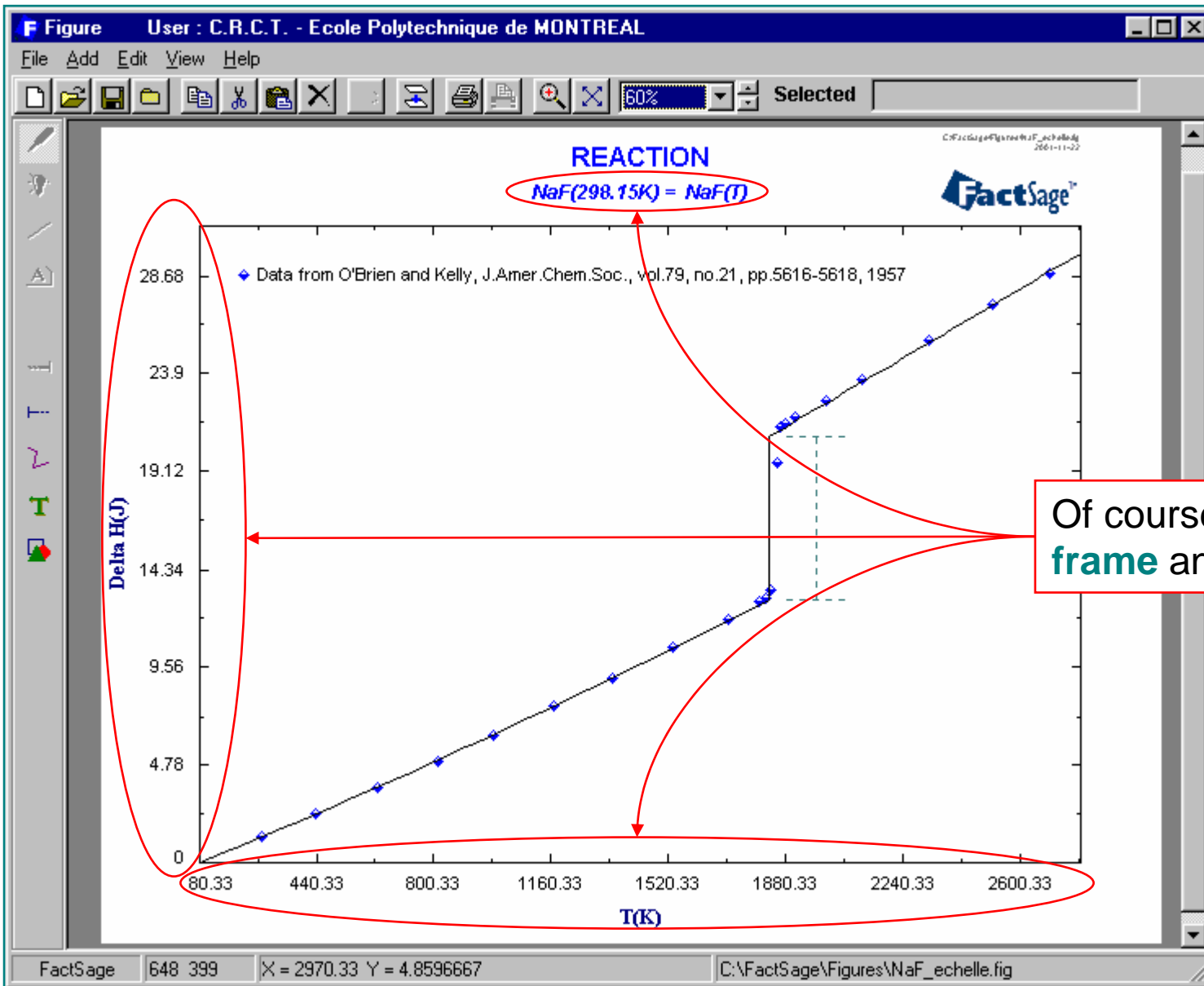
1. From the Menu bar, select:
Edit > Change Scale... to
open the **Change Scale**
window



3. Press «OK»

Figure 12.1

Change scale: Result



Of course, you can **edit** the **frame** and the **axes** again.

One of the major uses of the *Figure* module is in conjunction with the *Phase Diagram* module.

In that context the *Figure* module is called/opened automatically when the calculation of the phase diagram begins.

After the diagram is complete the *Figure* module is used to post-process the diagram on-line. Labels can be generated and fixed to a user selected position in the diagram, tie-lines can be calculated and plotted (if applicable), it is even possible to use the cursor to generate input for a point equilibrium calculation for a given x-y position in the diagram.

Calculating and drawing a binary *Phase Diagram*

Calculating the MgO-CaO phase diagram using the *Phase Diagram* program. (For details see *Phase Diagram* help, sections 4 and 15)

Parameters - Phase Diagram

Description	Used	Max
Reactant components:	2	8
Species retrieved from databanks:	26	no limit
Magnetic species retrieved from databanks:	0	no limit
Species selected for products:	6	692
Components (elements + electron phases):	3	32
Number of Gibbs energy/Cp equations for a constituent:		20
Total number of Gibbs energy/Cp equations:		2200
Selected species with volume or compressibility data:		100
Non-ideal solutions retrieved from databanks:	3	no limit

Target Limits

	min.	max.
T(K):	250	10000
P(bar):	1.0E-35	1.0E+08
V(l):	1.0E-08	1.0E+35
Alpha:	1.0e-5	1.0

Phase Diagram

Display
full screen: color:

Labels
size: 9 (5 - 20)
 chemical numerical

Show
status: labels:
 tie-lines warnings

Stop/Kill Window
 yes refresh: 2 sec

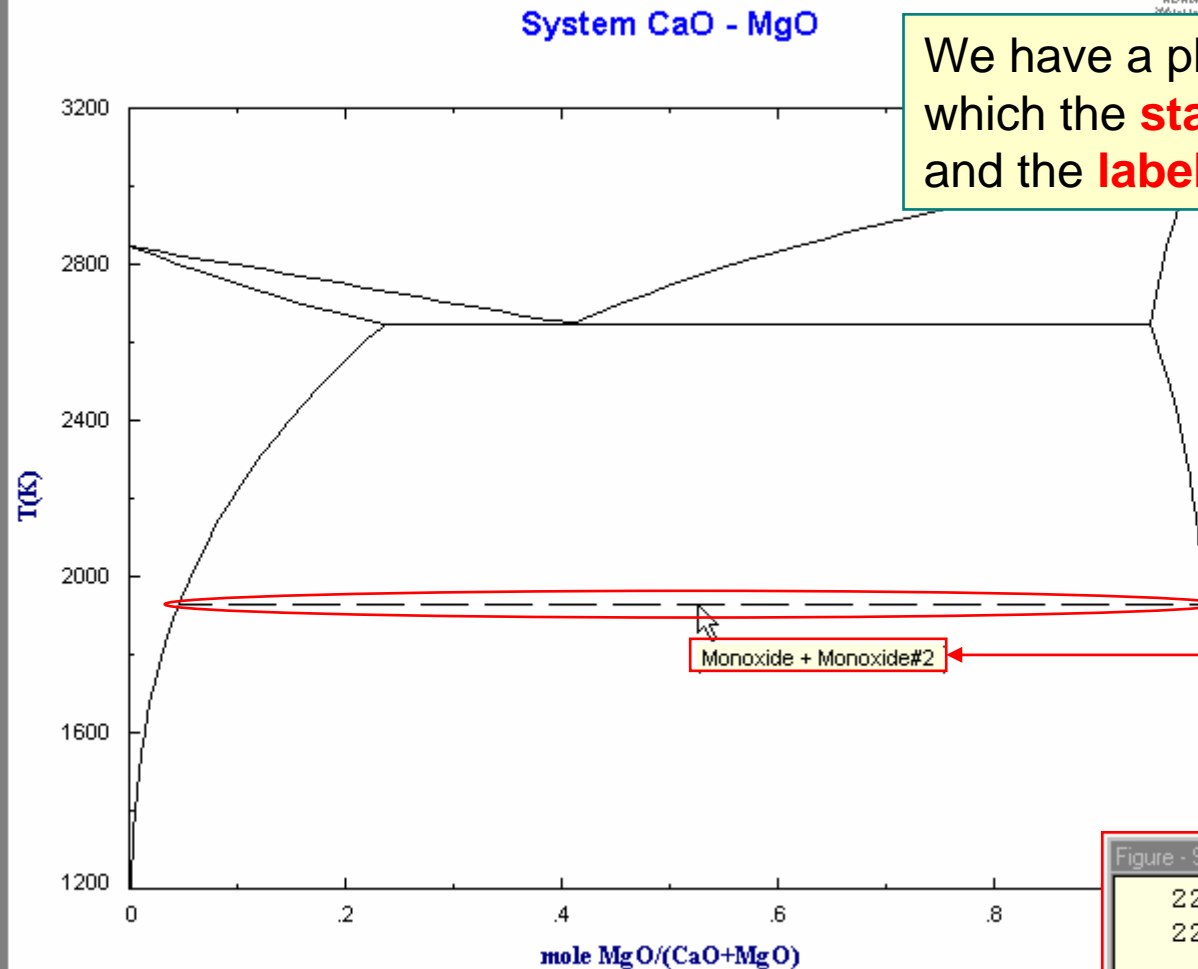
OK

Important:
To enable the 2-phases tie-lines mode, you must check the box show tie-lines in the Parameters window of the Phase Diagram program.

Phase diagram: **Figure** output

By default, the stable phases label mode is enable. Click on the figure to add the names of equilibrium phases at the cursor position.

We have a phase diagram in **color** in which the **status** window, the **tie-lines** and the **labels** are shown.



Phase Diagram

full screen: show status:

color: show tie-lines:

show labels:

Labels

size: (5 - 20)

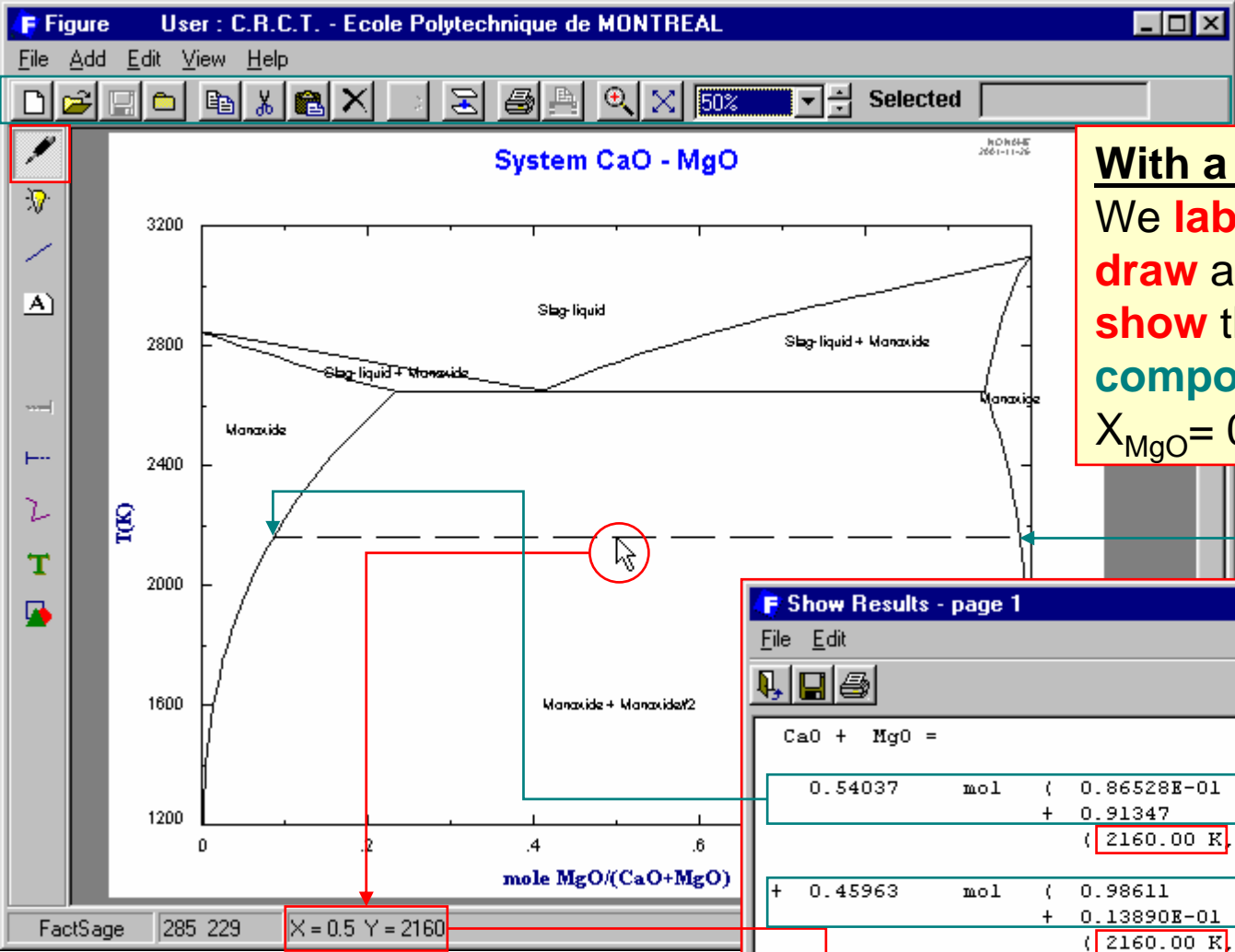
chemical numerical




Figure - Status : OK


223	9.9993E-01	1.2059E+03
224	9.9993E-01	1.2000E+03

- finished.

Labeling phase domains, drawing tie-lines and showing results of calculation



With a few mouse clicks,
 We **label** each domain ,
draw a tie-line at 2160 K ,
show the **proportion** and the **composition** of the phases at $X_{MgO} = 0.5$ and $T = 2160$ K .

The **normal edition mode toolbar** appears when the normal edition mode is **enabled** 

Show Results - page 1

CaO + MgO =

0.54037	mol	(0.86528E-01	MgO)
		+	0.91347	CaO)
			(2160.00 K	, 1.0000
				atm, Monoxi#1)	
+ 0.45963	mol	(0.98611	MgO)
		+	0.13890E-01	CaO)
			(2160.00 K	, 1.0000
				atm, Monoxi#2)	
+ 0.00000	mol	(0.37703	MgO)
		+	0.62297	CaO)
			(2160.00 K	, 1.0000
				atm, Slag-liq, a=0.34415	

where "A" on the reactant side is 0.5000

A Ternary (Gibbs triangular) diagram

The following two slides show how a ternary isothermal phase diagram (Gibbs triangle) is prepared and plotted.

It is also shown that a **group of items** (here **all phase boundaries**) can be treated with an **«ensemble» command**, for example to **change the color of all members of the group**.

Calculating and drawing a ternary *Phase Diagram*

Calculating the LiF-KF-NaF phase diagram using the *Phase Diagram* program.
(For details see [Phase Diagram help, section 12](#))

The screenshot shows the 'Phase Diagram' software interface with the following configuration:

- Menu - Phase Diagram** (Title bar)
- File Units Parameters Variables Help (Menu bar)
- Units: T(C) P(atm) Energy(J) Mass(mol) Vol(l)
- Components (3)**: LiF + KF + NaF
- Products**:
 - Compound species: gas (0), liquid (0), aqueous (0), solid (3) [checked]. Suppress duplicates: checked. Species: 3.
 - Solution species table:

*	+	Base-Phase	Full Name
	+	FACT-SALT	Salt-liquid
	+	FACT-AFA	Alk-F
	+	FACT-NLF	NaF-LiF
 - Custom Solutions: 0 fixed activities, 0 activity coefficients, 0 ideal solutions. [Details]
 - include molar volumes: unchecked.
 - Total Species (max 700): 10
 - Total Solutions (max 30): 3
 - [Default]
- Target**: Estimate T(K): 1000, Mass(mol): 0.
- Legend**: + - selected. [checked] Show all selected. species: 7, solutions: 3. [Clear]
- Variables**:

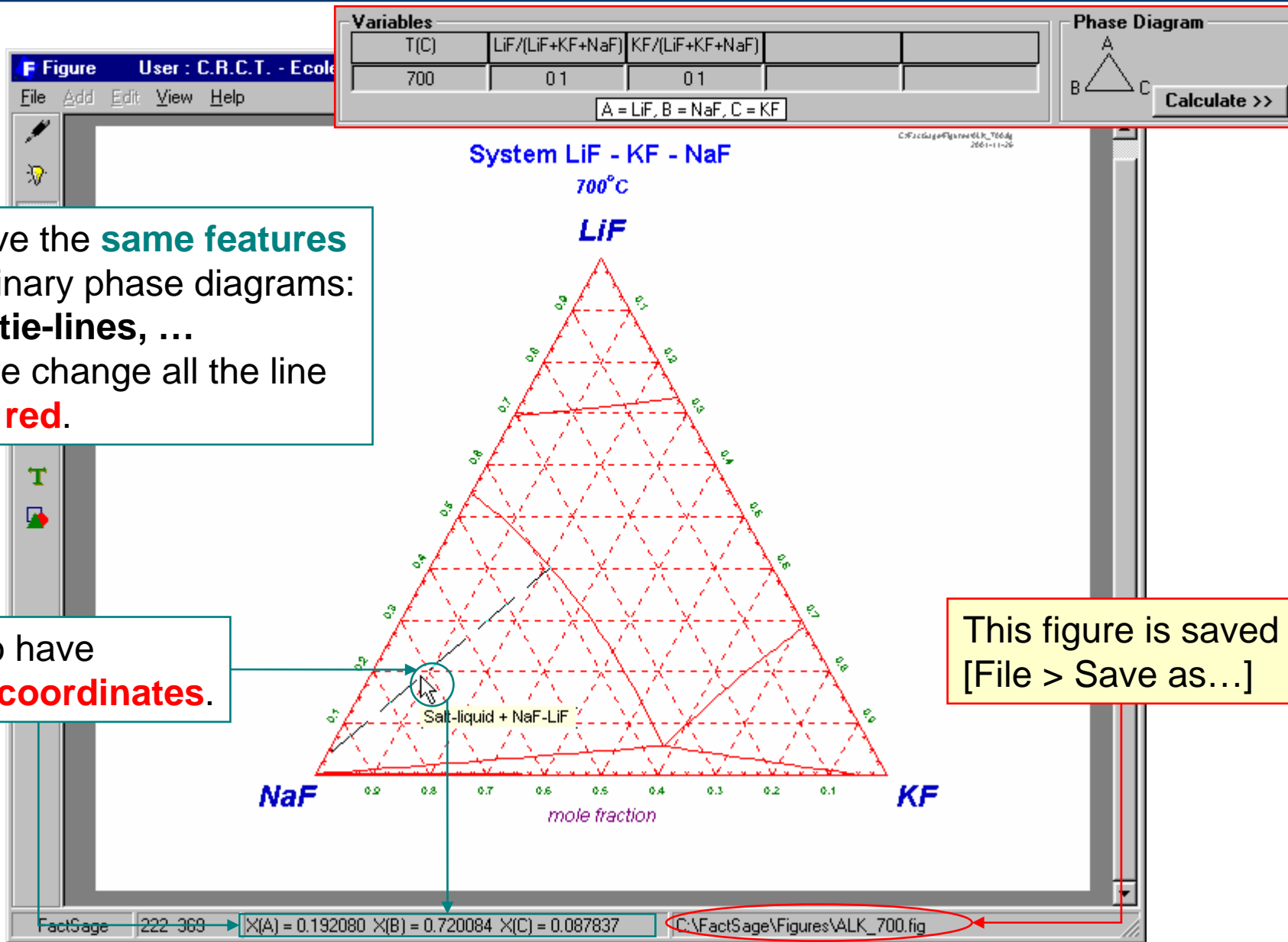
T(C)	LiF/(LiF+KF+NaF)	KF/(LiF+KF+NaF)		
700	0.1	0.1		

A = LiF, B = NaF, C = KF
- Phase Diagram**: Ternary diagram with vertices A, B, C. [Calculate >>]

FactSage 5.0 (25 May 01)

Figure 13.5

Ternary coordinates



You have the **same features** as on binary phase diagrams: **labels, tie-lines, ...**
Here, we change all the line color to **red**.

You also have **ternary coordinates**.

This figure is saved [File > Save as...]

Superimposed diagrams

The following two slides show how to make use of the **Superimpose** feature of *Figure*.

It is often useful to be able to draw diagrams in which a series of curves appear which depend on one particular parameter. The value of this parameter is different for each diagram, but the type of diagram is the same for a whole series.

As an example an overlay of two isothermal ternary phase diagrams is generated in which the temperature is the parameter.

NOTE that this feature is particularly useful if so-called **liquidus projections** are to be generated.

The **Superimposed Figure** feature

Variables

T (C)	LiF/(LiF+KF+NaF)	KF/(LiF+KF+NaF)		
650	0.1	0.1		

A = LiF, B = NaF, C = KF

Phase Diagram

Calculate >>

Figure User : C.R.C.T. - Ecole Polytechnique de
File Add Edit View Help


60%

Superimposed Figure LiF - KF - NaF
650°C
LiF

NaF mole fraction KF

FactSage 204 6 X = 0.24814815 Y = 1.1641026

Calculating another isotherm, at $T=650^{\circ}\text{C}$, of the **LiF-KF-NaF** phase diagram using the **Phase Diagram** program.

Select the «**Superimposed Figure**» fonction from the **normal edition mode toolbar**  or from the **menu bar: File > Superimpose...**

File

- New Ctrl+N
- Open... Ctrl+O
- Save Ctrl+S
- Save as...
- Close
- Superimpose...**
- Print... Ctrl+P
- NO NAME
- Exit

Superimposed figures

Select the figure to be superimposed on the previous one and press «Open»

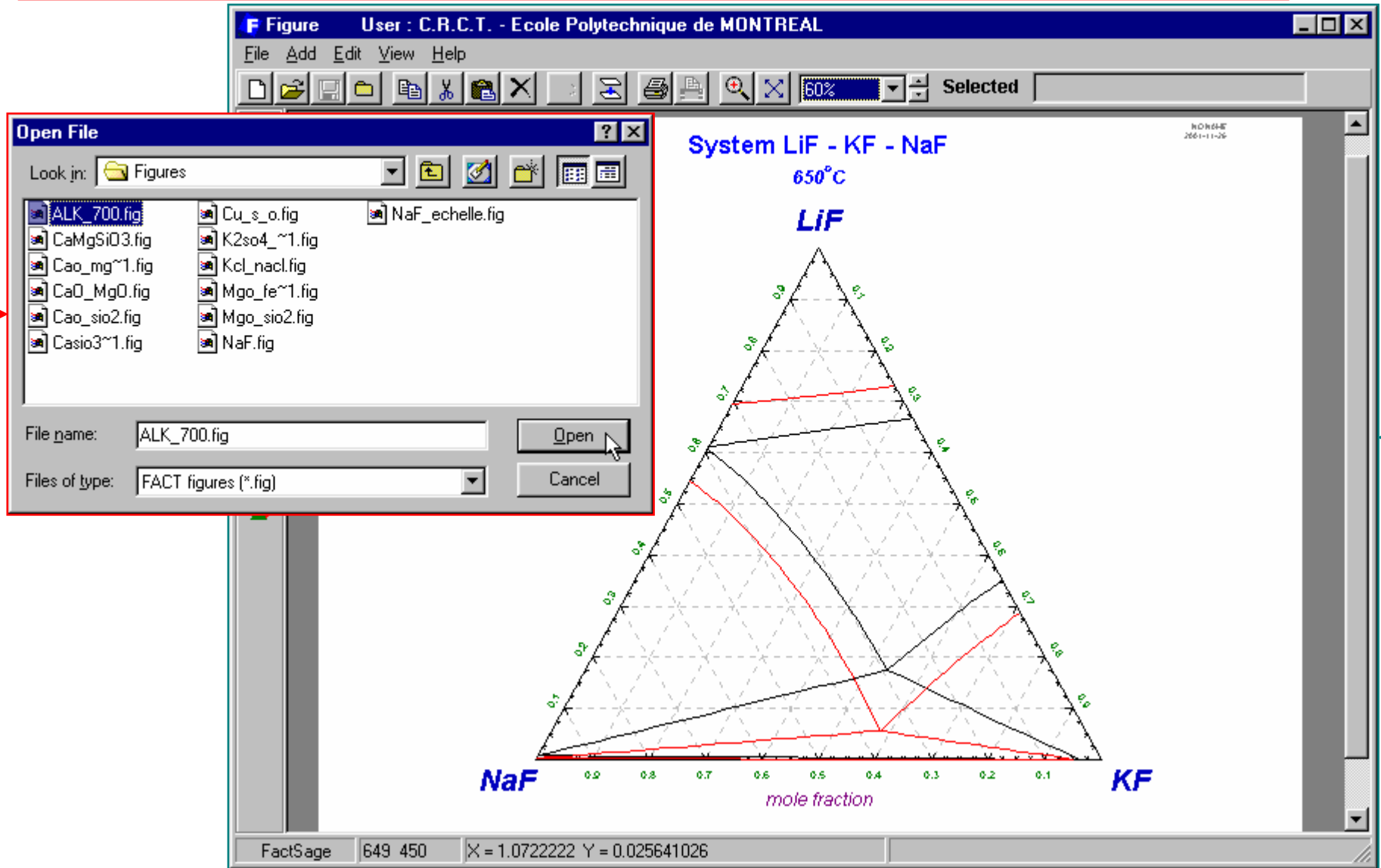


Figure 14.2