

# MyChemise

My Chemical Structure Editor

Software description

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## Introduction

MyChemise (my-chemical-structure-editor) is a 2D chemical structure drawing program that can present work in different ways. MyChemise is a Java-Applet. It runs as an application in a browser-window. MyChemise needs an up-to-date Java plug-in. If the plug-in has not already been installed it will normally install automatically into the Microsoft operating system being used when MyChemise starts for the first time. If this doesn't happen (e.g. under Linux) then the plug-in has to be installed manually (first try it with <http://java.com/en/download/installed.jsp>) There you can normally find a link for the plug-in. If not, browse for this Java plug-in).

Normally, for security reasons an applet is embedded in a 'sandbox' .

However, in MyChemise, you can use the clipboard to copy and paste. Files can also be saved on a computer's own hard disc.

For this reason, MyChemise is a signed applet with extended access rights.

Consequently, you will get a system-dependent security warning when MyChemise starts up.



**If you want to use MyChemise  
you have to agree to it**

The following text describes and presents the menu items in MyChemise. Well-known commands from standard-software (save, open etc.) or self-explanatory commands are not described.

## 1 The menu

file edit paste atom bond bond cross view presentation extras

When the mouse pointer is moved over each item the corresponding toolbar appears. Click on an item in the toolbar to fix it.

### 1.1 The file menu item

The screenshot shows the MyChemise software interface. The menu bar includes: file, edit, paste, atom, bond, bond cross, view, presentation, extras. The toolbar contains various icons for file operations, atom selection, bond types, and presentation options. A 'file' menu is open, showing options: new, open, save, save as, sketch area, page setup, print preview, print. Labels with arrows point to specific toolbar icons: 'print', 'open', 'save', 'new' point to the first four icons; 'atom symbol input' points to the 'C' input field; 'choice of bonds' points to the bond type selection icons; 'short notation' points to the 'C' input field; 'selects bond cross type' points to the bond cross selection icons; 'choice of atoms' points to the 'C H O N S Cl Br F CH<sub>2</sub> CH<sub>2</sub> more' selection area; 'cycl. hydrocarbons' points to the ring selection icon; 'undo set atom' points to the undo icon; 'undo set bond' points to the redo icon; 'colour' and 'repaint' point to the color and refresh icons.

file edit paste atom bond bond cross view presentation extras

print  
open  
save  
new

file edit paste a

new  
open  
save  
save as  
sketch area  
page setup  
print preview  
print

atom symbol input

choice of bonds

short notation

selects bond cross type

choice of atoms

cycl. hydrocarbons

undo set atom

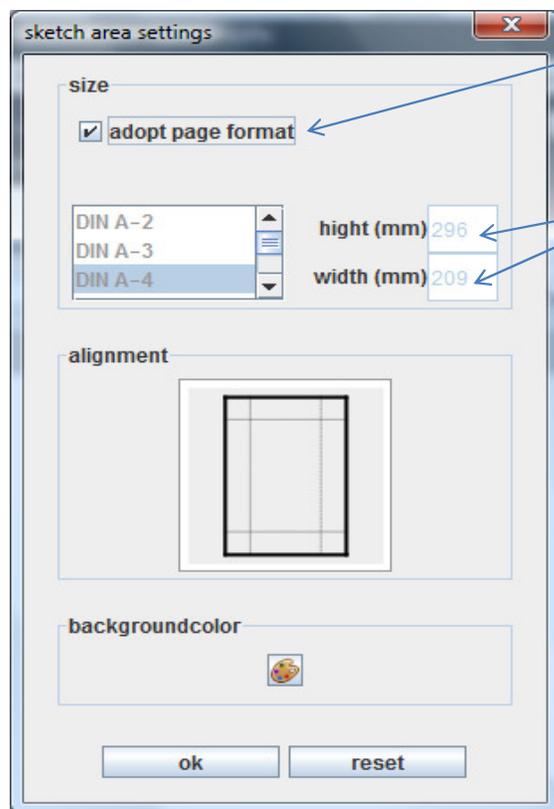
undo set bond

colour

repaint

Tip: for mol-files with a great number of atoms and bonds (e.g.: dna.mol [<http://www.chm.bris.ac.uk/motm/dna/dna.htm>]) select a small font size and set-up a atom-bond-distance of 1 px (Extras-options-atom) before opening it

### 1.1.1 The set-up sketch area window

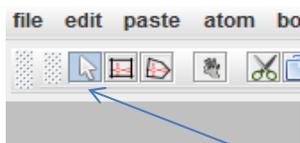


The adopt page format (file --> page set-up) is set by default. The standard setting is a DIN A-4 page in portrait format

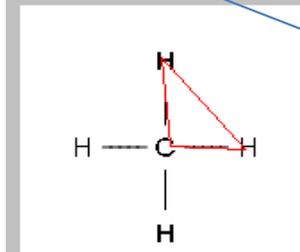
Can be changed

Tip: MyChemise is a drawing program. The dimensions of the sketch area directly effect the computer's speed. Therefore, select the smallest, necessary dimensions that you can use.

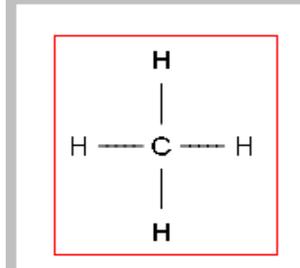
## 1.2 The edit menu item



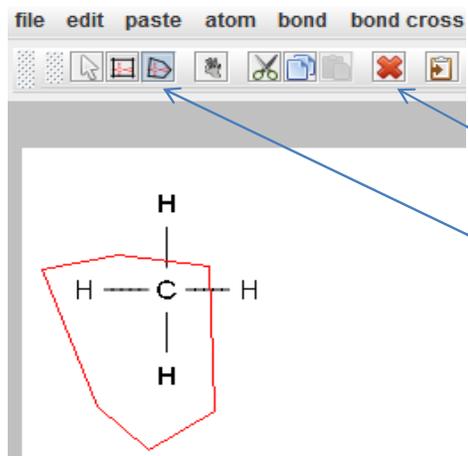
Note: in the edit menu it is impossible to set a new atom or a bond using a mouse click. To do this, you must first change back to the file, atom or bond menu.



to select specific atoms and bonds: click on each atom/bond

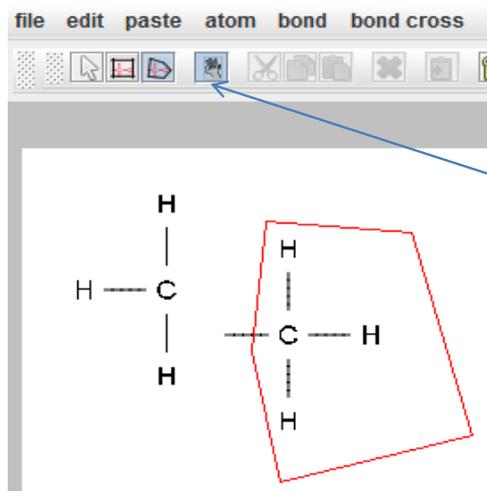


rectangular selection frame: press mouse and drag

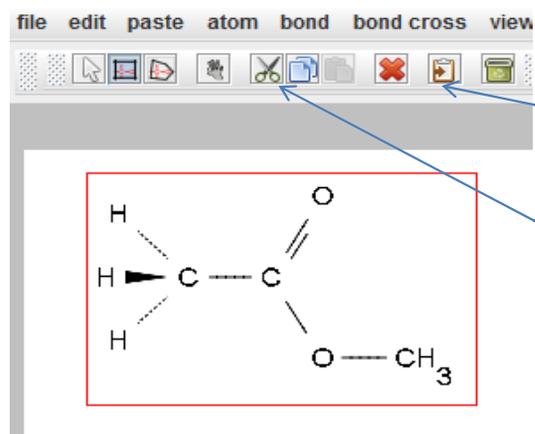


delete option

polygonal selection frame: every click is a vertex



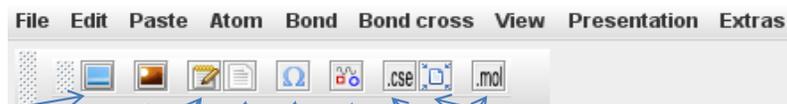
moves selection when mouse button is held down



copies selection onto clipboard  
(always produces a rectangular image. Can be pasted into other programs).

copies or cuts selection,  
can be pasted to the position  
of next mouse-click in the sketch area.

### 1.3 The paste menu item



Pastes an image from the clipboard  
(from other programs) onto the  
sketch area

opens the background window

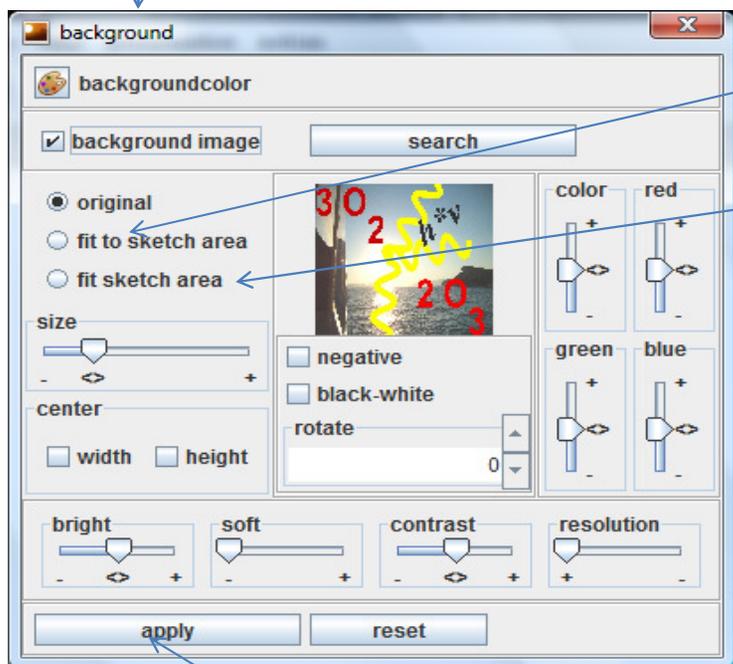
opens the editor

shows the text of the editor on the sketch area

opens the drawing window

opens the special-character window

a structure from a .cse or .mol file can be pasted to  
position of the next mouse-click. Linking atom is the atom  
on the farthest left side. Activate it to paste the structure  
at the original position.



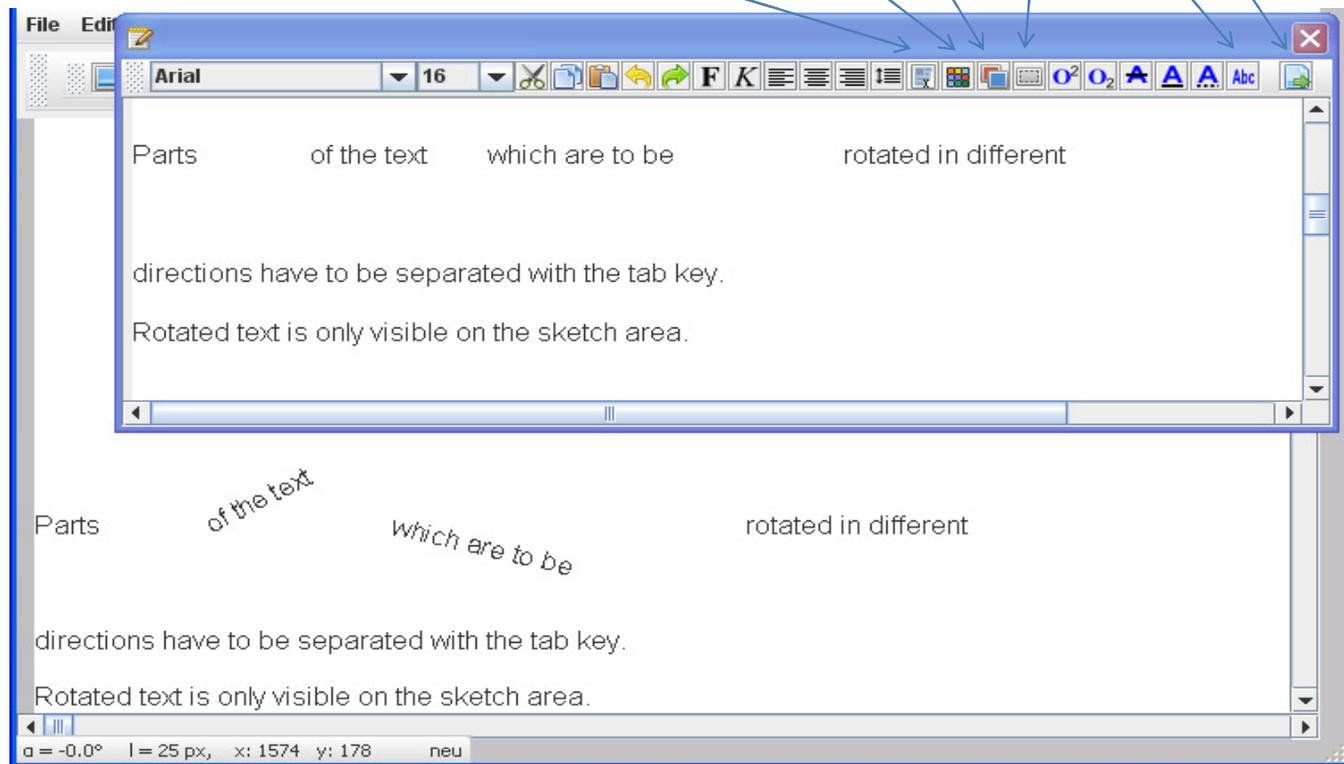
dimensions of the image are adjusted to the dimensions of the sketch area

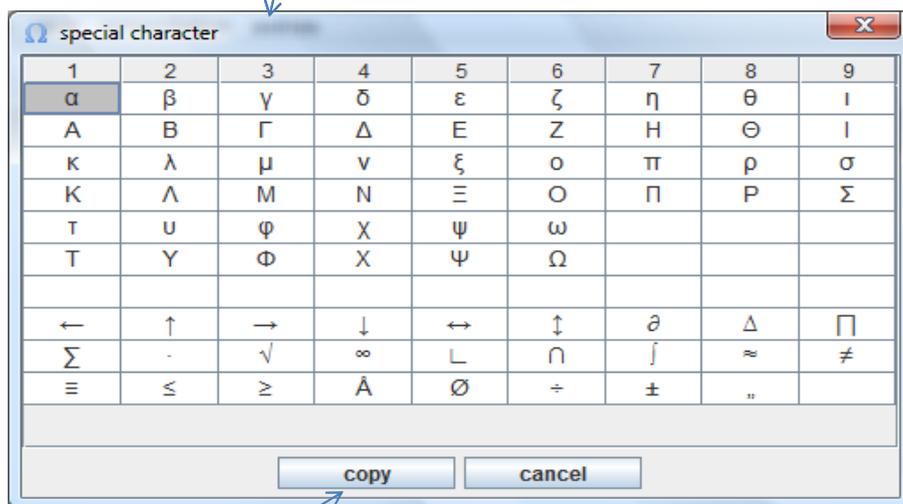
dimensions of the sketch area are adjusted to the dimensions of the image

pastes the image to the sketch area



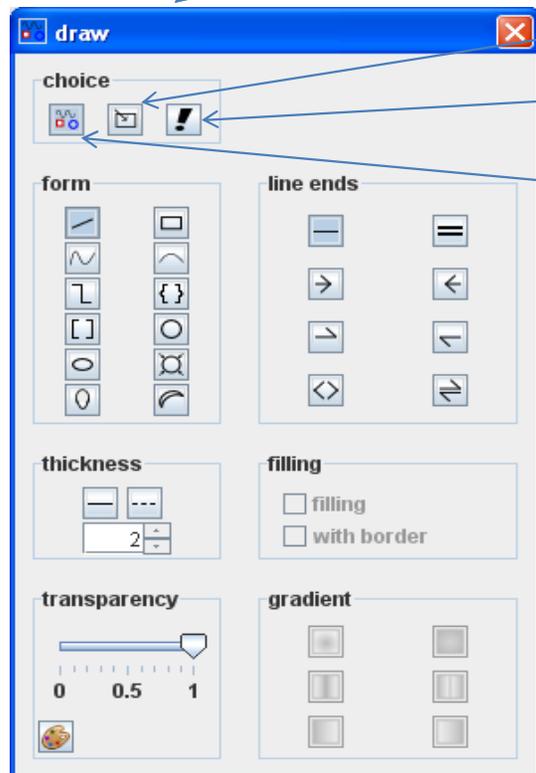
text colour  
transparent text background  
text background colour  
rotate text  
transfers the text to sketch area  
mark all





copy to the clipboard  
 (you can paste it into the editor or into the atom symbol input -->





select a form with a mouse click for changing the size, for moving etc.

repaint (sketch area will be refreshed)

you can draw by keeping the mouse button depressed while on the sketch area

## 1.4 The atom menu item



text box: you can e. g. place numbers close to atom symbols (you have to enter your input here and then you have to click the sketch-area)

atomic shells

text colour

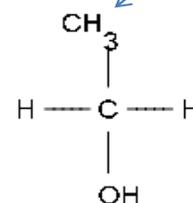
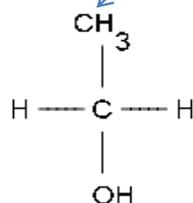
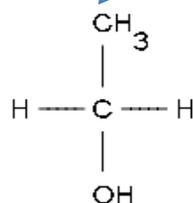
repaint (sketch area will be refreshed)

undo set atom

undo set bonds



input for atom symbols or short text  
 e.g.: (superscript with ^) O<sup>2+</sup>  
 (subscript with \_) O<sub>2</sub>  
 (write in left text direction with <) He<<sup>4</sup>  
 (marker sign for < set using #) ^4#He<<sub>2</sub>



Text alignment can only be adjusted before setting an atom.

Therefore, subsequent changes require that you first delete the atom, realign and then re-enter the text.



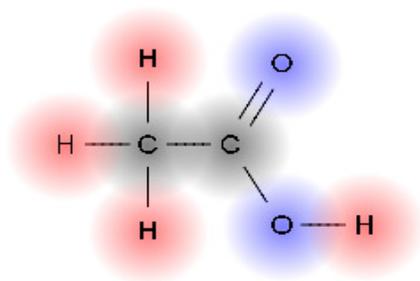
elements

1A	2A	3B	4B	5B	6B	7B	8B	8B	8B	1B	2B	3A	4A	5A	6A	7A	8A
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt									
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	

C   <sub>6</sub>C   <sup>12,011</sup>C   <sup>12,011</sup><sub>6</sub>C



bond bond cross view presentation extras



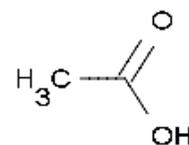
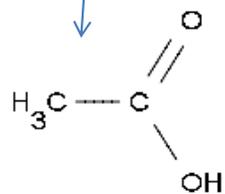
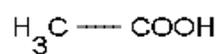
Property panel for a selected object, showing various settings:

- size**: A vertical slider ranging from 0 to 5.
- borderline thickness**: A horizontal slider ranging from 0 to 9.
- transp.**: A vertical slider ranging from 0 to 1.
- color**: A color selection palette with options for black, purple, blue, light blue, yellow, and green.
- gradient**: Three small icons representing different gradient styles.

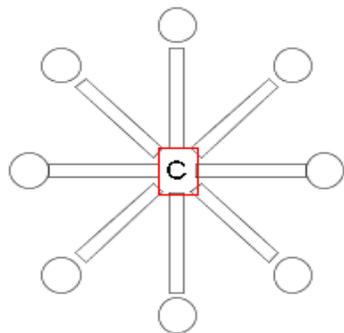
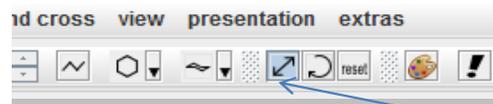


more functional groups

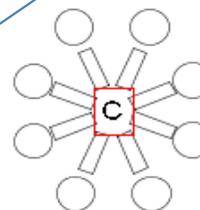
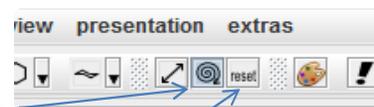
1	2	3	4	5	6	7	8	9	10	11
CH <sub>3</sub>	H <sub>3</sub> C	CH <sub>2</sub>	H <sub>2</sub> C	COOH	HOOC	OH	HO	NH <sub>2</sub>	H <sub>2</sub> N	C(2-bond)C
C <sub>2</sub> H <sub>5</sub>	H <sub>5</sub> C <sub>2</sub>	CH(CH <sub>3</sub> ) <sub>2</sub>	(H <sub>3</sub> C) <sub>2</sub> HC	CHO	OHC	SH	HS	SO <sub>2</sub> H	HO <sub>2</sub> S	C(3-bond)C
C <sub>3</sub> H <sub>7</sub>	H <sub>7</sub> C <sub>3</sub>	CH <sub>2</sub> CH(CH <sub>3</sub> ) <sub>2</sub>	(H <sub>3</sub> C) <sub>2</sub> HCH <sub>2</sub> C	CONH <sub>2</sub>	H <sub>2</sub> NOC	NCO	OCN	SO <sub>3</sub> H	HO <sub>3</sub> S	CN
C <sub>4</sub> H <sub>9</sub>	H <sub>9</sub> C <sub>4</sub>	C(CH <sub>3</sub> ) <sub>3</sub>	(H <sub>3</sub> C) <sub>3</sub> C	COO	OOC	SCN	NCS	NO <sub>2</sub>	O <sub>2</sub> N	NC
methyl	ethyl	propyl	i-propyl	n-butyl	i-butyl	tert-butyl	phenyl	benzyl	R(alkyl)	R(aryl)



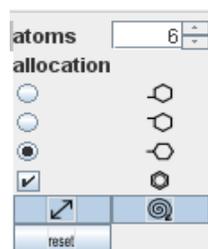




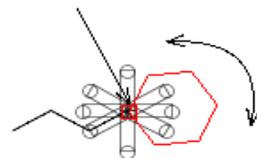
turns or drags the bond cross  
for changing the angle or  
bond length



resets the bond length to standard value (extras - options)  
and turns the bond cross to 0°



first press here then turn resp. drag

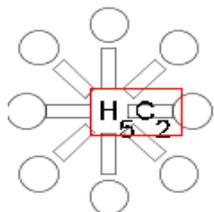


## 1.6 The bond-cross menu item

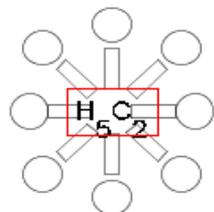


Setting the position of the bond cross:

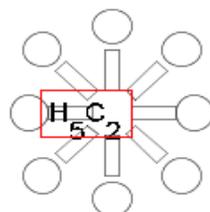
shifted to the right



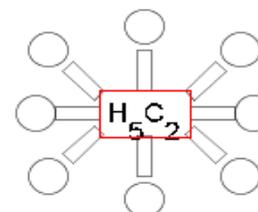
centralised



shifted to the left

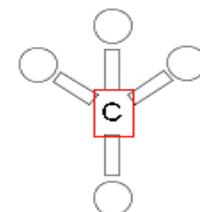
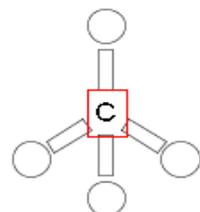
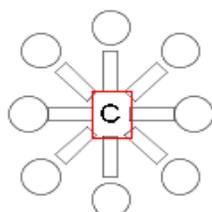
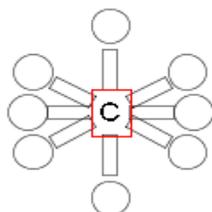
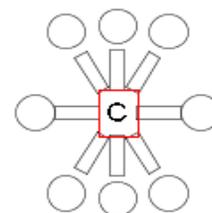
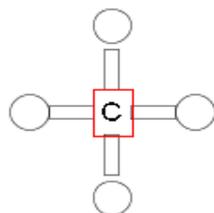
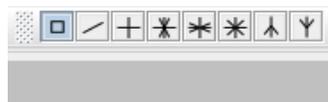


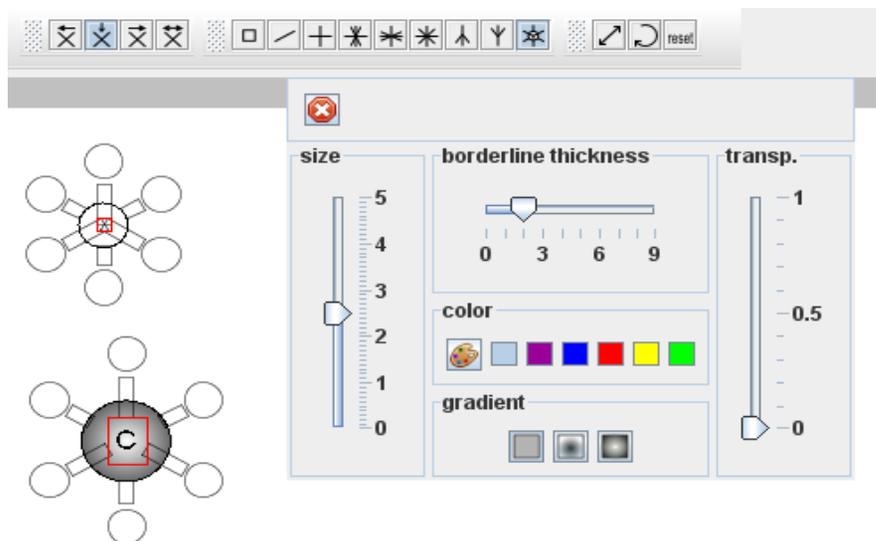
stretched



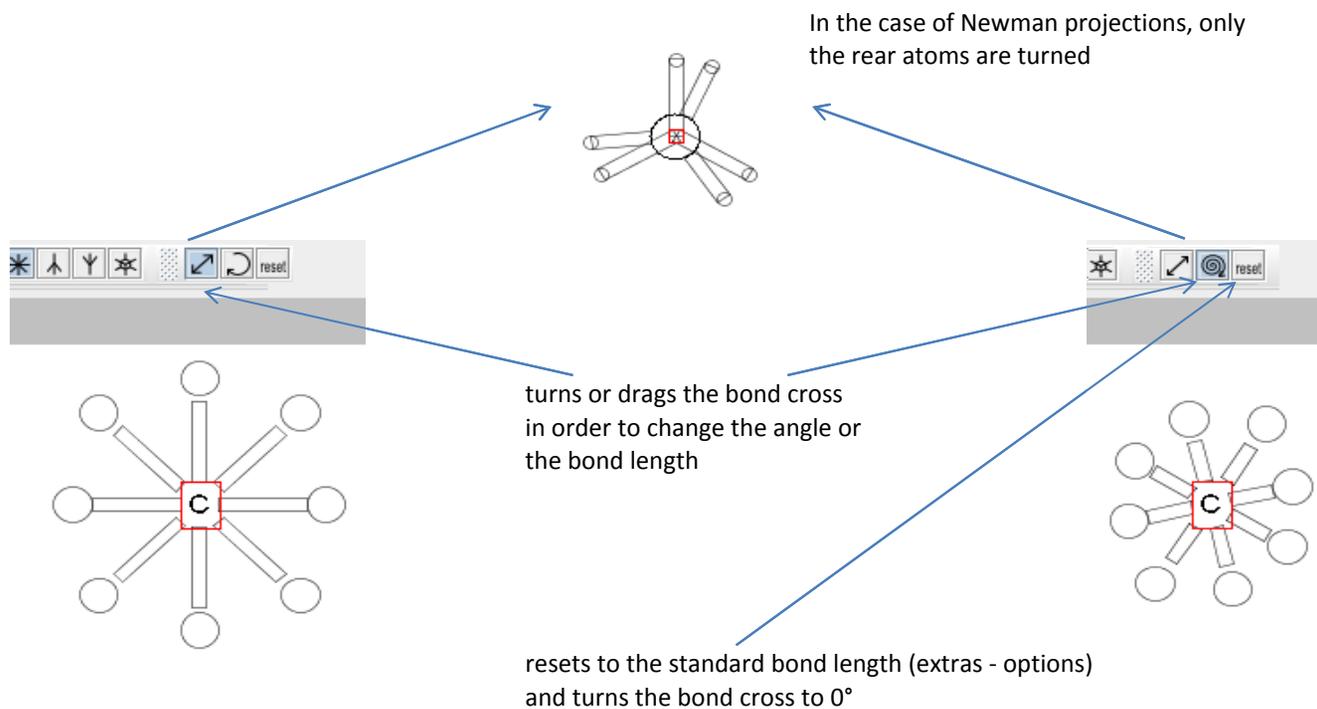


Selects type of bond cross:

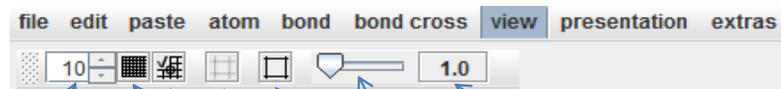




for Newman projections you can change the appearance of the circle using the atomic shell panel



## 1.7 The view menu item



- spacing of the grid
- show grid
- show margins
- show page breaks
- zoom
- adjust zoom factor 1
- show grid (new atoms which are not fixed by the bond cross)

## 1.8 The presentation menu item

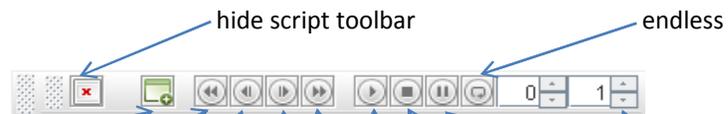


script dialog window

morphing window

animation dialog window

### 1.8.1 The scripting toolbar



hide script toolbar

endless

start script in new window (click left mouse to show next slide)

to the beginning

back

forward (next side)

to the end

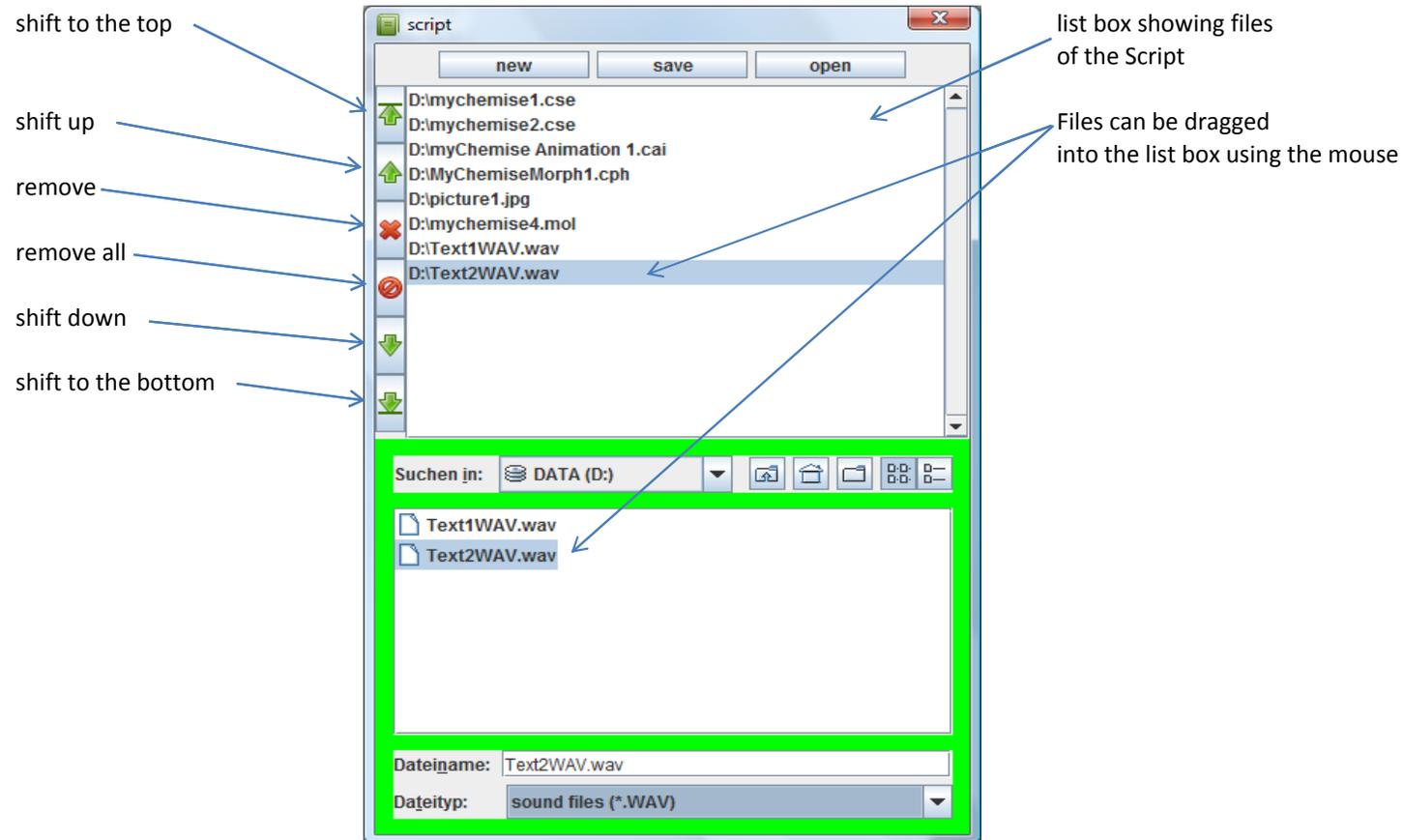
start script

stop

break

seconds } per side  
minutes }

### 1.8.2 The windows scripting dialog



### 1.8.3 The animation dialog window

Annotations for the animation dialog window:

- shift to the top
- shift up
- remove
- remove all
- shift down
- shift to the bottom
- Files can be dragged into the table using the mouse
- table showing the files that should contain the animation
- input for the (theoretical) time between image changes (the real duration depends on file size and hardware)
- opens the animation in a new window. The files are always reopened from new every time
- opens the files before the animation has started and stores them as jpg-files. Advantage: image changing is much quicker. The animation then opens in a new window
- shows all images side by side in a new window

no.	file	milli-sec.
1	D:\mychemise1.cse	100
2	D:\mychemise2.cse	300
3		50

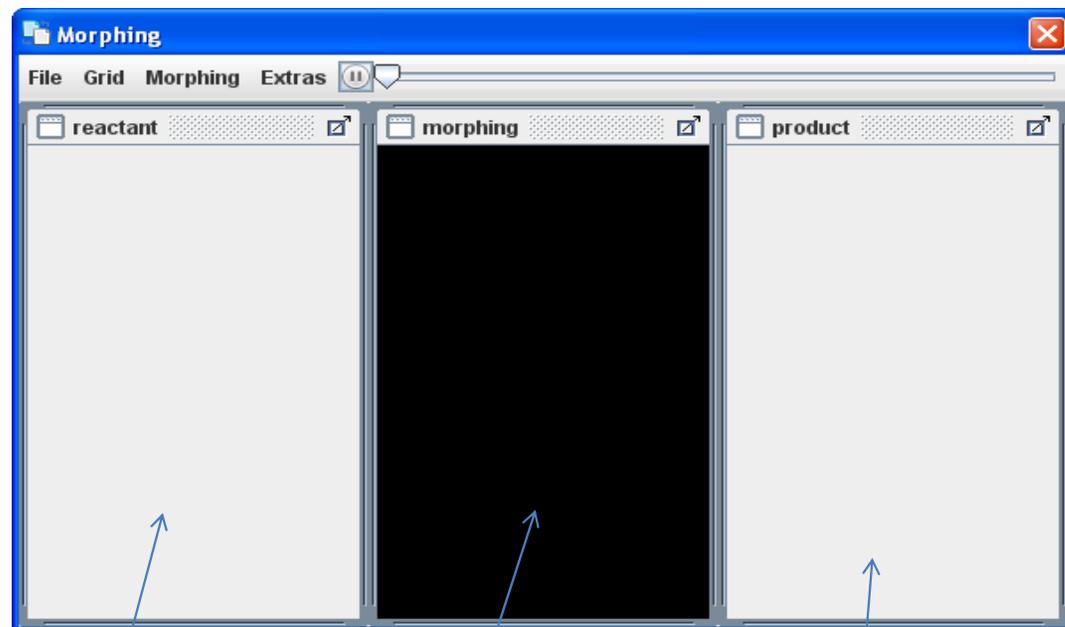
Look In: DATA (D:)

- mychemise1.cse
- mychemise2.cse
- mychemise3.cse

File Name: mychemise2.cse

Files of Type: mychemise (\*.cse)

#### 1.8.4 Morphing window



reactant window

morphing window

product window

### 1.8.4.1 Set-up (morphing) dialog window



choice of grids for defining the morphing areas

behaviour of the morphing areas

behaviour of the background (non-morphing areas)

process behaviour

set-up

progression

10 steps 300 delay(ms)

grid

3-point-affine transf. 2 rows

4-point-affine transf. 2 columns

from .cse/.mol-file

free rectangles 5 width

fixed size 5 length

morphingareas

reactant  single  morphing

background

reactant  single  morphing

white  colored  without react. m.areas

cycles

single  inv.  cycl.  acycl.

ok cancel

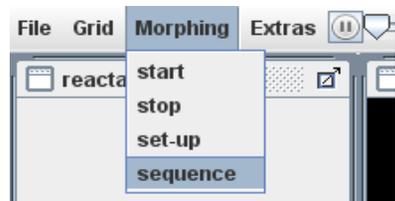
number of intermediate steps calculated

input for the (theoretical) time between image changes (the real duration depends on file size and hardware)

number of rows and columns for 3 and 4 point affine mappings

Set the size - this is for freely placeable rectangles

### 1.8.4.2 Sequence dialog window



shift to the top

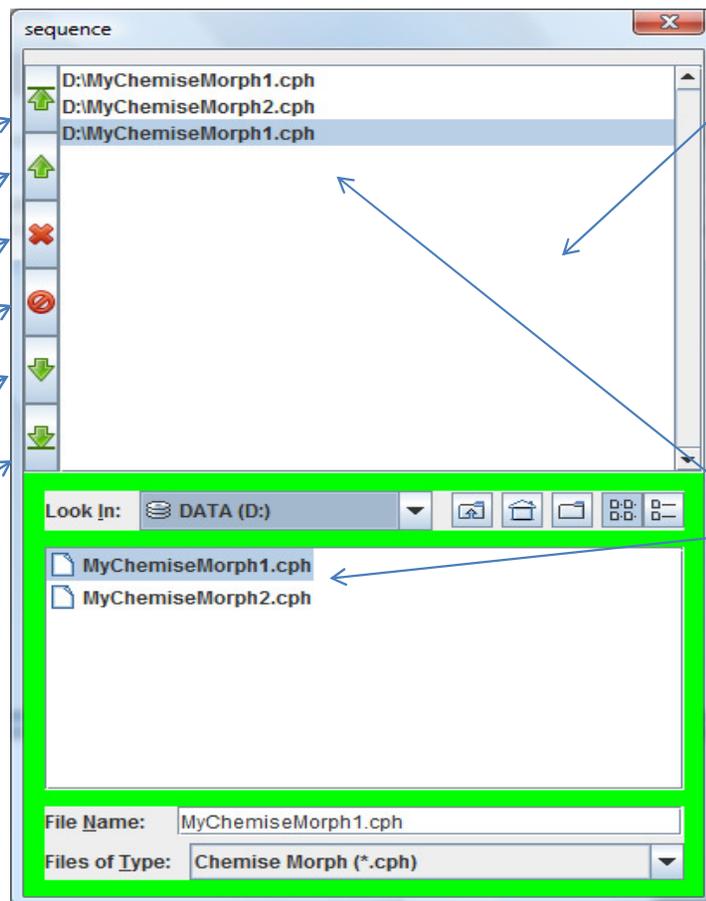
shift up

remove

remove all

shift down

shift to the bottom



list box showing those morphing files that are to be combined into a sequence

drag files into list box using mouse

### 1.8.4.3 Allocation dialog window

File Grid Morphing Extras

show grid  
new  
allocation

allocation

adapt positions

0 shift x 0 shift y

reactant area 0 >> productarea 0  
reactant area 1 >> productarea 1  
reactant area 2 >> productarea 2

sequence

Fries\_4.cse Fries\_5.cse

Annotations:

- shift to the top
- shift up
- corner points of areas:
  - move clockwise
  - for one position
  - permute upper/lower
  - permute left/right
- add new area
- copy area
- delete area
- shift down
- shift to the bottom
- open previous file of the sequence
- file which is visible in the reactant window
- file which is visible in the product window
- open next file of the sequence
- if .cse-/.cph-files are opened which were made using a different operating system the positions of the areas can show an offset. With shift x and shift y it is possible to resize all areas in one step.
- if the morphing settings are set to "grid from .cse-/.mol-file" then the list box shows morphing areas from the reactant window and product window

Diagram illustrating area mapping:

1 2  
4 3

1 2  
4 3

1 2  
4 3

4 1  
3 2

2 1  
3 4

4 3  
1 2

### 1.8.4.4 The Export dialog window

select the file to be exported

input field for the filename of the new imagefile(s)

animations (e.g. animated.gif) can run faster than morphing does. So it's possible to set more steps if desired. (e.g.: .cph-file with 5 steps, step-coefficient: 2 --> 10 images)

number of repeats of the gif-animation

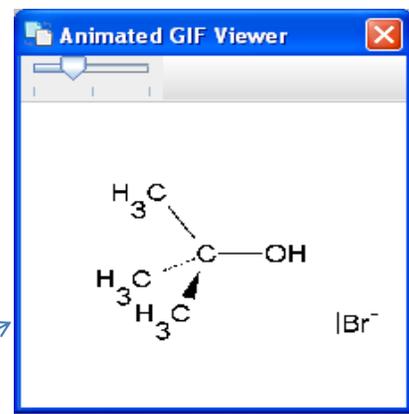
with a trial run it's possible to find out how many images are created during export

manually adjustable delay for gif-animation

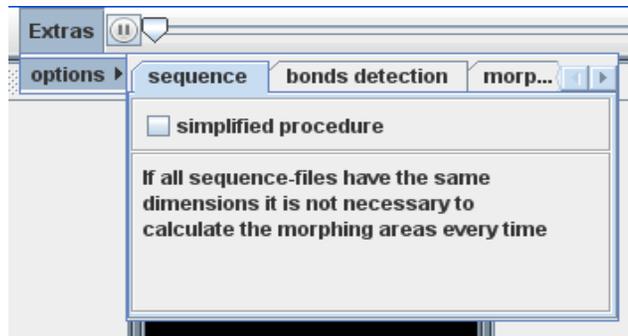
endless gif-animation

the delay is adopted from the .cph-files

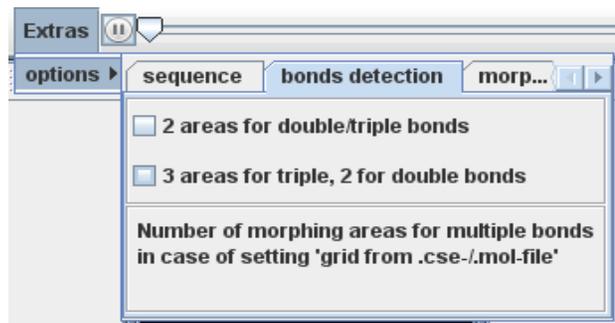
the animated.gif creates only one file at the end. So it's not necessary to save the intermediate steps.



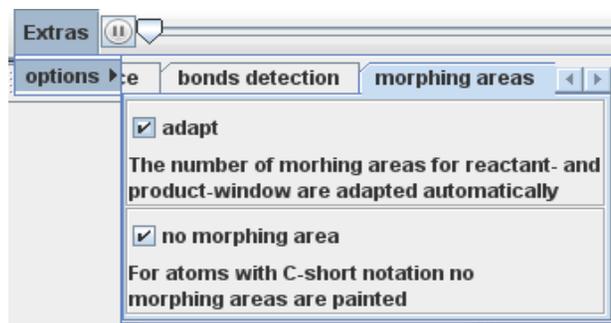
#### 1.8.4.5 The Extras menu item



Makes morphing sometimes more quickly.



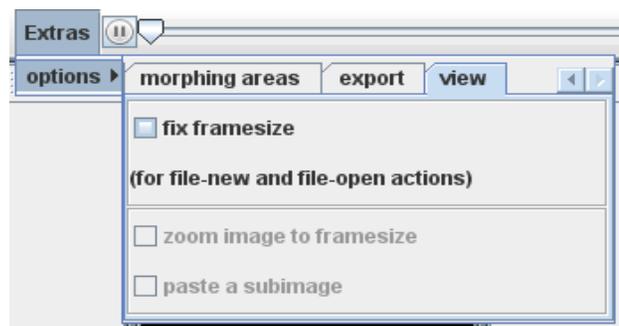
It's possible to preselect the number of areas for double and triple bonds.



This default-settings simplify the beginning of the procedure to make a morphing file.



For export it's necessary that all images have the same size. This is essential to avoid flickering.



If chemical structures are painted on a great sketch area it is better to minimize the size before it is applied for morphing if only parts of the images are used for it. In this case activate 'fix framesize' and 'paste a subimage' boxes.

## 2 Procedure for writing a script

1. Open the script dialog window 
2. Drag files into the list box using the mouse
3. Arrange the files in the correct sequence (     )
4. Save as a MyChemise script (.csp)
5. Close the script dialog window; the script toolbar appears
6. Move using buttons     of the script-toolbar in the script

The next page is always opened using 

The contents of the files are shown on the drawing area or in a new window (  ).

In the new window, you can open the next page by clicking with the mouse.

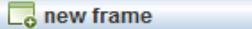
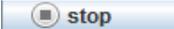
MyChemise files (.cse), MyChemise animations (.cai), image files (.jpg, .jpeg, .gif, .png, .bmp) and mol files (.mol) are shown directly in MyChemise.

Other files (e.g. .xls) are opened using other programs that are registered in the operating system software (e.g. Excel).

8. The script can be run as a slideshow (  )

The time until the next image is displayed is set using 

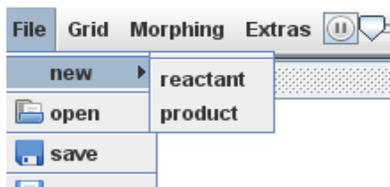
### 3 Making an animation

1. Open the animation dialog window 
2. Drag files into the list box using the mouse
3. Arrange the files into the correct sequence (     )
4. Enter the time delay between image changes
5. Save as a MyChemise animation (.cai)
6. Start the animation using  (in most cases it's better to activate  )  
If it is necessary to show the animation in a new window, try it out using  or  
using  to see which option gives the best results
5. Close the animation dialog window
6. To end the animation close the window in which it is running or  
open the animation dialog window and use stop 

## 4 Morphing

You can use morphing to transfer areas of the reactant window stepwise into areas of the product window

1. Open the morphing window 
2. Create a new morphing file.



MyChemise files (.cse), image-files (.jpg, .jpeg, .gif, .png, .bmp) and .mol-files. can be used in both the reactant window and product window,

If necessary files can also be opened in their original sizes.

For good morphing effects files of the same size should have already been created (for .cse-files use drawing areas with the same (small!) size).

During morphing every pixel is recalculated. Therefore, the processing speed is dependant on the image size. Therefore set the image size (sketch area) to be as small as possible and not bigger than necessary.

3. Open the set-up (morphing) dialog window.  
Set the numbers of steps (always start with 3 to 5 steps) and the (theoretical) delay time .

progression	
<input type="text" value="5"/> steps	<input type="text" value="100"/> delay(ms)

Choose the grid type (for image files - above all 3-point and 4-point mappings and free rectangles are used). Cse and .mol files are directly morphed from 'from cse-file' created grids or 'from free' rectangles.

Also the following applies:

The calculation time needed increases according to the number of areas.

grid		
<input type="radio"/> 3-point-affine transf.	<input type="text" value="2"/>	rows
<input type="radio"/> 4-point-affine transf.	<input type="text" value="2"/>	columns
<input checked="" type="radio"/> from .cse/.mol-file		
<input type="radio"/> free rectangles	<input type="text" value="5"/>	width
<input type="checkbox"/> fixed size	<input type="text" value="5"/>	length

Set-up the behaviour of the areas and that of the background (areas which are not to be morphed):

- reactant: only what is visible in the reactant window is moved.
- single: as for reactant but in the last step that what is visible is shown in the product window.
- morphing: shape and colour are been morphed
- white: white background
- colored: coloured background
- without react. m.areas: make sense if only a few bonds and atoms of the structural formula have to be morphed. Atoms and bonds which are not moved can be treated as background (without frame). In this way morphing is faster.



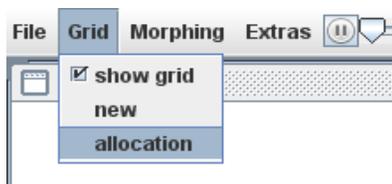
Set-up the time progression:

- single: one pass
- inverse: morphing from product to reactant
- cyclic: pass changes direction at the end, endless
- acyclic: restarts at the beginning again, endless



Close set-up (morphing) dialog window using OK

4. For .cse-/.mol-files allocate the areas (for image files carry on from point 5)



Arrange the files in the right sequence

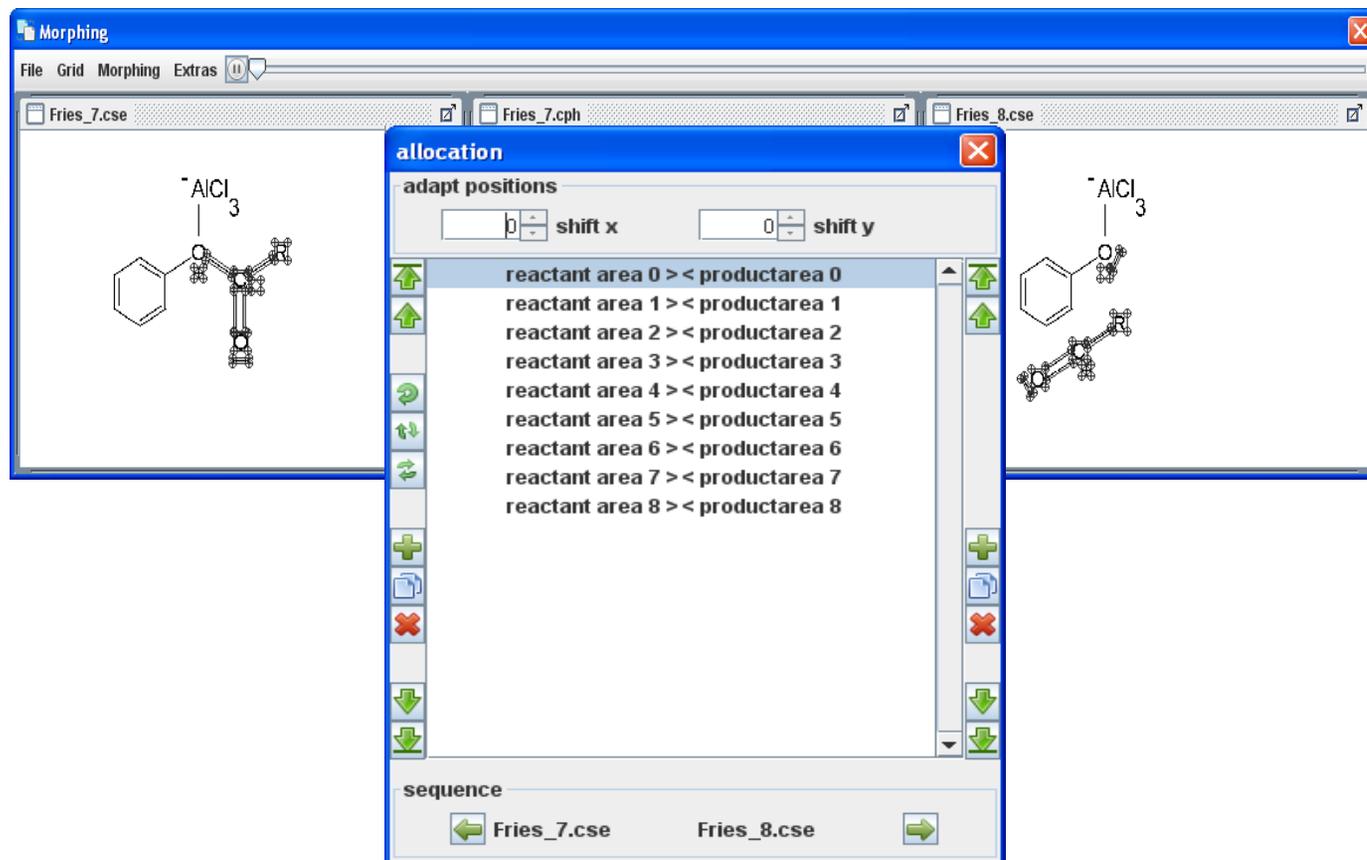
Open allocation dialog window:

Arrange the reactant and product areas using the arrow buttons  in such a way, that the areas to be brought together face each other.

Tip: when creating the cse file (sketching the product) by adding and deleting, it is helpful to change the .cse file of the reactant so that the product or an intermediate step is achieved. This prevents those atoms and bonds from being morphed (change of their positions on the screen) that should not really be moved.

Areas can be added or deleted. 

There must be the same number of areas in both the reactant and product windows.



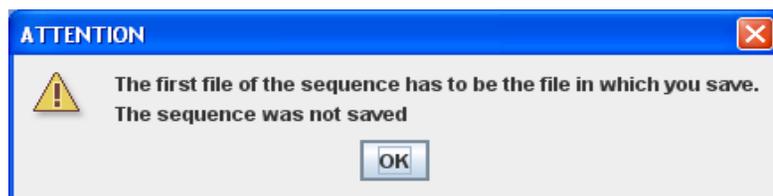
Sometimes an unwanted turning of single areas is visible later during morphing.  
 These areas then have to be turned. 

All areas can be resized in one step using  shift x  shift y

This can be helpful if .cse-and .cph-files from different operating systems are used.

If a morph sequence (-> 4.1) has been created then the names of the predecessor and the follow-up files in the sequence are visible in the lower part of the allocation dialog window. You can open them using the arrow buttons (if .cse files).  

If you make changes (e.g. shifts the morphing areas with the mouse) you have to save the file. If the file you are working in is not the first file of the sequence you will get an error message:



You can ignore it because the sequence is already saved in the first file of the sequence.

Close the allocation dialog window.

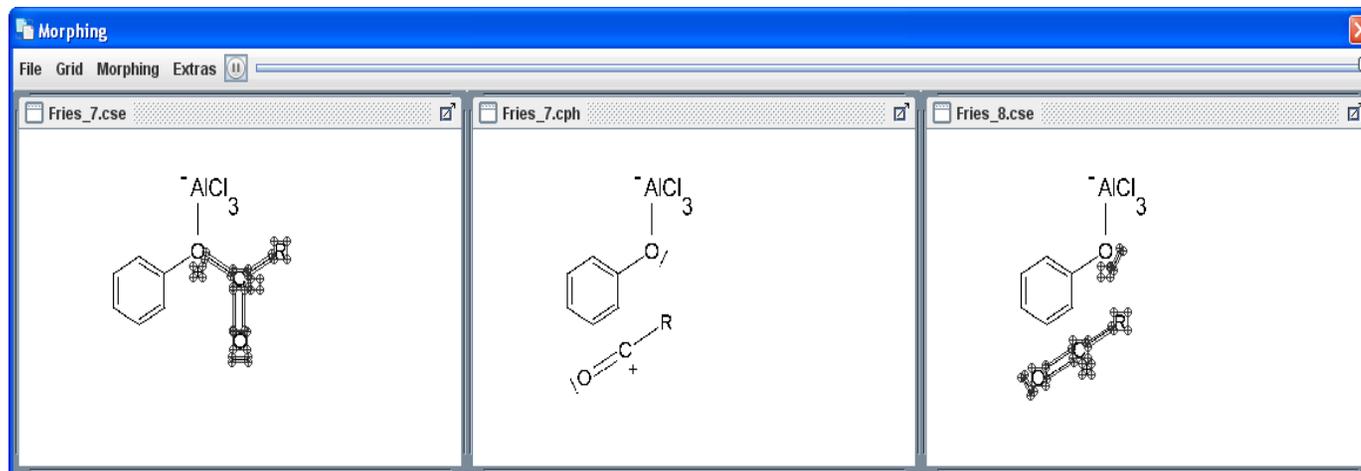
Tip: you can preset the number of morphing areas for multiple bonds (1 or 2 for double bonds, 2 or 3 for triple bonds) in the extras-options menu.

In some cases it is necessary to set 2 areas for double bonds if you want to show the differently movements of the electrons.

In the extras-options menu it is also possible to set an automatic adaption of the number of morphing areas for the reactant and the product window created with a new grid.

5. Change areas if necessary:

Clicking in the areas enables you to mark allocated areas in both windows.



Areas can be moved using a depressed mouse button. If the shift key is also simultaneously held down then the areas in both windows are moved to the same place at same time.

If the alt key is used instead of the shift key the movement is relative to the start position.

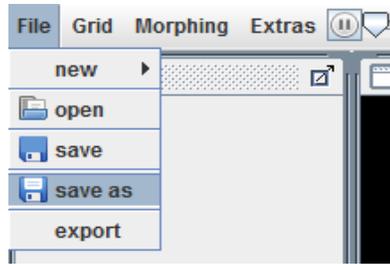
Areas can be moved with the arrow-keys (left, right, up, down), too and can be rotated with the page-up- and page-down-keys.

The same is valid for single points. Using the ctrl-button it's possible to mark several points at the same time.

In the same manner it is also possible to edit the grids of 3 and 4 point mappings.

For the grid choice 'free rectangles' it is possible to set areas as pairs, in both the reactant and product windows. Marked areas can be deleted using the Delete key.

6. Save the file



7. Start morphing



#### 4.1 Making a morphing sequence

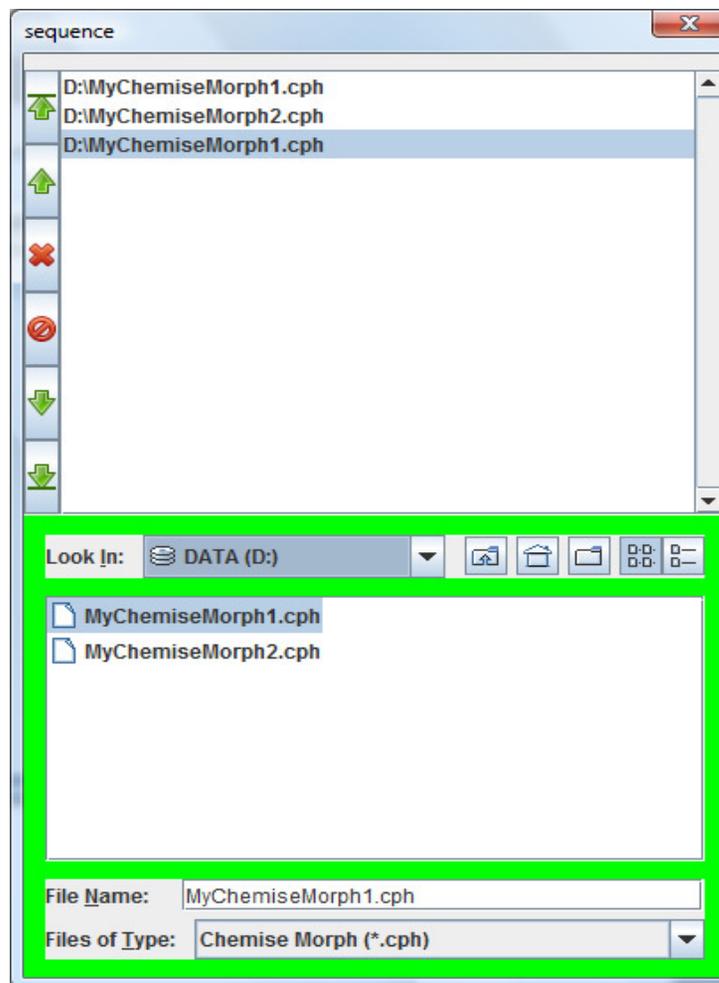
Using the mouse, drag the morphing files (.cph), which are to be made into a sequence, into the window.

Top priority is to name the file in which the sequence will be saved (the just opened file; in the example shown on the right MyChemiseMorph1.cph)

If this file is entered at the end again this produces an endless sequence and morphing starts from the beginning again.

Using the arrow buttons,  files can be moved to the correct position.

Don't forget to save the file at the end (as a morphing file (.cph)).



## 5 **Note for Linux users**

Linux users experience a problem when copying using the system clipboard. This problem is well-known for java-programs and is discussed in web forums. If you want to export a structure as an image into other (text processing) programs, first save your MyChemise file as an image file and then paste the structure directly or with a graphic program into your (text processing) program.