ScienceWord and Class

Chemical formulae and structures

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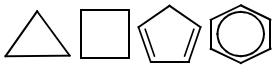
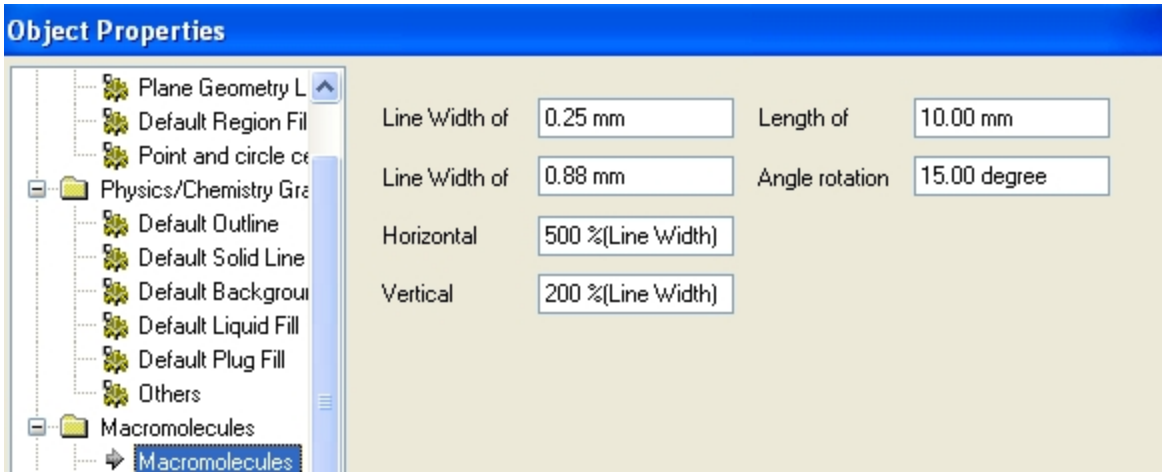
Chemical formulae

I) General view

Chemical formulae consist of chemical symbols (C, O, CH_2 , OH, Br etc.) and simple chemical bonds in the form of lines ( etc.) , and other chemical groups in the form of polygons ( , etc.) which we name polygonal chemical group

Writing of chemical formulae is simplified thanks to insertion techniques of symbols and chemical bonds developed in ScienceWord. For example, simple chemical bonds are carried out in the same way we do when we are drawing them with a pen! Hence, the characteristics linked with carrying out a simple chemical bond are pre-defined in the dialogue box below



To go to this dialogue box, click on **"Default Drawing Settings"** within the **"Format"** menu**.**

Line : 0.25 mm is related to the thickness of the simple chemical bond.

Wide : 0.88 mm is related to the size of the vertical lines in a bond of the type ( ) .

Horizontal :500 % is related to the space between the vertical lines in a bond of the type ( ) .

Vertical : 200 % is related to the space between the horizontal lines in a bond of the type ( ) .

Length: 10. 00 mm is related to the length of the simple chemical bond.

Unit : 15^0 is related to the angle of rotation of a rotating thrust of a simple chemical

bond .

Note: The colour of the simple chemical bonds can also be predefined by means of the ***"Default Color"*** *sub-menu of the "Macromolecule" menu.*

II) Inserting chemical bonds and chemical symbols

1) Inserting chemical bonds in a regular direction

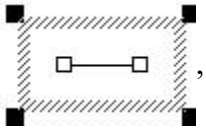
Click for example on "***Single Line Chemical Bond***" ( ) in the Macromolecules toolbar. The pointer would take the shape ( ) on the workspace. Click on the workspace without releasing the left button of the mouse. Move the mouse gently in a rotating movement whilst holding the left button down, then you would see a line appear whose direction changes according to the movement of the mouse. The figure below is an illustration of this.

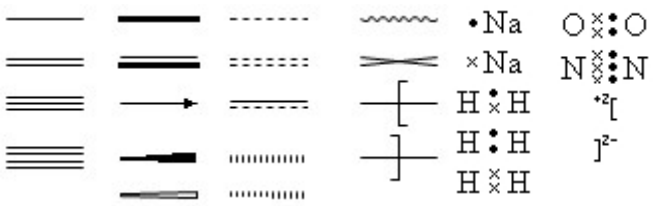
This illustration shows in fact the sequences of rotating thrusts in the positive direction.

2) Inserting chemical bonds in a controlled direction

You may vary the length of the bond and the angle of rotation by pressing the **"Alt"** key during the rotating thrusts:  .

Note

The macromolecules toolbar shows some of simple chemical bounds available in ScienceWord. To accede to the other simple bounds, first insert from this macromolecules toolbar any simple chemical bound., for example the bound ——— , then whilst this chemical bound appears as follow selected  , , bump into "Object Properties" dialog box through contextual menu, where it is possible to make a choice of one of the following eighteen simple chemical bounds



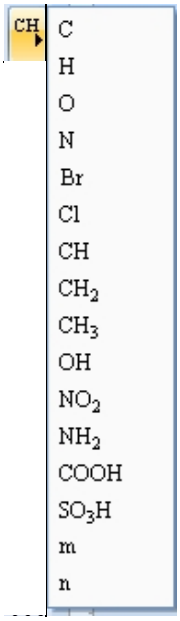
- A simple bond links up with another bond through one of its ends (such a combination is obtained by clicking with the mouse when a red cross appears) .

- A polygonal group links up with another group either through a vertex (a red cross appears during the linking up) or through one side (a yellow line appears during the linking up) .

3) Inserting a chemical symbols

Draw a chemical bond as follows ——

Click on the chemistry label button  in the toolbar of macromolecules located beside the vertical ruler. The menu of chemical symbols shown below opens up.



Click on " CH_3" and then move the pointer to the end of the chemical bond:

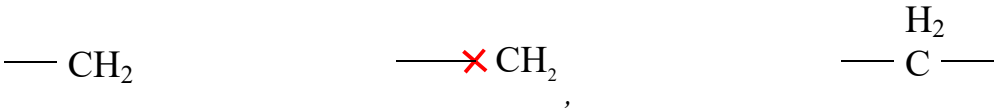
Click when a red cross appears (see the illustration below) .

Whilst "CH_3" symbol appears in a rectangular grid, you can shift it using the directional keys (→, ←, ↑, ↓) or the mouse. This method also helps to modify the length or the direction of the chemical bond.

Notes :

A chemical symbol can be inserted at a point of linkage of two chemical bonds

A chemical bond can link up with another chemical bond at a point having a chemical symbol .



It is possible to arrange the chemical symbol " $\overset{H_2}{C}$ *" via object properties dialog box .*

For example, it is possible to obtain the arrangement CH_2 *by applying the "Right Arrange" option of "Label property" text orientation option*

4) Examples

Example1:

Let's write the chemical formula $CH_3-\underset{\displaystyle CH_2-CH_2-CH_2OH}{\overset{\displaystyle |}{CH}}-CH_3$.

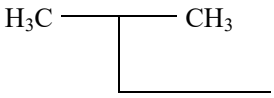
To do so, follow the steps below:

i) Enter the Continuous Mode (Click on  button in the "Geometry Toolbar") and then click on "  Single Line Chemical Bond" button in the "Macromolecules Toolbar".

ii) Use the procedure of linking bonds to draw the five bonds of the chemical formulae as shown below (make sure that the red cross appears during the linkage of two bonds)

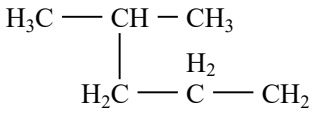
iii) Thereafter, without leaving the "Continuous Mode", click on  button in the Macromolecules Toolbar and then click on "CH_3" in the labels list that opens up. On the

workspace, whilst the cursor changes into "" shape, insert continuously the "CH_3" label at the suitable places (remember that a red cross appears to show that the linking could happen) . Then you get the result below :

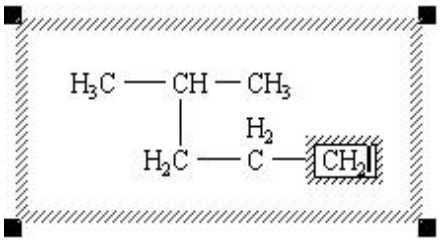


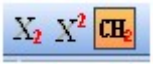
iv) Follow the same method of insertion to insert the "CH_2" and "CH" labels.

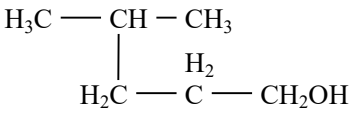
You therefore obtain the following result:



v) In order to write "CH_2OH", double click on "CH_2". Then you obtain the following result:



vi) Notice that the cursor blinks in the " CH_2" box and that the useful tools  are available in the chemical toolbar. Make sure that the tool that helps Normal writing is active, then write OH.

You obtain this result  .

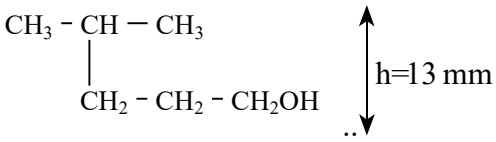
vii) Now, in order to arrange the labels, double-click on any bond to select the molecule, then right-click and in the contextual menu that opens up click on Properties to access the Object properties dialog box. Then click on "Label Properties " and tick off the option

"Right Arrange" and click "OK" to get tha appropriate arrangement.

viii) Insertion into text only when working in ScienceWord

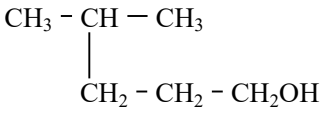
- Click on any label or any bond and right-click ; then in the contextuel menu that opens up click on "insert into text"

The following is obtained

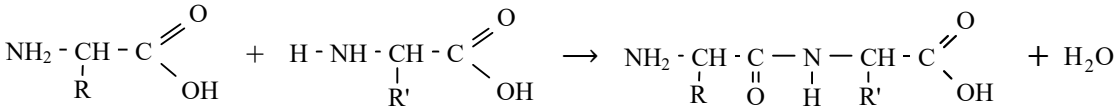


The right insertion into text should be done at the level of CH_3 presently located at 13mm to the text level as illustrated. (In practical way to get this measure, click on line icon in the Geometry toolbar, draw a vertical segment as shown and check its size through object properties dialog box) .

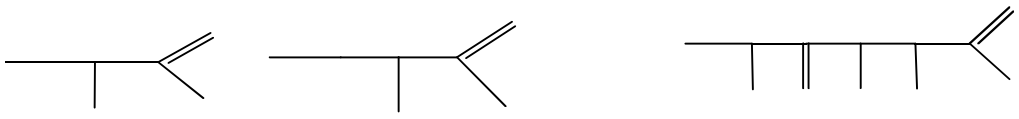
- Again Click on any label or any bond and right-click. In the contextual menu that opens up, click on "Set object layout style". Then in the dialog box tha opens up, enter the figure 13 in the "Down Margin" box and click on "OK". Then the expected result is obtained as follow .



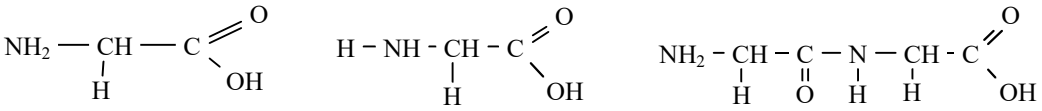
Example 2 : Let's write the chemical equation below



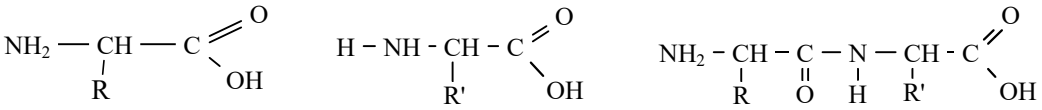
i) First activate the "Continuous Mode" and then draw continuously the bonds of the three molecules as shown below:



ii) Without leaving the "Continuous Mode", proceed to insert the labels. Notice that you can not insert directly labels such as R or R' . For the purpose, you just need to fill their corresponding locations with any label, H for example; You would get the following.

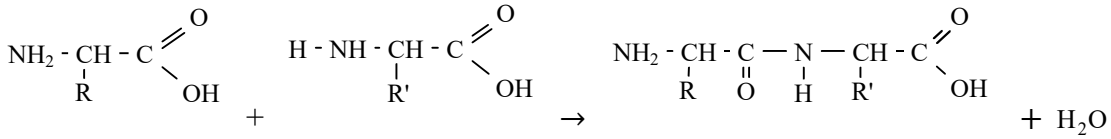


Then double-click on the H that should be replaced by R or R' to enable the replacement. The new result is shown as below.



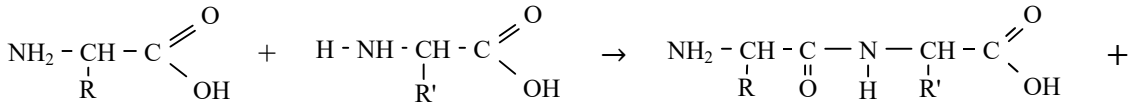
iii) When working with ScienceWord, the reaction can be inserted into text. To get this insertion done on one ligne we can reduce the labels font size.

iii) Insert the first molecule into text and type the sign "+"; then insert the second molecule and insert the symbol "⟶"; then insert the third molecule and type the expression "+ H_2O". Then you would get the following result.



iv) Note that the right insertion into text of the first and the third molecules should be done at the level of the label NH_2 and that of the second molecule at the level of the label H and all these labels are located at the distance 8mm to the level of the text.

Then select each molecule and through "Set object layout style" dialog box, set 8mm for the Down margin option. The result is as follow



H_2O

Note1:

- *In order to keep the equation written on one line you may need to reduce the labels font size of each molecule. To do so,* double-click on any bond to select the molecule, then right-click and in the contextual menu that opens up click on Properties to access the

Object properties dialog box. *Then select Label font and set the new font size and font color and click OK. In this example the chemical label font size is 10.*

- *Instead of inserting one by one molecules into text, you could use the grouping option. But first make sure that the sign "+", the symbol "⟶" and the expression "+H_2O" are written in text box (with invisible ligne). Then select these text boxes and macromolecules, get the appropriate alignment and click on Group tool "" from format menu to group them. Then the insertion could be done at once.*

Note2:

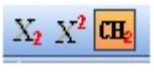
You can just use ordinary text and mathematical formulae templates to write simple chemical equation such as:

$$NaOH + HCl \longrightarrow NaCl + H_2O \; ; \quad 2H_2O_2 \xrightarrow[\text{☆}]{FeCl_3} 2H_2O + O_2\uparrow$$

5) Modifying chemical formulae

- You could also, as in the case of drawings, hold any one of the four black big squares that surround a macromolecule and stretch its selection region in order to reduce or increase its size. If the "Ctrl" key is depressed during this stretching, then the chemical bonds would maintain the same proportion of shrinkage or enlargement.

- When a part of a macromolecule or the whole macromolecule is selected, you can hold on a blank square in order to strech, enlarge in one direction or flip that part or the whole macromolecule. When the flipping is happening from the left to the right or from the bottom to the top, you can hold down Ctrl button to flip towards both horizontal and vertical directions.

- If you rather want to modify the chemical symbol, for example instead of OH you would like to write OH^-, then, just double-click on OH. Three tools would appear within the macromolecules toolbar as the following illustration shows  *(up to down, the first one is activated for the subscript, the second one is activated for the superscript and the third for the normal writing). Just click once on the suitable button (in this case the second button for the superscript) in order to enable it. Note that you can apply Lucida Console font to the chemical label OH^- to get a good appearence in superscript*

of the minus sign "−" .

6- Two major kinds of selection of objects in a drawing zone

Note that in any case, after the needed selection is done, you have right-click. Then contextuel menu that opens up click on properties to access object properties dialog box where modifications be done on the items selected. In the particular case where a drawing zone is selected, modifications can be done in all items of that drawing zone!

Note:

When two or more objects belong to the same drawing zone, the selection of any one produces a grid surrondings all the objects.

To merge two or more drawing zones, just hold down Shift key and click on a single of each, then click on the Combine " tool that appears automatically in drawing toolbar.

a) Selecting macromolocelues within the drawing zone

- You can just double-click on any bond of a group of linked bonds to select these bonds and their associate chemical elements. If you are selecting different groups, then just hold down the Shift key when double clicking on one bond of each group.

- To select any single empty bond end or any single empty vertex (ie non linked to any chemical element) just click on that end or that vertex. But for a series of selections, hold down Shift key when clicking on each of these ends or vertice.

- To select any single charged bond end or any single charged vertex (ie linked to a chemical element) hold down Ctrl key and click on that end or that vertex. But for a series of selections, hold down both Ctrl and Shift keys when clicking on each of these ends or vertice. This technique of selection can also be applied to the previous case of selection of empty bond ends or vertice.

b) Selecting of the whole drawing zone

There are three methods

Method 1: Click on any single element (simple chemical bond or chemical symbol) . The grid of the common selection region appears. Hold down "Ctrl" key and click on this grid to select it.

Method 2: Click on any single element (simple chemical bond or chemical symbol) . The grid of the common selection region appears. Then to select the drawing zone, just hold down "Shift" key and click again on the same element to unselect it.

Method 3: Click on the button within the geometry toolbar to activate the drawing mode. The pointer changes to the shape on the workspace. Then, hold down the left button of the mouse and slide the mouse in such a way to draw a rectangle encompassing the set of items in the drawing zone.

III) The general process of linking two chemical objects

Let's call chemical objects the set of chemical symbols, chemical bonds, chemical group, macromolecules.

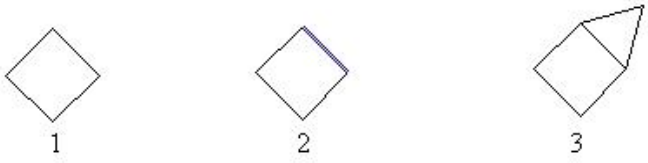
1) Through a direct linkage:

The same technique is used as in linking two chemical bonds. The linkage has thus taken place at one end, at the side or at a vertex of a chemical object. An automatic arrangement of these chemical objects is the result from such a linkage.

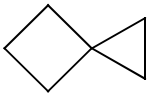
a) The process of linking two polygonal groups

This process of linkage is explained as follows:

- Click on the cyclobutane " " button, then click on the workspace to get (1) .
- Click on the cyclopropane " " button then move the pointer to one of the sides of cyclobutane. A yellow line as shown in (2) appears to indicate that a linkage can be done.
- Click when the yellow line appears to get (3) .



Attention: *You could change the direction of insertion of cyclopropane (triangular) to (3) by keeping the key "Ctrl" depressed whilst clicking with the mouse on the side of cyclobutane (square) . You would get the following result:*  .

The linkage has taken place on one side of cyclobutane. It could also take place at a vertex as shown in the following illustration:  . *In this case it is a red cross, which indicates that a linkage can take place.*

b) Linkage of macromolecules

All the objects of chemistry templates library also use the same techniques of linkage as described in a } !

2) Through the use of the combine tool

a) General concept

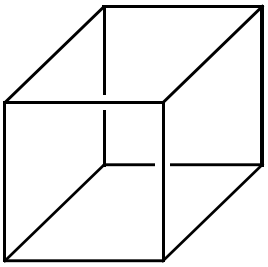
Let's call chemical objects the set of chemical symbols, chemical bonds, chemical groups, or macromolecules.

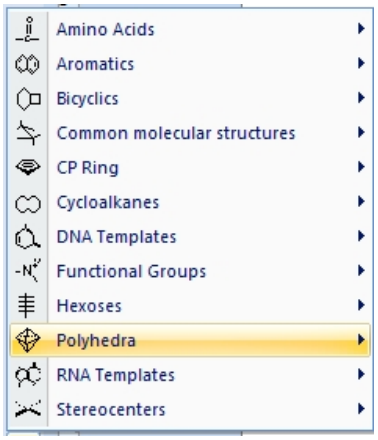
- Apply the "Combine " tool to these two chemical objects.

- Use the arrow keys (or the mouse) to relocate and move these objects in order to join them. A red cross or a yellow line will appear when the joining occurs.

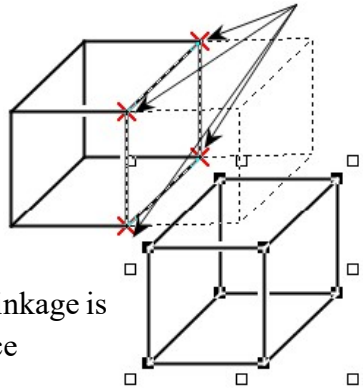
b) The crystalline example

Click on to acces macromolecules templates, then draw from polyedra templates the following element .





Press Ctrl key and drag this polyhedral to get a copy of it. Use "Combine " to group the two identical polyhedral and link them by their lateral face (04 red crosses appear at each vertex of theses faces when the linkage is taken place see fig1) .



Figl : The linkage is taking place

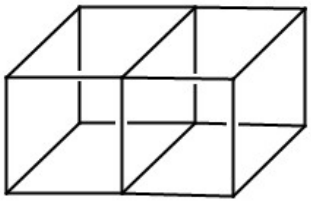
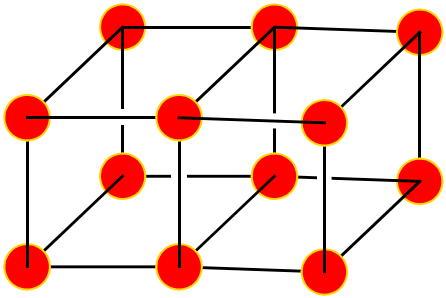


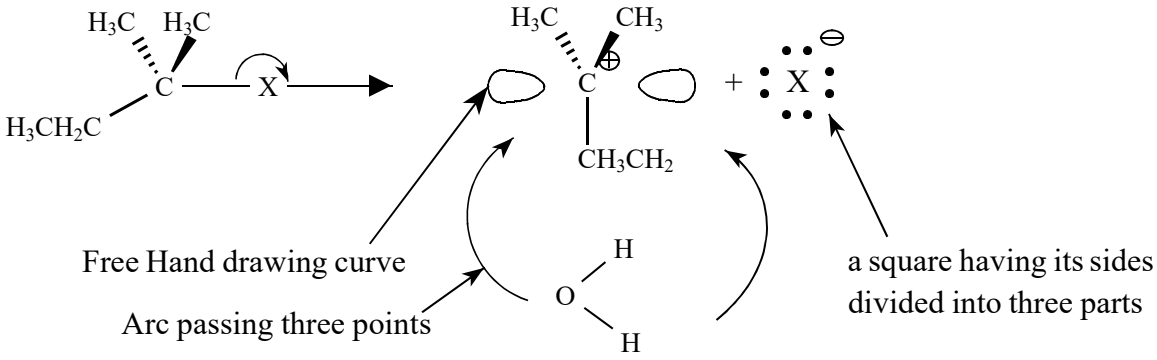
Fig2: The final result

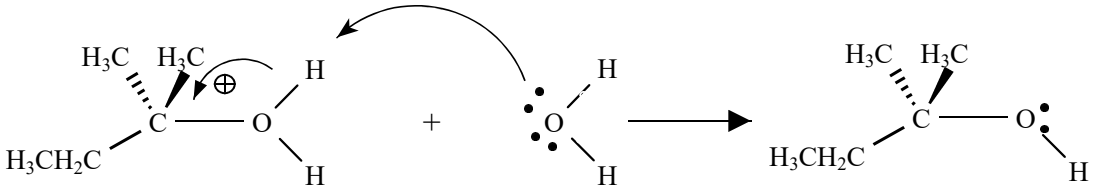
Now select the grid surrounding the final result, right-click and from contextual menu go to properties. From point properties, set 3mm for the radius, yellow line and Point inside fill red color. Then you get the following result.



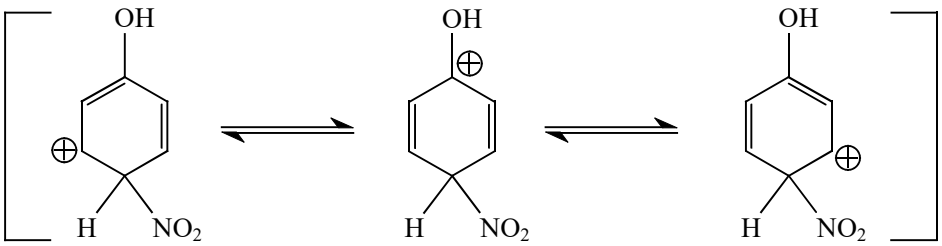
IV) Mixing chemical objects with other graphics

The need of aditional geometry tools or text boxes is real to complete some chemical objects. For example, the following chemical objects are a combination of chemical structures and geometrical objects such as two symmetrical block free hand drawing curves, square, arc passing three points, text boxes. They have been selected and grouped with the Group of objects tool that can be found in format toolbar.

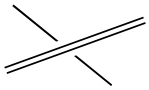




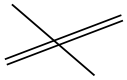
Para attack



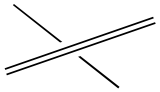
V) 3D effect

The "3D" effect of the property of chemical bonds is noticeable in the case of two combined chemical bonds crossing each other. That particular kind of effect helps hiding part or several chemical bonds laying in background. 

Example 1:

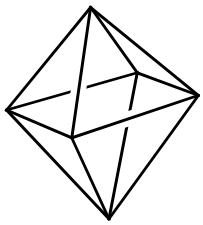
Draw two chemical bonds as follow  and group them with the tool "

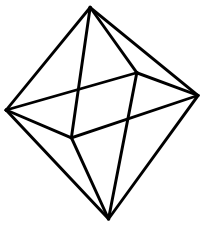
Combine"

Select any of the bonds, then access to "Object Properties". Click on "Optional Future" and tick off "3D Effect". You will obtain the following result  (The order in the drawing of the bonds is very important. Here, the second drawn bond is the double chemical bond) .

Example 2

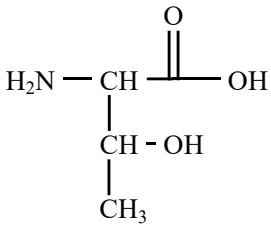
Draw from chemistry polyedra template the following two polyedrons, where the 3D effect is applied. to the first one and not to the second one

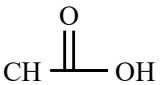




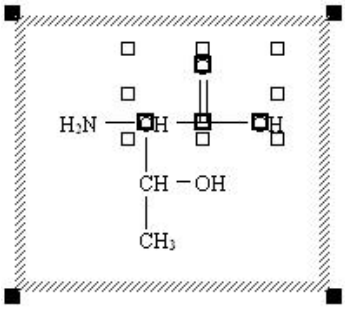
VI) Rotation of a chemical object part

To make rotation, make sure that the chemical object is not inserted into text.

Let's consider the following chemical object: 

Select only the following part:  of the chemical object above.

To do so, use "Ctrl" and "Shift" keys to select each of the symbols or bonds of this part. The principle of selection is the same as for any drawing. You can also make such selection by activating the " Drawing Mode"; and thereafter, slide the mouse in such a way to draw a rectangle encompassing the set of the part to be selected. After the selection you obtain the result as shown in Fig1.:



Figl

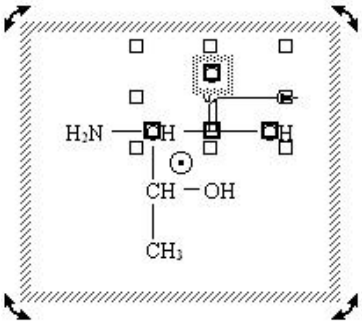


Fig2

Click on " " button in the drawing toolbar. Then the chemical object appears as shown in Fig2.:

The left end of the next arrow:  is the centre of rotation of the selected part. To rotate such a part, take the arrow by its right end whilst the pointer takes the  shape

and then shift the mouse conveniently. To move the centre of rotation, take the arrow by its left end and shift the mouse to position the centre at the suitable place.

The surrounded point "⊙" is the centre of rotation of the whole chemical object. It can be also moved.

To rotate the whole chemical object, click on any arrow and shift conveniently the mouse whilst the left button of the mouse is held down.

During the rotation, you can hold down the Ctrl button to have a better view of objects being rotated.

Remark 1:

While the whole chemical object is selected, the two centres of rotation mentioned above are merged as follow: ; but you can move them using the mouse to other location. The two types of rotation coexist.

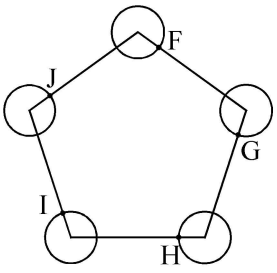
Remark 2:

The same principle of rotation can be applied to chemical objects belonging to the same selection region; then to chemical objects combined with "*Combine*" function.

VII) Drawing chemical polygonal group made of bicolor bounds

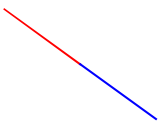
There are several techniques that can be used to draw chemical groups with bicolor bonds.

Here, we have to produce a pentagon and find the direction of each side with positive values in degrees according to clockwise, as shown below:

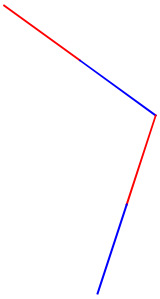


Measure 11295: Measure of F = 36.0°
Measure 11309: Measure of G = 108.00°
Measure 11325: Measure of H = 180.00°
Measure 11341: Measure of I = 252.0°
Measure 11357: Measure of J = 324.00°

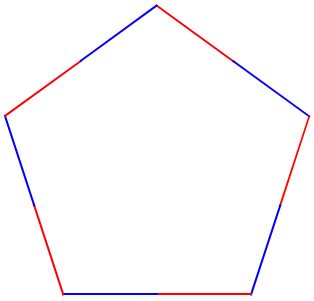
For this method, you have to set from the default drawings properties dialog box, the length (for example 5mm) and the rotation angle value, which first is 36°. Then you draw the first two chemical bonds. As you complete the first step, you get the following result:



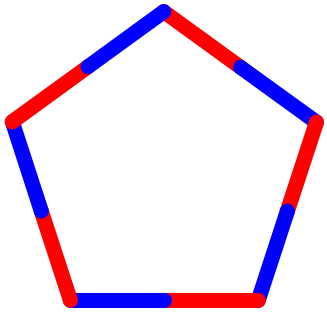
Next you set the angle value of 108° as default value. When you complete the second step, you get the following result:



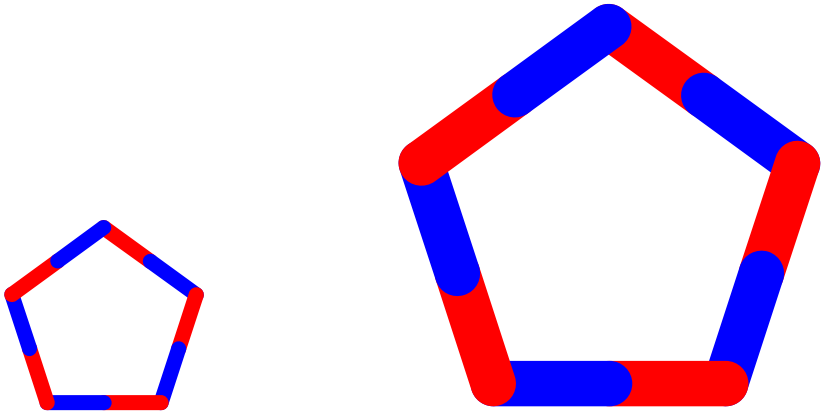
Next you set the agle value of 180° to draw the two related bonds. Then you repeat the same process using the angles values 252° and 324°.
Finally, you get the following result:



Now you can first select all the red bonds and set the width of the line to 2mm and check the box for the round angle; then you select all the blue bonds and make the same settings .
Finally, you get the following result.



You can adjust the chemical group to get it smaller or larger, even with a thicker line as shown below.



Important note:

(i.) Conveniently, the user can create a new menu for "Drawings Default Properties", having it handy somewhere on the interface from which he could quickly access the corresponding dialog box.

The user can also create a shortcut key for "Drawings Default Properties" to quickly access the corresponding dialog box.

(ii.) Drawing this type of chemical group is easier when the continuous mode is kept activated throughout.

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