

Introduction to FX ChemStruct 1

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User's Guide

by Efofex Software

Efofex Software

Always check our website for our current postal, phone and fax details

Email: info@efofex.com

Web: www.efofex.com

Intoduction to FX ChemStruct 1

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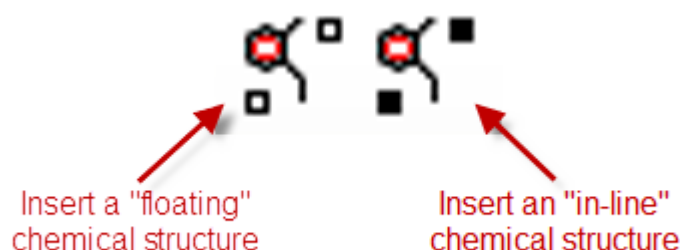
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1 Using FX ChemStruct From Within Word

Even though FX ChemStruct adds itself to your Start menu, the best way to use it is from within Word.

To use FX ChemStruct in this manner...

- Load Word
- When you wish to insert a diagram, push one of the FX ChemStructs button that has been added to your toolbars. (If you have not got an FX ChemStruct button, see the note below.)



- "Floating" and "In-Line" are Word concepts. A floating object can be freely moved around the page and text can be wrapped around it - this is what you will normally use. An in-line object sits in a line of text - like a character. It will follow the line of text around and the line height will be increased to accommodate the diagram.
- Enter and format your structure.
- Once you are happy with your structure, PUSH THE GREEN TICK on your toolbar. This is the most important step - if you do not push the green tick, your structure will not be returned to Word.



- You should now be returned to Word and your structure should be on your page. If you wish to edit your structure later on, DOUBLE-CLICK on it. FX ChemStruct will reopen and let you edit the structure. To return to Word, you PUSH THE GREEN TICK again and your changes will be shown in your Word file.

IF YOU DO NOT HAVE AN FX CHEMSTRUCT TOOLBAR BUTTON

Firstly check that you have not just missed it. If you are using Word 2007 or Word 2010 it will be in the Add-Ins tab of the ribbon.

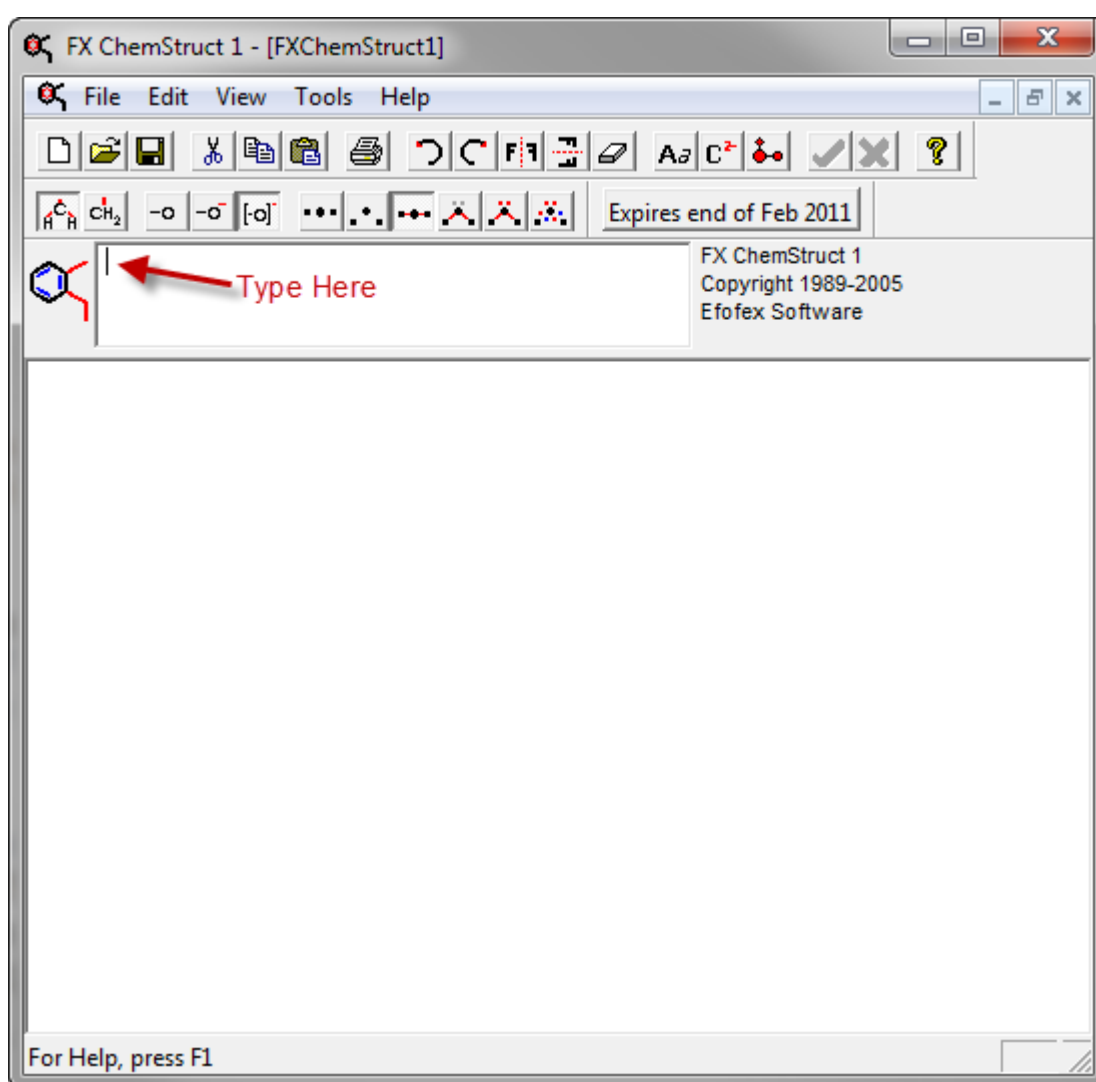


If it is not there, you should reinstall FX ChemStruct taking particular notice of when it asks you if it should integrate with Word. Make sure that you select the correct version of Word.

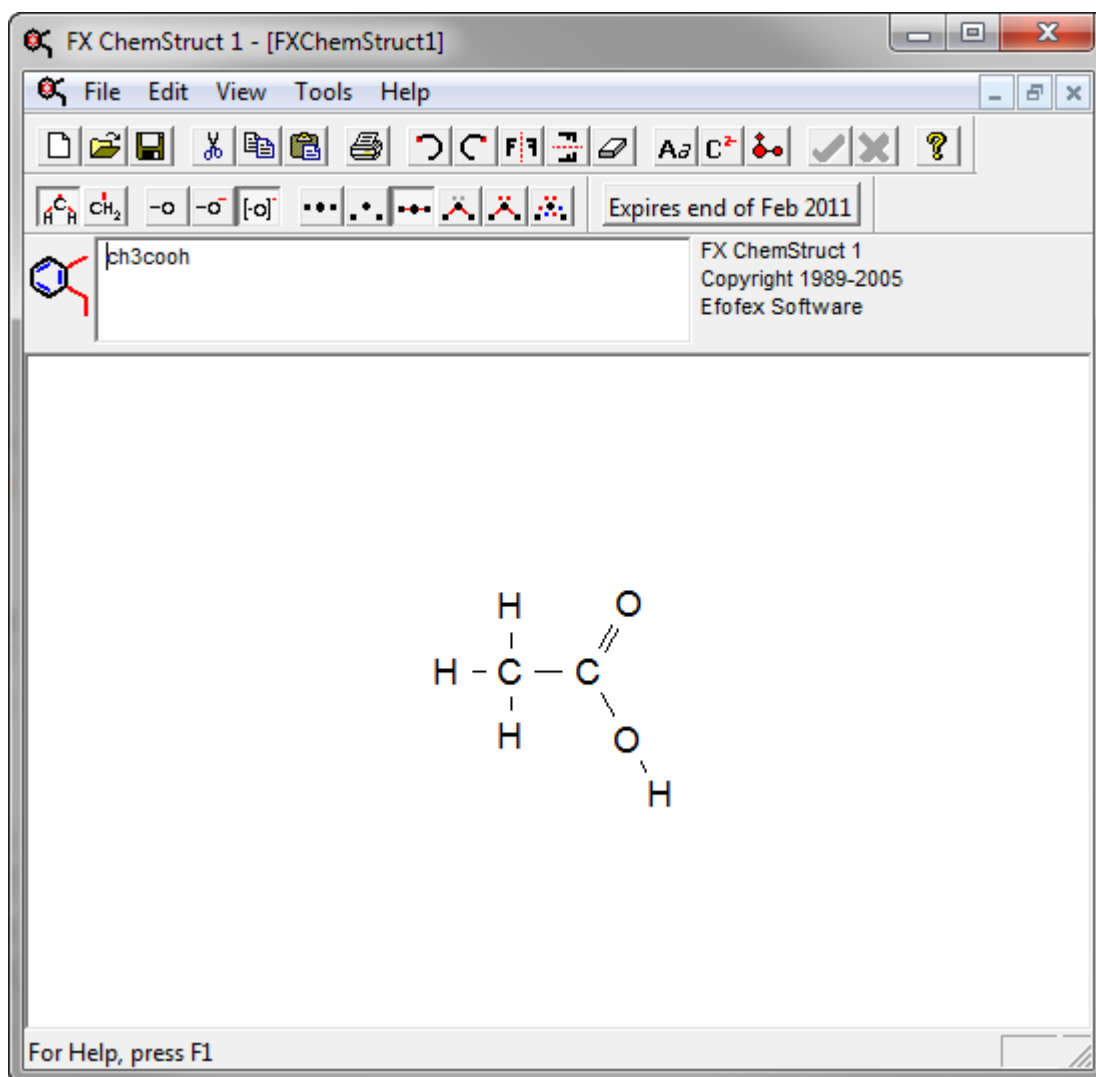
2 The Basic Idea

FX ChemStruct is designed to make the drawing of most chemical structures as EASY as possible. FX ChemStruct CANNOT draw every possible chemical structure but it can draw most structures required by secondary chemistry teachers – amazingly quickly.

When you first start FX ChemStruct there is not much to see.



To start using FX ChemStruct – just start typing. Try this:



Notice that we have **NOT** capitalized the elements.

That is nearly all there is to using FX ChemStruct.

Try typing the following:

- **ch3ch2ch2ch3**
- **ch3(ch2)4ch3**
- **ch2ch2**
- **chch**
- **ch3ch2coh**
- **ch3cooh**
- **ch3coch3**
- **ch3och3**
- **ch3conh2**
- **ch3cooch3**

All of these compounds are organic but FX ChemStruct is capable of more than just simple organic molecules. We will look at the extra features later.

You might notice that the compounds are entered in **STRUCTURAL** form (where the structure is implied in the formula). FX ChemStruct **REQUIRES** that you enter molecules while providing structural information.

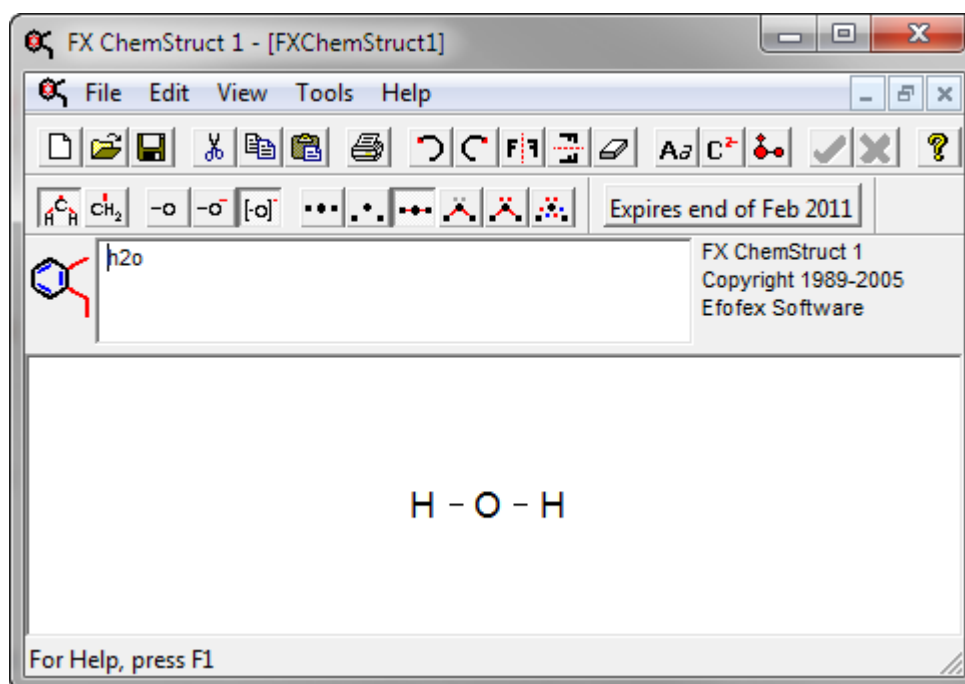
For example: A compound with the molecular formula c_3h_6o could either be an aldehyde (ch_3ch_2coh) OR a ketone (ch_3coch_3). FX ChemStruct has **NO WAY** of determining which one is the desired molecule. You need to give FX ChemStruct more information to work with.

3 Display Options 1

FX ChemStruct has a number of display options that are controlled using the display toolbar. The display toolbar has lots of “structure” type buttons. We will be concentrating on the buttons on the right hand end of the toolbar in today’s lesson.

Open FX ChemStruct and type:

h2o



The 6 right hand buttons control how this simple water molecule will be displayed.



From left to right:

1. Show structure of molecule **WITHOUT** showing any bonds and taking

no account of any unbonded electron pairs. This option can be useful for designing questions for students.



2. Show structure of molecule WITHOUT showing any bonds but taking account of any unbonded electron pairs. This option will put the “bend” in the water molecule.
3. Show structure and bonds of the molecule taking no account of any unbonded electron pairs. The molecule will jump back to being straight but this time the single bonds will be shown. $\text{H} - \text{O} - \text{H}$.
4. Show structure and bonds taking account of unbonded electron pairs. Same as 3 but with the bend.
5. Take unbonded electron pairs into account AND display them. Same as four but the two pairs of unbonded electrons are displayed.
6. Show all electrons.

Experiment with these display options and how they affect different molecules.

4 Display Options 2

The five left hand buttons in the display toolbar control how atoms and charges are displayed.

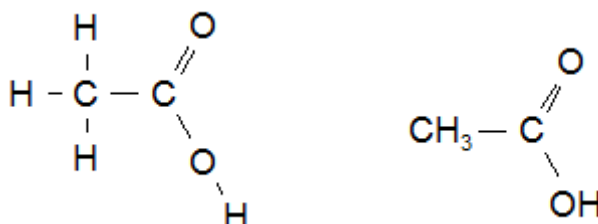
For example:

Start FX ChemStruct and enter

ch3cooh



The first two buttons determine how hydrogen atoms are displayed – either summarised or as separately bonded.



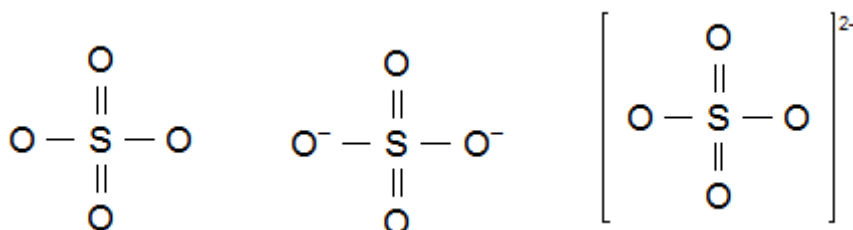
Now clear FX ChemStruct and type

so4



The next three buttons determine how charge is shown on structures.

- The first button does NOT show charge
- The second button shows the charge on each individual atom
- The third button shows the OVERALL charge of the structure.

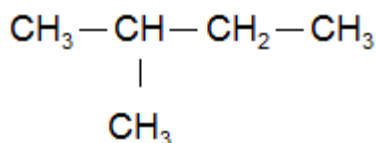


5 Branched Structures

Entering most simple compounds is easy with FX ChemStruct – you simply enter them the way you would write them down, starting at one end and moving to the other. Branched structures provide a bit more of a challenge to enter.

For example, 2 methylbutane

ch3chch3ch2ch3



You will notice that when entering this molecule, we started at one end and worked our way across. When we got to a “fork”, we entered the whole of one branch and then went back and entered the second branch. We have annotated the entry below.

ch3ch (a “fork” in the structure) **ch3** (one branch) **ch2ch3** (second branch).

We could have started from the other end and got the same result.

ch3ch2chch3ch3

ch3ch2ch (“fork”) **ch3** (branch) **ch3** (branch).

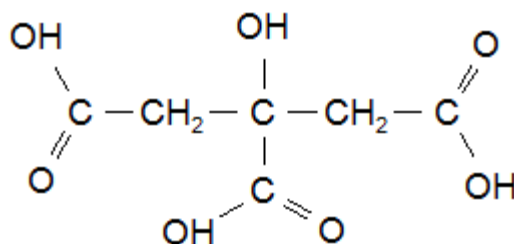
The golden rule is

Completely enter one branch before you start on the next branch.

Take some time to study how the two formula above work.

Branched structures can get quite complex.

coohch2coohch2cooh (citric acid)



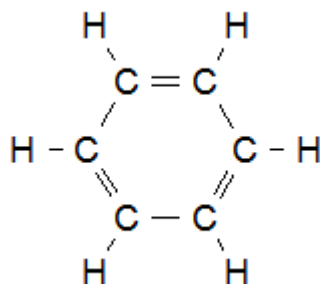
Take a moment or two to make sure you understand how the formula produces the structure.

6 Benzene Rings

Benzene rings are central to organic chemistry but they would be fairly tedious to draw using FX ChemStruct.

You CAN create a benzene ring by typing:

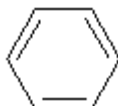
chchchchch



and sometimes this is the best way of doing it – you get to see all of the individual atoms and their bonds. **Note that this will only work if FX ChemStruct is set to automatically detect rings (see below).**

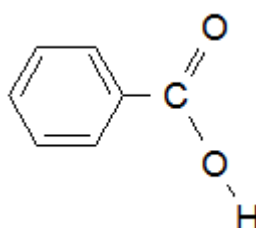
Most the time you will want to create a benzene ring using a quicker approach. Quick entry of benzene rings can be done using

bz or **ph** (Note: the use of ph is OPTIONAL and can be turned off)



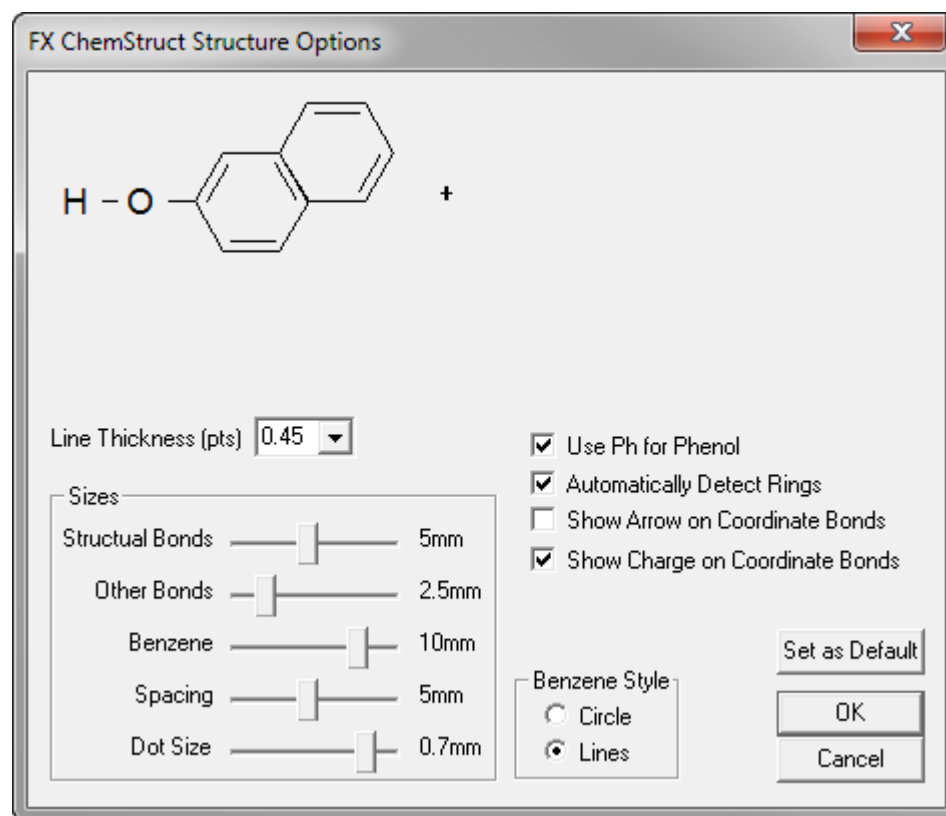
For example, benzoic acid can be entered as

bzcooh or **phcooh**



Benzene rings have a number of formatting options that are controlled using the structure options dialog box. You open this by clicking on this button.





Notice the Automatically Detect Rings option

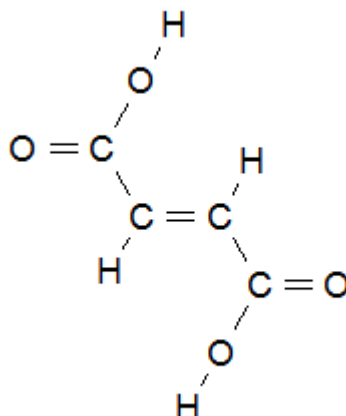
7 Clicking on Elements 1

In lesson two, we discussed how you needed to enter STRUCTURAL formulae because simple molecular formulae (such as c_3h_6o) did not contain enough information to allow FX ChemStruct to create the structure.

Another problem emerges with geometric isomers. For example, cis-butenedioic acid and trans-butenedioic acid.

Enter this formula into FX ChemStruct

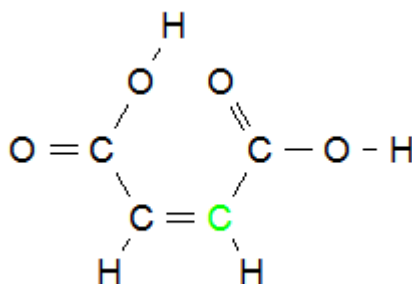
chcoohchcooh



This is the trans isomer – where the cooh groups are on opposite sides of molecule.

The big question becomes – how do we get the cis isomer? Let's start clicking!

Click the left mouse button ONCE on either of the two carbons joined by a double bond. FX ChemStruct will swap the bonds around the carbon atom – producing the cis isomer.



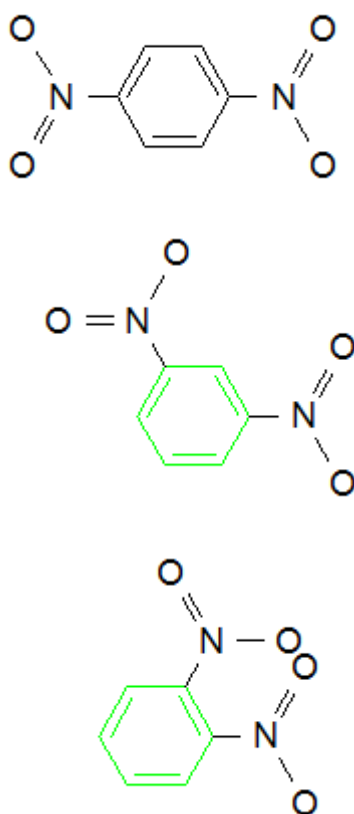
You will notice that the atom you clicked on turns green. This will NOT affect the structures that you put into Word. We colour the atom green because when you click on some big structures, the resulting change can be so large that it is easy to get confused about what you have done. Colouring the atom green makes it much easier to track what has happened.

You can click on any atom that has three or more bonds emanating from it. Unbonded electron pairs count if you have chosen to take them into account. Every click will shuffle the bonds through a cycle of possible arrangements.

Try this structure:

bzno2no2 (dinitrobenzene)

Clicking on the benzene ring allows you to produce the ortho, meta and para isomers of dinitrobenzene.



Sometimes, after merrily clicking away, you might decide to just start again. You can undo ALL the clicks (as well as any rotations or reflections) by clicking on the eraser button.



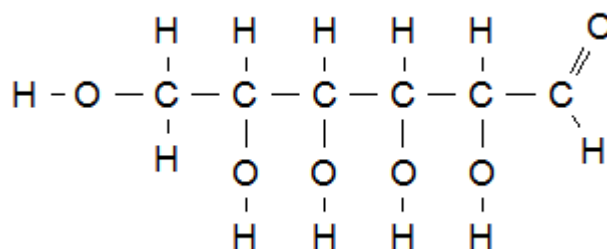
8 Clicking on Elements 2

There is a problem with clicking on elements to rotate bonds – as the number of bonds increases, the number of permutations skyrockets. Most of these permutations just “get in the way”.

To overcome this problem, FX ChemStruct ignores many of the permutations.

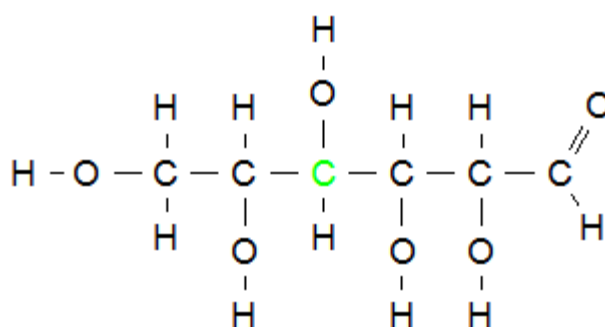
For example, start FX ChemStruct and type the following:

ch2ohchohchohchohchohcoh (glucose)



In this molecule, all the OH groups are on the same side.

Click on one of the C's that an OH group is attached to. The OH group will jump to the other side.



Click on the C again and the OH will jump back. If you keep clicking, the OH will keep swapping sides. There is a cycle of arrangements that repeats every TWO.

There are of course OTHER permutations that you might want access to.

Click the Eraser button to clear all of the clicks you have made.

Now click on the same C, this time holding down the SHIFT key as you do it.

The first click will make the OH swap sides – just like before. The difference is that subsequent clicks will access all of the other permutations. There is now a cycle of permutations that repeats every SIX.

Clicking provides access to common arrangements. Shift clicking provides access to all arrangements.

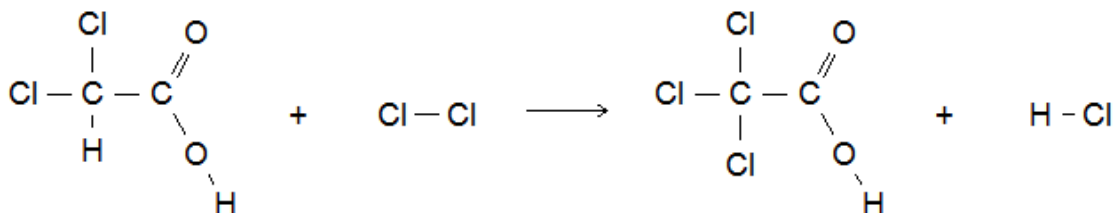
PLEASE NOTE: FX ChemStruct can only process 100 clicks per molecule. Any more than that are ignored. You can reset the click count by pressing the eraser button.

9 Reaction & Equilibrium Arrows

FX ChemStruct can produce equations involving structures and uses the same conventions as FX Chem.

For example, start FX ChemStruct and type

chcl2cooh+cl2=>ccl3cooh+hcl



This is a fully formatted equation with each structure formatted individually and a reaction arrow. You have access to a full range of reaction arrows.

- =>** gives you a single arrow
- <>** gives you a double arrow
- ="above">** adds a message above the arrow
- ="above","below">** the comma allows information below the arrow as well

If you do not include the quotes, FX ChemStruct will interpret the text on the arrow as a chemical equation (NOT a chemical structure)

There are a few important points regarding arrows:

You have a choice of four different styles of equilibrium arrow. Go to the equation options screen to select the one you want. The equation options screen is discussed later.

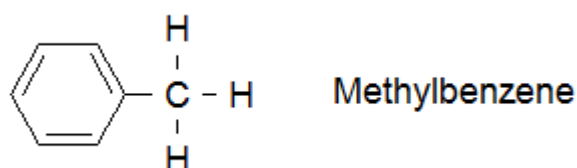
You CANNOT have structures above or below an arrow. You can have chemical formulae.

We have included comments above and below the arrow in the instructions above. Comments are discussed in a later lesson.

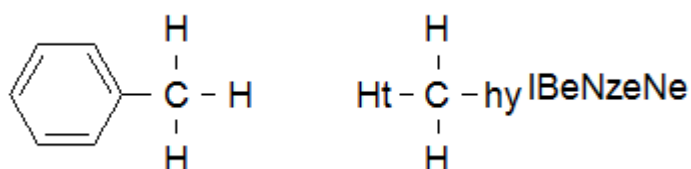
10 Adding Comments

Comments can be added to any equation. Anything surrounded by quotes will be ignored by FX ChemStruct and just displayed as text.

For example, start FX ChemStruct and type

bzch3 "Methylbenzene"

Now remove the quotes and try again

bzch3 Methylbenzene

FX ChemStruct will try to interpret the letters methylbenzene as a structure and it is fair to say that it gets terribly confused!

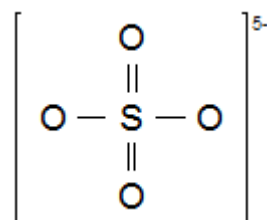
Comments can also be added above and below arrows.

11 Phase & Charge

FX ChemStruct will automatically calculate the charge for a polyatomic ion and can display it in a number of ways. Sometimes, you may wish to OVERRIDE the automatic calculation. This can be easily done using the same conventions as FX Chem.

For example, suppose you wish to have a sulphate ion with a charge of 5-. You can force FX ChemStruct to produce this anomaly by typing

so45-



We agree that there would seem to be little educational benefit from a structure such as this but we do not like restricting use of our products.

A much more important use is for metallic ions.

For example, type **fe**



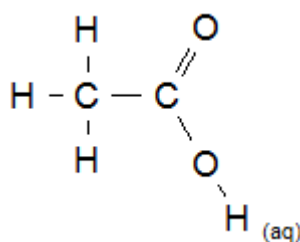
FX ChemStruct will produce Fe²⁺. If you want Fe³⁺, you need to explicitly tell FX ChemStruct the ion's charge.

fe3+



You can also add phase information to a structure. For example, if you want to indicate that acetic acid is in an aqueous solution, type

ch3cooh(aq)



Anything in brackets will be treated as phase or state information.

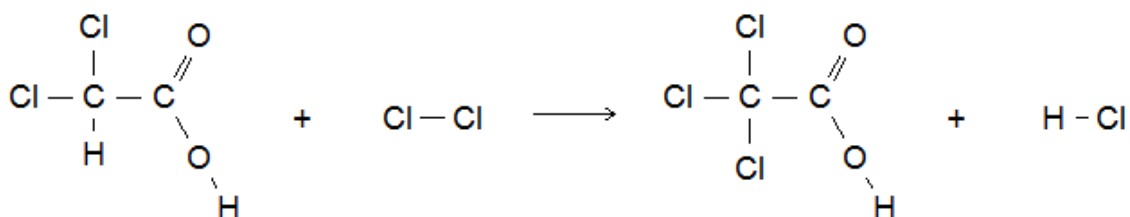
12 Spaces

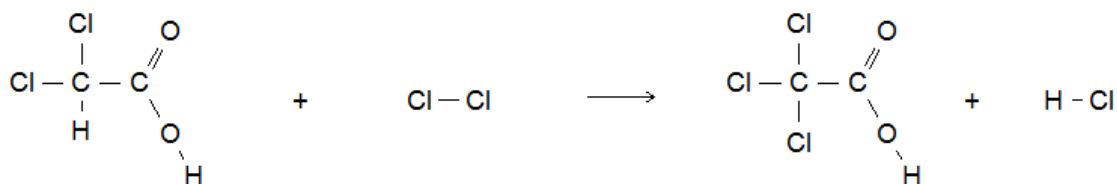
Spaces have two important uses in FX ChemStruct.

Firstly, you can use them to add white space between structures. FX ChemStruct automatically adds some white space between structures (and this amount can be set in the structure options dialog box) but you can add space yourself.

For example,

chcl2cooh+cl2=>ccl3cooh+hcl



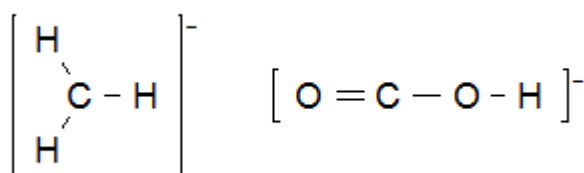


display quite differently.

The second use for a space is to break a structure into bits. A space indicates to FX ChemStruct that a compound is complete and it needs to start a new one.

Try typing

ch3 cooh



the structure is broken into two pieces.

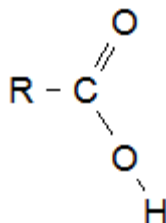
The second use of a space is very important when drawing ionic compounds.

13 R & R'

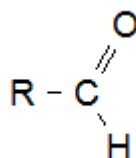
A nice simple lesson for today.

FX ChemStruct treats R and R' as elements that can support a single covalent bond. This allows you to show functional groups such as

rcooh



rcoh



ror'



14 Polyatomic Ions

FX ChemStruct was originally designed to draw organic compounds and this is still its prime focus. We have added the ability to draw polyatomic ions.

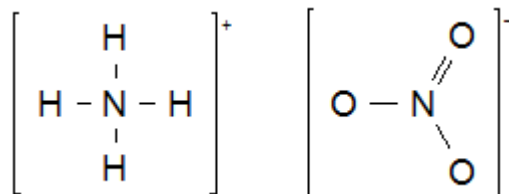
To draw a polyatomic ion, just type it in normally. FX ChemStruct should recognise it and display it appropriately.

When you are trying to draw ionic compounds, it is necessary to separate the ions with a space so that FX ChemStruct can treat them separately.

For example, ammonium nitrate.

Type

nh4 no3



rather than

nh4no3

15 Rotation & Reflection - Resonance Forms

FX ChemStruct can rotate and reflect structures. First draw the structure and then push the rotate or reflect buttons.

The rotate buttons are on the top toolbar and are curved arrows.



The reflect buttons have capital F's reflected over a vertical and horizontal axis.

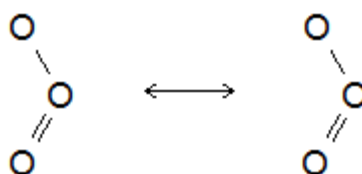


The rotation buttons rotate the structure in 15 degree intervals clockwise and counterclockwise.

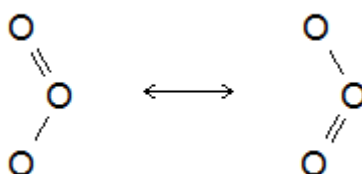
One of the main uses of these features is to draw resonance forms of structures.

For example, ozone.

o3 <> o3



Now push the reflect over horizontal line button and the first ozone molecule will flip over – producing the resonance form.



16 co & ph Causing Problems?

Typing co can cause problems. FX ChemStruct will ALWAYS interpret co as carbon/oxygen – which is usually exactly what you want. What do you do when you REALLY want cobalt?

If FX ChemStruct gets the capitalisation wrong, you need to capitalise that structure yourself. In this case, you need to type Co rather than co. If FX ChemStruct finds ANY capitals in a structure, it will assume that the entire

structure is capitalised correctly.

ph can also cause a problem if you have set the option that turns this into a benzene ring. You will NOT be able to draw any structure that has phosphorus and hydrogen together UNLESS you capitalise the structure yourself. In other words, typing PH will produce the desired result.

17 Ring Structures

There is limited support for ring structures in FX ChemStruct. FX ChemStruct can handle ring structures automatically - which provides limited functionality - or the user can explicitly indicate the rings

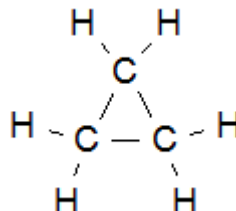
You can turn automatic recognition on and off using the Structure Options screen.

Automatic Recognition

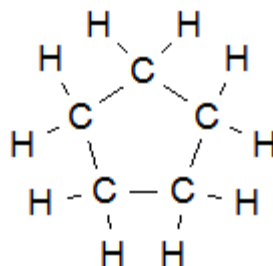
If automatic recognition is turned on, FX ChemStruct will look to see if the elements entered can be formed into a ring. If possible, FX ChemStruct will automatically "link" the ring. Automatic recognition is very limited and is best used for carbon-based rings.

For example:

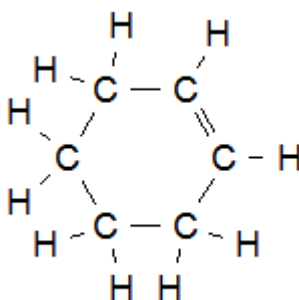
ch2ch2ch2



ch2ch2ch2ch2ch2



ch2ch2ch2chch2

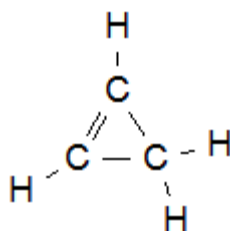


Explicit Indication

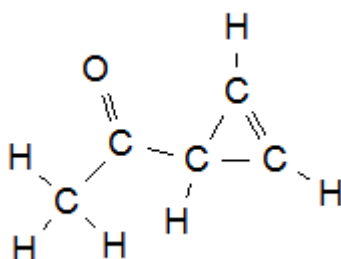
If automatic recognition is **NOT** turned on, you can explicitly indicate ring structures. Surround the elements in the ring structure with curly brackets and FX ChemStruct will attempt to form them into a ring.

For example:

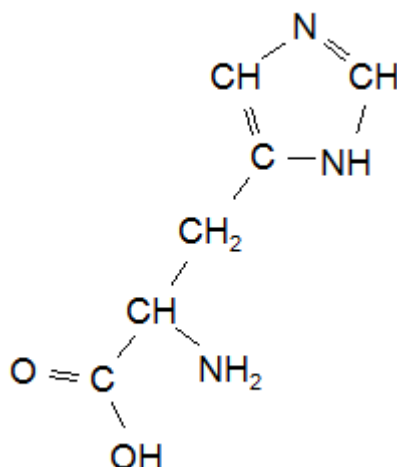
{chchch2}



{chchch}coch3




{cchnchnh}ch2chnh2cooh





Explicitly indicating rings allows many more structures to be drawn but it is important to note that not all structures can be entered this way.

18 Drawing Options

FX ChemStruct allows you control over many aspects of your equations and structures. These options can be accessed through the Tools menu (Tools/Font, Tools/Options/Equations and Tools/Options/Structures) or through three buttons on the top tool bar.

The  button lets you change the font used for your structure.

The  button allows you to change the format of any chemical equations – in much the same way as FX Chem.

The  button allows you to set structural options.

Both the equation options screen and the structural options screen give you a lot of control over how your structures appear and SHOW you the effects of your changed options as you make them.

It is worthwhile taking some time to explore these options and ensure that you understand the options available.

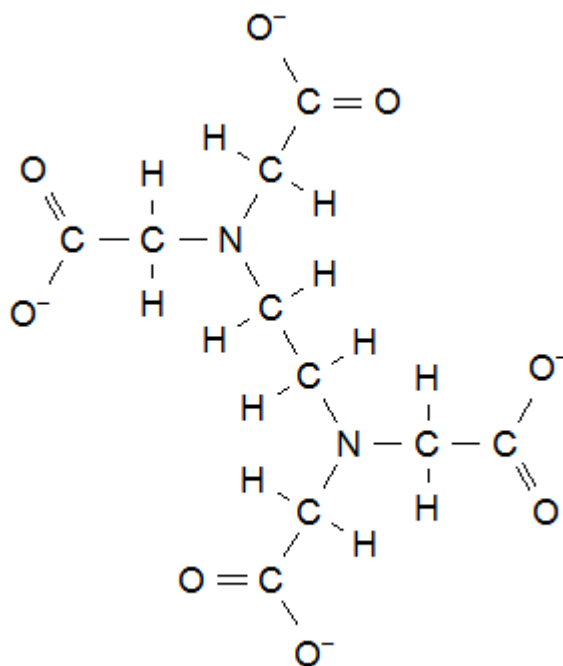
19 Preventing Bonding

FX ChemStruct uses a complicated algorithm to determine where the "next" element is attached to the existing structure. Sometimes this can cause problems if you want to leave a "bonding site" unbonded.

For example:

EDTA – EDTA is a complicated four-branch structure with unbonded oxygens at the end of each arm. You can see it by copying this into FX ChemStruct V1.1 or later.

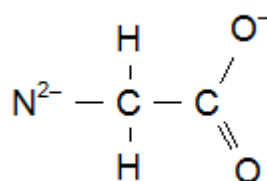
nch2ch2n(ch2coo*)4



To fully understand this lesson, you need to be typing things into FX ChemStruct as you go.

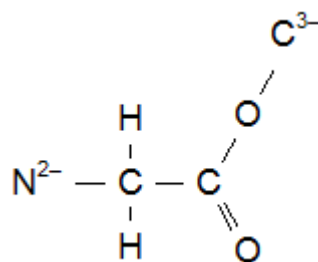
Imagine you are trying to enter this structure into FX ChemStruct (forget about the * for the moment). You might start with one of the N's and move out one of the arms

nch2coo



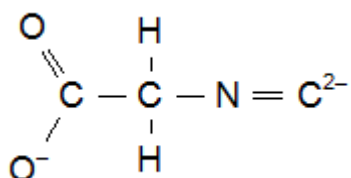
So far so good. Now if you attempt to start another arm - by typing a C - things start to go wrong

nch2cooc



FX ChemStruct has no way of knowing that you have finished the first arm and attached the C to the remaining bonding site on the O. Oops! What we need is a way of telling FX ChemStruct to stop there. You can do this using the * key.

nch2coo*c



The * has prevented the C from bonding to the O so FX ChemStruct bonds the C to the N instead.

To enter EDTA we can use

nch2ch2nch2coo*ch2coo*ch2coo*ch2coo* or **nch2ch2n(ch2coo*)4**

Note: There are other possible ways of entering EDTA - but all require the use of the * key.

20 What To Do When FX ChemStruct Gets It Wrong

FX ChemStruct is a VERY complicated piece of software. Why is it so complicated? Because it is trying to interpret ambiguous information to produce what you want. The FX ChemStruct technology is designed explicitly to service SECONDARY school level chemistry and makes some assumptions based on this. It is these assumptions that allow FX ChemStruct to do things so fast. The net result of this complexity and assumptions is that sometimes FX ChemStruct will get things wrong. It also means that FX ChemStruct is not infinitely extensible – there are some things that FX ChemStruct will NEVER be able to do.

If you find things that are incorrect, TELL US!! All that we ask is that you realise that what you are requesting may just be impossible. There is also a trick to telling us.

1. Include EXACTLY what you have typed to get FX ChemStruct to make the mistake.
2. Include EXACTLY the output you would expect – you may need to use

a drawing program to produce the diagram.

We will always attempt to get FX ChemStruct to produce what you are after or explain to you why it is not possible using the FX ChemStruct technology.

That brings us to the end of the FX ChemStruct email lesson series. We hope that you have learnt something about the product and we welcome any suggestions that can help us improve the quality of the lessons.