

Kludging BKChem.

by

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Introduction.

This doesn't pretend to be a correct guide to the art of using BKChem (look up the word "kludge" online if you don't know what it means); neither have I made any attempt to be comprehensive. I'm working on the assumption that, like me, you've started using the program to help neaten up a chemistry assignment or something like that, so you're using it simply as a "word processing tool", and don't have time to investigate the more interesting features right now.

This is what I'm going to do: I'll answer the sketching part of some chemistry problems actually posed in a UNISA assignment, and as I go along, I'll make screen shots of the BKChem interface to show what I'm doing. So the format will be:

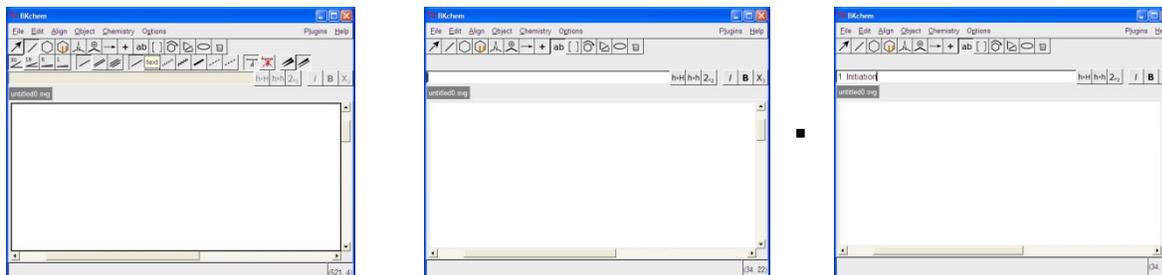
Synopsis of question (A)

Pictures showing progress in attempting an answer (B)

Please note that the chemistry herein is to be treated as highly suspect. I'm not producing model answers, just whatever answers I come up with; and the answers I come up with are frequently wrong - and seldom a suitable model. The point is to demonstrate BKChem in as lazy a way as possible, with the byproduct of a set of assignment answer components on file at the end of it all.

I'm no expert, and I'm sure there are better ways to do all the things I show here, but those are for you to find out. This booklet will just give you a quicker start than I had, and get you up to "advanced beginner" level quicker than otherwise (or so I hope).

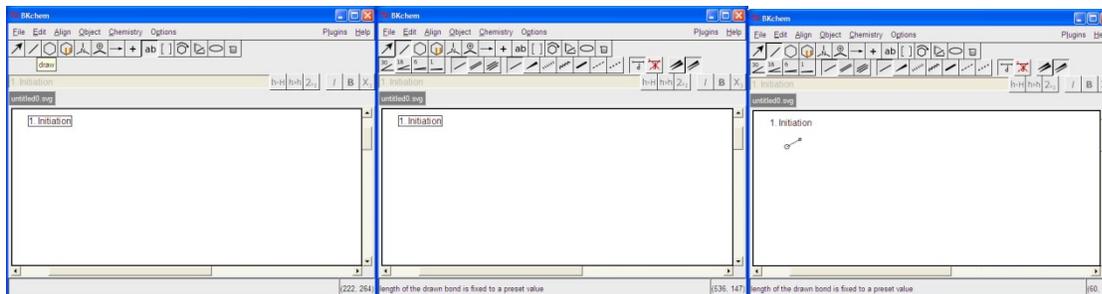
1. Free Radical Reaction (that'll do for a "synopsis")



Select the text button **ab**. (Sorry, the screenshots don't show the mouse).

- Now your cursor is in the edit field, and you can type something.
- I can't show you this, but all you do is click the page wherever you want your text to appear, and when you hit Enter, that's where it will appear.
- Naturally *you'd* have never gotten stuck on something like this, but for those like myself, who have, here's a "trick": **Don't go clicking on the page again after you've hit Enter**. If you do, you're going to have to hit Enter again, because BKChem now thinks you want to insert yet another text field. If you don't now hit Enter a second time (and delete your unwanted entry, obviously) BKChem is going to appear to be "stuck". The safest way to deal with text is to immediately click on "Edit" (the Select arrow's popup hint says "Edit") as soon as you've Entered your text - either that or immediately select your next action eg. Atom, Mark etc.
- Don't fuss about getting it perfect. It's very easy to select, move, rotate, etc. things with BKChem if you don't "get it stuck". Just click on text later, and then move it about at your pleasure till it's perfectly placed to the exact millimetre.

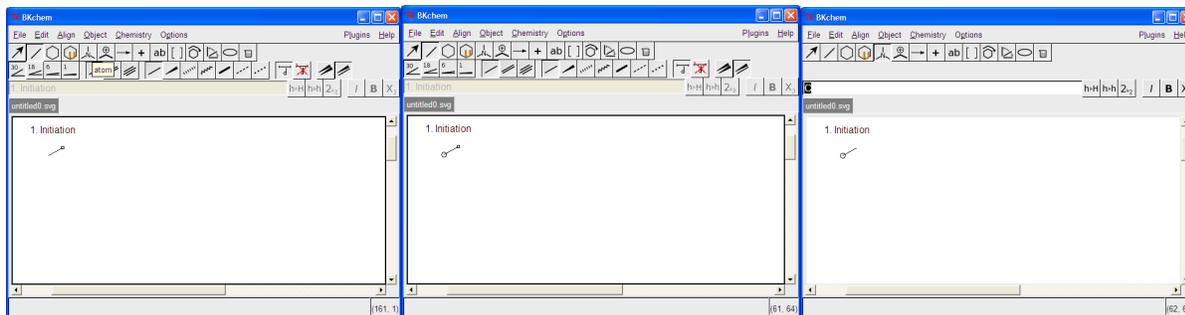
Now we'll click just once to make the skeleton of a Chlorine atom, straight after hitting Enter.



Click up the Draw mode toolbar, then click approximately where you want your molecule on the page. By default you'll get a two-carbon line drawing for your click... and now we'll make it Cl_2 ...

Select "Atom Mode" (not Text mode, but BKChem will tell you so, anyway). The same line editor you used for text is activated when you do so.

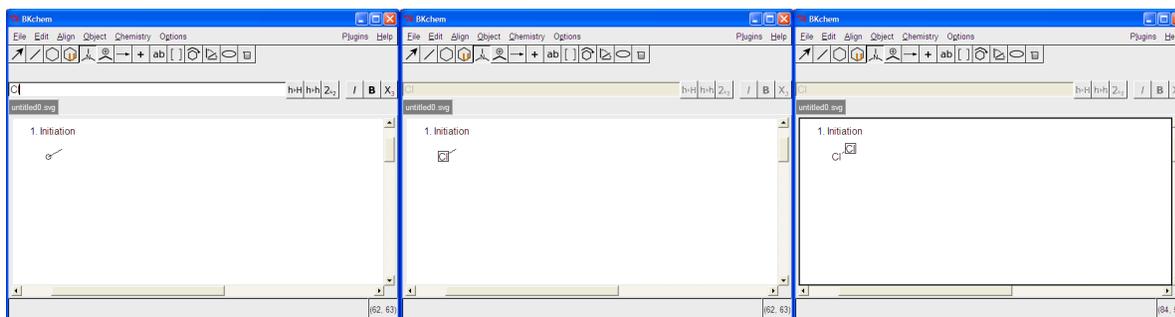
Then pick a side of the molecule, and follow the pictures on the next page.



Atom Mode

Pick a side ("hover" there)

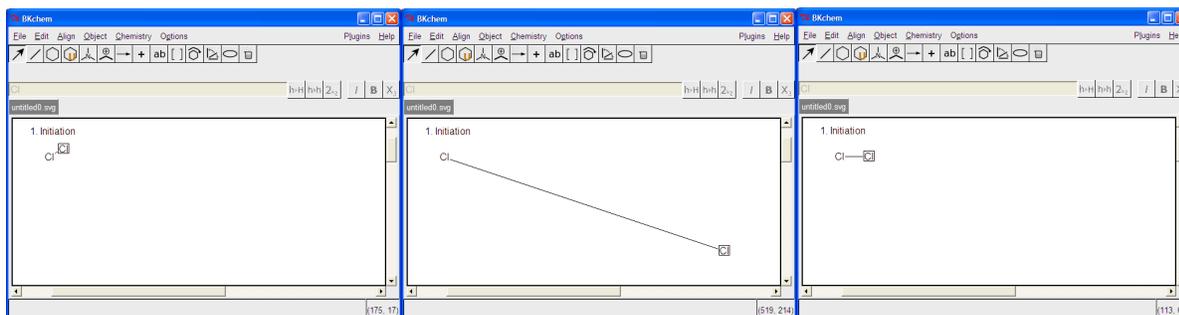
Click a side (see the C?)



Type "Cl" in the box

hit Enter

and do the same on other side.

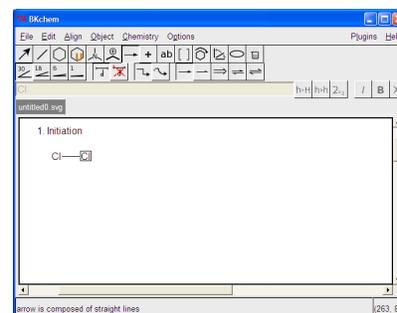


Quickly change to "Edit" (select) arrow and stretch and drag to taste.

Remember that you're going to have to fit in reaction arrows, so don't make it too cramped... Let's do that: Heterolytic cleavage of the bond, shown with "fishhook arrows".

All arrows are under the horizontal arrow button. As happens in DrawChem mode, clicking on the button opens a contextual tool bar, which we won't do that much with here. If you were starting to fall asleep by now, it could be an idea to wake up for a bit. If you're an old hand at using drawing programs, and playing with splines go straight back into mellow mode, but otherwise prepare for some incredibly exciting pictures.

First klikki klikki on that arrow thingy.



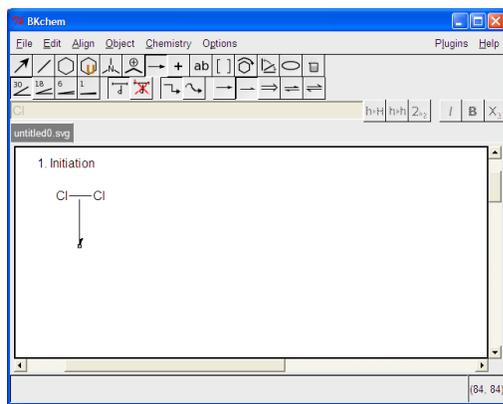
Here you must make **TWO** choices.

The number of choices you shall make shall be TWO, not One, nor Three, but TWO. in principle anyway. In fact if you choose to make all your arrows "splines" then you'll be fine most of the time. To choose splines, push the curvy-arrow button that pops up the hint "spline".

The second choice, of course, is the type of head the arrow has. Look at the other buttons and work it out for yourself.

Now I did mention somewhere that I'm no expert, didn't I? Unfortunately I can't give the definitive guide to splines here; however, I do know a few kludges one can perform upon a spline...

Anyway, let's stop the jabbering and have a look at some:



A single click-and-short-directional-drag gives you the beginnings of your spline (*you need to drag a little* because the default direction is right-horizontal).

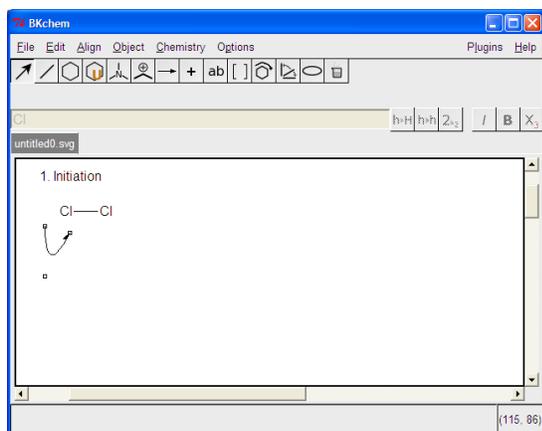
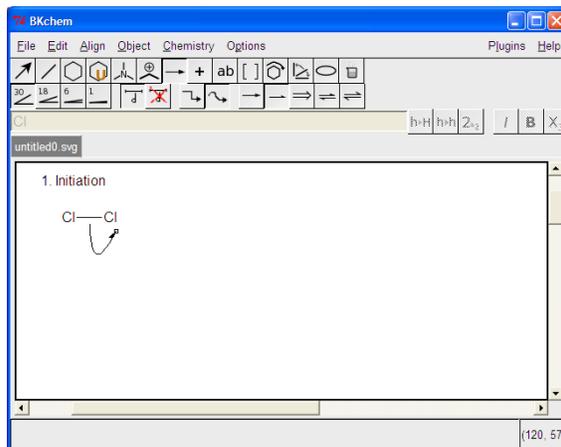
(and please pretend not to notice that I've mucked up here in a way I'll leave you to guess).

Now drag

that square handle on the arrow head around to point in **More or Less the Right Direction**.

This is a good tip: Don't try to perfect your splines right away. Just get them more or less right, and then go into select mode and fiddle further to the extent of your own fussiness.

This is where my inexpertitudinousness begins to show up: I don't really know for sure how to give shape to splines. I think (but I don't know for sure) that to move just a part of the spline you need to click quite accurately IN THE SQUARE, however.



I'm getting ahead of myself here, but this needs to be said reasonably early on: Until you've found your own way with splines, just accept that occasionally you're going to do things like try to drag the arrow head closer to an atom, and instead end up dragging the whole arrow off and out of position.

Relax. It's not a train smash. It's quite easy to to just shift it back and try again. Generally when your mouth is

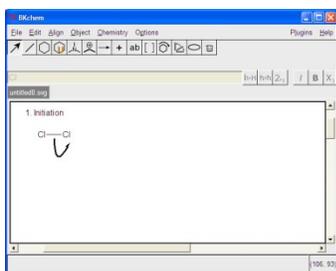
shouting is when your brain is doing the least thinking. Remain calm, and you remain intelligent. Lose it, and you must expect that what an orangutang attempts in the line of the rational sciences is never going to amount to much. So treat the little misbehaviours of your splines as useful practice in the art of keeping your brain switched on and your temper switched off. The two can't work in tandem, and better you learn that with something harmless like a spline than with that bomb you're busy making in the garage.

You've forgotten where we were, too?

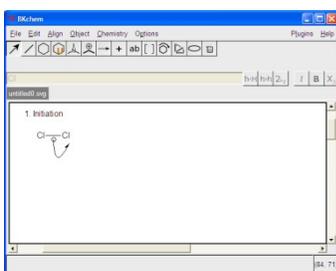
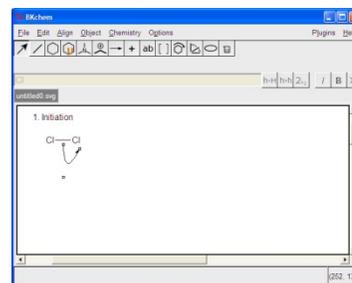
A recapitulation: You click and drag just a little bit, and you get part of your spline. Then you click and drag the head round into more or less the right position. Don't try to make it perfect.

Now, you go into select mode, and with a lot of experimentation you'll eventually find yourself producing splines that could only be worthily described as "masterpieces" or as objects of exquisite beauty that bring tears to the eyes of the stone hearted. I will defer the masterclass till later for now, though.

Some experiments you will probably make with splines:

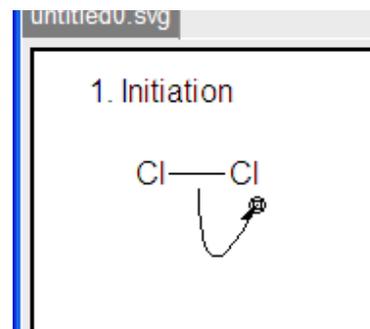


Selecting the whole spline. First it darkens while you hover, then all three handles show when you click it.



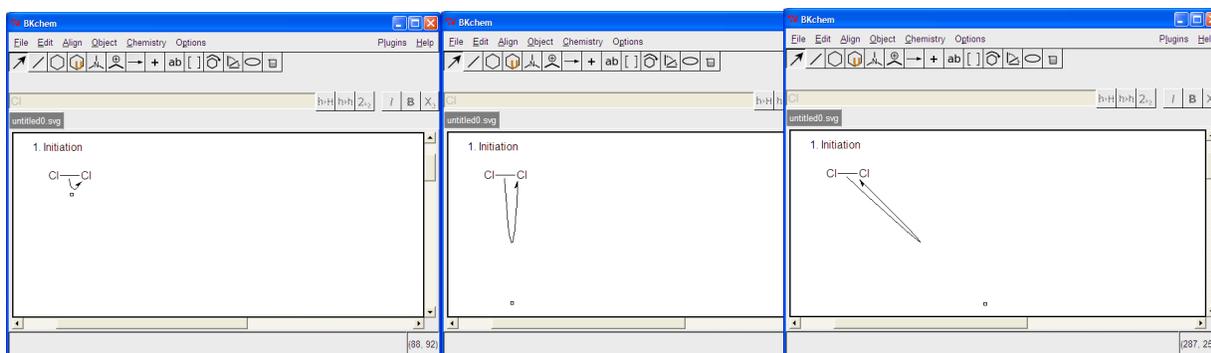
Selecting either end.

Notice how the circle gets a square inside it? If you accurately click in the square it seems to drag just that tip, but if you only catch the circle, you tend to move the whole arrow, as previously depicted.



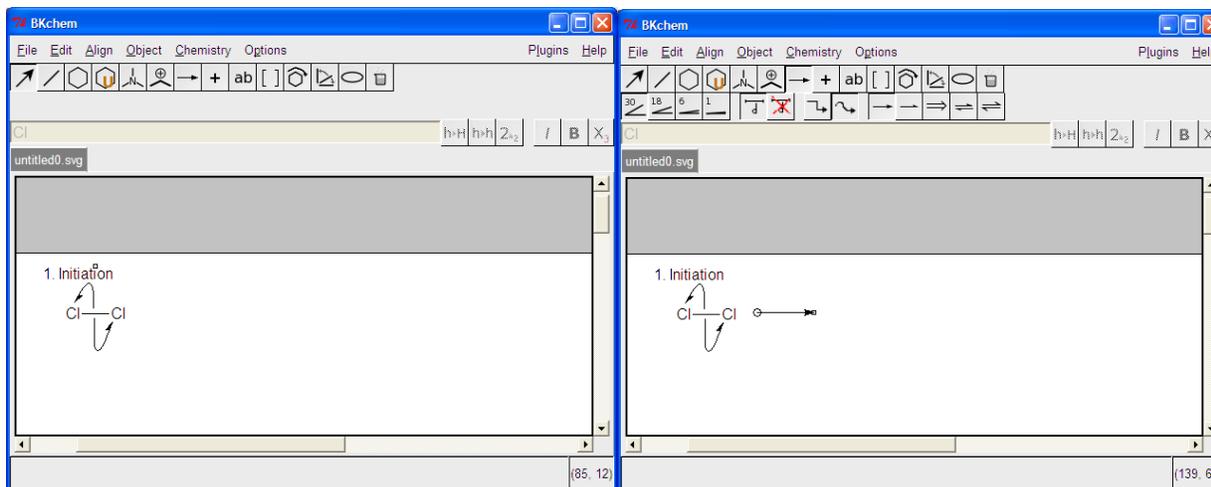
This vagueness is one of the imperfections in this otherwise perfectly good set of BKChem kludges, and the only advice I can give on how to deal with it is ... work it out for yourself. Better still, work it out, and then write an appendix to this, or edit my literary prose up to a higher level of technical accuracy.

Let's have a look at the central handle. Unless you select the whole spline, it's usually as invisible as a ghost, though it does make apparitions if your mouse pointer strays over it. Generally to get a grip on the central handle you need to select the whole spline, then click on the central handle's square. I think then you need to click again. You can't just "grab and drag" without dragging the whole arrow around, losing your temper, and blowing up the neighbour's house in retaliation.



That should give you a rough idea of what you can do with the central handle. (If you're one of those ignoramuses like me who hasn't drawn things with Paint etc. before).

So you can drag the ends around to wherever you like, and you can make the loop big, small, or a bit skew. That's enough to get you started on taking control of your reaction arrows, but I know you're already bored with all this. Deep down inside there's only a chemist within; let other people have their artists. What happened to that lovely **REACTION(!!!)** we were looking at???

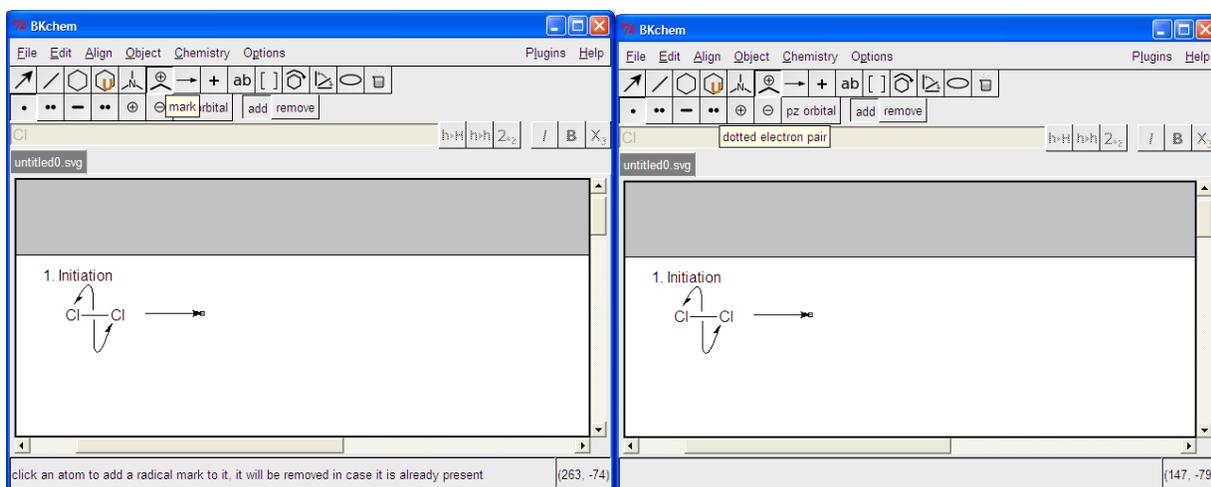


Homolysis

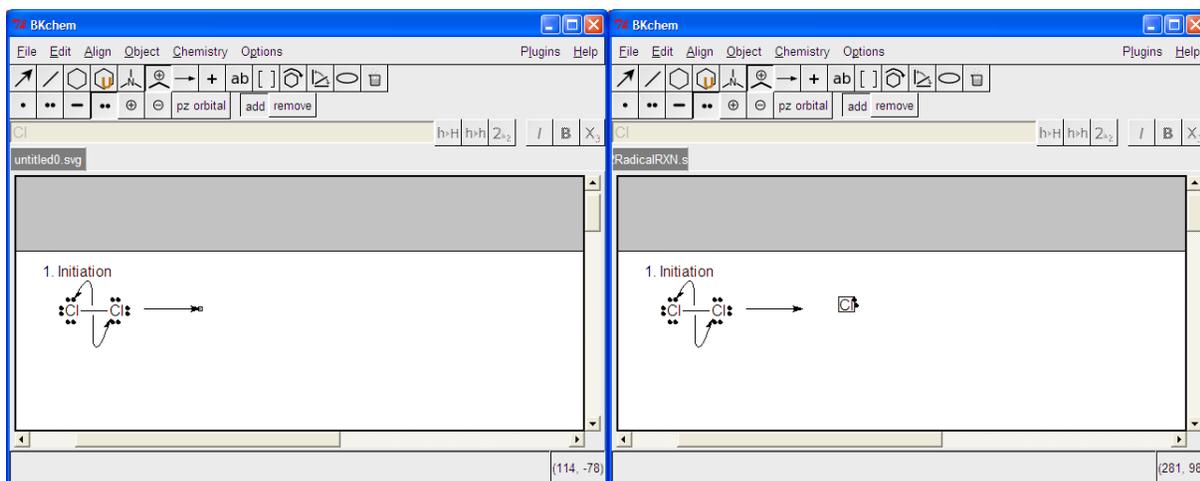
A one-click reaction arrow... .. progress at last...

Notice that the reaction arrow is really a spline. As long as you don't go putting interesting curves in it, no-one need ever know.

But hang on, what about dots for the nonbonding electrons? Easy. Click on the "Mark" button and look what's under it.



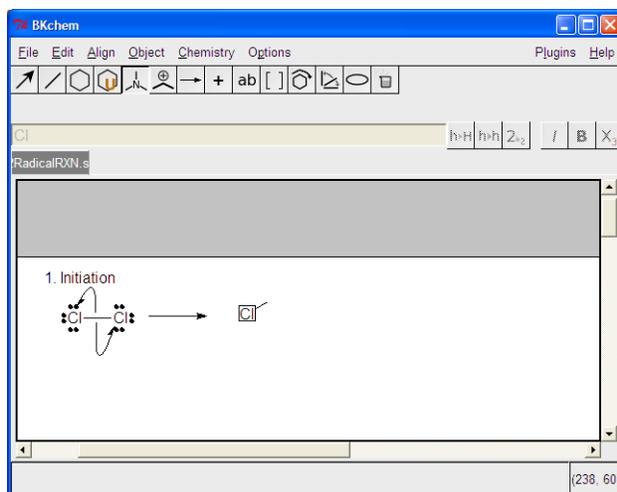
These dotted pairs don't always behave exactly as one who hasn't read the manual properly would hope, but in this case, all it takes is three clicks per Cl atom, and there you have your electron pairs all dotted in. Easy, like I said. Most of the time BKChem works just fine without kludges of any kind.



Great! ... but what's with the Cl on the RHS of the RXN? I went Atom|Mark|electron pair was already set, so went click, click, "?".

Firstly I have only one electron pair on that atom (what matters); and secondly, that pair is skew. I assume the assumption is that you can take it as given that the other valence electrons will all be present(☺), and that the only one of interest is the radical electron - thence the program's noncooperation in supplying additional electron pairs. (In this case it's actually quite courteous of it to supply even one pair). As for the skewness, that's simply because the program is set up for line drawings of a certain angle, so the electrons are nicely aligned, and our Cl₂ is the one who is skew.

Good and well, but how to make up a radical with all valence electrons showing, then? (This is what our lecturers require). Well I'm sure there must be a civilised way of doing this, but ...



... but wouldn't it be nicer to just Kludge together a solution?

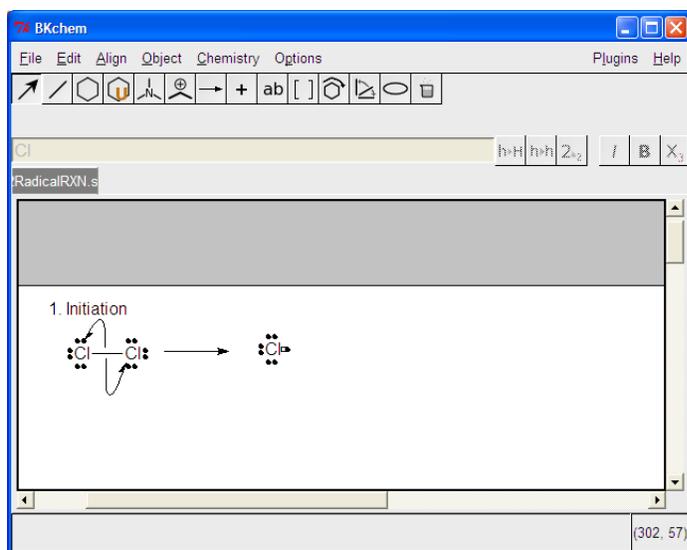
... like clicking in a single bond, then designating one end of it as a Cl atom ...

... and then twisting it to force it into the horizontal plane (totally unnecessary, really, because the program does allow for changes in bond angles) ...

Once you've done that, you can put three easy klikki klikki electron pairs onto the Cl, and then turn the hidden Carbon into a radical. (Well it will

be hidden when I'm done with it).

This does work, and it really is a kludge, with all the ugliness that that word connotes. Here it is:

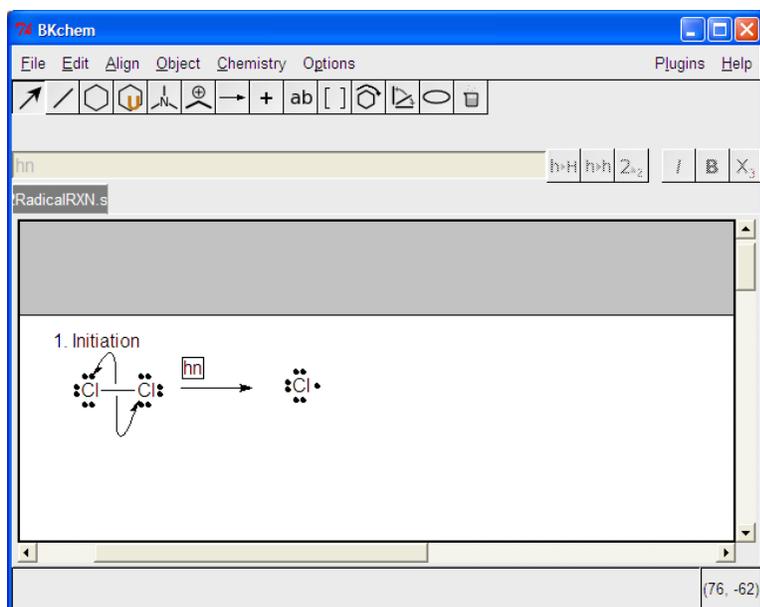


... and don't you worry your pretty little head about that square you see; it'll vanish as soon as the next object is selected.

The tragic thing about kludges is that they're one-off solutions, generally. For instance, in this case, when I try to copy and paste my kludged radical to the Propagation reactions later, BKChem will try very hard to insist on it's nonetheless behaving itself in a civilised manner. Civilised sigma bonds must have the decency to flash a little bond to show its existence. So BKChem will bravely insert a tiny little length of bond between the Carbon and the Chlorine, and will fight

back if I make attempts to scrunch it up and make it vanish again. So the only way to perpetrate the kludge later on is to go through the whole schlepp of making the bond, twisting it in a direction it has no desire to go in, clicking in a Cl, etc. etc. etc.

So there's much that can (and has been said) against the kludge. However, if you're pressed for time, and are too lazy to RTFM to boot, they have their virtues. They get the job done. Sort of like the chewing gum that held Chernobyl together I suppose... On we go! Forget this philosophy! Leave it to others to have a philosopher within. We are chemists at heart with little concern about rubbish like that. More Chemistry! More Chemistry! ... How about putting a nice little $h\nu$ on top of that reaction arrow, then? Go on! I dare you. Before going on to the next page, have a go at putting the expression $h\nu$ on top of that reaction arrow. !

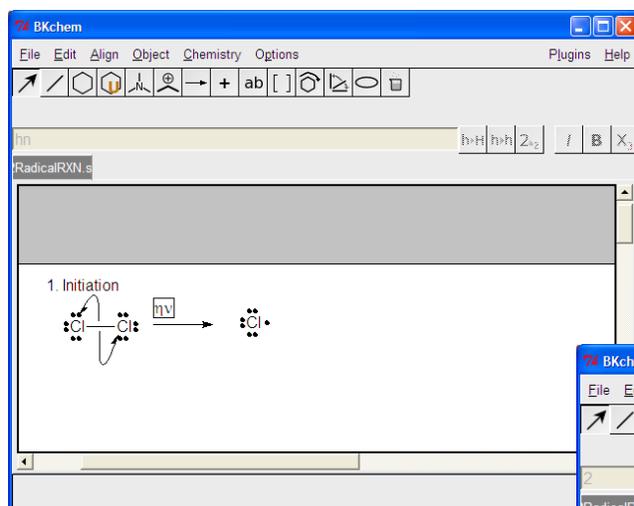


Yes! You're absolutely right! That's how you start.

But how do you then make the "n" Greek?

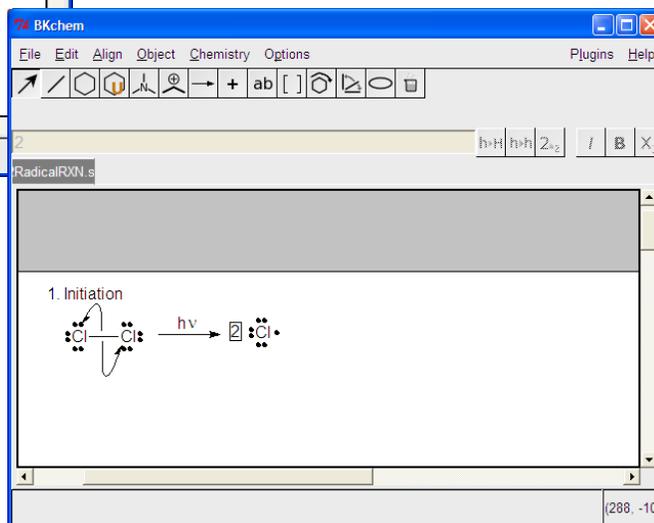
(BTW - there being space for an aside here- v isn't Ancient Greek. The symbol is a later European invention. Greeks just used N. It was either Biblical scholars or mathematicians who invented lowercase Greek much later on-- and, typically, I can't remember which. Take this with a pinch of salt. On rare occasions I'm less perfectly right than usual).

Come on Watson, when all reasonable possibilities have been excluded, the other reasonable one must be true. Just change the font. How do you do that with say a Word document? Right click, ja? When in doubt, Right Click. This is going to get you out of another pickle quite shortly - and it's not a kludge, just a hidden feature of the software, to be used with all the blessings the programmer can bestow.

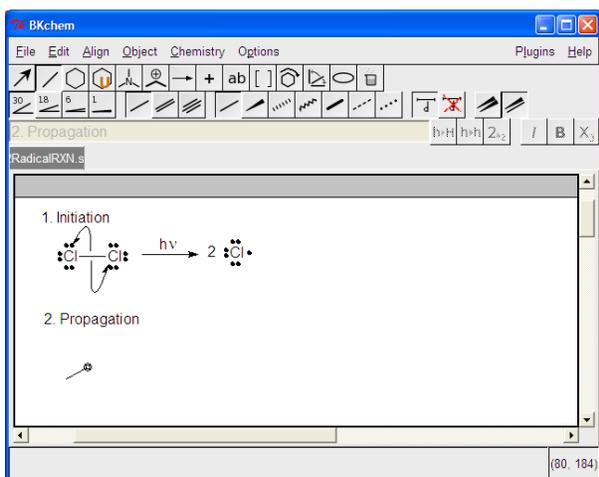


Eyish! So near and yet so far...

Set your font to Symbol, and you're nearly there. Those with a deeper knowledge of fonts would follow the basic principle but produce a more civilised solution to this last little problem, but mine is such an obvious kludge I'll keep it a secret and just show you the result.



(Tip: Stop ~~double-clicking~~ that text selection box, and just **click the text button** instead, to call up the text entry box, where all editing is done).

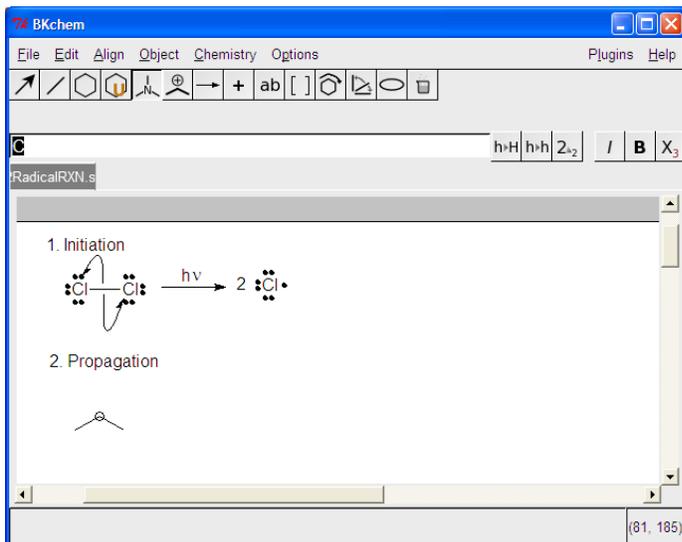
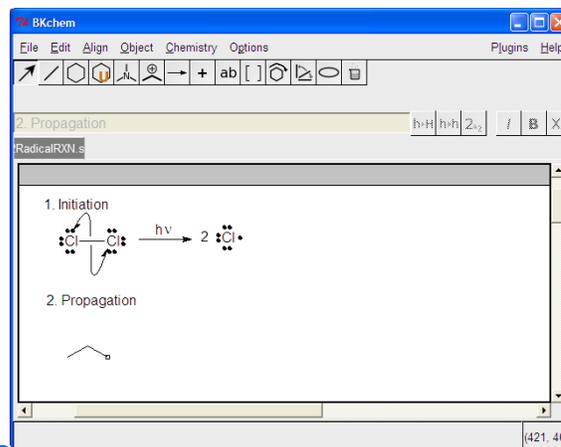


For starters, let's have some propane for the Chlorine radicals to assault. Just click once for one bond, then select one end (the circle round the square indicates that the unseen mouse pointer is hovering, ready to click at any moment)... another click, and it is done.

There's our propane, but the lecturers would like to see a Lewis structure, rather than a line structure.

No problem, let's edit the atoms as before, and put some Carbons in...

...

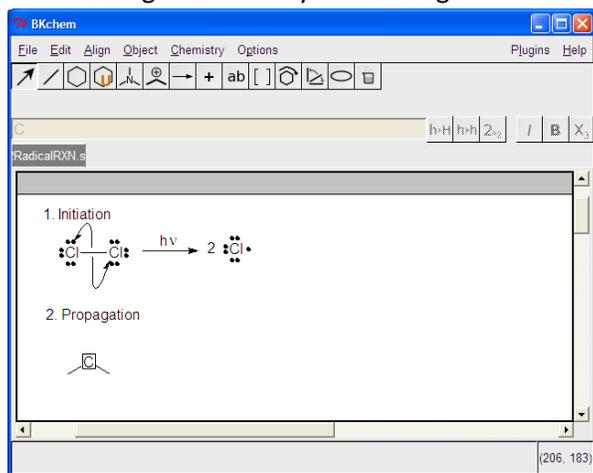


only problem is the carbon I've Entered here refuses to show. Oh dearie, dearie me...

tut tut

I really did push Enter - Really Hard, TOO. Nothing. Nada.

Ah! The program is set up for line diagrams, which is what you graduate to once you know what you're doing in Chemistry. Fair enough....



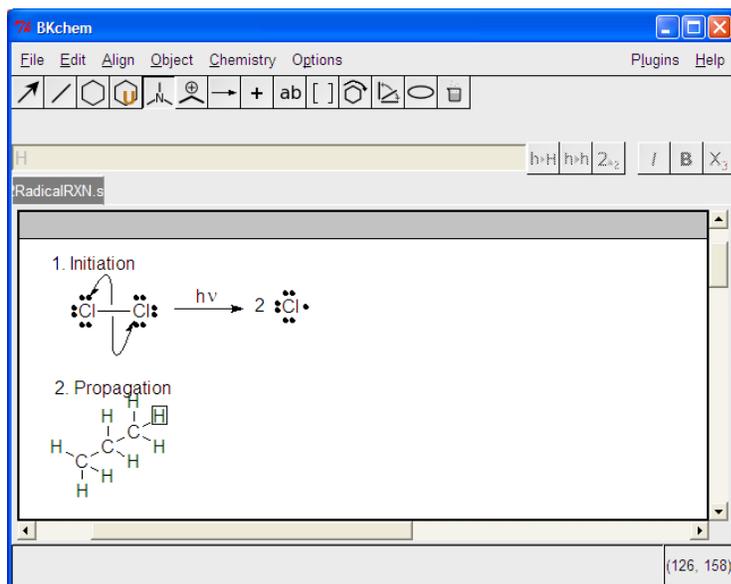
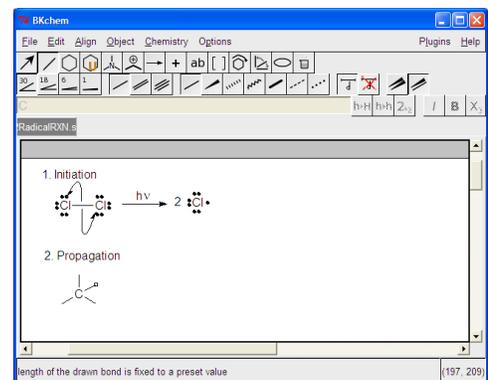
But I want Carbons, and there seems no kludge at hand to fix this one...

No kludge required. Just **right click** on that selfsame junction of the lines that you tried hammering Carbons into, and examine the options that pop up. When you find one that appears to be a solution to your problem, choose your solution and see what happens... and so on ... the technique should be quite familiar to you...

There seems to be a Carbon SHOWing (nudge nudge wink

wink) now. Good. And BKChem is very clever, too. If you click repeatedly on the same Carbon/Line Junction, the program will keep adding sigma bonds, radiating out from that point. However, if you exceed the permissible valency you will get a warning. Sometimes when you've made it do a whole lot of things it was never designed to do it will give false warnings, but more about that later. (I have to first remember how to replicate the errors that lead there).

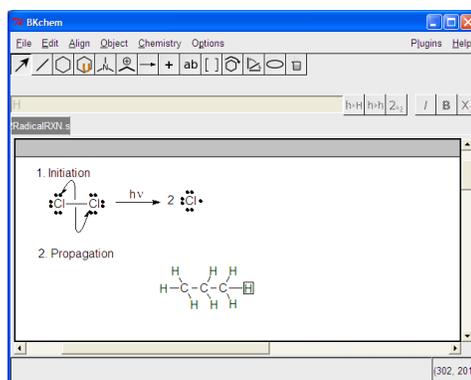
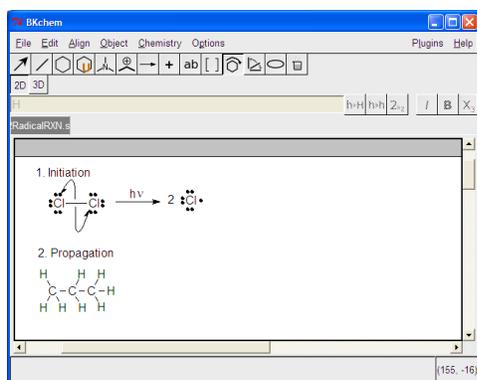
Yes it's a little bit ugly, but that's how to start. It can all be fixed up nicely later.



There we go. Beautiful full Lewis propane... what do you mean it's "still ugly"?

To Rotate, click on the cyclohexane that appears to be rotating. Then click a centralish bond. Then rotate. It's that simple. In Rotate mode, the molecule needn't be "fully selected" - so to speak. I think later I'll just do a picture to explain what I mean. In Rotate mode there's no indication that you've made any selection after your click, but you can rotate the molecule. Just try it and you'll see. Don't be put off by the lack of

feedback. Who needs it when something works that simply?

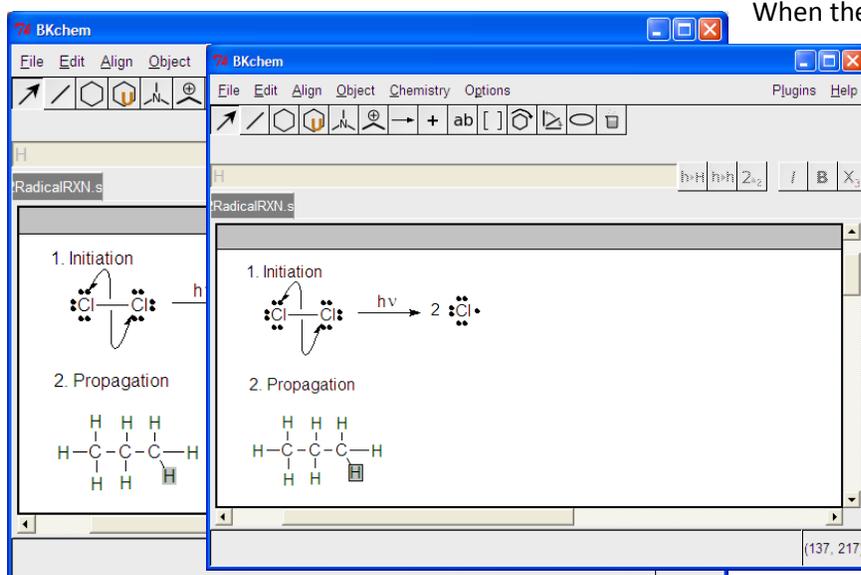


But what happens if you just Pounce upon a Hydrogen and forthwith commence to drag it across the screen? The whole molecule will move

and rigidly maintain its shape.

Solution? Well it's obvious, isn't it? Just chuck all your toys out of your cot and start screaming very loud. That normally fixes things pretty well...or...

1. Select (klikki). Treat that as a kind of "knock on Hydrogen's door". ie. *let go*.
 2. Click and drag. Start to stretch out the Hydrogens to wherever your Creative Impulse drives you to drag them. Let some or other thing be your guide or something like that. .. Or just do what makes sense.
- (Notice that you now have a nice easy trick for moving molecules around: Just Pounce on an atom, and immediately start to drag it, without waiting and clicking a second time).

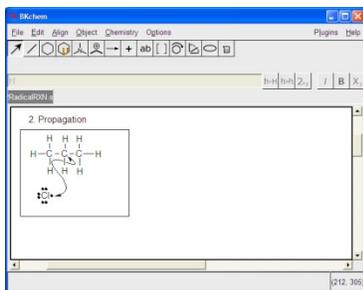


When the hydrogen is grey (no little box around it), then dragging it as is will drag the whole molecule, without altering the molecule's shape.

When the hydrogen has a little box around it, if you drag it it will "stretch away from" the rest of the molecule, which will stay exactly where it is.

Best to reduce such things to simple rules such as these.

Now we're ready to start using the "Edit" (or select) arrow to avoid unnecessary work (and I've skipped a few steps ahead to do the same):



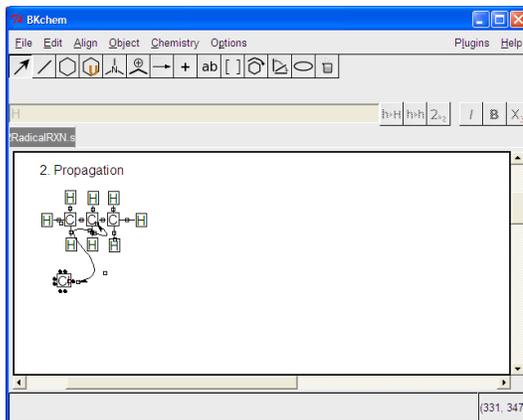
Drag a box right round the edges of any region you want to copy as a whole. (ie. do exactly what you'd do in any other program). Rather make the box too big than too small, otherwise you end up missing bits you wanted to keep. (It's as easy as clubbing baby seals to delete any superfluous bits you copy, so don't concern yourself with selecting "too much"). Then do

the usual ctrl-c, ctrl-v copy and paste.

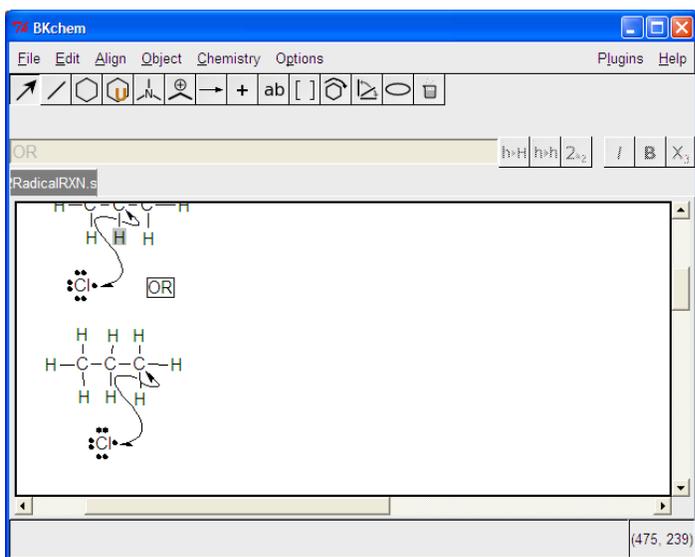
This is what you'll see when you release your mouse at the end of dragging your box. Grab any piece and you can move the whole lot anywhere.

You'll get no feedback when you click on the spot you want to copy to, but don't let that phase you. Believe me:

You can trust BKChem to behave beautifully in copy and paste operations. (It even went and refused to ruin the radical I copied - possibly because I dragged a big enough box round it).



As you well know, in this reaction there are two possible reaction paths, with the radical attacking either the secondary Carbon in the middle or one of the primary Carbons on the ends. I can't think of a nice way of presenting that using split reaction paths, so I'll just copy and paste, and then simply drag the existing reaction arrows to a new location. Again, I'll jump straight to the result.

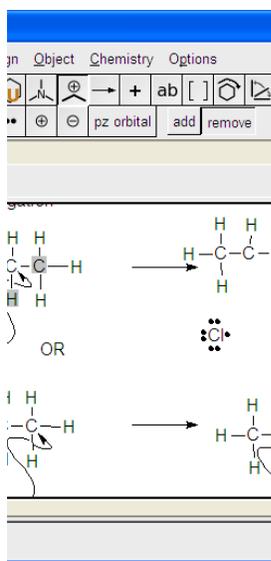


Easy kapeazy. Though my copy does appear to have suffered some damage - probably due to violent mishandling of some or other handle on landing. Don't blame BKChem for your own mistakes.

But I suppose that bloomin' inner artist of yours is so distracted by now by the beauty of the left hand arrow, that you're scarcely paying attention to the chemistry any more.

"How'd he get it all nice and curvy like that?" is all you can think of. Well put it this way: you can put an arbitrary number of

handles on a spline. Keep clicking beyond what's absolutely necessary, and you get a more complex spline. I don't think I need say any more than that. Play with your splines if you get the urge, and you'll quickly have it all figured for yourself.

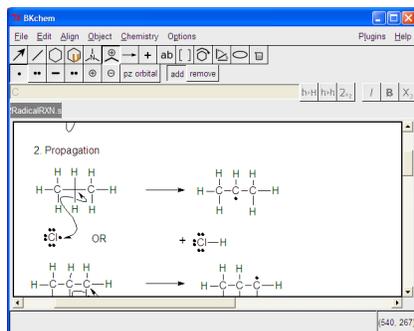


Notice that if you want to remove dots and other marks, you can't just delete them somehow. You have to select the REMOVE button under the Marks toolbar. With this selected you just click to remove the mark selected on the left. BKChem will complain at you if you use the facility incorrectly, so the only remark I'll make is simply that you have to use the Remove button to remove things.

You can see I've just left the copy of the propanes, arrows and Chlorines on the clipboard, and have pasted them across for amputations of divers kinds. Some odd little artifacts like the greyed out atoms, I can't explain.

There's no feedback from this kind of cut and paste, but as I've said before, that's nowt to worry about.

Now let me try removing that radical from the ghost carbon (if it's still there).



There we are. All neat and tidy, and ready for the next step:

Copy and Paste each of the radicals, and then Copy and Paste a Cl₂ for each one, to participate in the radical recycling step of the chain reaction.

The artifacts are easily removed by selecting and then selecting a blank space. I think they result from my touchpad "snagging" things accidentally, occasionally.

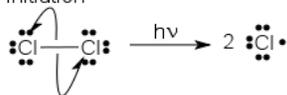
There's nothing more to learn from the processes, so I'll just go and finish up my question, and then show the final result .. Oh yes ... once the .svg file is done, you have to Export it as a .png file (or some other graphic file if you know of a better one) if you want to paste it into eg. a wordprocessor document.

File | Export -- and select from the popup that appears. I just accept the defaults BKChem offers, but if you know better, once again you can please yourself.

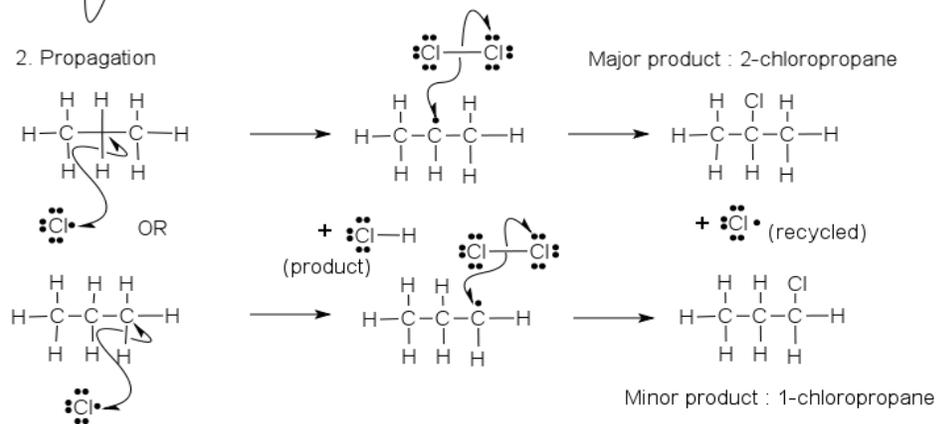
The radicals let me down by refusing to produce false errors, so for now I'll just tell you how to sort out those, as well as little minus signs that suddenly appear, and stick like glue to your Carbons. RIGHT CLICK. The problem concerns Charge, so look for a menu option to do with Charge.

In fact this particular example has worked so well as a "demo model" that I wonder if I'll ever do a "Problem 2"...

1. Initiation



2. Propagation



3. Termination - radical to radical reactions eg.



And here's that .png file that I pasted into my assignment document (at long last).

Long live BKChem!