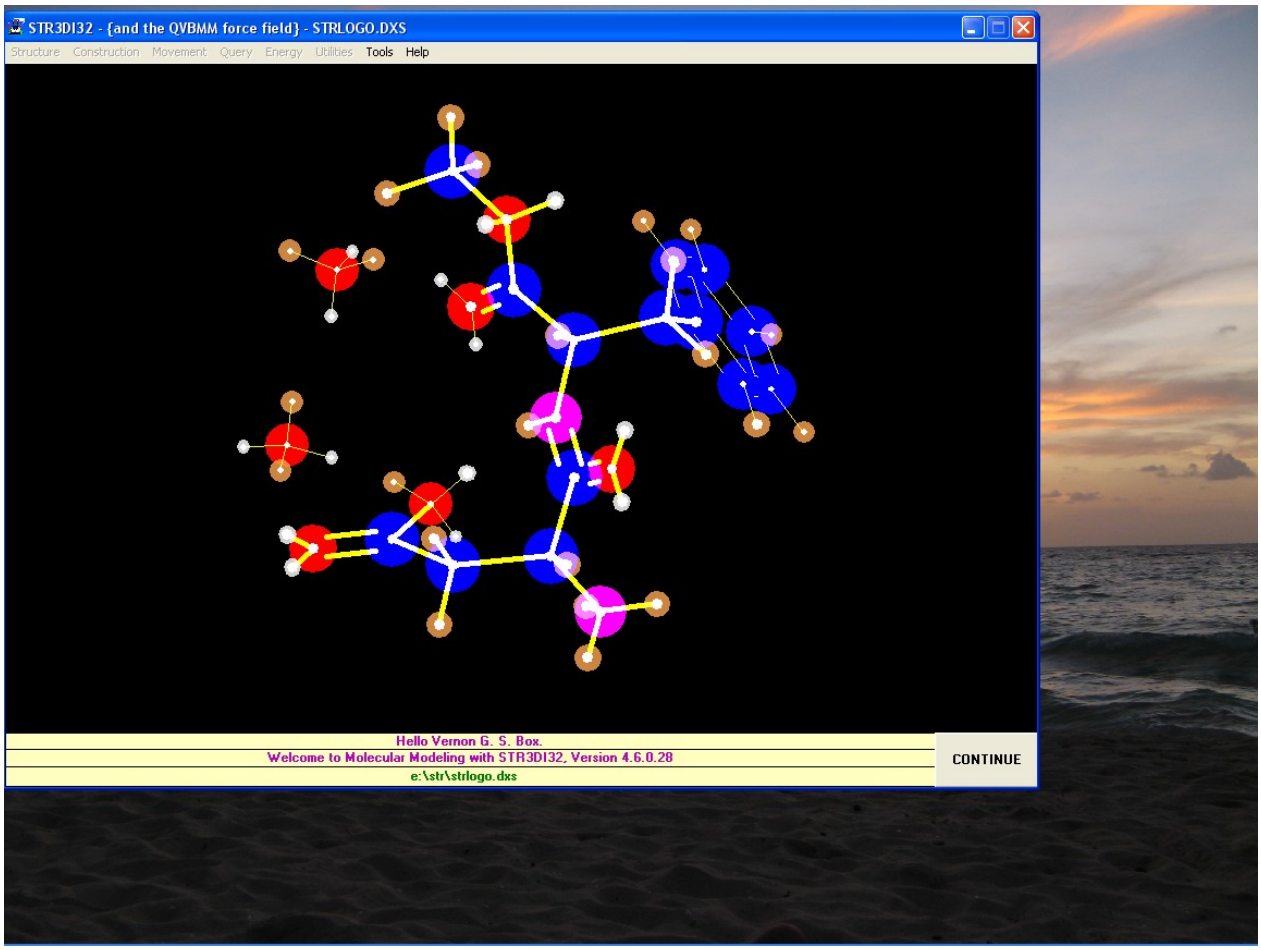
Welcome to StruMM3D



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Introduction

We have put together a short sequence of graphics showing StruMM3D being used to construct a simple monocyclic molecule, piperidine. This exercise should illustrate the uses of the various controls in the CONSTRUCTION window, that is accessible from the CONSTRUCTION main menu option. It will also show how one can use the other options in the CONSTRUCTION menu to convert the piperidine template into a variety of structures.

Before We Begin

There are a few things to remember before we embark on the exercise.

StruMM3D does not normally allow users to draw single, unattached, atoms as "stand-alone" entities. A single "atom" in a cluster, e.g. a chloride ion will be acceptable, but not a single chloride ion, by itself.

StruMM3D requires the user to create molecules with specified geometry. StruMM3D therefore suggest appropriate bond lengths, bond angles (and dihedral angles whenever appropriate) that can form the bases of the user's specifications. Thus, these suggested numbers can be replaced by the user by values that are desired. This will be illustrated below.

It is best to plan to create/draw ONLY the core skeleton of the molecule. Exiting from the CONSTRUCTION window takes the user back to the main menus where the molecular skelton that was created can be "fleshed" out with hydrogens and lone pairs. These appended atoms can then be transformed into other atoms, e.g. hydrogens to carbons, hydrogen to halogen, etc., in order to further elaborate the created molecule into more highly substituted, or complex, systems.

The CONSTRUCTION window has "boxes" to be filled in to specify the type of new bond to be drawn. These text boxes can be filled from the keyboard, or by clicking on the symbol of an atom or bond type in the lower part of this window.

The host bond (the bond carries the host atom), will always be horizontal, with the host atom (that will be a part of the new bond) to the right. The new atom will be located on an arc the goes clockwise (above the host bond), or anticlockwise (below the host bond) with the bond angle defined by the sweep of that arc. Dihedral angles are measured with respect to the host bond and a flanking coplanar reference atom.

At the top of the CONSTRUCTION window there are controls that specify the direction in which the new bond will be drawn. We have tried to make these as intuitive as is possible.

R- to the right,
C - clockwise from the already drawn host bond,
A - anticlockwise from the already drawn host bond,
I - inwards (from the host atom into the screen),
O - outwards (from the host atom towards the user),
UI - upwards (from the host atom) and into the screen,
DO - downwards (from the host atom) and out of the screen (towards the user), and so on.
UO - upwards (from the host atom) and out of the screen, towards the user
DI - downwards (from the host atom) and into the screen (away from the user).

All of the controls in the CONSTRUCTION window are mouse-active, so you can enter data with either the keyboard by a click on an appropriate CONSTRUCTION control.

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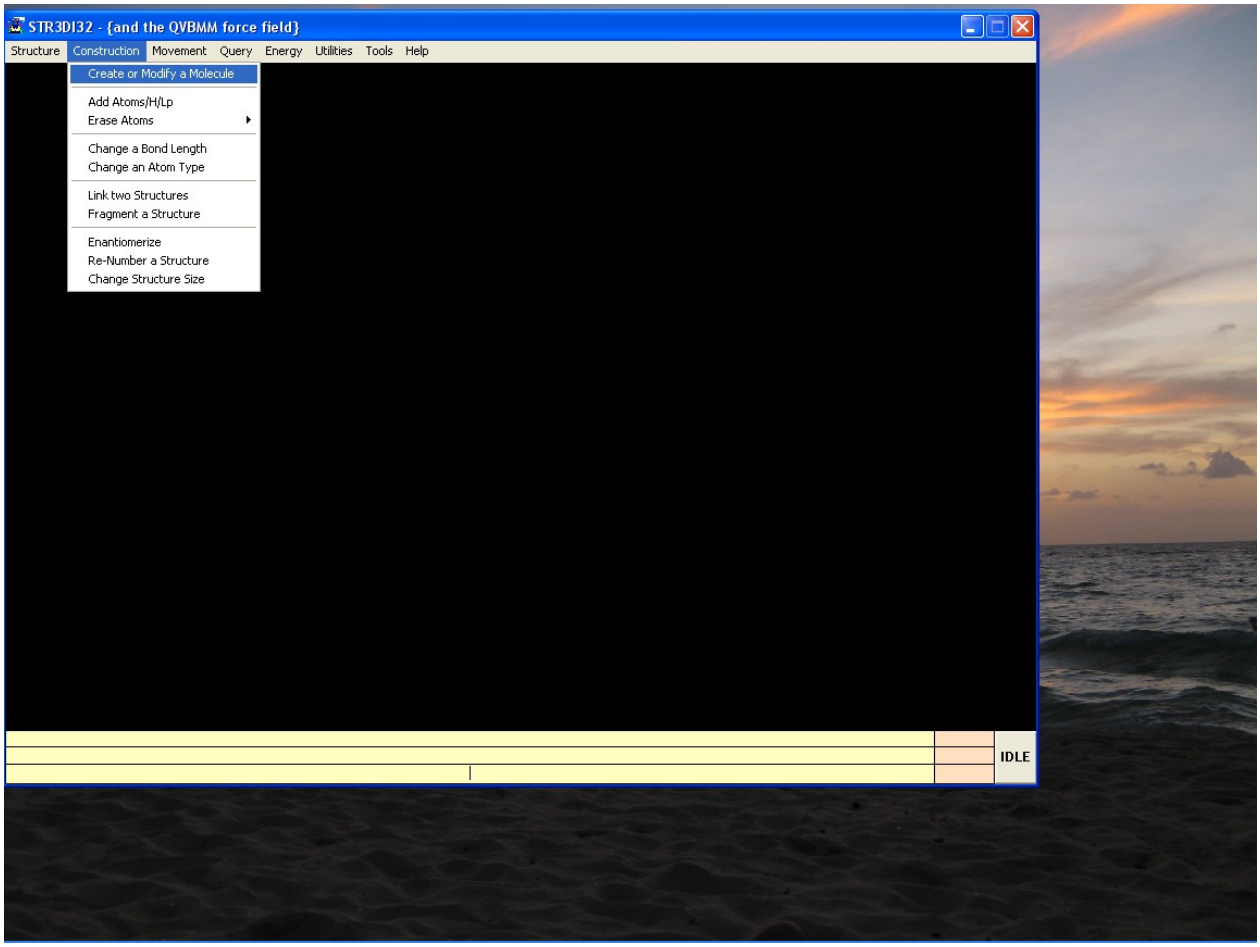
Launch StruMM3D and, after the greeting screen, click on CONSTRUCTION, then in the drop-down menu, click on CREATE OR MODIFY A MOLECULE.



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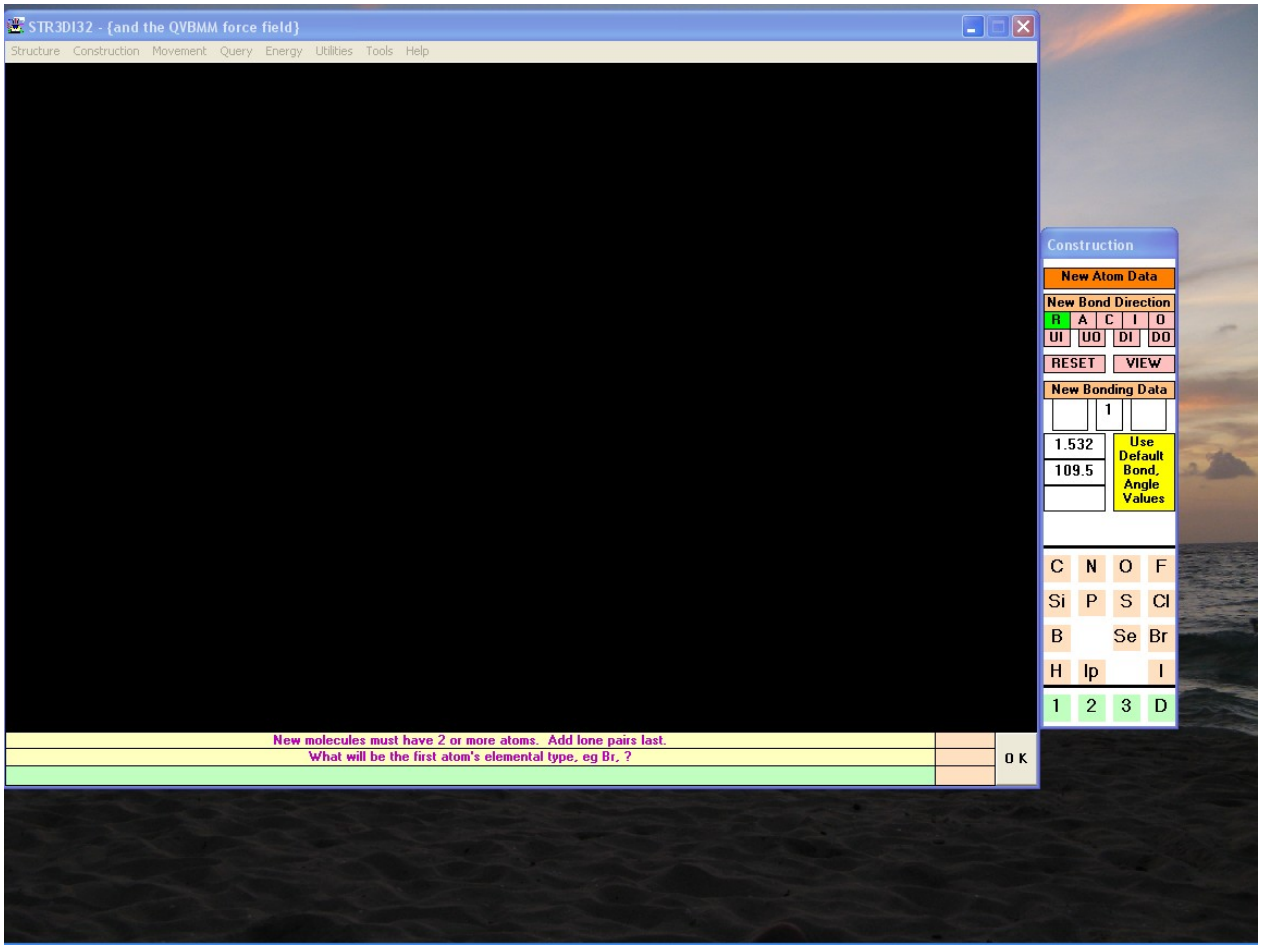
The CONSTRUCTION window is opened, and a set of prompts, which will appear at the bottom of the main screen, will guide you through the processes. Remember to look at BOTH windows as we go along.

The main screen prompts you to decide what type of atom to start the new bond with. Fort the exercise we can enter, from the keyboard, “C”, then click on OK, in the main window, or click the “C” control in the CONSTRUCTION window.



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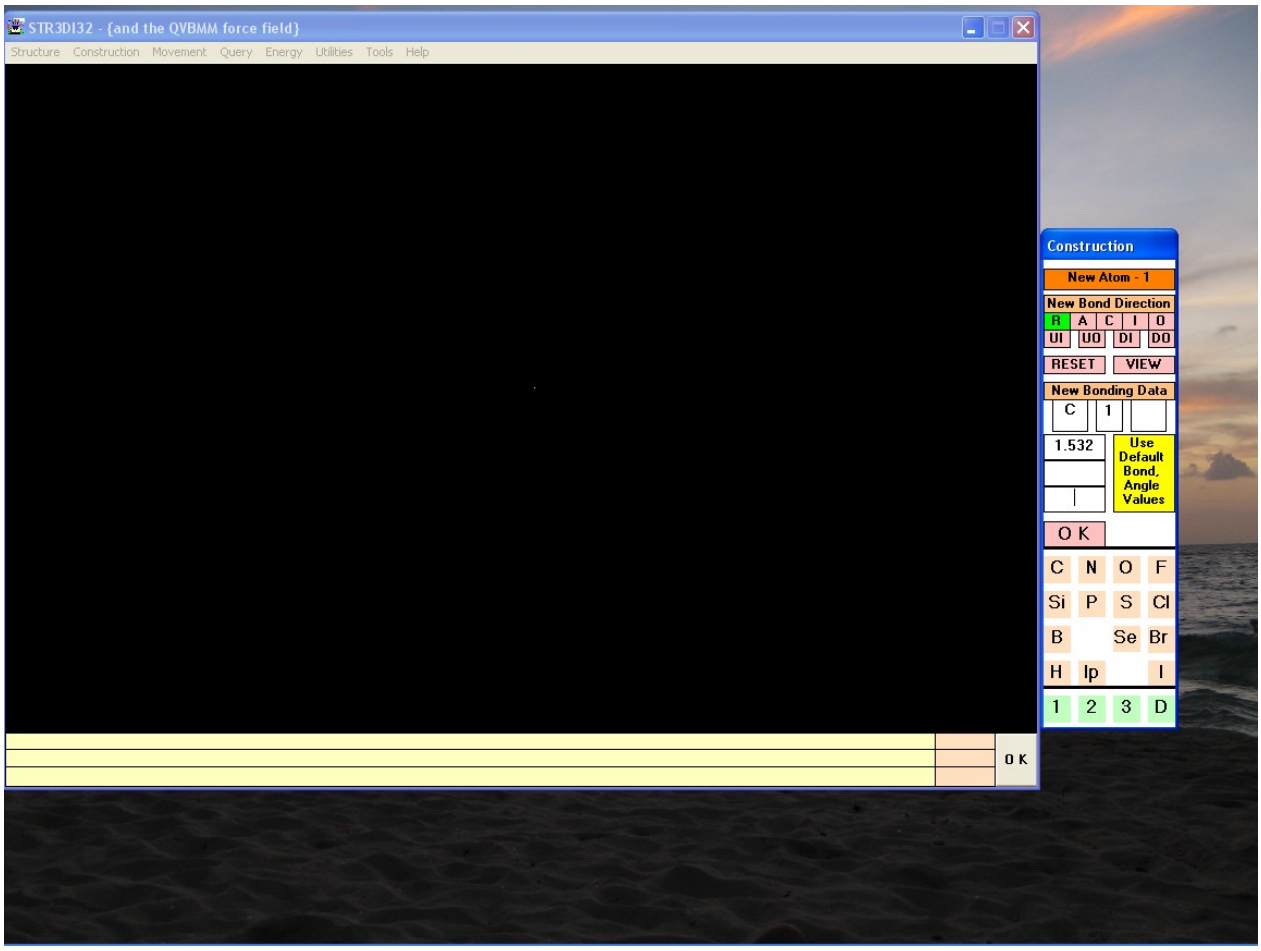
Notice that the “C” now appears in the leftmost textbox of the “New Bonding Data” boxes, in the CONSTRUCTION window. The “1” suggests a single bond, the other box is empty and awaits an atom type to complete the new bond’s data.

Now click on a control at the bottom of the CONSTRUCTION window to select the next atom in new the bond, or you can click on the empty “New Bonding Data” box and enter the atom type from the keyboard.

Any of these parameters can be changed before clicking OK.



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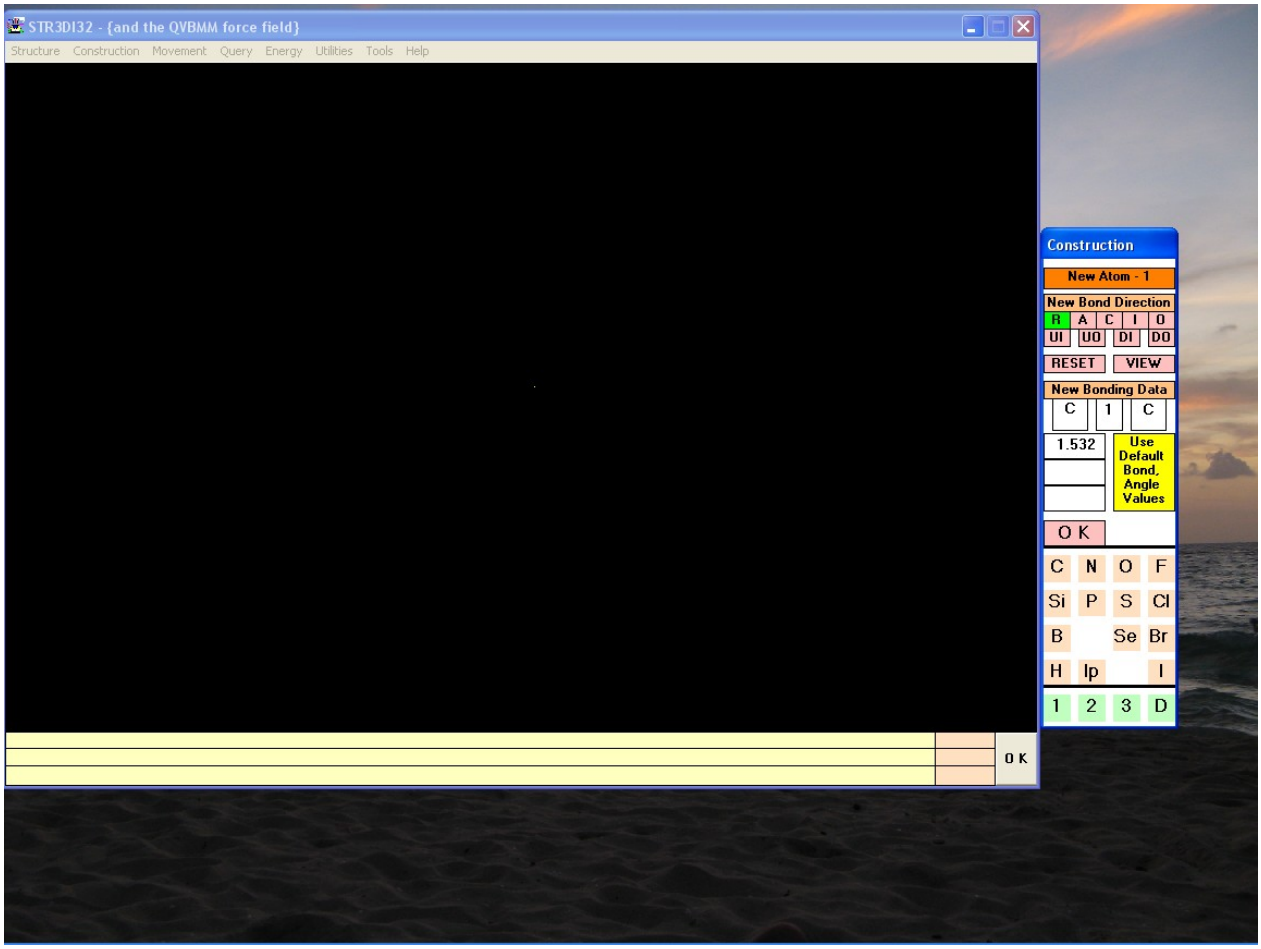
If we enter another “C”, to draw a carbon - carbon single bond, notice that the topmost box below the “New Bonding Data” boxes shows a suggested bond length. This can also be changed.



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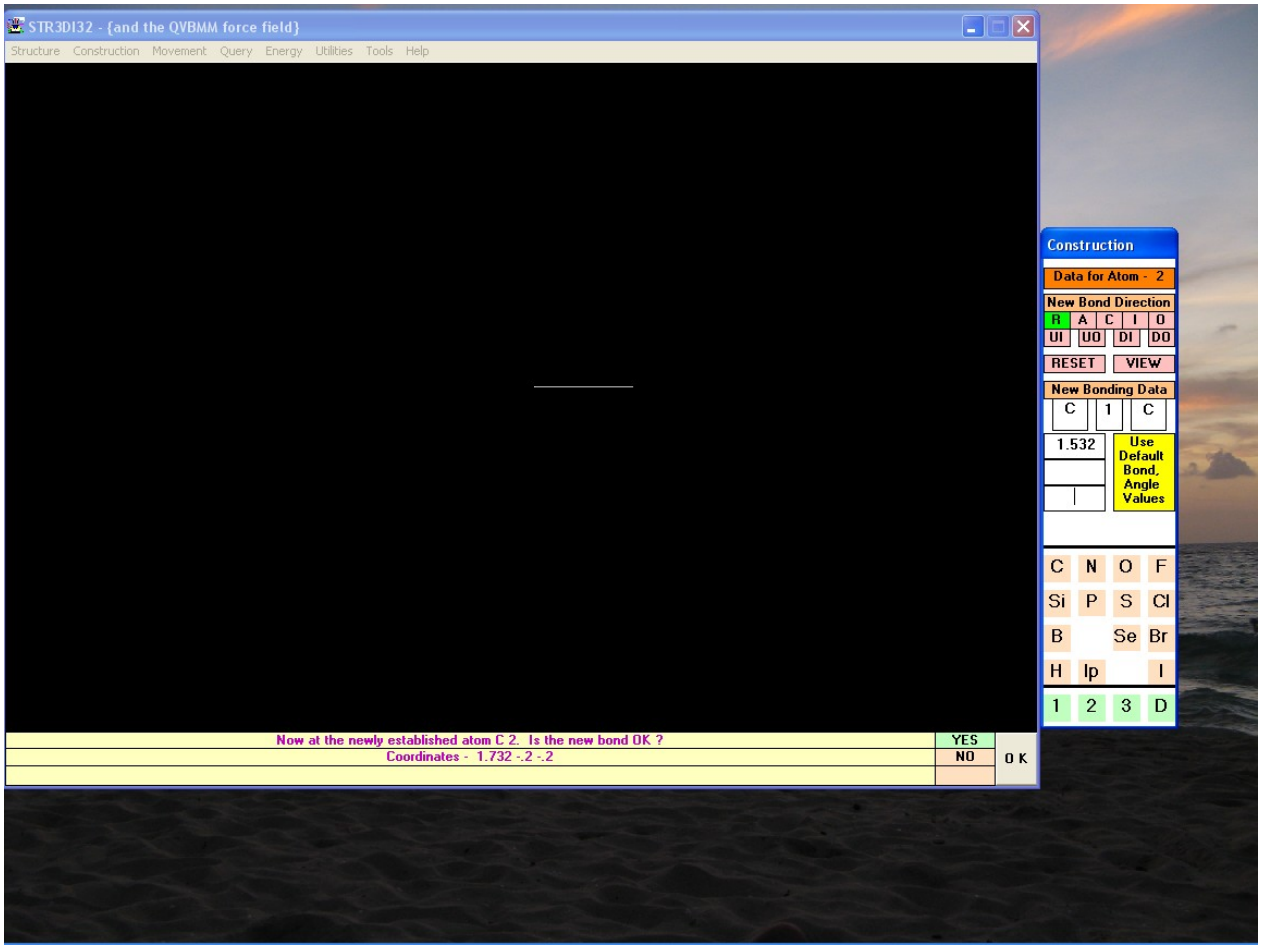
However, we accepted the data, by clicking on OK, and the program draws the new bond. The main screen asks if you really want this bond, and tells you that you are at atom #2. We accept and then …



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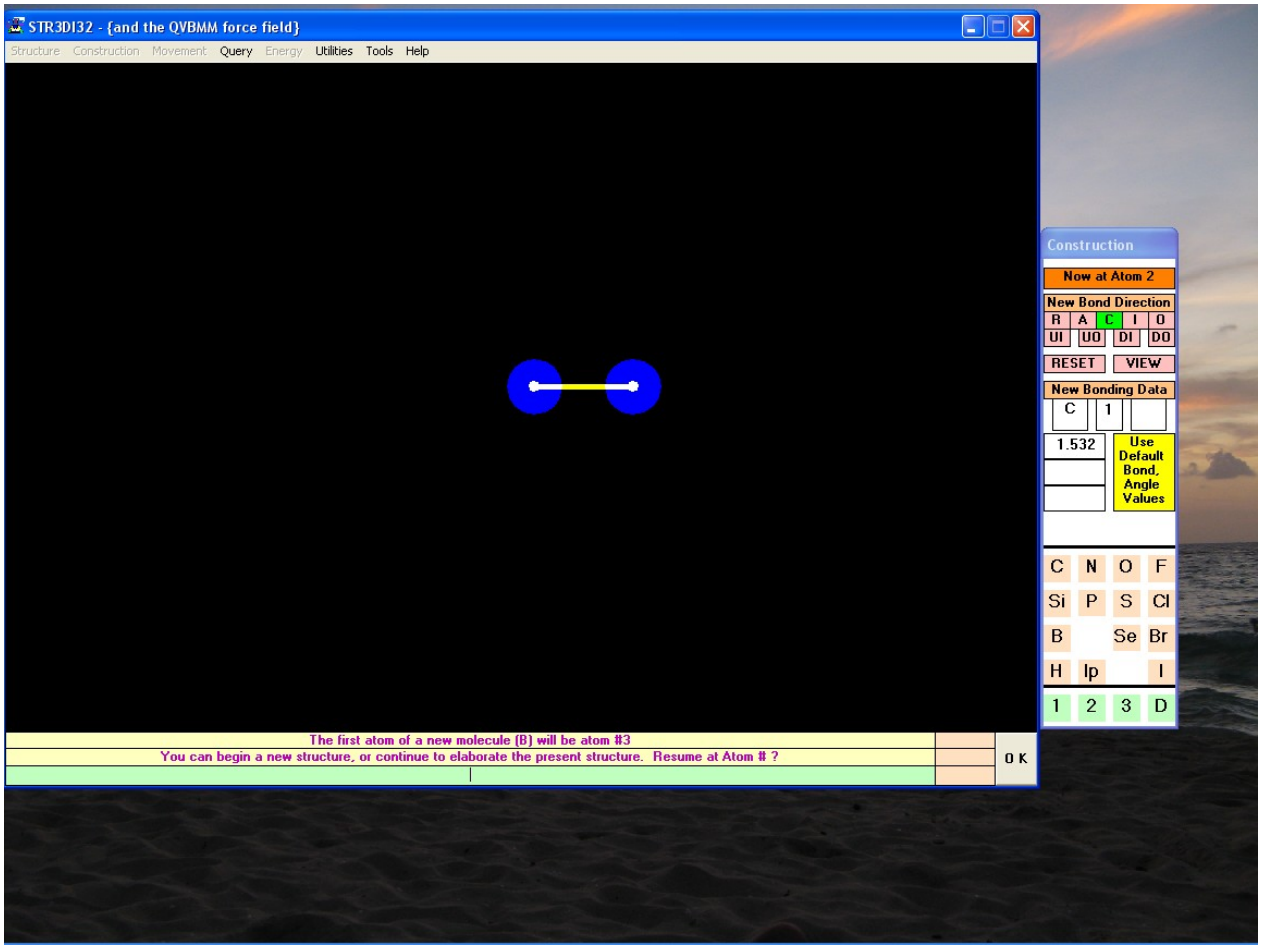
StruMM3D shows the atoms' type colors, and asks which atom you wish to continue drawing from. You now either click on the atom to continue drawing from, or enter a number in the INPUT TEXTBOX of the main window, followed by clicking OK.

This is obviously useful when modifying existing structures. Since the new atom was carbon, the "New Bonding Data" leftmost box, of the CONSTRUCTION window, shows carbon in anticipation of your continuing to draw from that atom.



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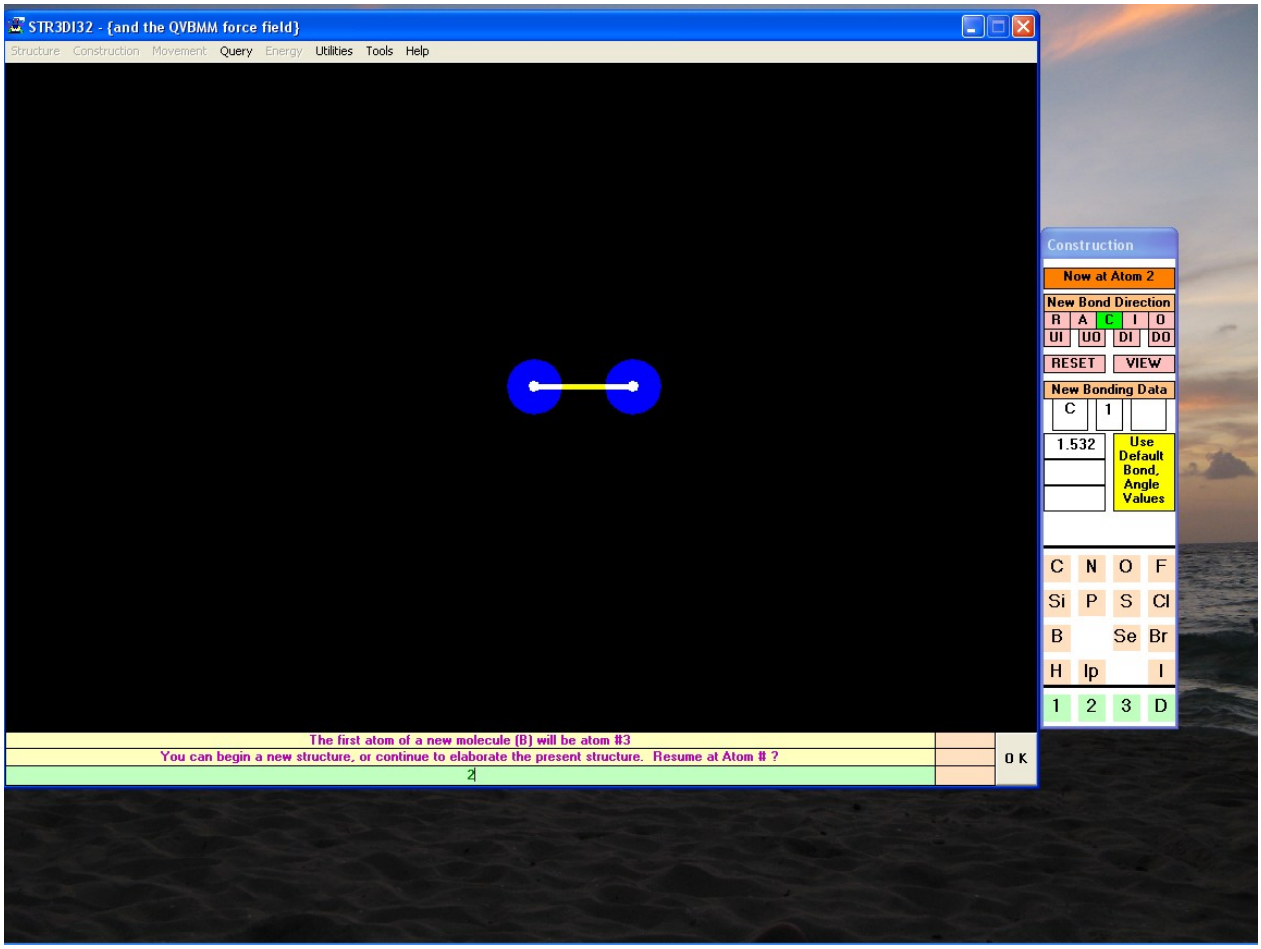
We selected, by clicking on, OR by entering 2 in the main screen's input textbox then clicking on OK, Carbon #2 as the new host atom.



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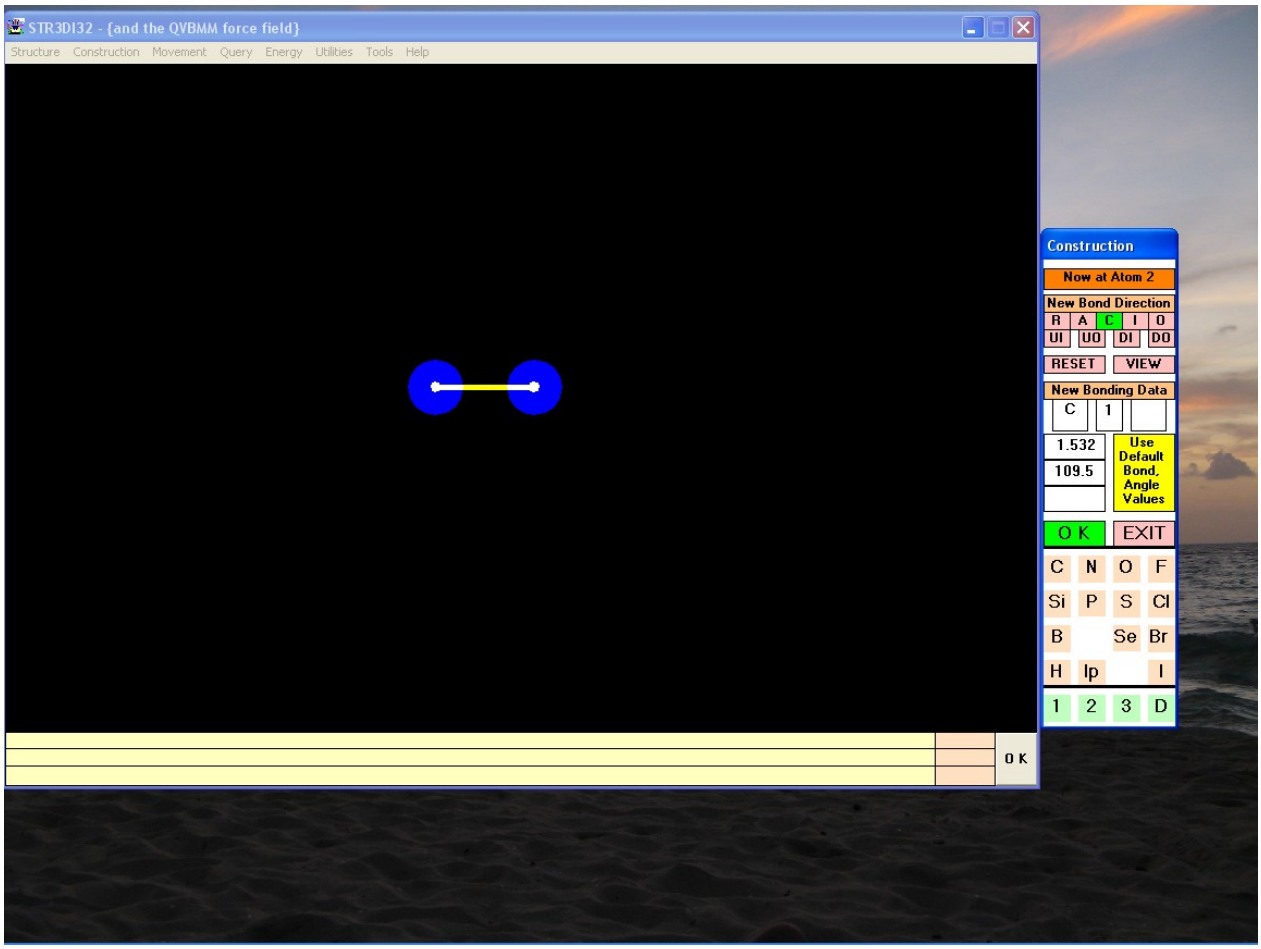
Now we have to provide the next new atom type for the “New Bonding Data” rightmost box, and you will also notice that a suggested bond angle of 109.5 degrees is shown. You can simply click on any of the atomic symbols in the lower part of the CONSTRUCTION window, or click on the empty box and then, from the keyboard, type the new atom symbol, and it appears in the rightmost box of the “New Bonding Data” information set.



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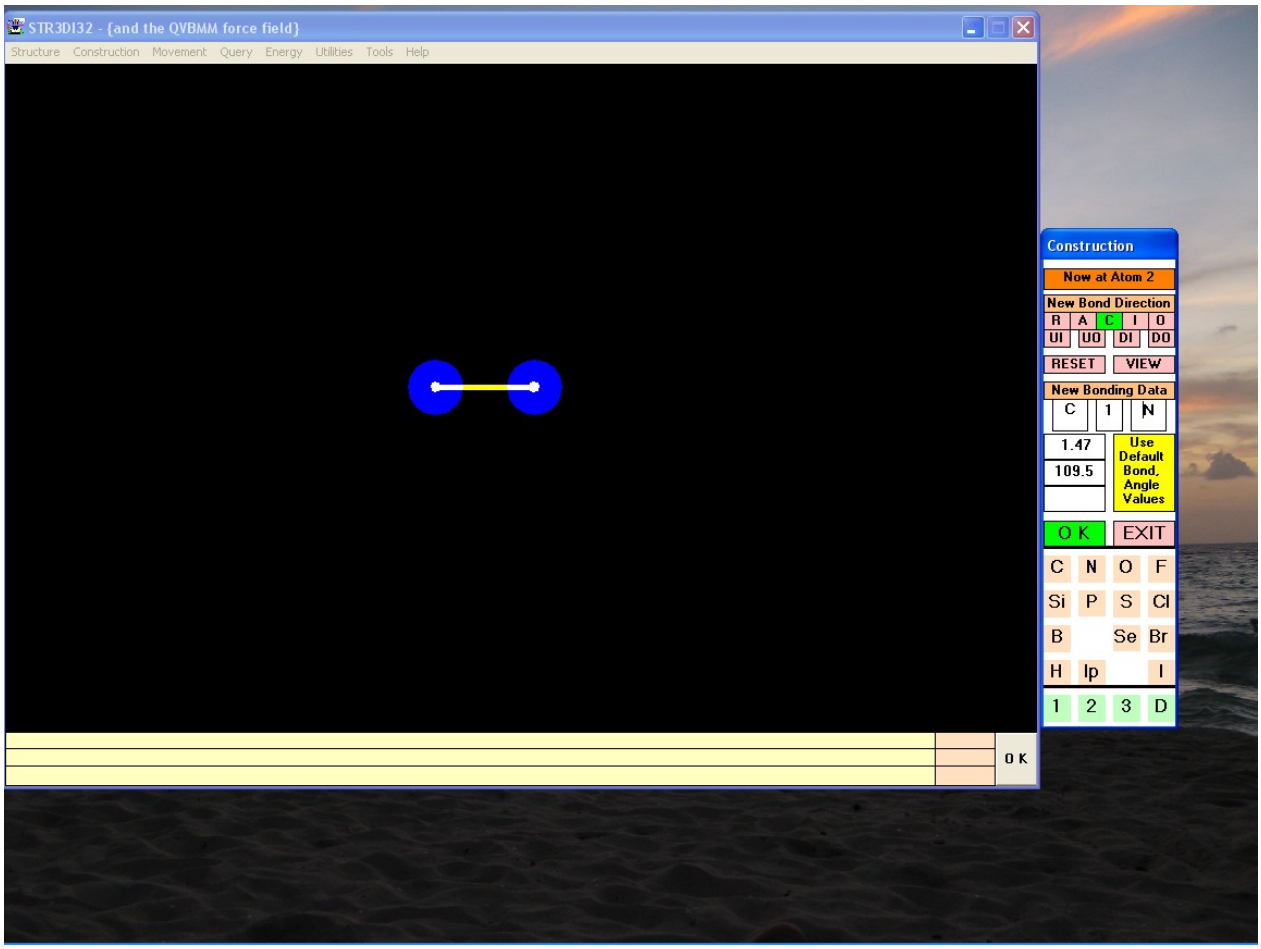
We selected a nitrogen atom. The “New Bonding Data” information updated to show the normal C-N single bond length, which you can alter if you wish.

We also need to tell StruMM3D where to place the new nitrogen. In the “New Bond Direction” set of symbols we clicked on “C”, for clockwise, starting from the recently drawn horizontal bond, linked to the host atom #2. Then we click OK.

Remember that if you change the data in the “New Bond Data” set of boxes several times, you can ensure that the correct bond length and angle data are suggested by clicking the yellow control “Use Default Bond, Angle Values”, which will update all the suggested information.



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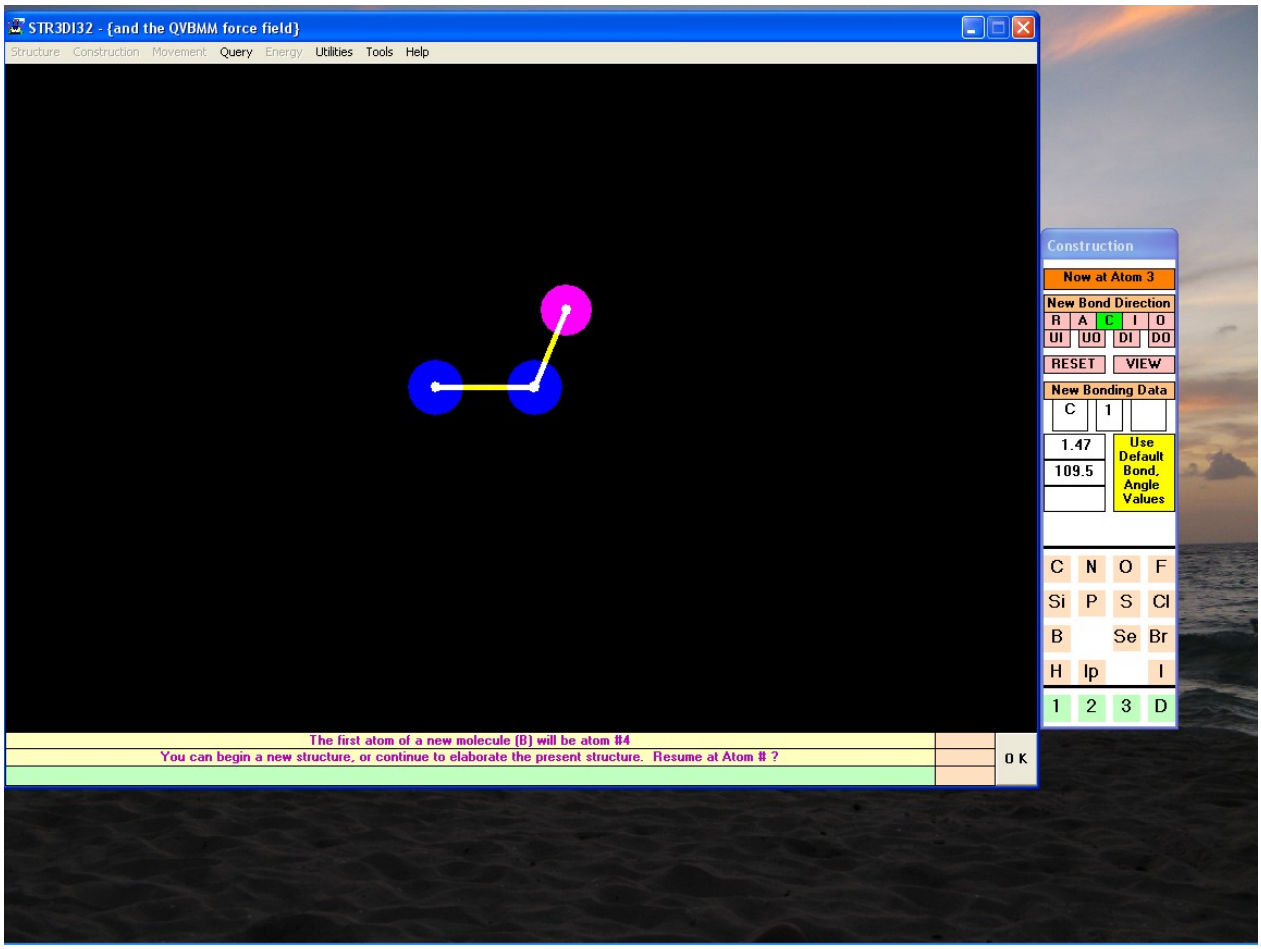
The new C-N bond appears with the new nitrogen at “1 o’clock”, clockwise from the horizontal bond that was pointing to 9 o’clock. This position will vary, of course, depending on the bond angle you select. If we had selected “A” from the “New Bond Direction” set of symbols then the new nitrogen would have been placed at 5 o’clock.

The main screen asks if you are happy with the new bond. If so click on “Yes”, then OK and the atom color appears for nitrogen atom #3. If you had selected “No”, then the bond would have been erased, and you would have the opportunity to do the bond again, with the proper/desired data.

Now you have to decide which atom to continue drawing from. We selected, by clicking on, atom #3.



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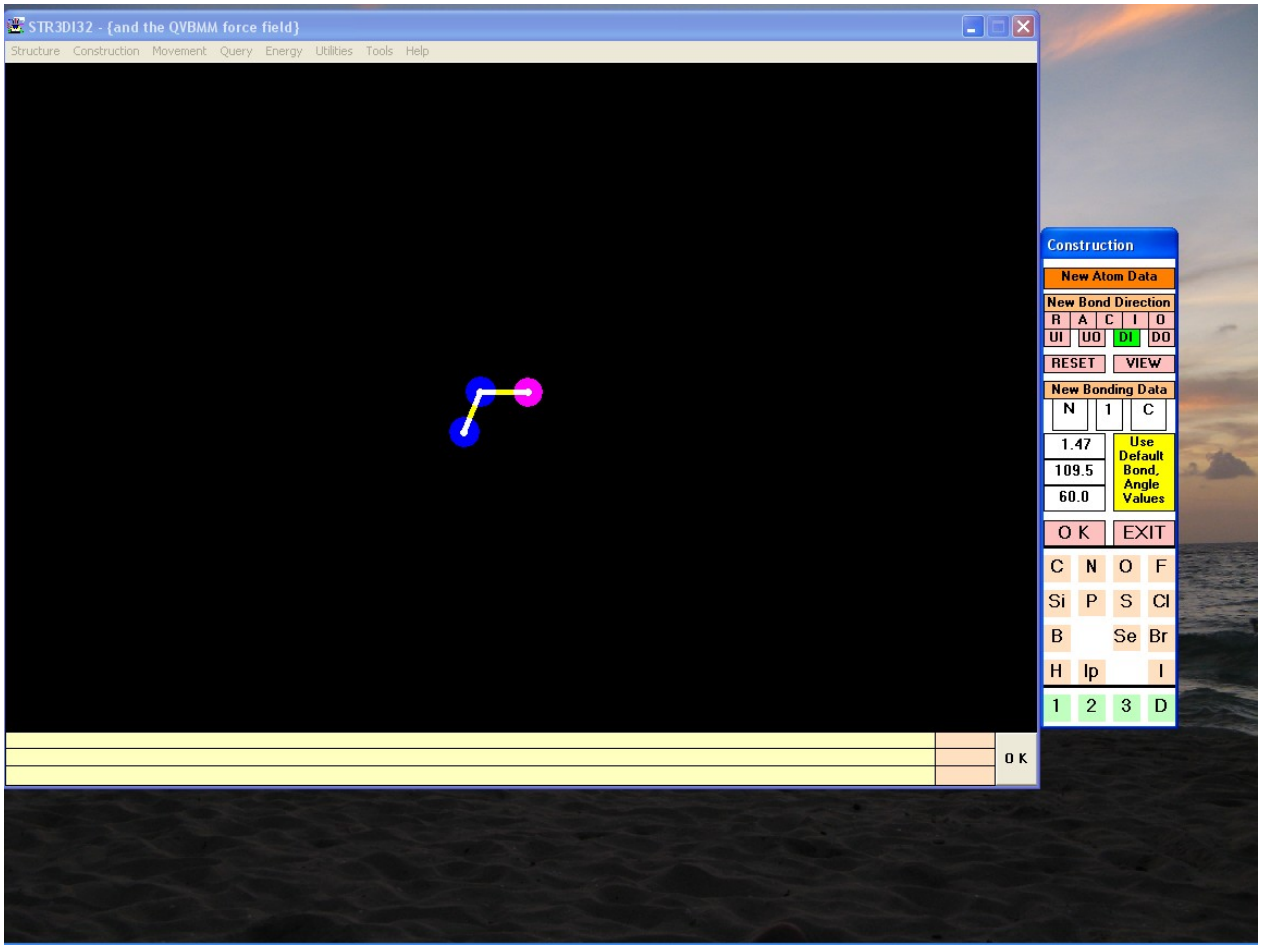
StruMM3D re-orients the 2-3 bond horizontally, with atom #3 to the right, since it will be the host atom.

The nitrogen is now in the leftmost "New Bonding Data" information box. We selected a carbon to complete the new bond data. StruMM3D suggested the new bond length. Now we have to select the new bond's direction. The three dimensional directions are the UI (upwards in), UO (upwards out), DI (downwards in), DO (downwards out) controls in the "New Bonding Direction" information set.

Since we are drawing a ring, then this new atom must be gauche (and on the same side) with the atom #1. So we select DI for the new direction.

Notice that if you select a 3D direction control (UI, UO, DI, DO) then StruMM3D will suggest a dihedral angle value of 60 degrees, which you can also alter. This dihedral angle is measured with respect to the 1-2 bond with is coplanar and to the left of the host bond.

We click OK in the CONSTRUCTION window, the new bond is drawn, and we complete by accepting it at the main screen's prompt…



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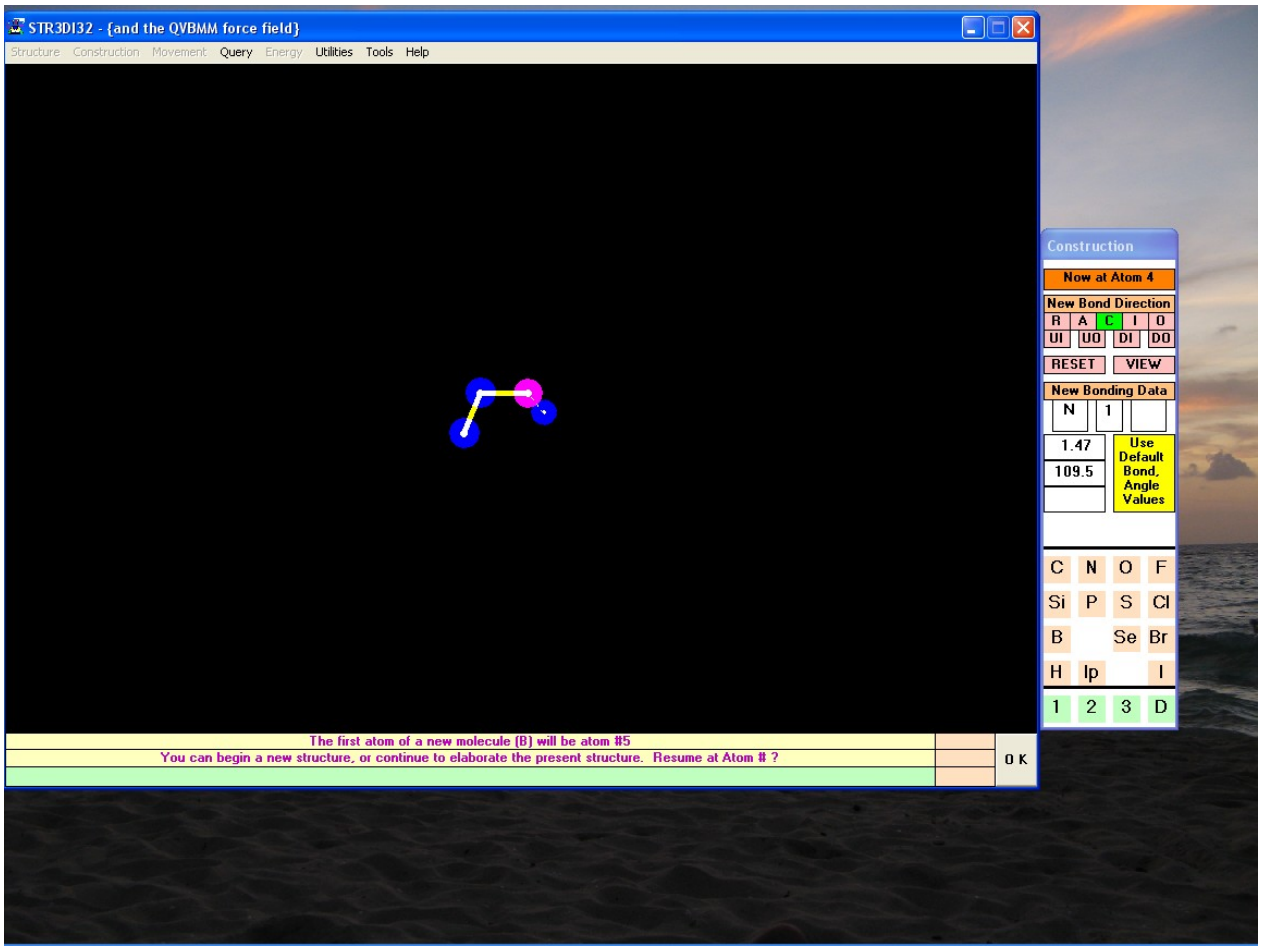
And now we must continue to cycle through these processes described above to complete the structure.

We select atom #4 as the host



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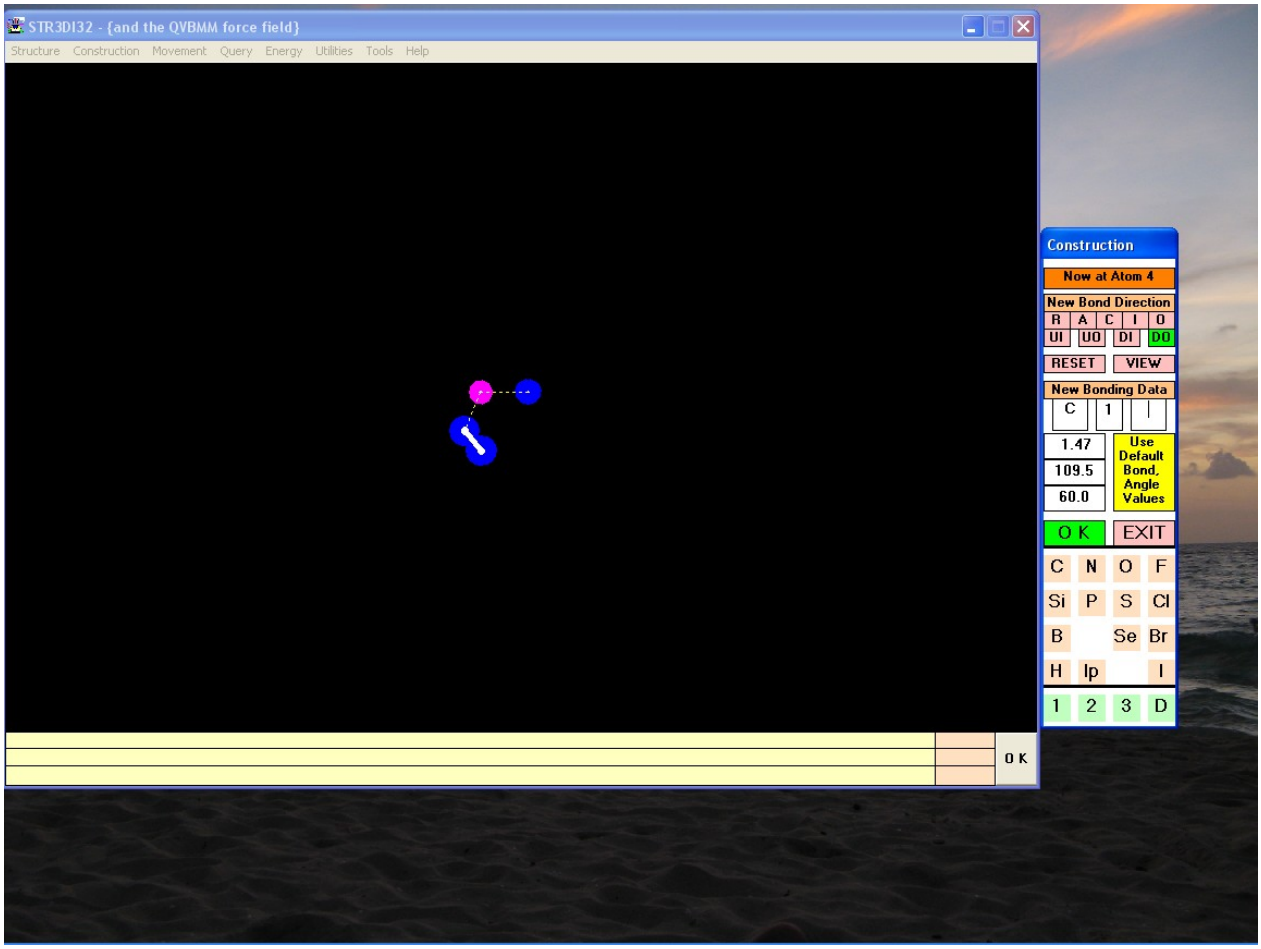
StruMM3D now re-orients the structure already drawn to place the 3-4 bond horizontally.

We are creating piperidine, and so the remaining 2 atoms will be carbons. Since we are creating a ring, then the new atom directions must curl back towards C-1. In six-membered rings, trans-annular bonds are always parallel, and so the new C-C bond will be in the DO (downward and outward) position.

We insert the new data…



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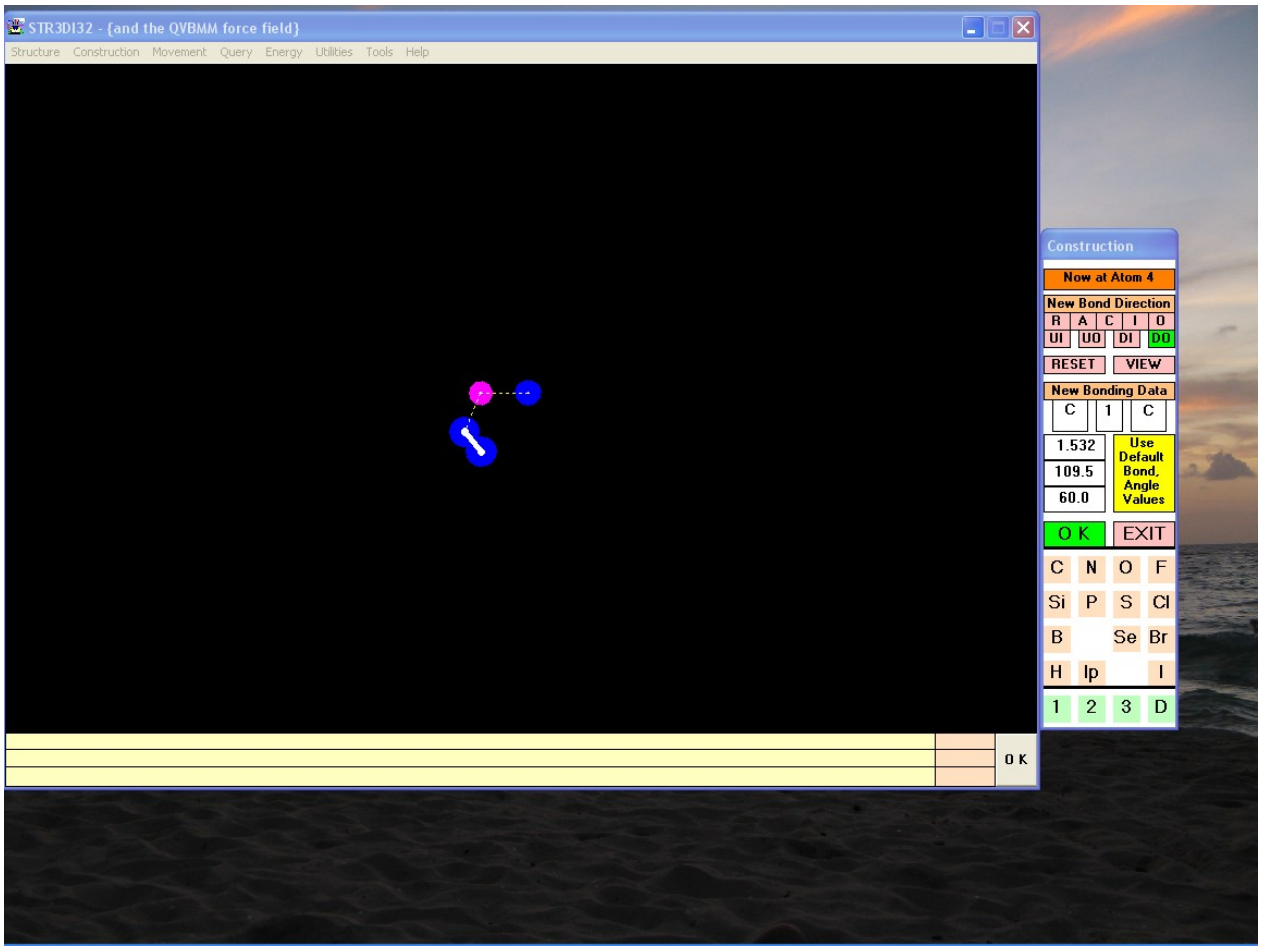
As shown, then click OK.



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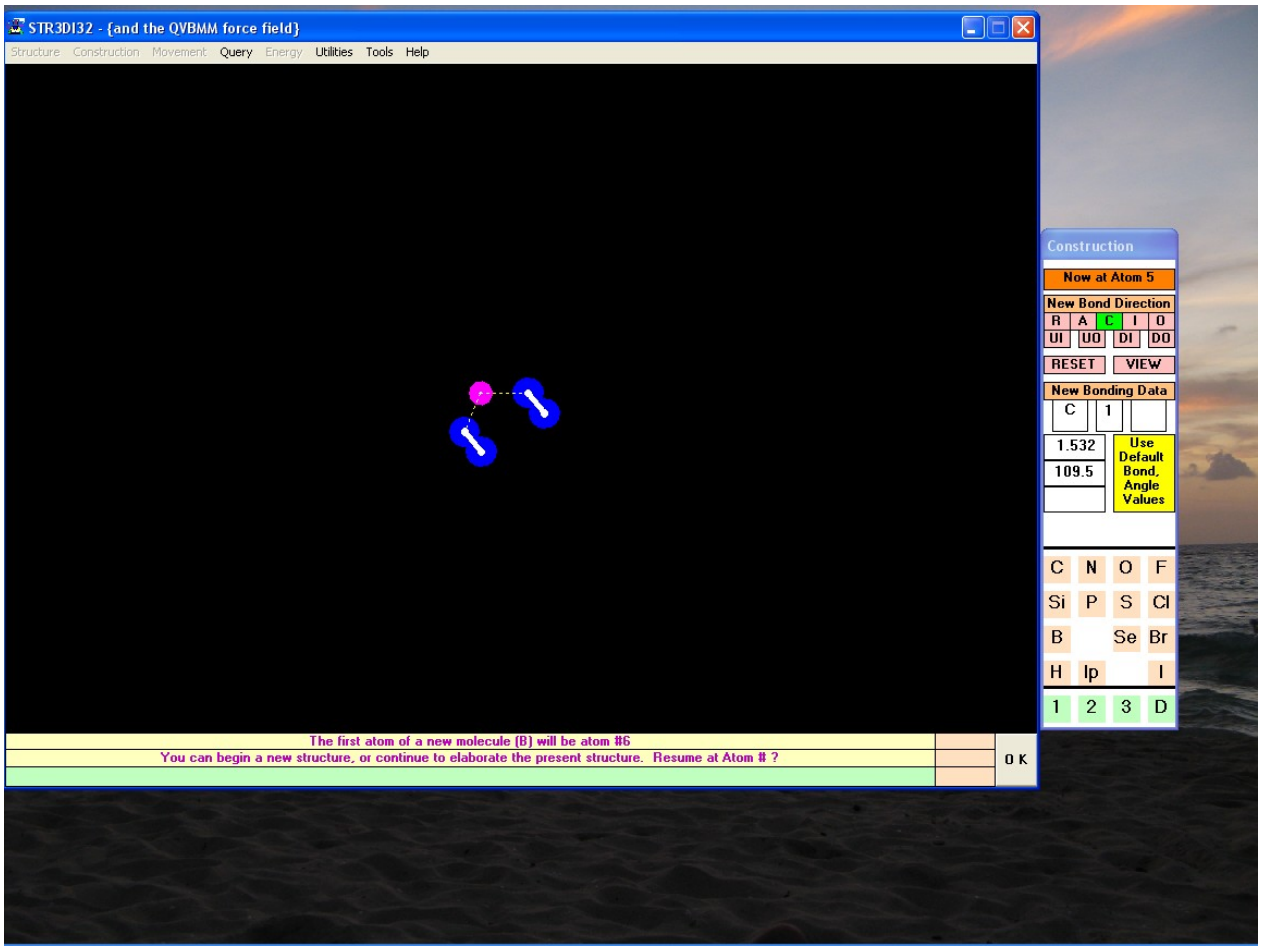
StruMM3D draws the new bond, the main screen asks if you like it. If yes, then it completes the draw and atom color, as is shown below.

We need to put in one more carbon.

We select the atom #5 as the new host atom.



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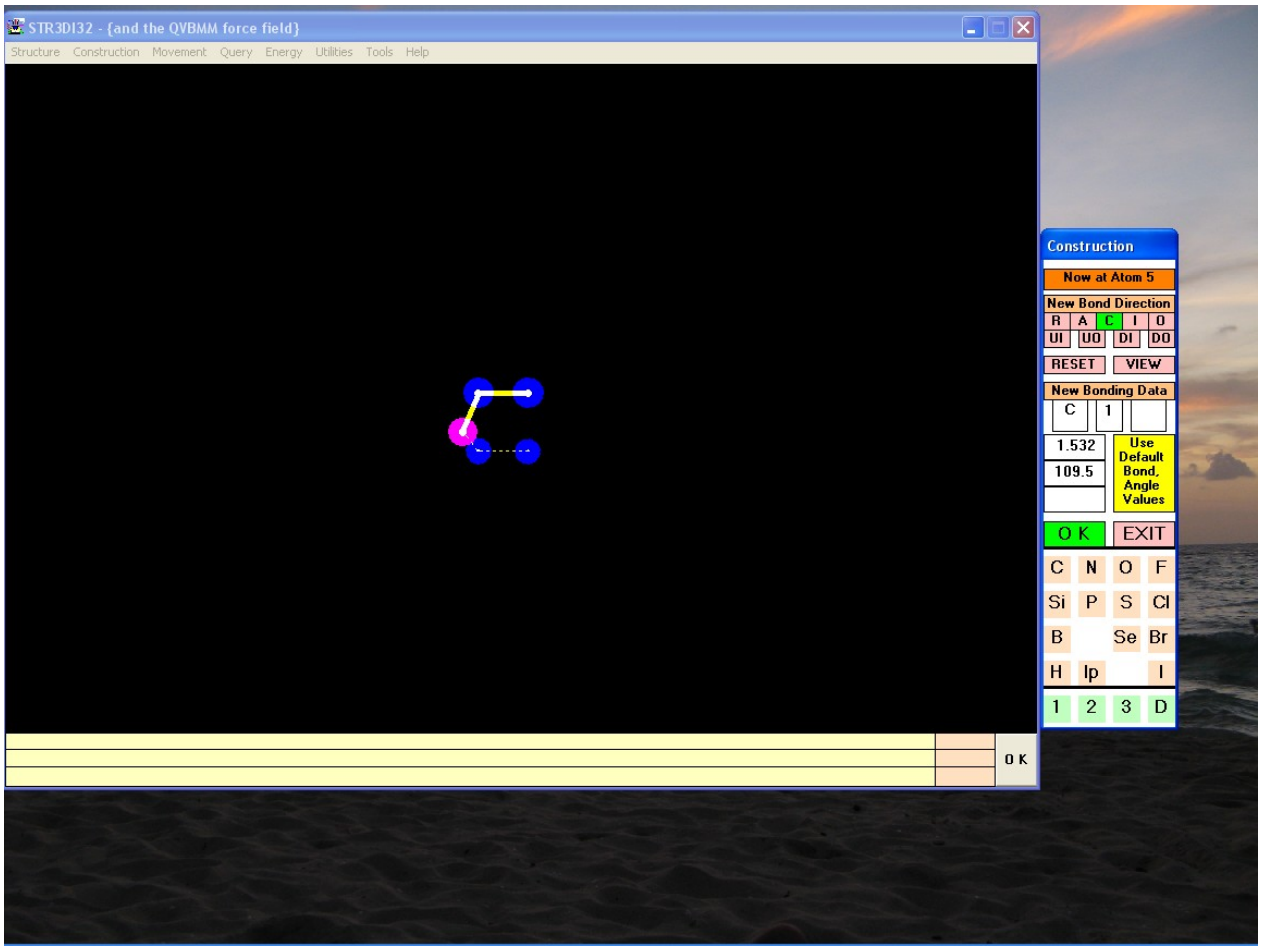
StruMM3D re-orients the molecule, with the 4-5 bond in the drawing position. The new carbon must go into the DI position to complete the ring, since C-1 is inwards (shown in dotted lines) behind the front of the screen.



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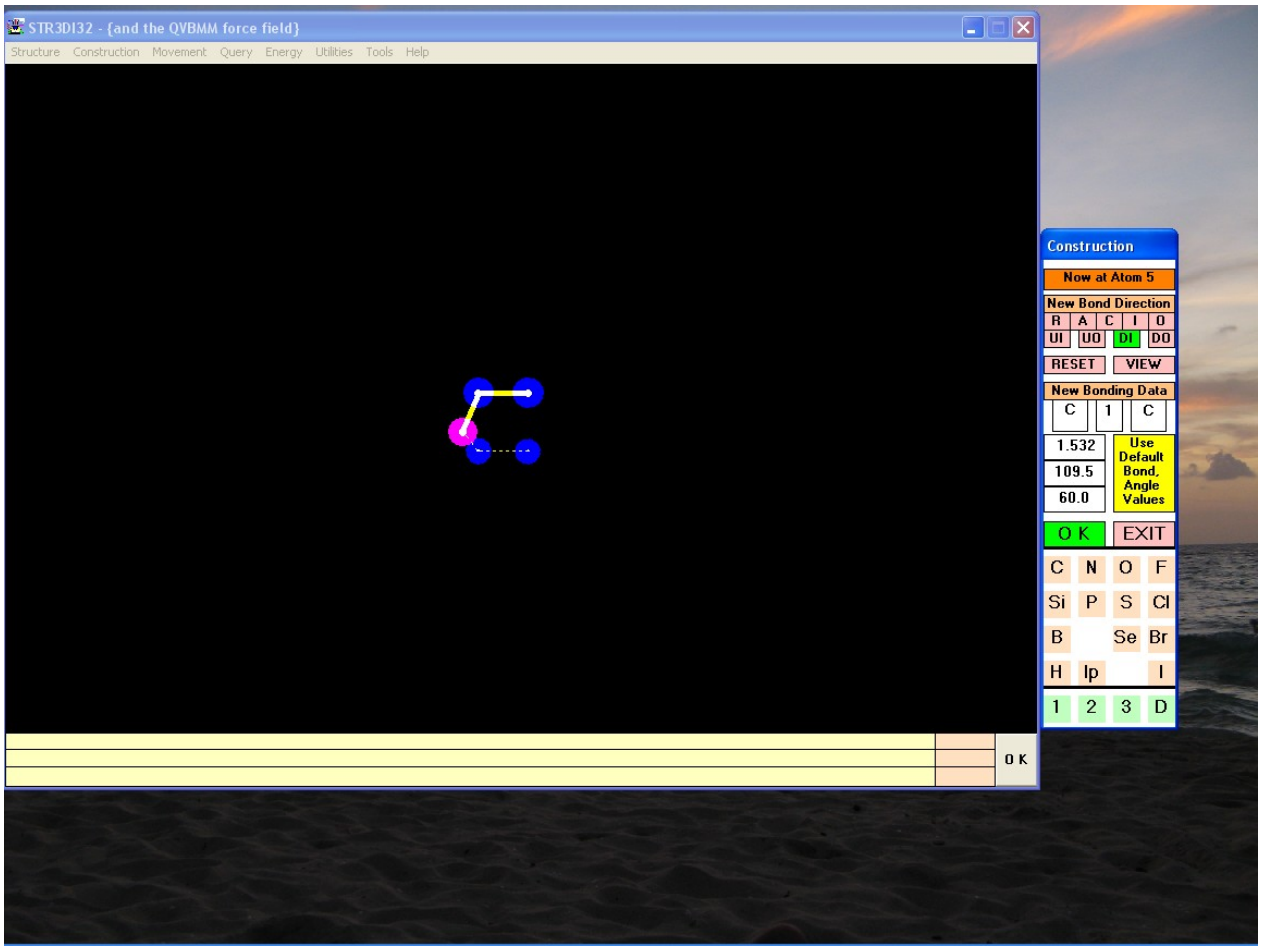
We insert the new data, as is shown below, then click OK on the CONSTRUCTION window.



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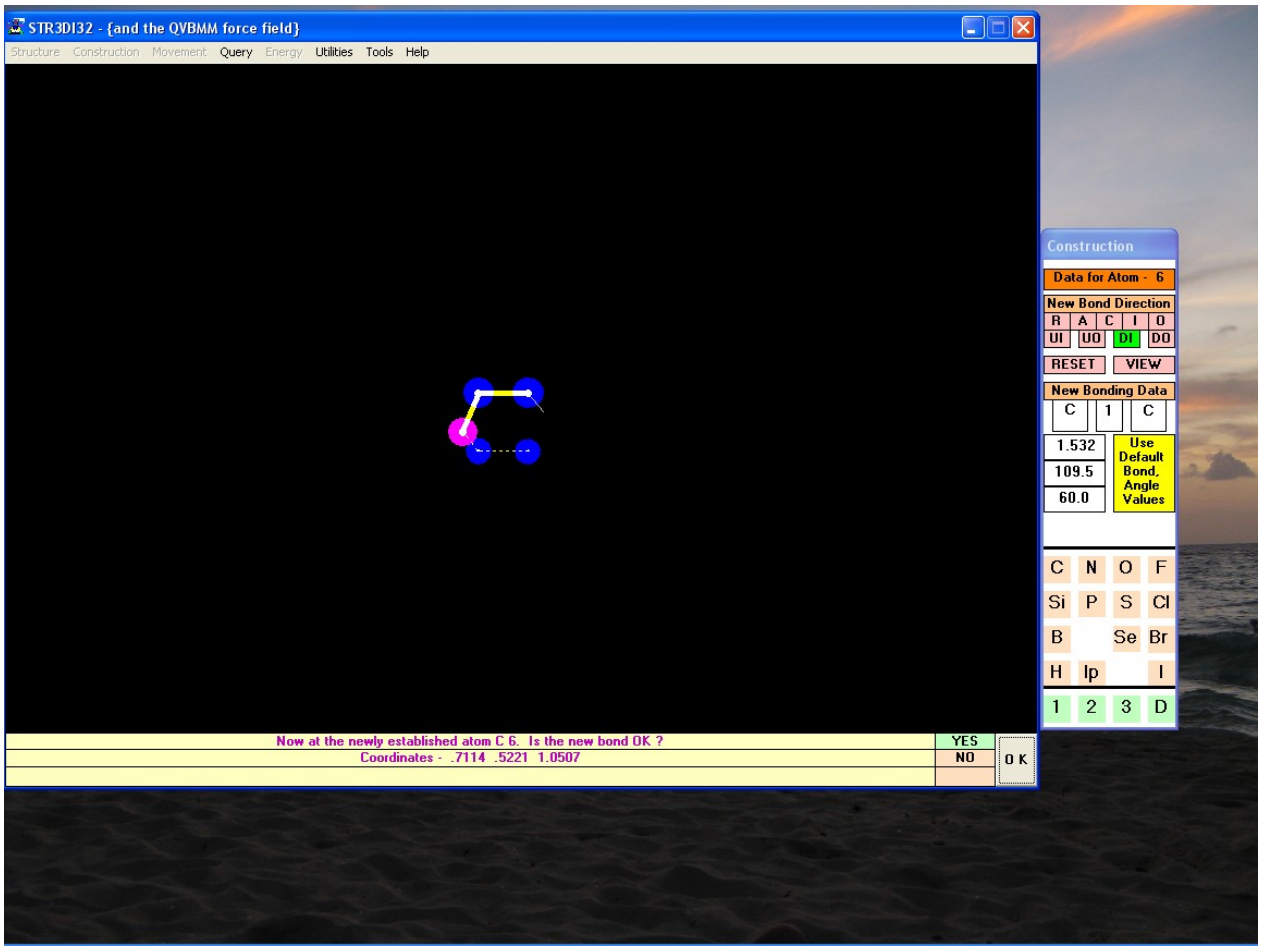
StruMM3D draws the new bond, and asks if it is OK.



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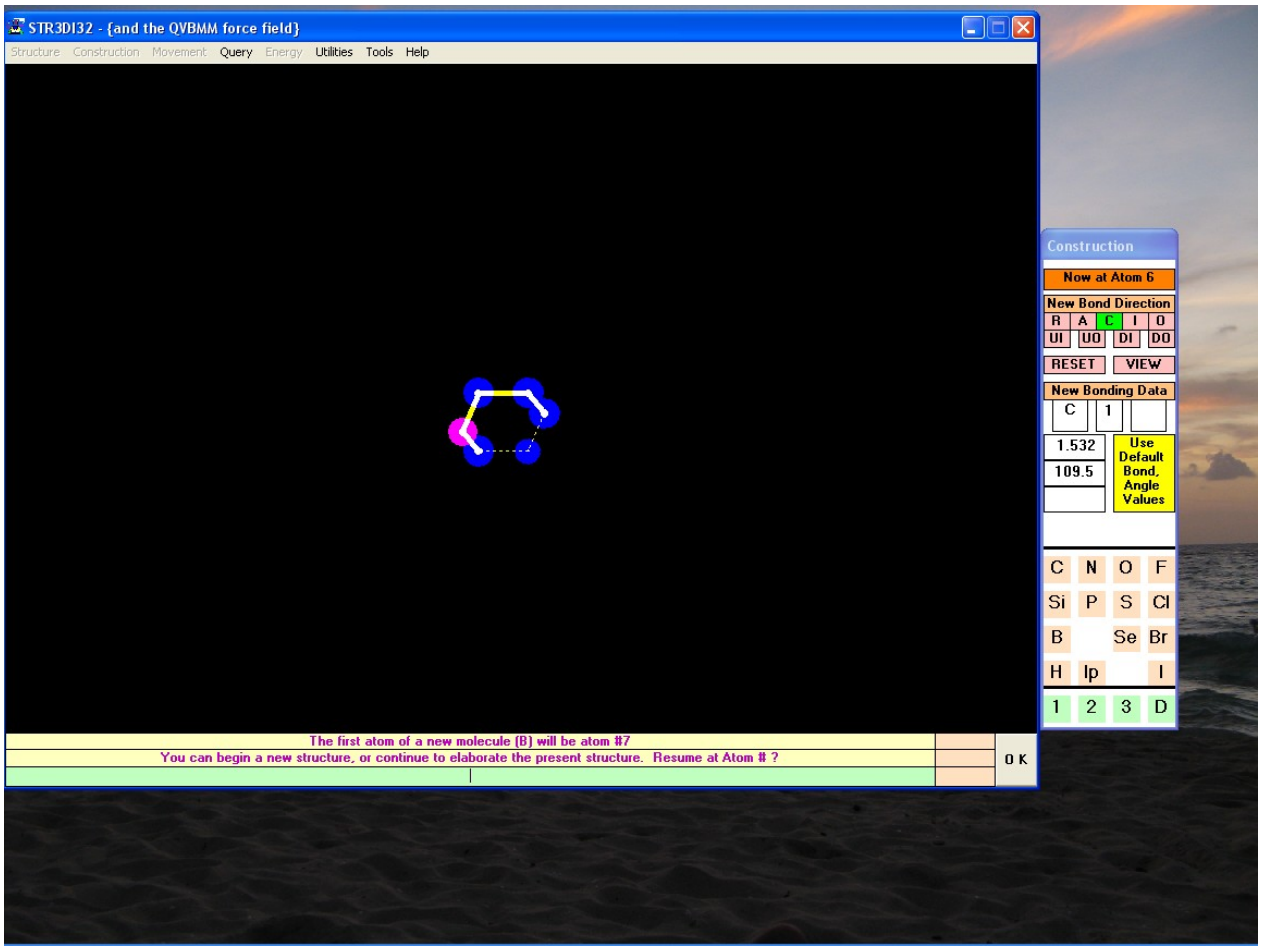
You select “Yes”. StruMM3D recognizes that the new atom #6 is within single bonding distance to the atom #1, and completes the ring for you. Voila!

Since the skeleton of the ring is complete, you want to stop drawing. So, at the prompt for selecting which atom is to be new host atom, you simply make no entry and click on OK.

StruMM3D terminates the process and send you back to the main screen, closing the CONSTRUCTION window.



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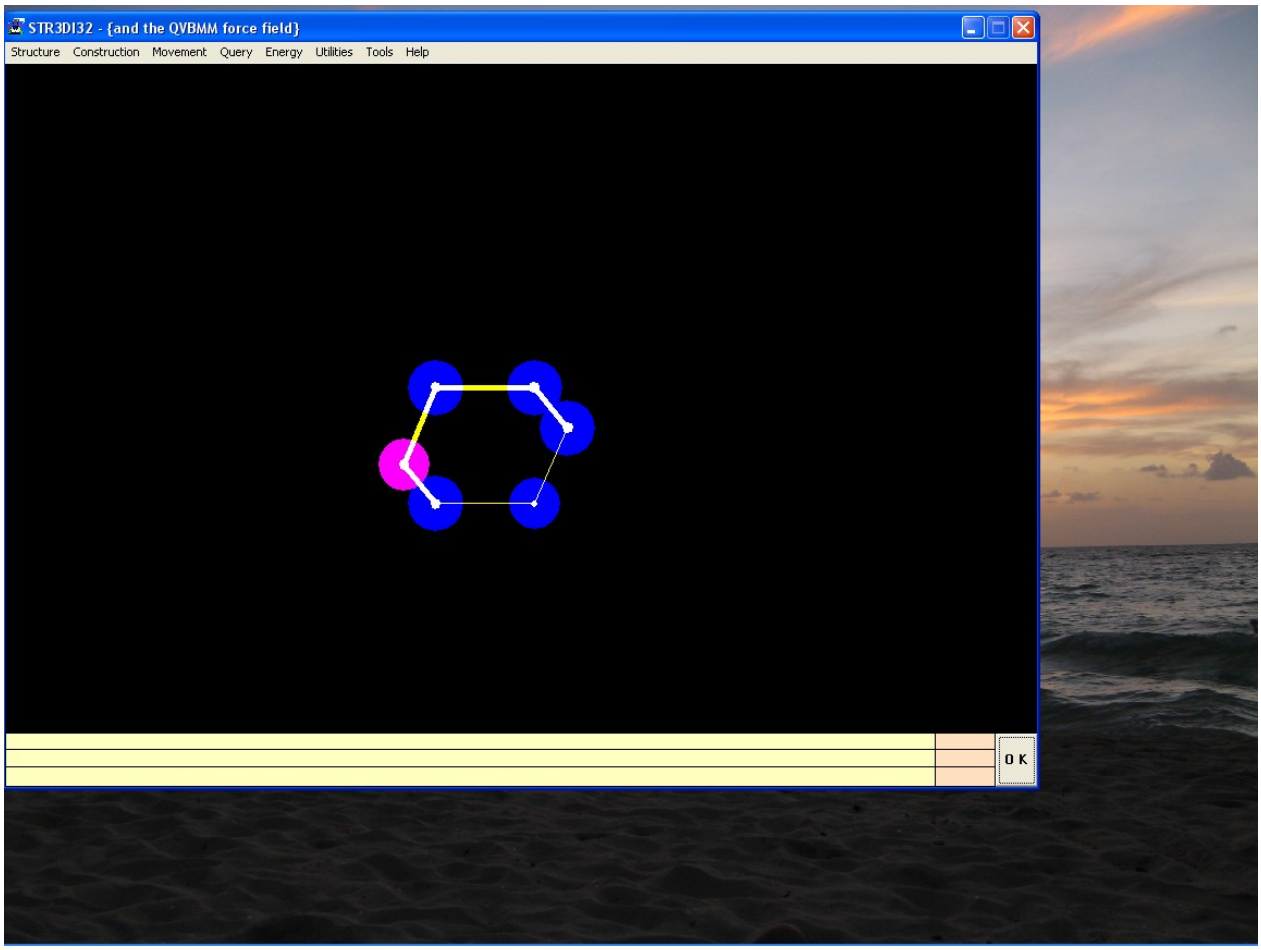
STR3DI32 - {and the QVBMM force field}
Structure Construction Movement Query Energy Utilities Tools Help
OK

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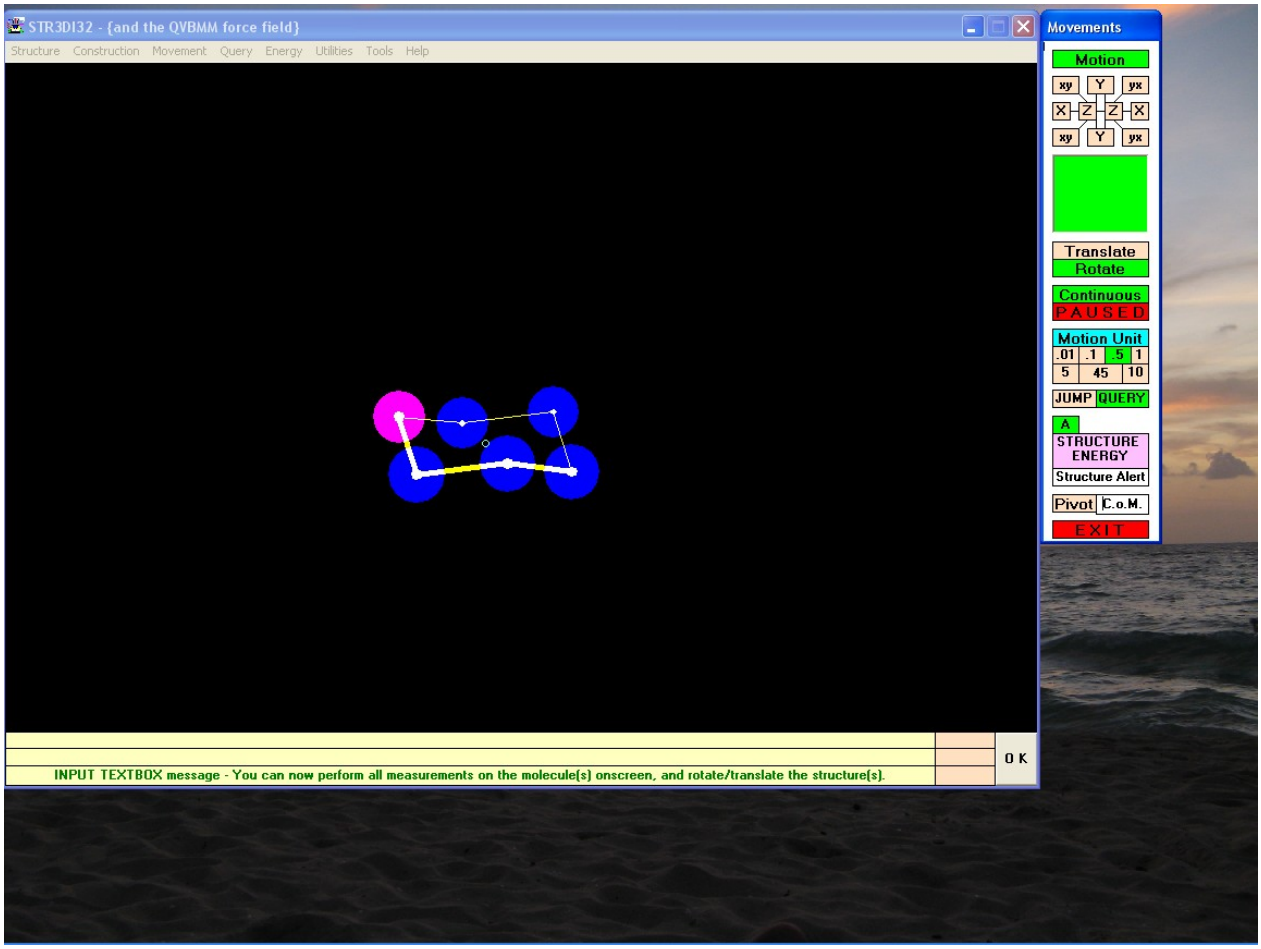
We can use the MOVEMENT menu MOVE option to re-orient the new molecule. Then exit the MOVEMENTS window.



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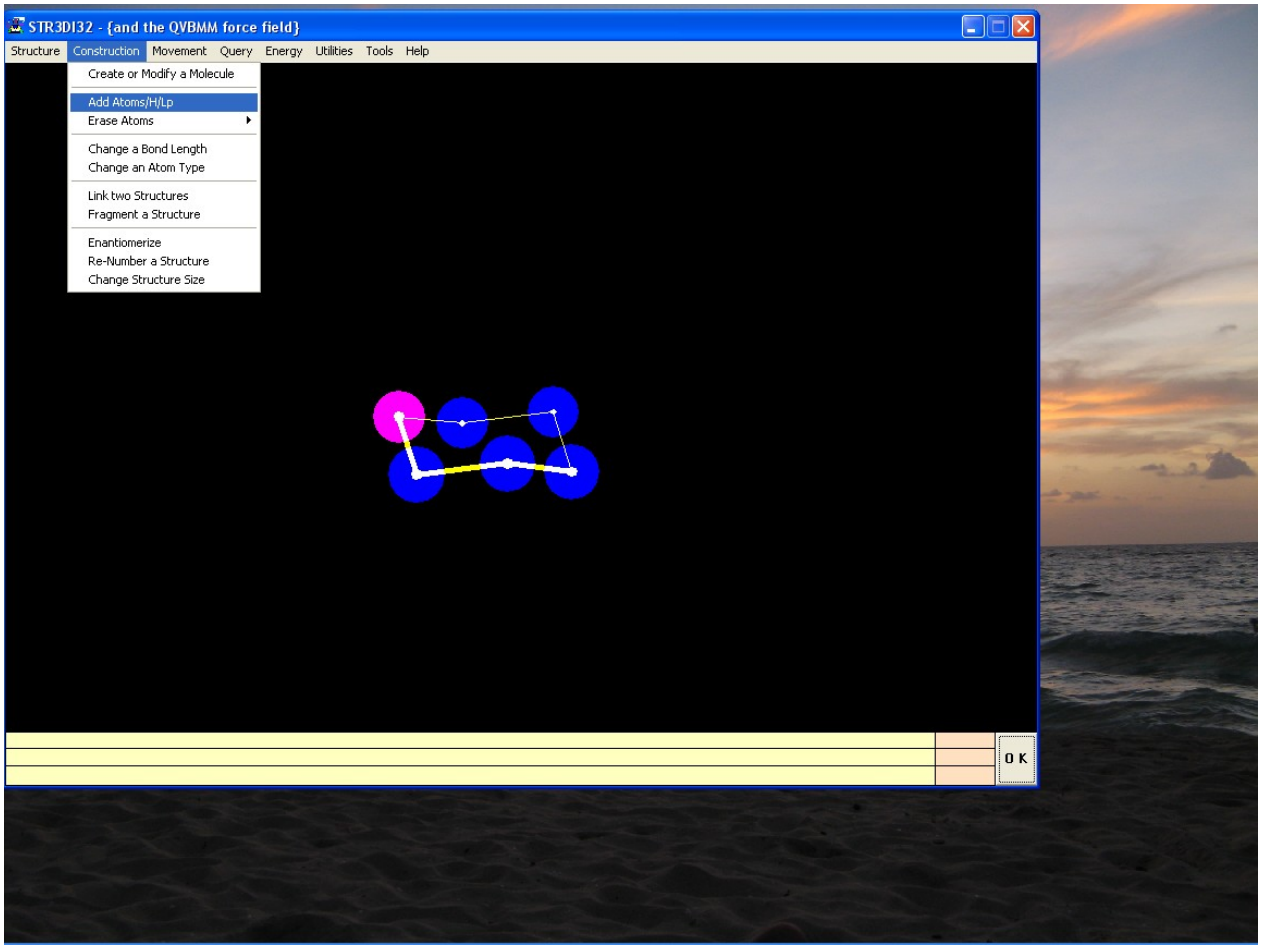
We now select the CONSTRUCTION option, and then ADD ATOMS/H/LP.

You will subsequently see a set of prompts asking for the mode in which to elaborate the skeleton. Remember to use STR Mode. MM2 and MMX modes do not use lone pairs the way StruMM3D does.



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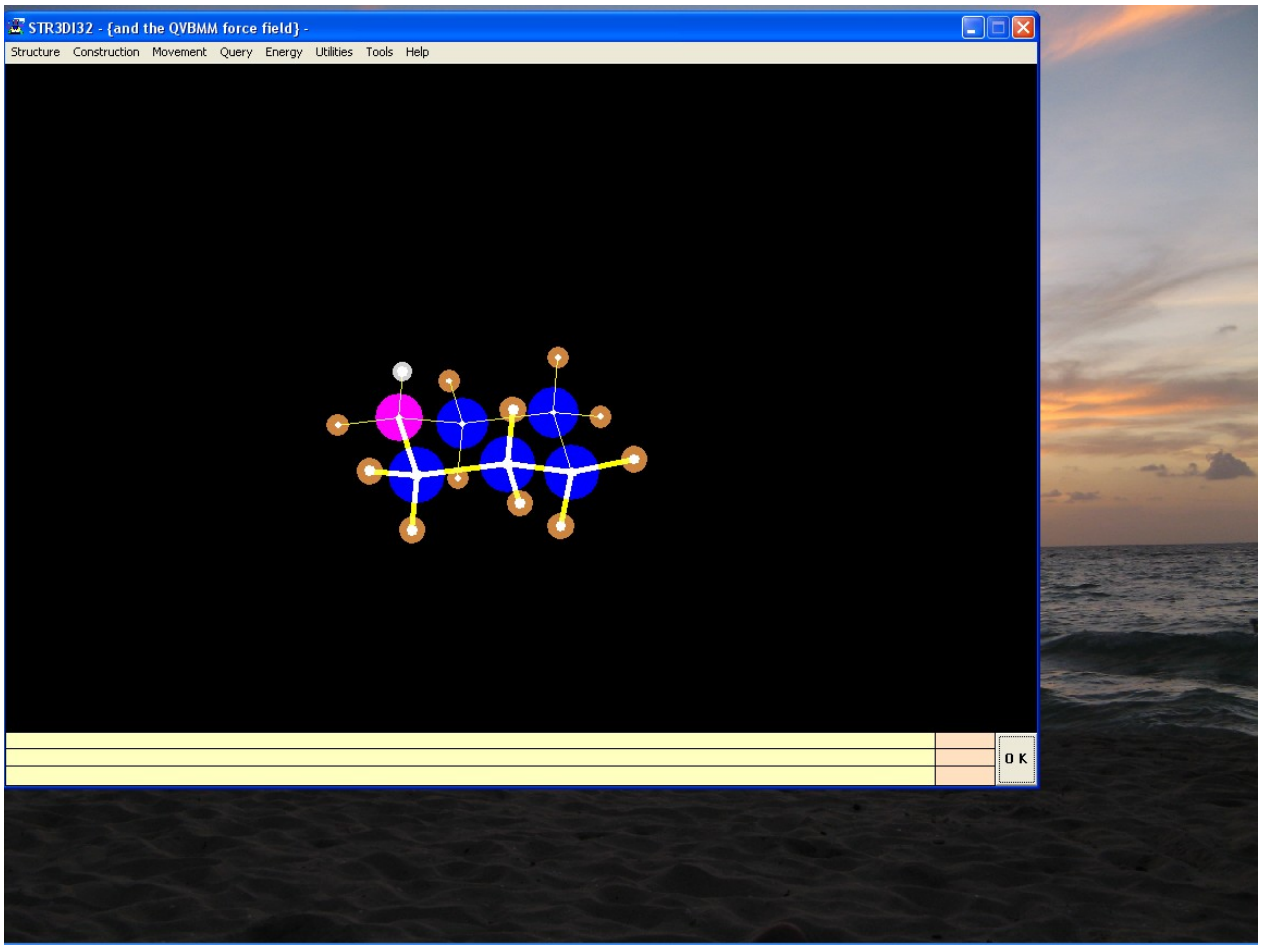
Here we are!

Remember that on the CONSTRUCTION sub-menu there is an option to CHANGE AN ATOM TYPE which we can use to convert any hydrogen into any other atom, to introduce new axial or equatorial atoms. We can convert any ring bond into any other atom type, to make diazanes, or thiazanes, or whatever. We can place the axial lone pair into the equatorial position by successively changing the equatorial hydrogen to lp and then the axial lp to H.

This new structure is in fact a template that you can use to generate scores of new structures which have a vague similarity to the original six-membered ring.



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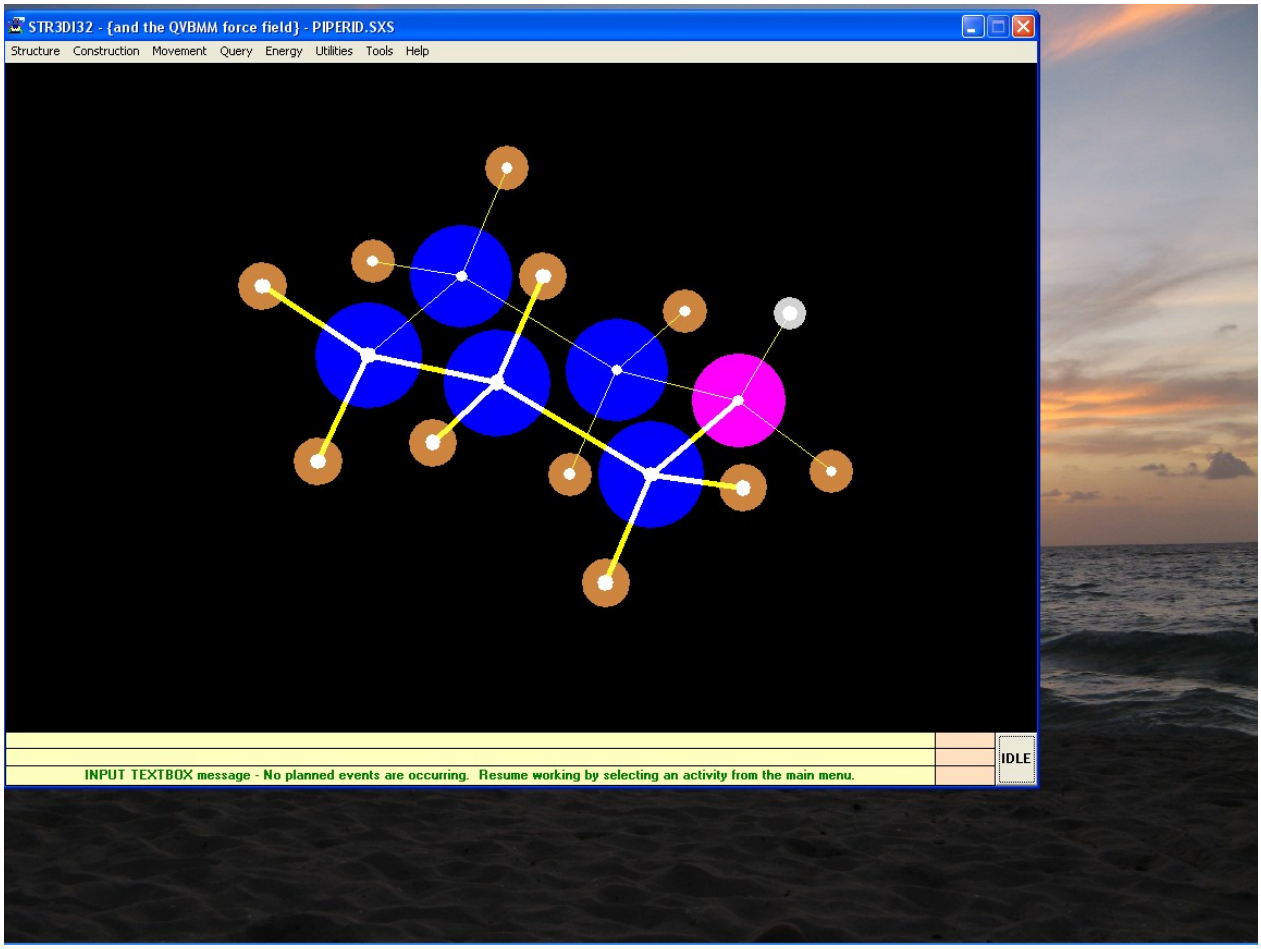
Let’s say that we want to generate the structure of (equatorial)-2-ethyl-(axial)-4-fluoro-piperidine from our template.

We are going to convert the appropriate hydrogens in sequence as follows.



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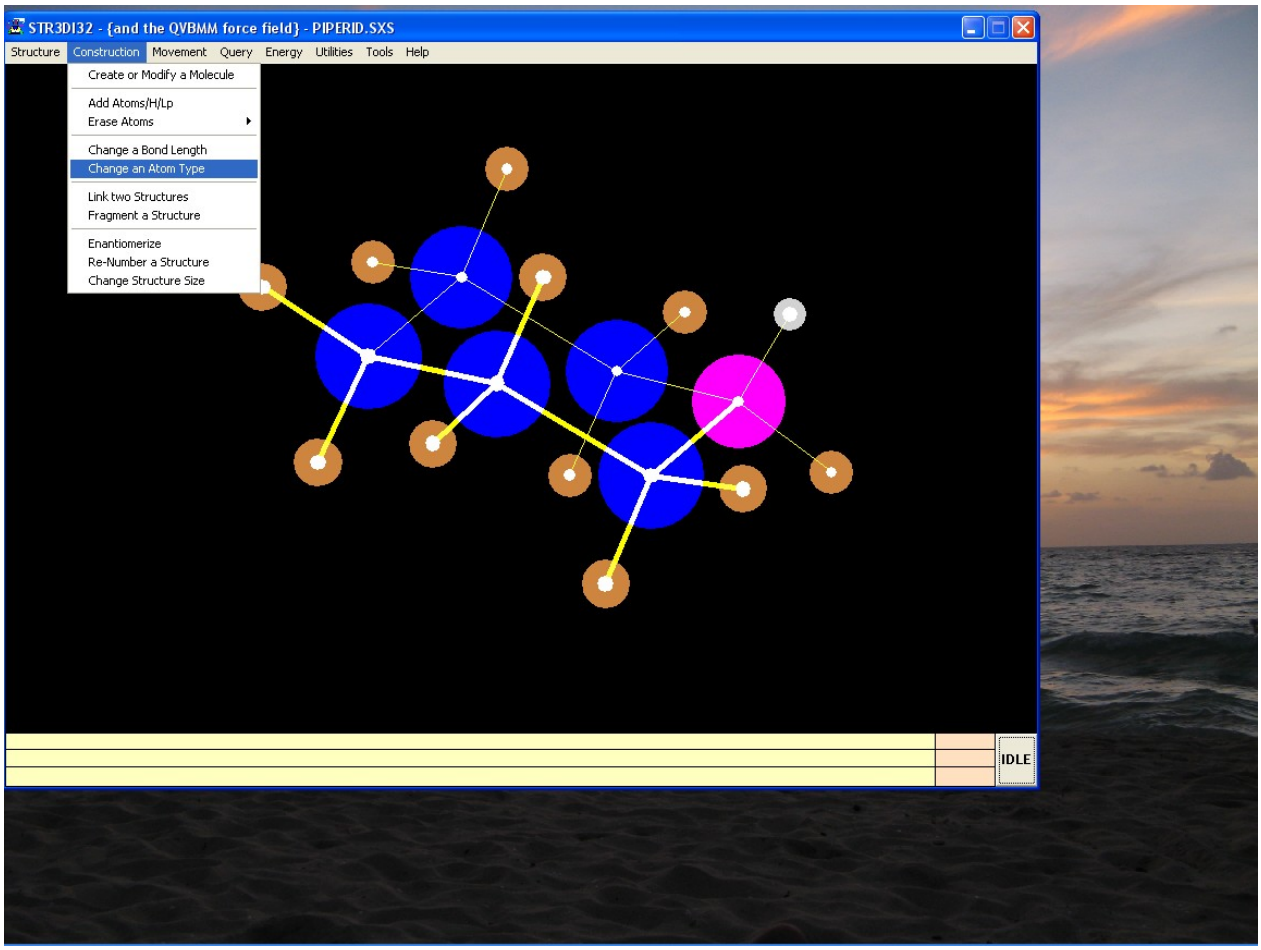
STR3DI32 - {and the QVBMM force field} - PIPERID.SXS
Structure
Construction
Movement
Query
Energy
Utilities
Tools
Help
Create or Modify a Molecule
Add Atoms/H/Lp
Erase Atoms
Change a Bond Length
Change an Atom Type
Link two Structures
Fragment a Structure
Enantiomerize
Re-Number a Structure
Change Structure Size
IDLE

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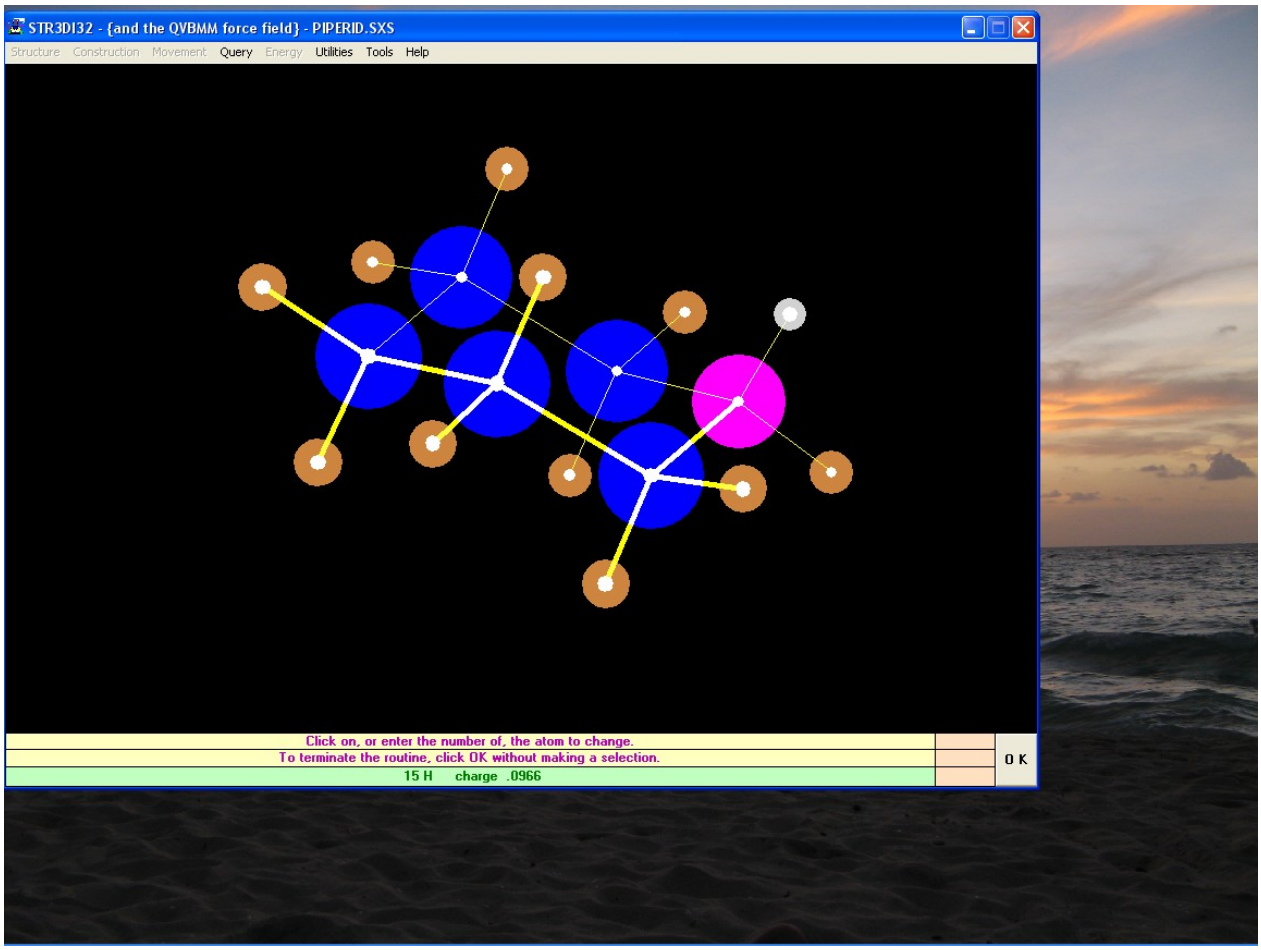
We click on the front, C-2, equatorial hydrogen. Its data appears. Then we click OK



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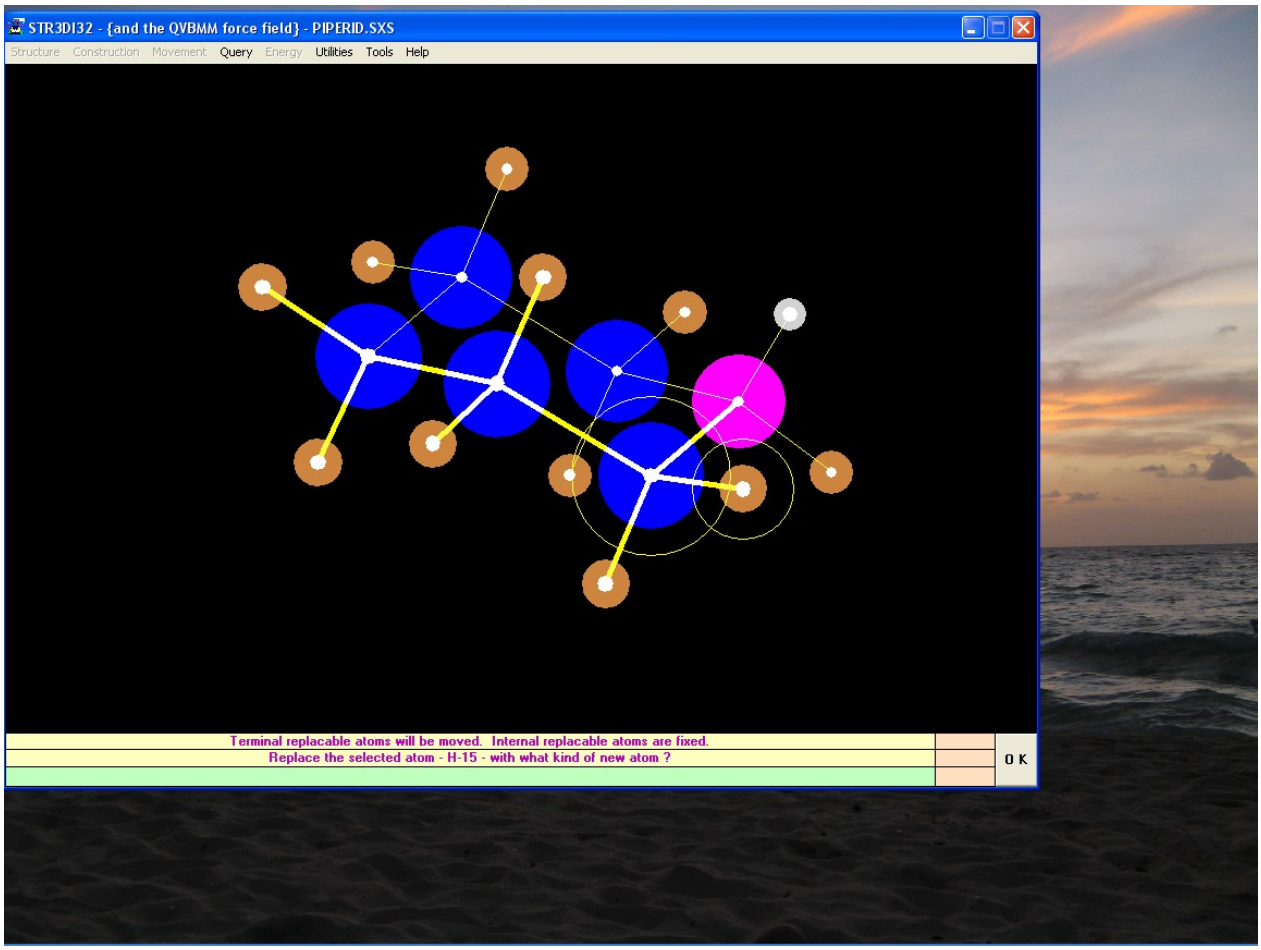
StruMM3D circles the important atoms, especially C-1 since the new atom's bond length to C-1 will be different from the C-H bond length. StruMM3D asks for the type of the new atom. We will enter "C" and click OK



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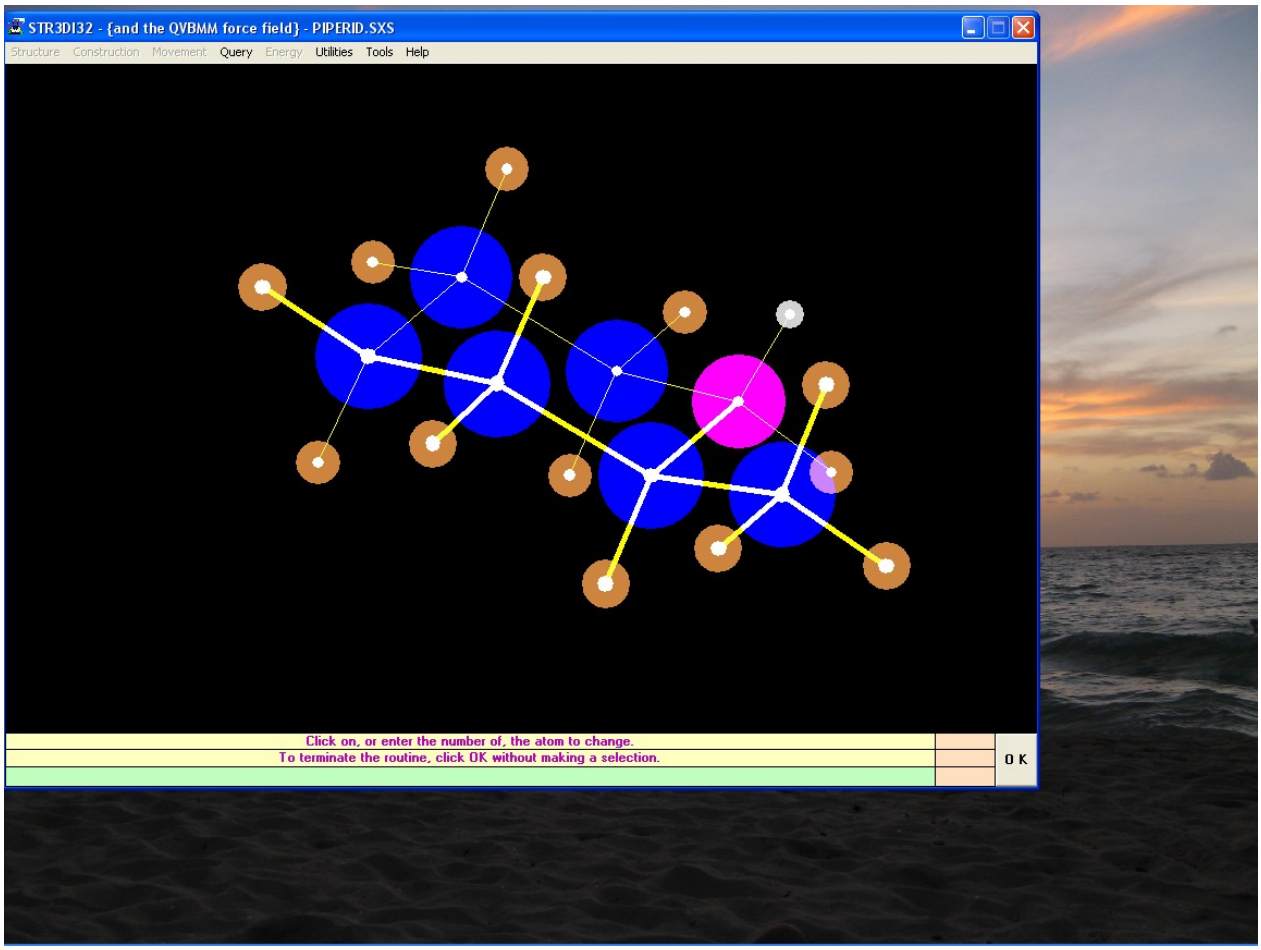
StruMM3D replaces the hydrogen with a carbon and adds the hydrogens to complete a methyl group.

We will replace one of the new methyl group's hydrogen with a carbon to make an ethyl group.



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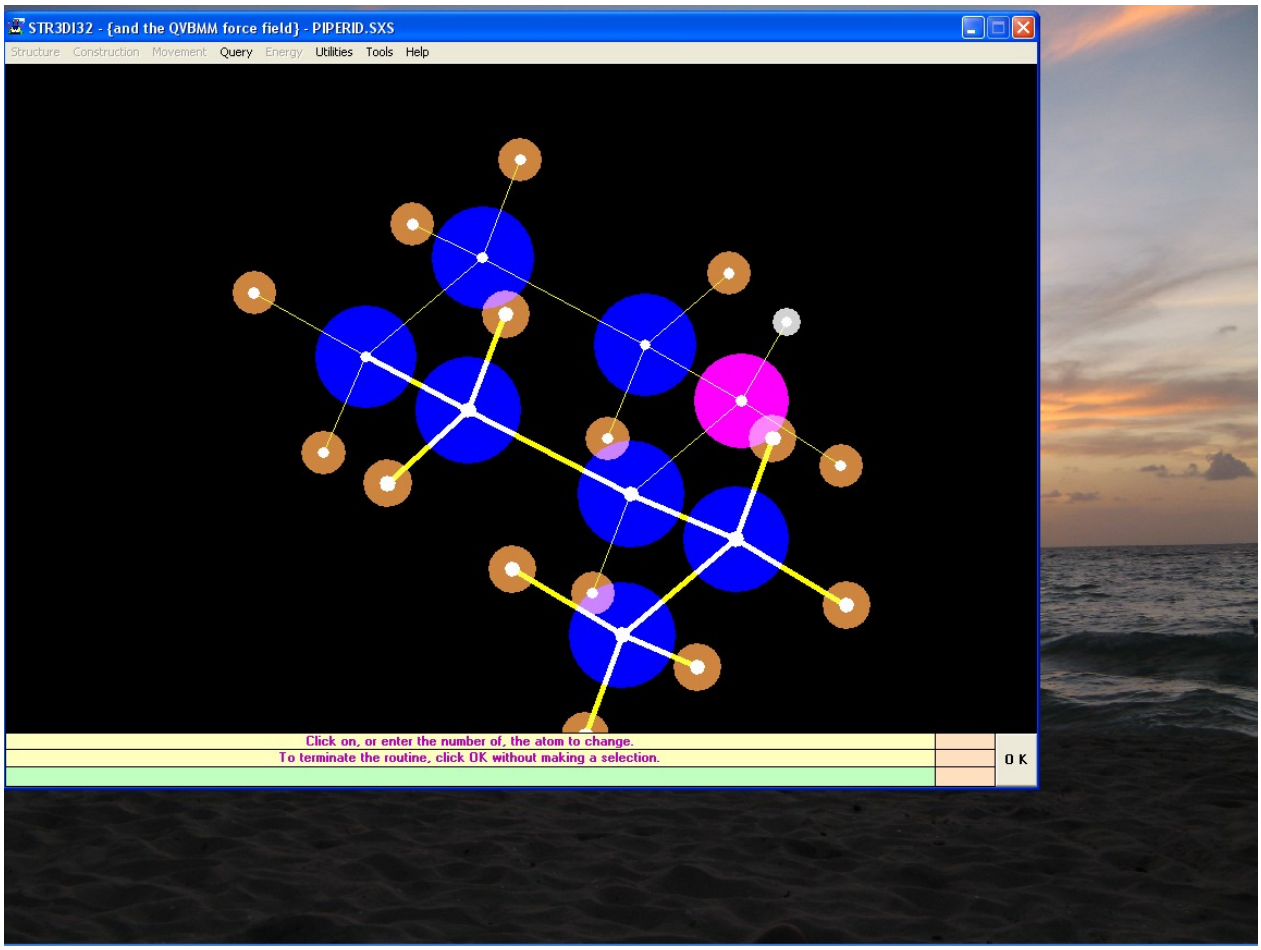
Now we will change the axial H-4 to a fluorine atom.



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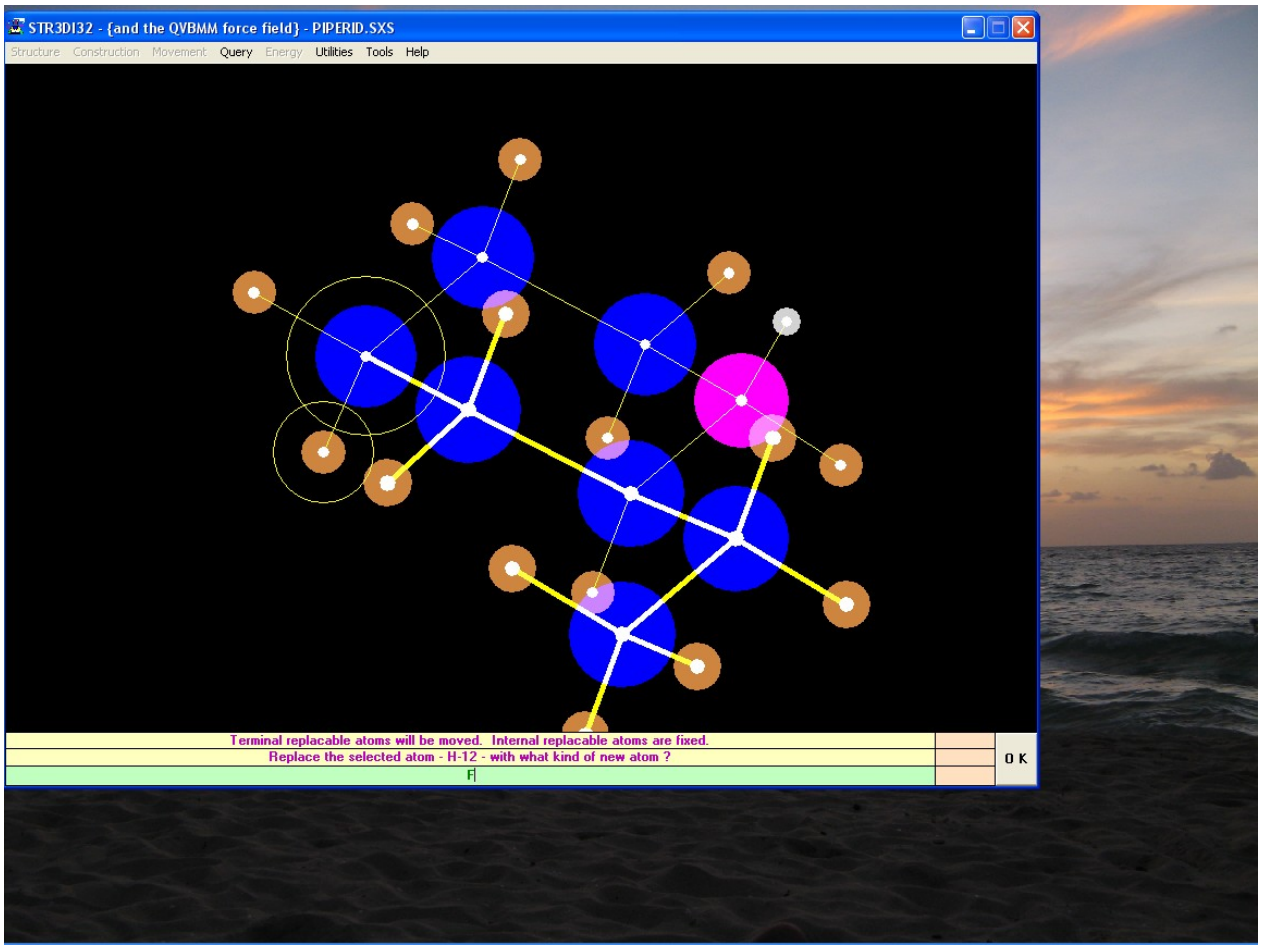
STR3DI32 - {and the QVBMM force field} - PIPERID.SXS
Structure Construction Movement Query Energy Utilities Tools Help
Terminal replacable atoms will be moved. Internal replacable atoms are fixed.
Replace the selected atom - H-12 - with what kind of new atom ?
F
O K

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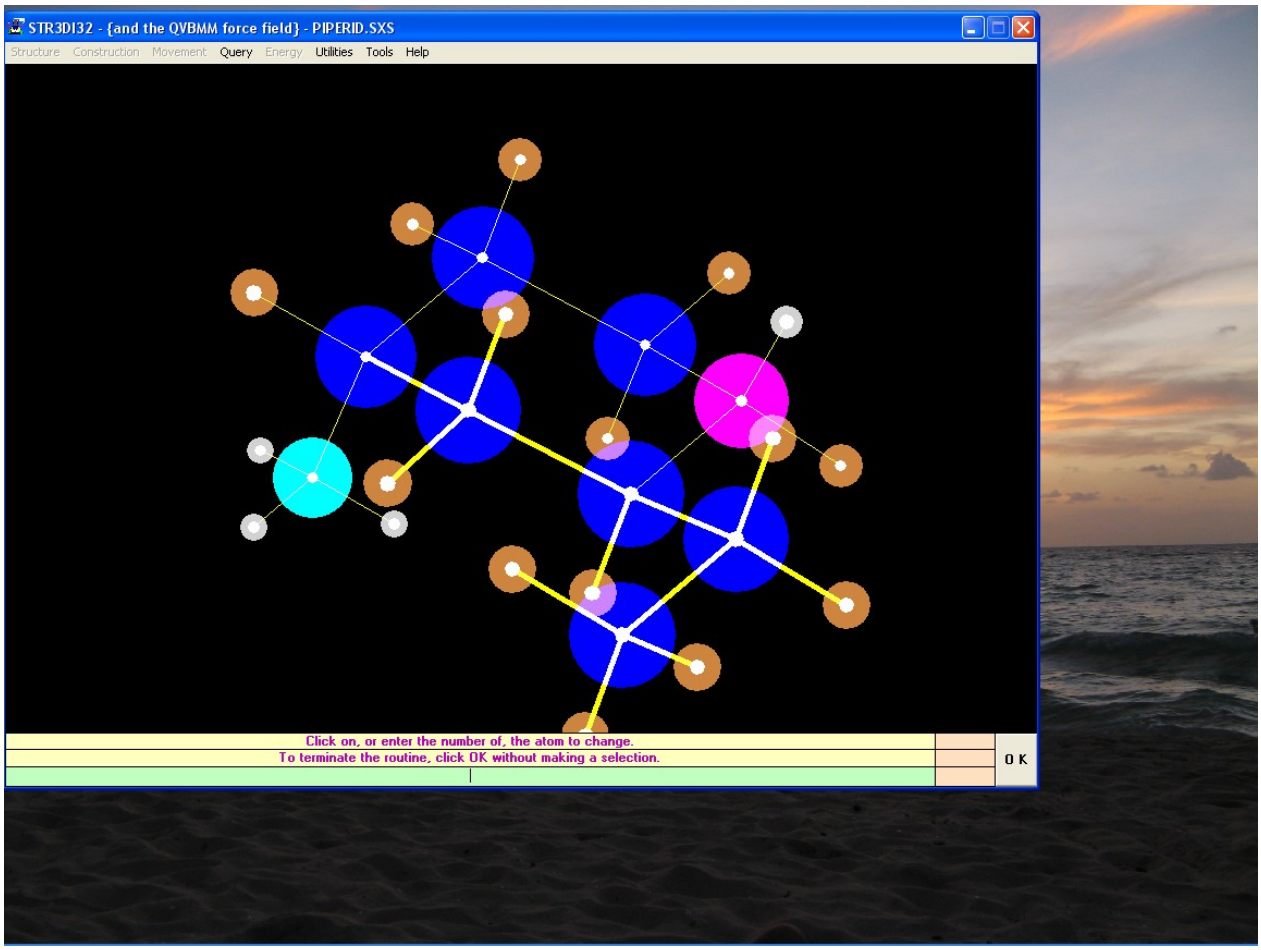
The hydrogen is replaced by a fluorine atom, complete with its lone pairs



Notice that we had absolute control of all stereochemistry, and all new bond lengths were controlled by the program. This relatively crude, but carefully drawn structure, will now be usable for further work, or will only require a brief structure energy minimization to make it perfect.

To exit from this change atom routine we just click OK without selecting any atom to be changed.

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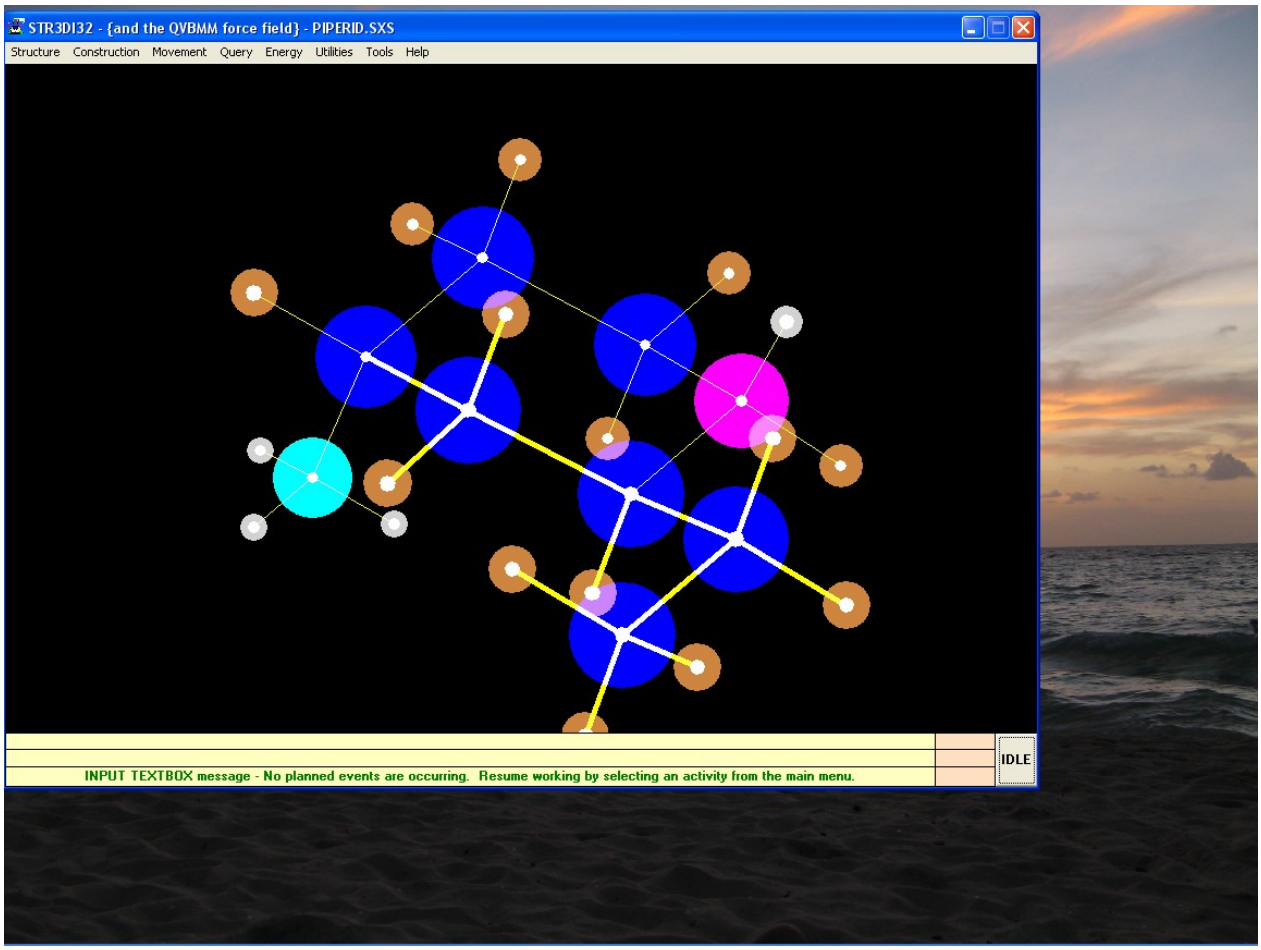
The StruMM3D INPUT TEXTBOX tells us that we are now idling, doing nothing.



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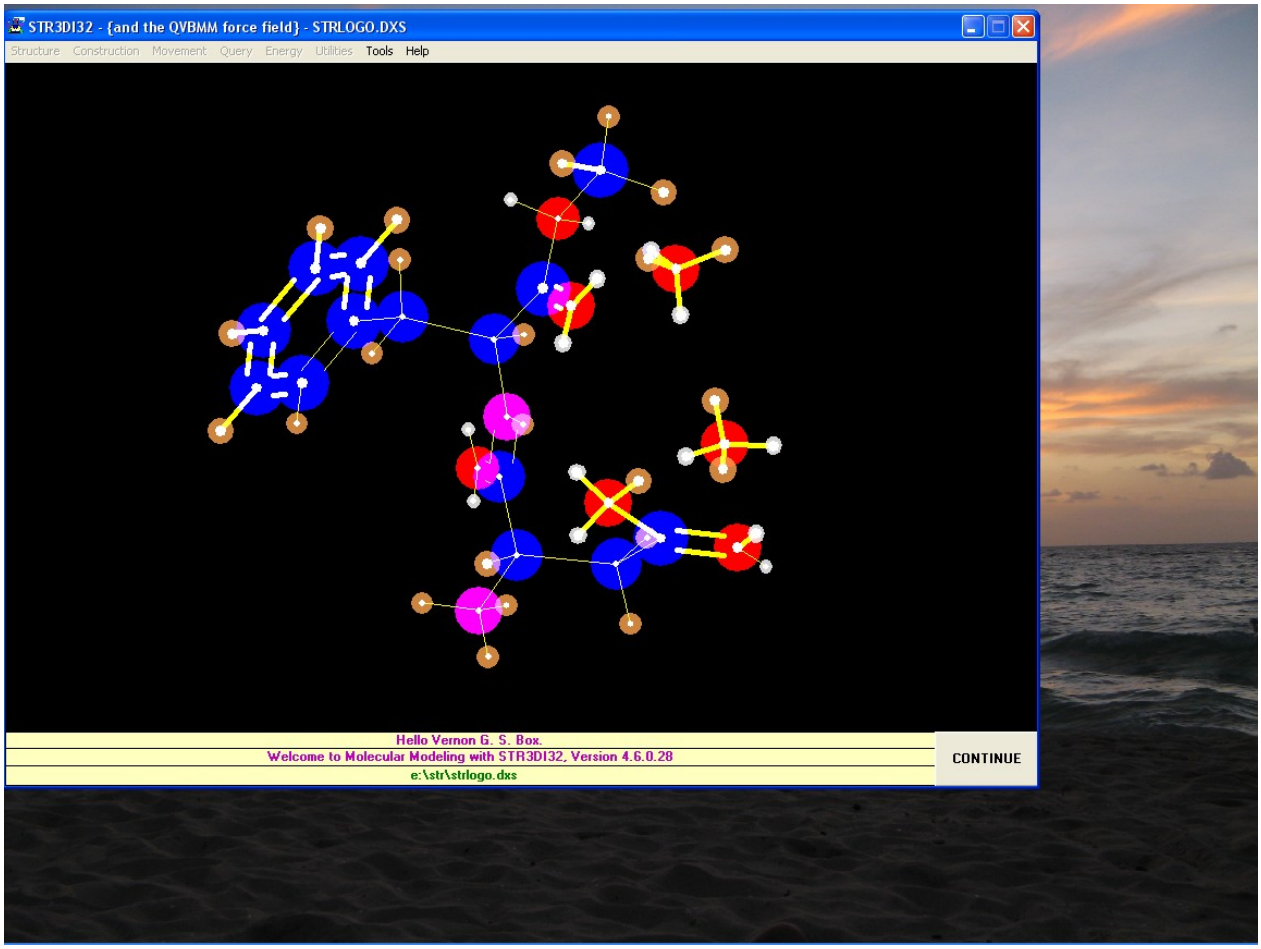
We can use this combination of CONSTRUCTION routines to create/draw almost any template's core (basic) skeleton) and then to elaborate that skeleton into really complex structures

With a bit of practice, we can become really adept at using this highly prompted sequence of routines to draw/create any molecule we might desire.



Thanks for using StruMM3D

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