

ADFinput

Tutorial and

Reference Manual

ADF Program System
Release 2003.01

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INTRODUCTION

ADFinput is a utility program, which enables ADF users to easily create ADF jobs. You can use ADFinput to define your molecule (geometry), pre-optimize it, and to set details of your ADF job using an easy-to-use graphical user interface. ADFinput will generate the complete job script for you. This script takes care of running ADF and property programs as required.

The documentation of ADFinput consists of two main sections.

The first part is a very basic hands-on tutorial. Its purpose is to make some simple job scripts, and to have a simple and fast tour of the main features of the utility. We estimate that you should be able to finish this section including the hands-on activities within 30 minutes.

The second part explains in detail many of the possible options, buttons and so on. This material is mainly included as a reference. We hope that the utility is easy to use, and that the options, together with the help information popping up, will not require you to use the reference manual.

At this point in time, ADFinput is still under development and is being tested. It is now released as a first version as a service to our customers. Your suggestions and bug reports are valuable to us for making an improved and extended next release available as soon as possible.

Please enable the automatic mailing of bug-reports. These reports contain detailed information about the internal state of ADFinput, but do not contain personal information.

You can enable this by setting the global environment variable `SCM_ERROR_MAIL`, for example in your login script:

```
SCM_ERROR_MAIL=errors@scm.com  
export SCM_ERROR_MAIL
```

This will ensure that the bug report will be sent to the mail address you specify. If you specify your own email address you can see exactly what kind of information is contained in the error report. And of course we would like you to forward that report to `errors@scm.com`.

Your comments and bug reports are very welcome. Please send them to `support@scm.com`.

TUTORIAL

This tutorial will help you to:

- create a molecule with ADFinput
- make some changes to the molecule
- set up an ADF calculation with ADFinput
- perform the actual ADF calculation
- visualize some results.

We will assume that you have installed the ADF package on your machine, and that you are familiar with running ADF jobs.

On all UNIX platforms, including Mac OS X, ADFinput is an XWindow program. Your environment should have been set up correctly to run such programs. In particular, you need to make sure that your DISPLAY environment variable has been set properly.

You can test this easily by starting a simple X program from your shell:

```
xclock &
```

Assuming the xclock program is in your \$PATH, a small window should appear with the image of a clock. If not, please consult your local system administrator for additional help. Typical problems have to do with your DISPLAY variable, and with security issues when trying to connect to the X server.

ADFinput is available for all platforms for which ADF 2003.01 is available.

STEP 1: START ADFINPUT

Make a directory for the tutorial

We prefer to run the tutorial in a clean directory. That way the tutorial will not interfere with other projects. Thus:

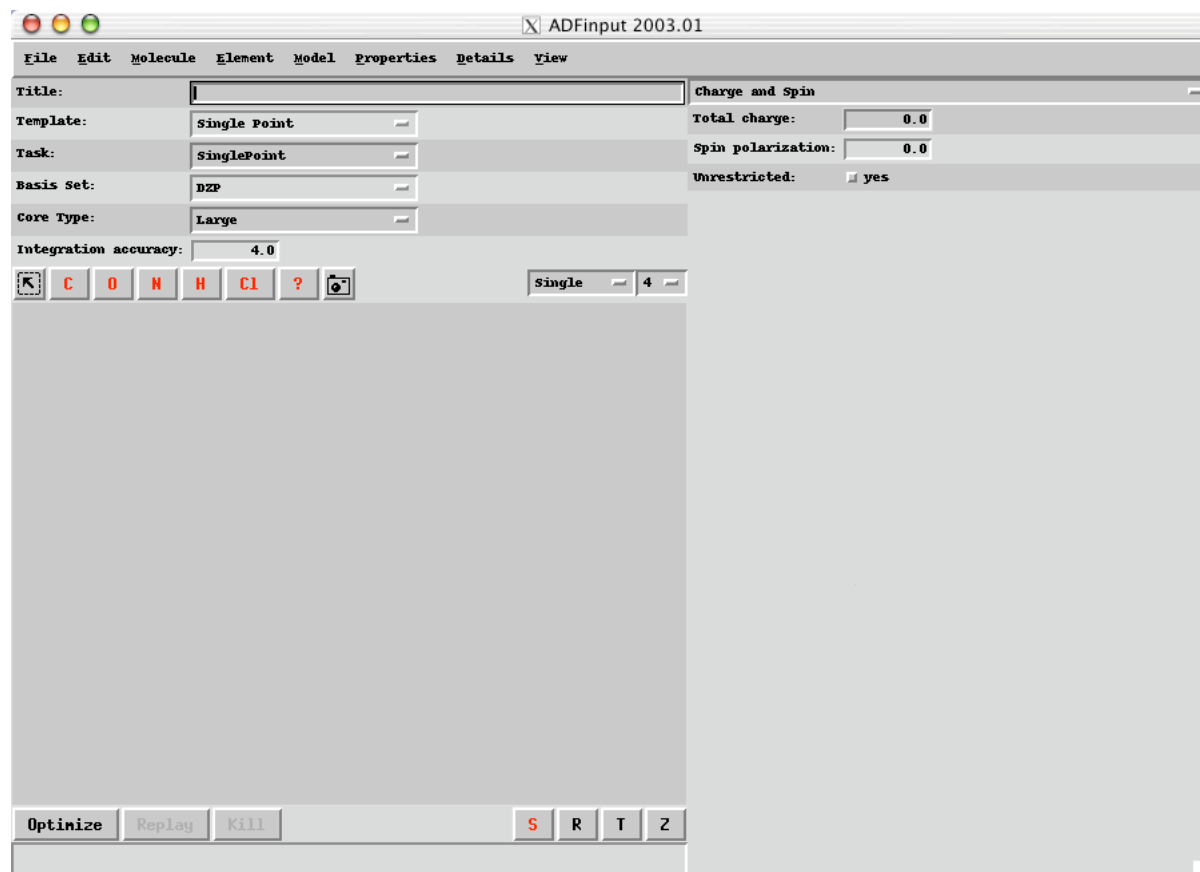
```
mkdir $ADFHOME/demo  
cd $ADFHOME/demo
```

Start ADFinput

Enter the following command:

adfinput&

This will start the ADFinput program in the background:



The main window consists of the following main parts:

- the menu bar with the menu commands
- the main options (on the top left side)
- the molecule editor with some tools (on the middle left side)
- the status field (on the bottom left, currently empty)
- a set of selected other options (currently 'Charge and Spin')

STEP 2: CREATE YOUR MOLECULE

Create a molecule

Next we are going to create an ethane molecule:

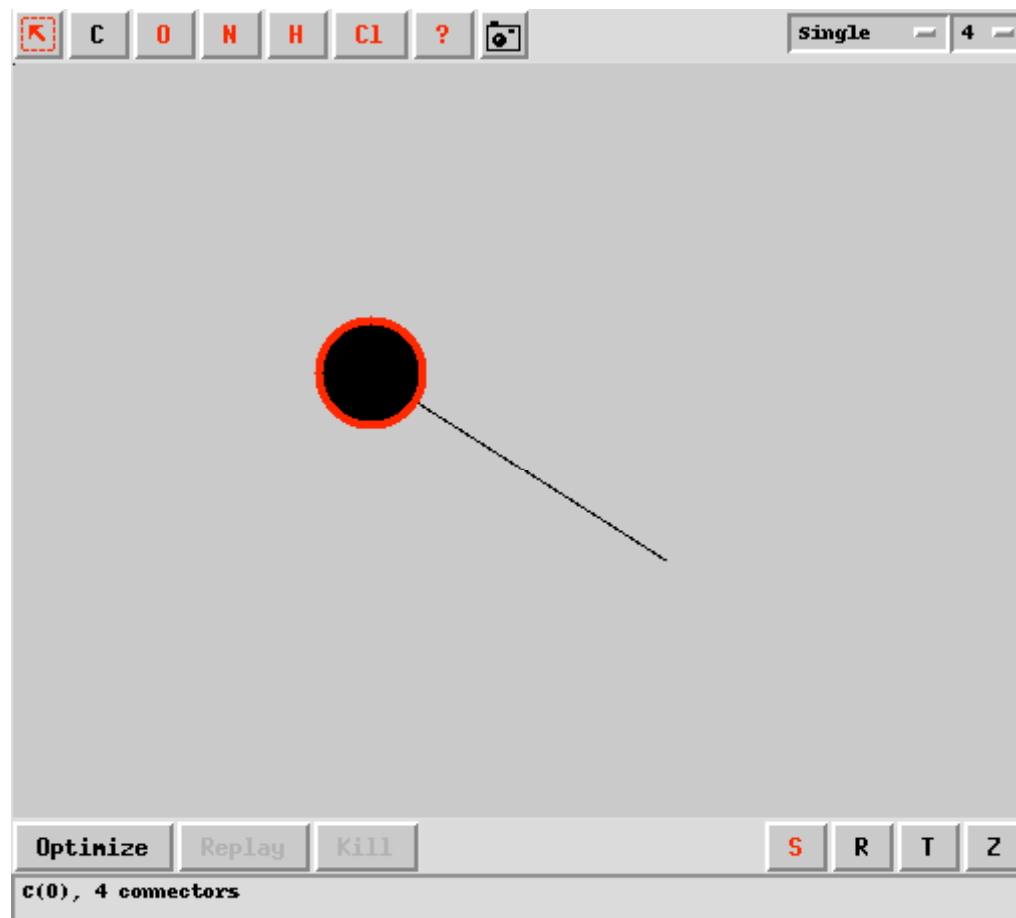
Select the C-tool

Select the C-tool by clicking on the 'C' button, just above the big empty drawing space.

The 'C' button is now black to indicate that you are using the C-tool.

Create the first carbon atom

Click somewhere in the dark-gray empty space below the buttons.



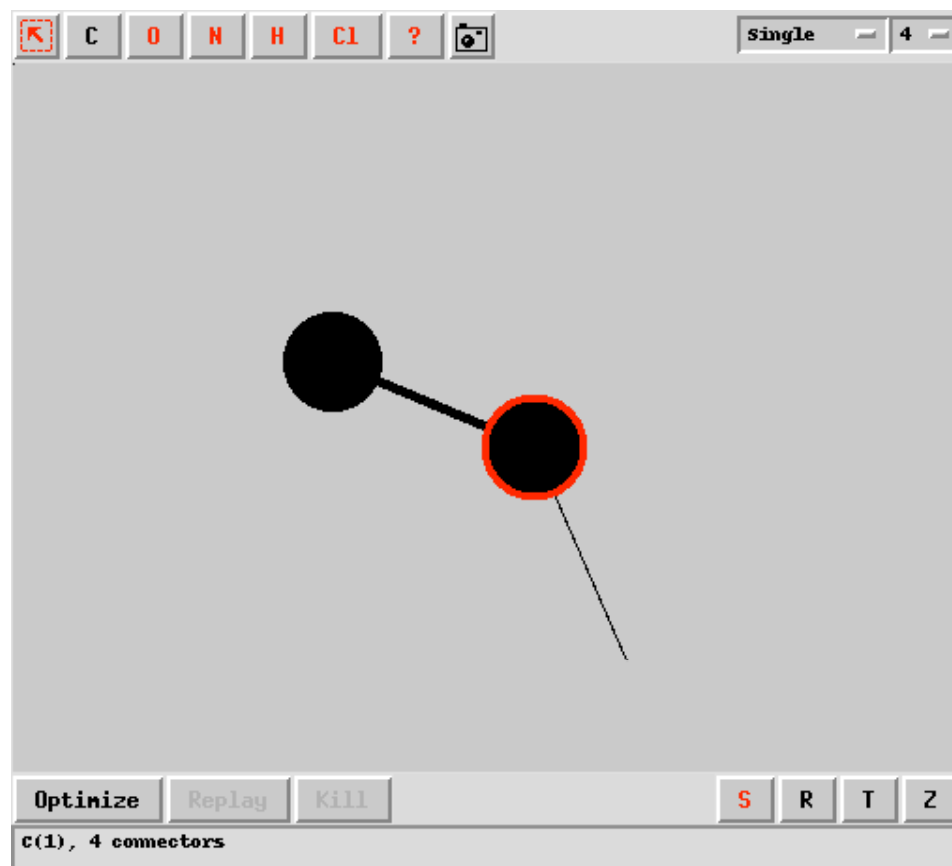
One carbon atom has been created.

Note that:

- If you move the mouse you will see a line from that carbon atom to the current mouse position: this shows you are in 'bonding' mode, and that the bond will be made to the atom just created.
- The 'C' button is black, indicating you are still using the C-tool.
- The red circle around the carbon atom indicates that the carbon atom is the current selection, of one atom only.
- Look at the status field, you can read some information about the current selection: it is a Carbon, number 0, with 4 'connectors'.

Create the second carbon atom

Click a second time somewhere in the empty space.



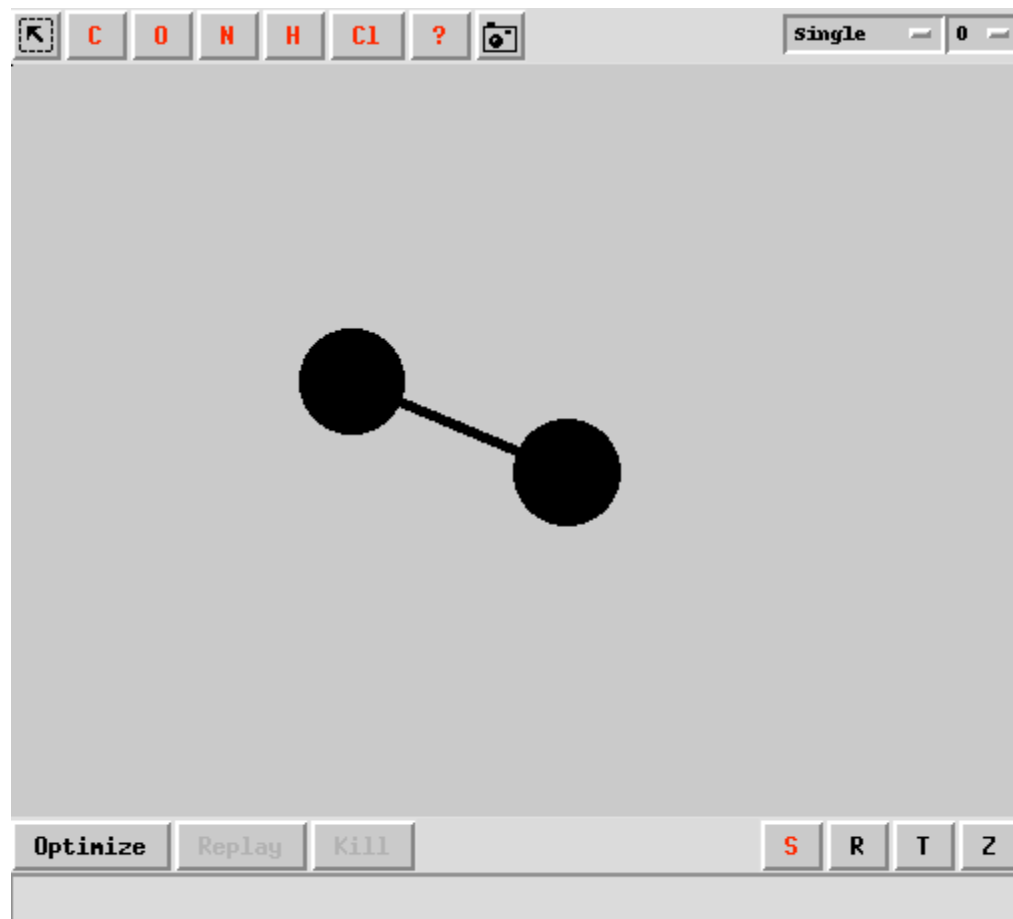
A second carbon atom will be created, bonded to the first atom.

The atom will be created along the 'bonding line', at a distance that corresponds to a normal C-C single bond distance. That is, the bond length is constrained while drawing.

The newly created atom becomes the new selection, and you are still in bonding mode. The next bond will be created to the carbon atom just created. And you are still using the C-tool.

Finish the C-tool mode

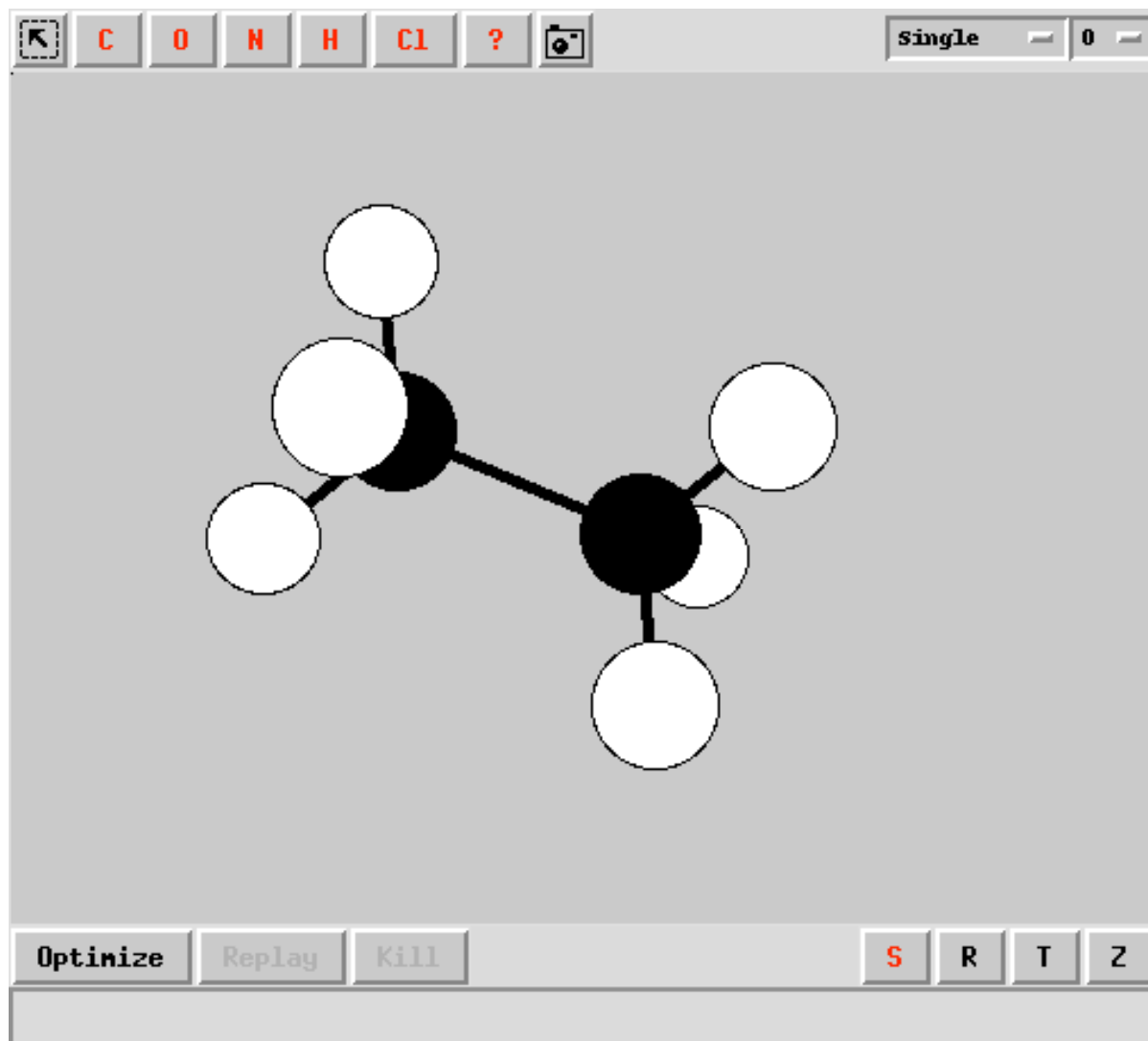
Click once on the currently selected carbon atom.



This ends the C-tool mode, as you can see you are now using the select-tool again.

Add the hydrogens

Select the 'Add Hydrogen' command from the Molecule menu.



You have created an ethane molecule.

Viewing the molecule

The following instructions assume you are using a three-button mouse. If you have a mouse with one or two buttons, check the description of the S, R, T, and Z buttons in the reference manual to learn how to achieve the same effects.

Rotate the molecule

Click in the picture and hold down the right mouse button.

A red rectangle appears for help with rotation.

Move the mouse around (still pressing the right mouse button!).

You will rotate your molecule, and will continue to do so until you:

Release the mouse button.

Rotating works using a 'virtual trackball': when you move the mouse somewhere in the center, the picture changes as if you were rotating by pushing the top of the ball. If you move the mouse near the edge of the picture (outside the rectangle), the rotation will be around an axis perpendicular to the screen.

Zoom the molecule

Press and hold the control key, click in the picture and hold down the right mouse button.

Move the mouse to the right (still pressing the right mouse button and control key!).

As the picture of the molecule will show, you are zooming in.

Move the mouse to the left (still pressing the right mouse button and control key!).

You are zooming out.

Release the mouse button and the control key.

Translate the molecule

Click in the picture using the middle mouse button, and hold down the mouse button.

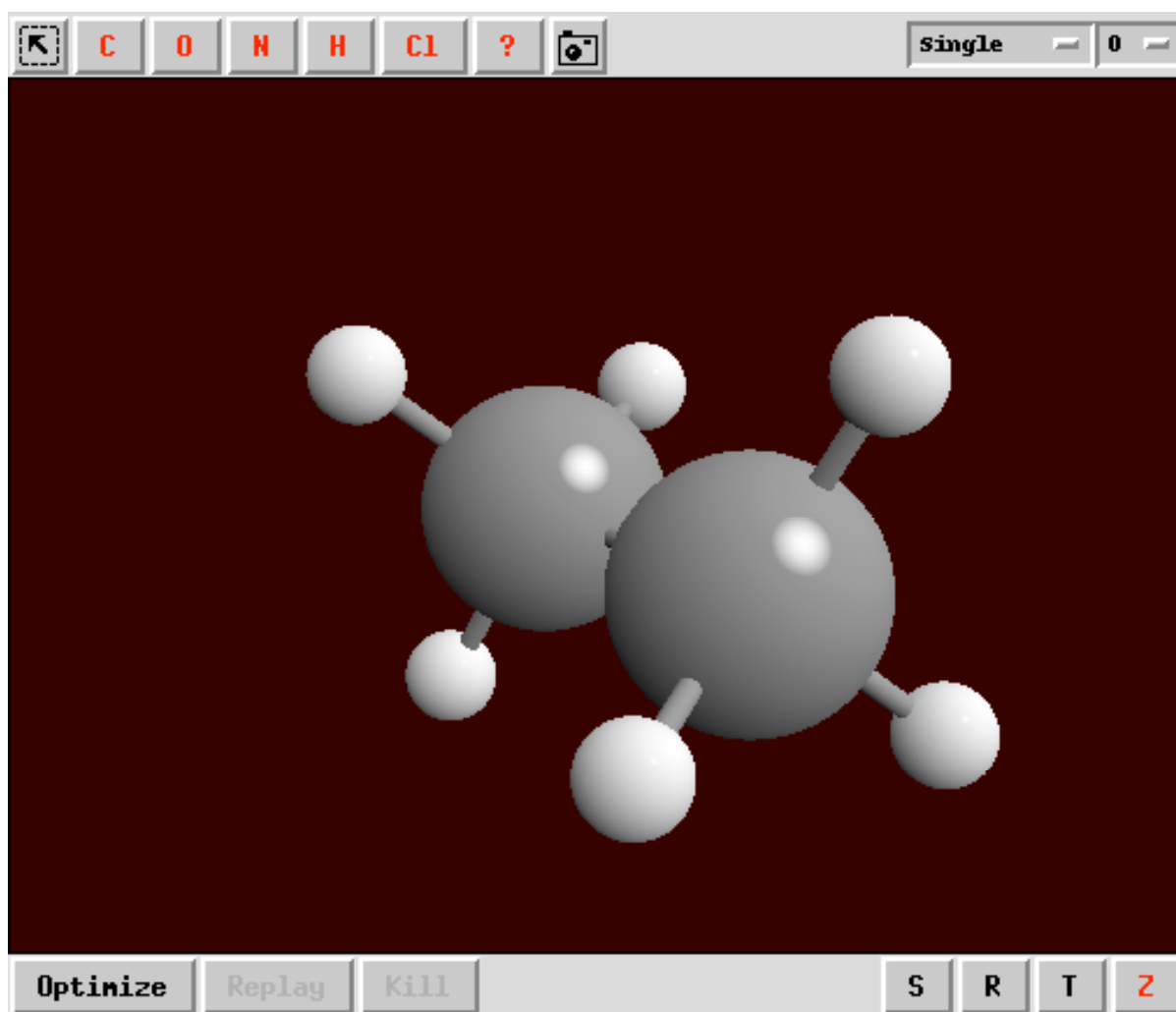
Drag the mouse in some direction.

The molecule will be translated following the mouse.

High quality image

You can also change the picture of the molecule to a high quality picture. This looks much better, but is also much slower. For that reason you will probably want to edit and move your molecule using the simple (default) display mode.

Press the button with the camera icon, next to the button with the question mark.

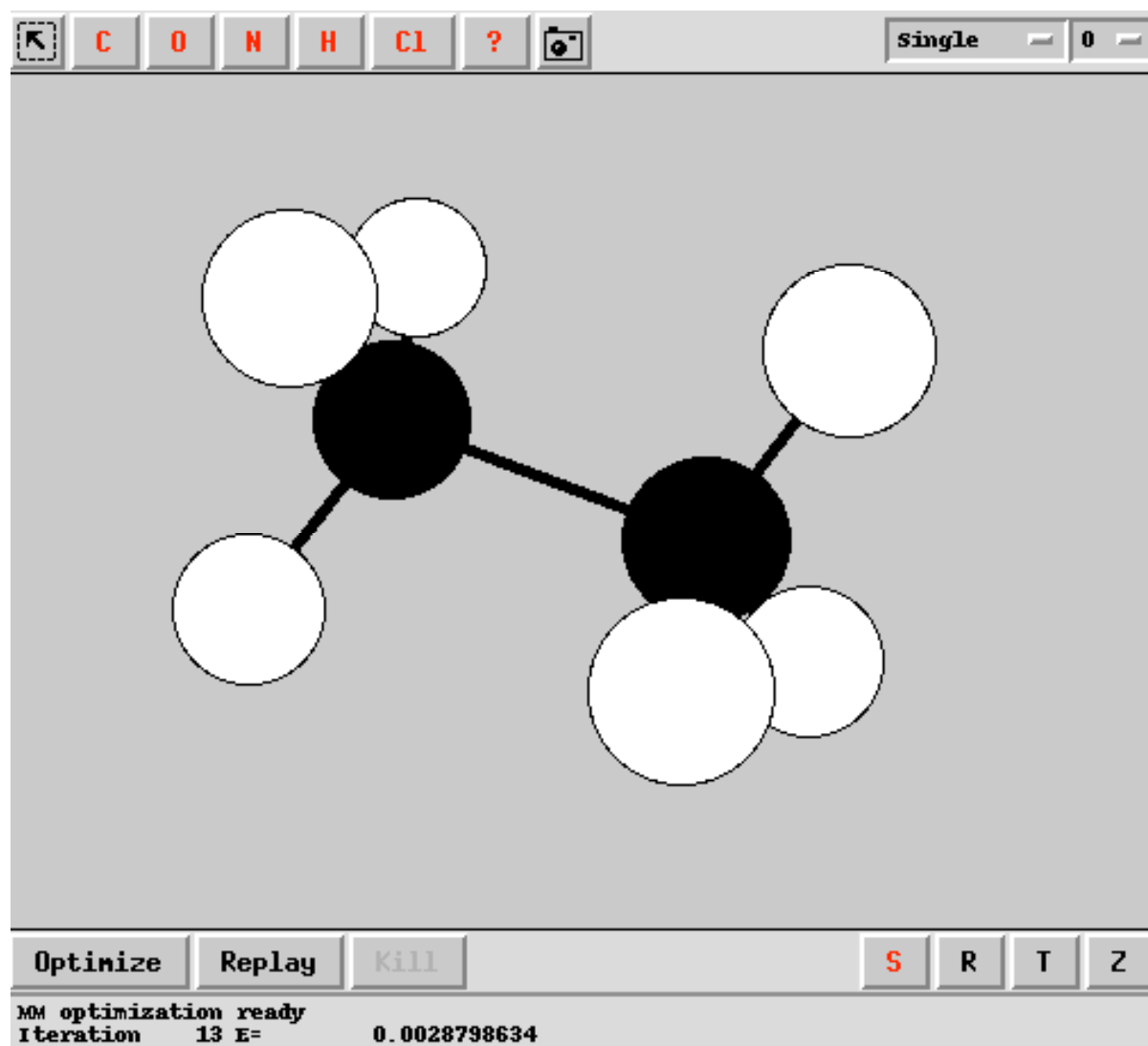


This toggles between the nice and fast picture modes.

Pre-Optimize Geometry

Click on the Optimize button in the lower part of the editing window.

This will optimize the geometry of the ethane molecule.



The method used for this optimization is a very simple (and not very accurate) optimization using a force field.

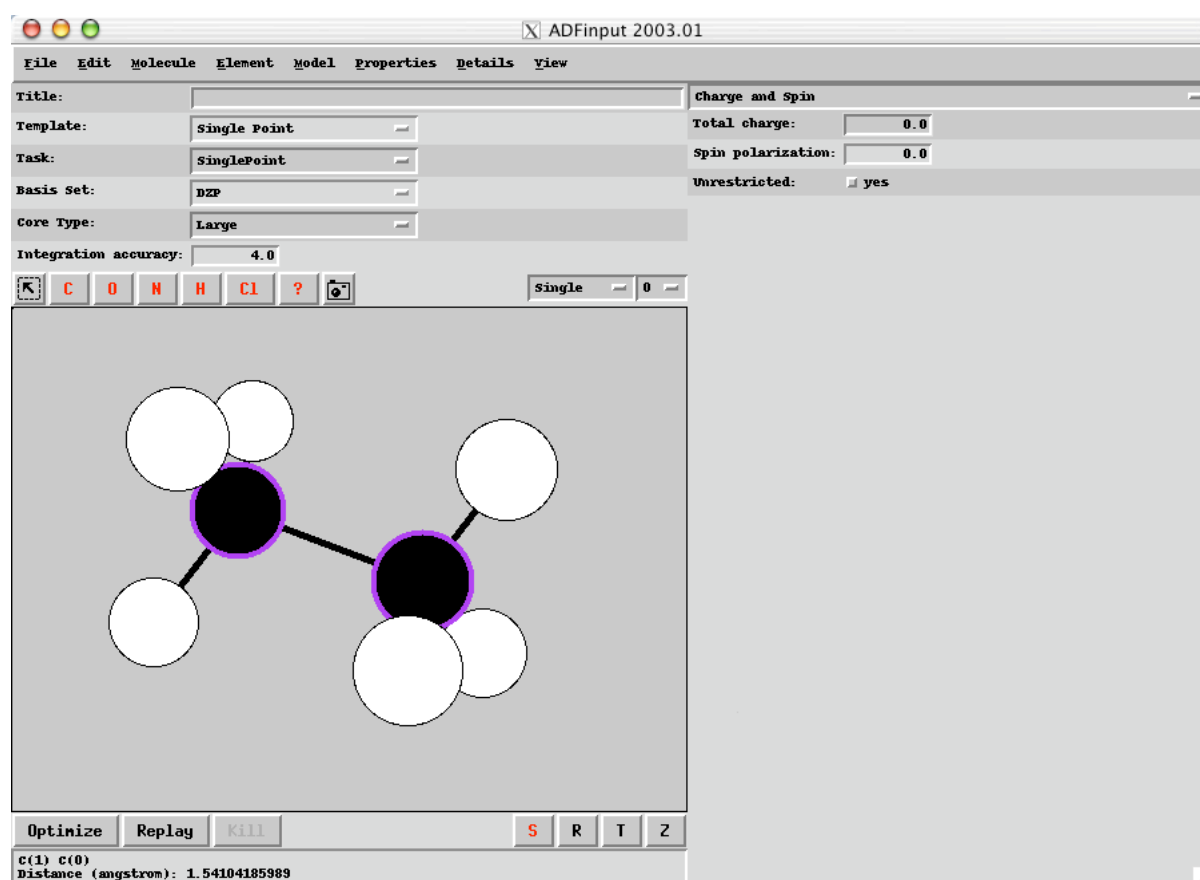
In the status field you can see the results of the optimization. The energy reported is just the force field value and has no physical meaning.

Geometry information

Bond length

Select the two Carbon atoms:

Hold the shift key, and click once on both carbon atoms.



In the status field you will find the bond length between the two selected atoms, and the names of the two selected atoms.

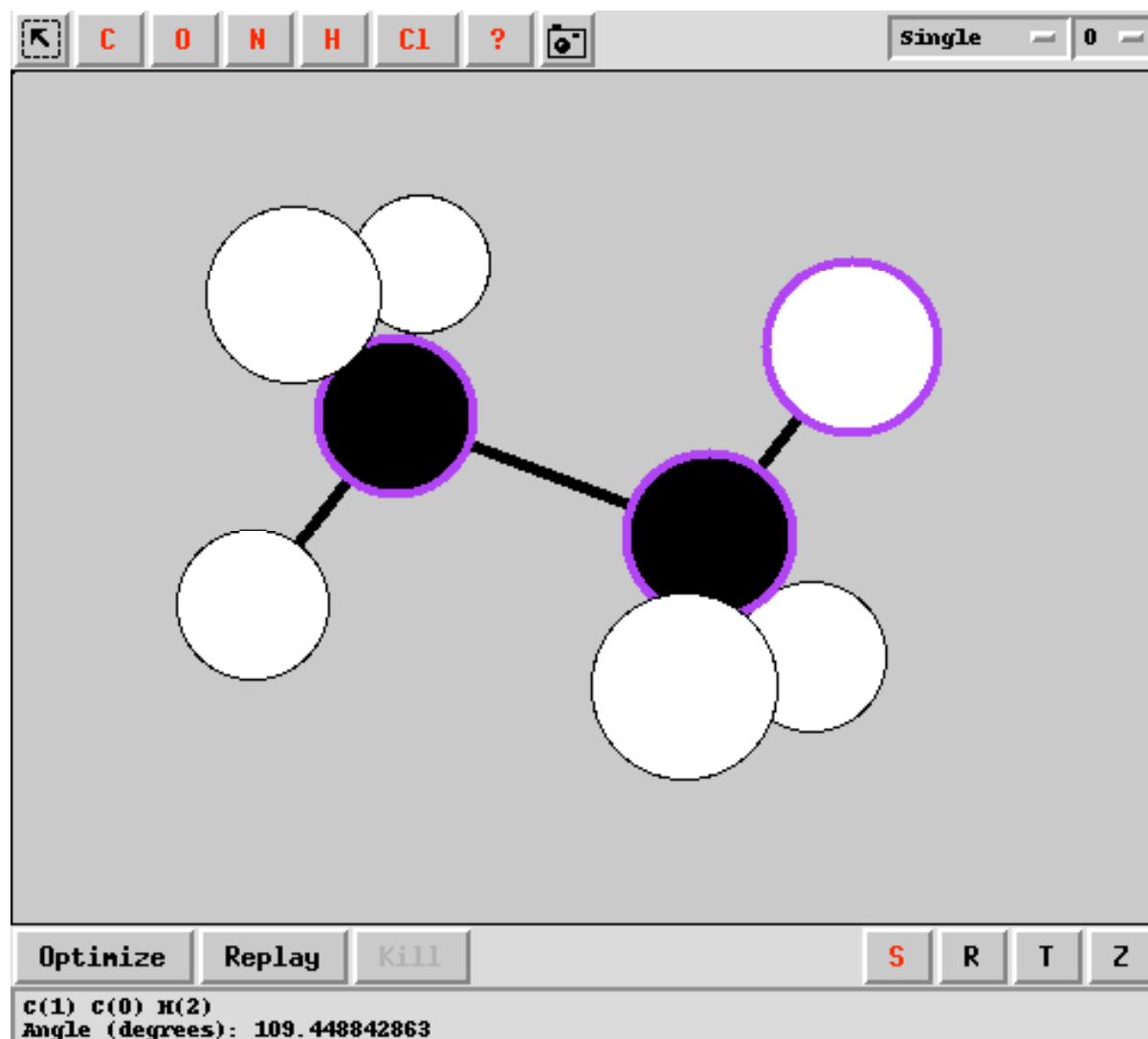
Bond angle

First clear the current selection

Click once in empty space.

Select three atoms:

Hold the shift key, click once on each carbon, and on a hydrogen.



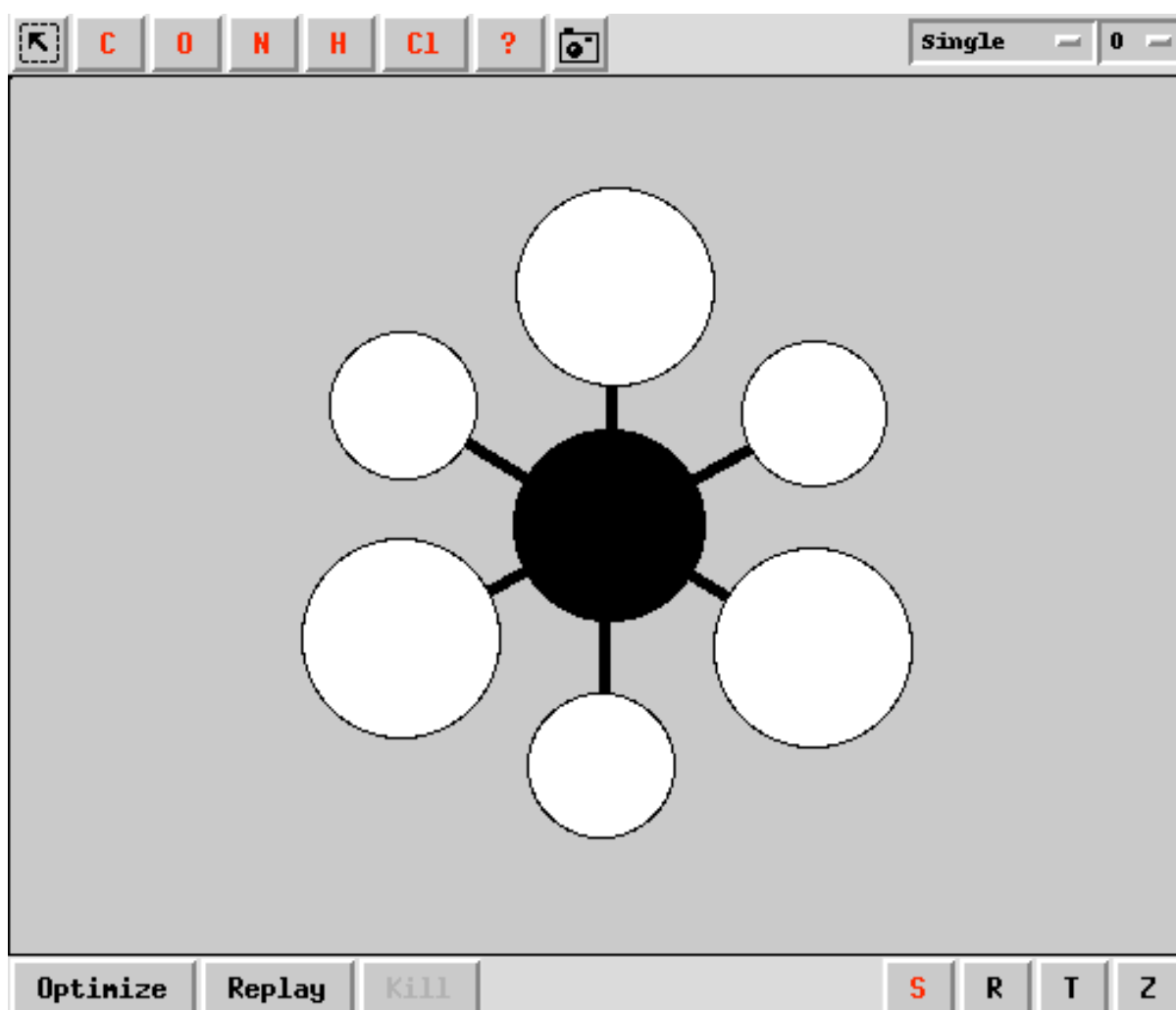
In the status field you will read the names of the three selected atoms, and the angle between these atoms. The order in which you select the atoms is important.

Changing the molecule

Rotate such that you look along the C-C axis

Clear the selection (click in empty space).

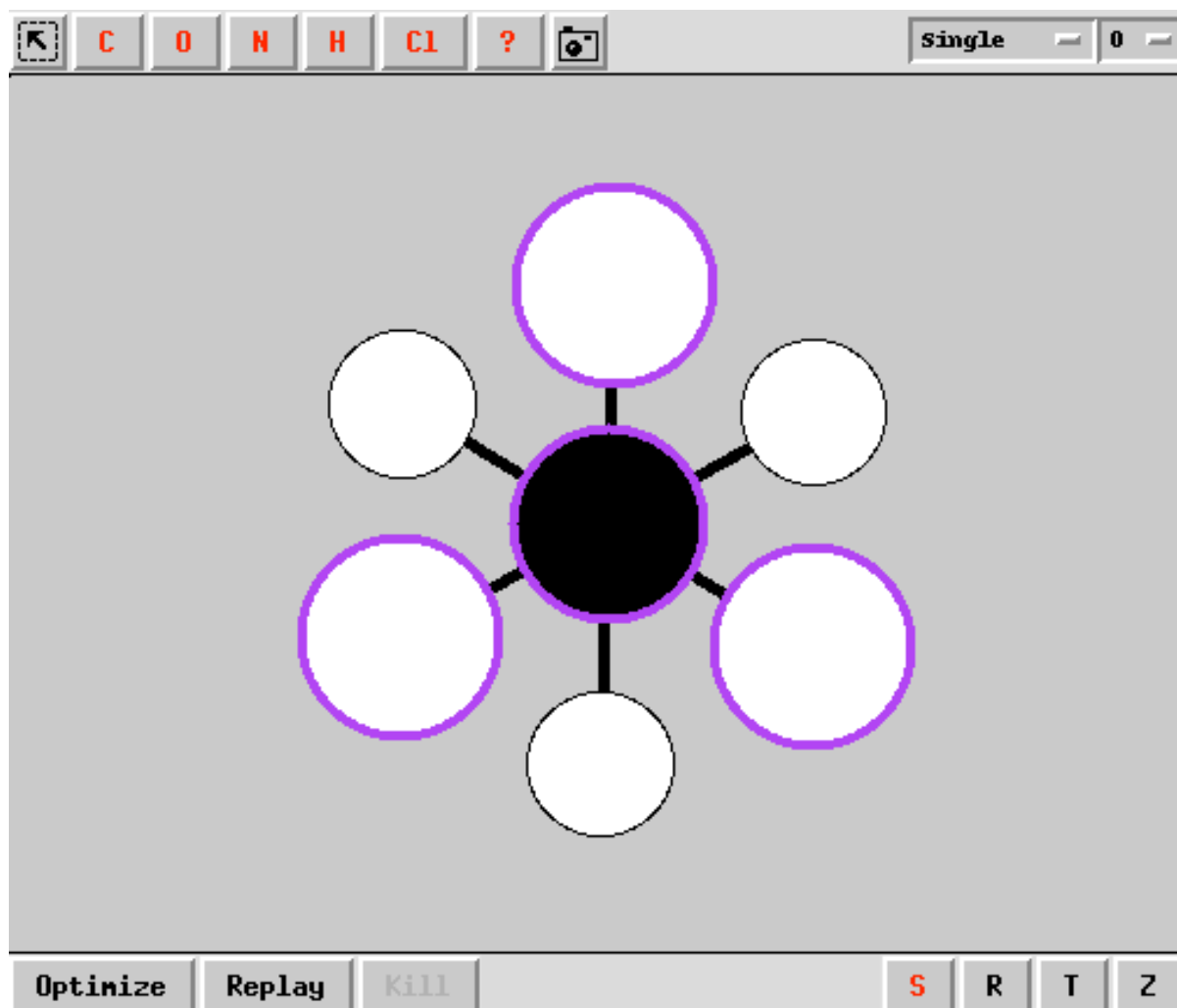
Rotate as described before (with right mouse button) such that the two C atoms are on top of each other.



Note that atoms far away are smaller than similar atoms closer to you.

Select the top CH3 group

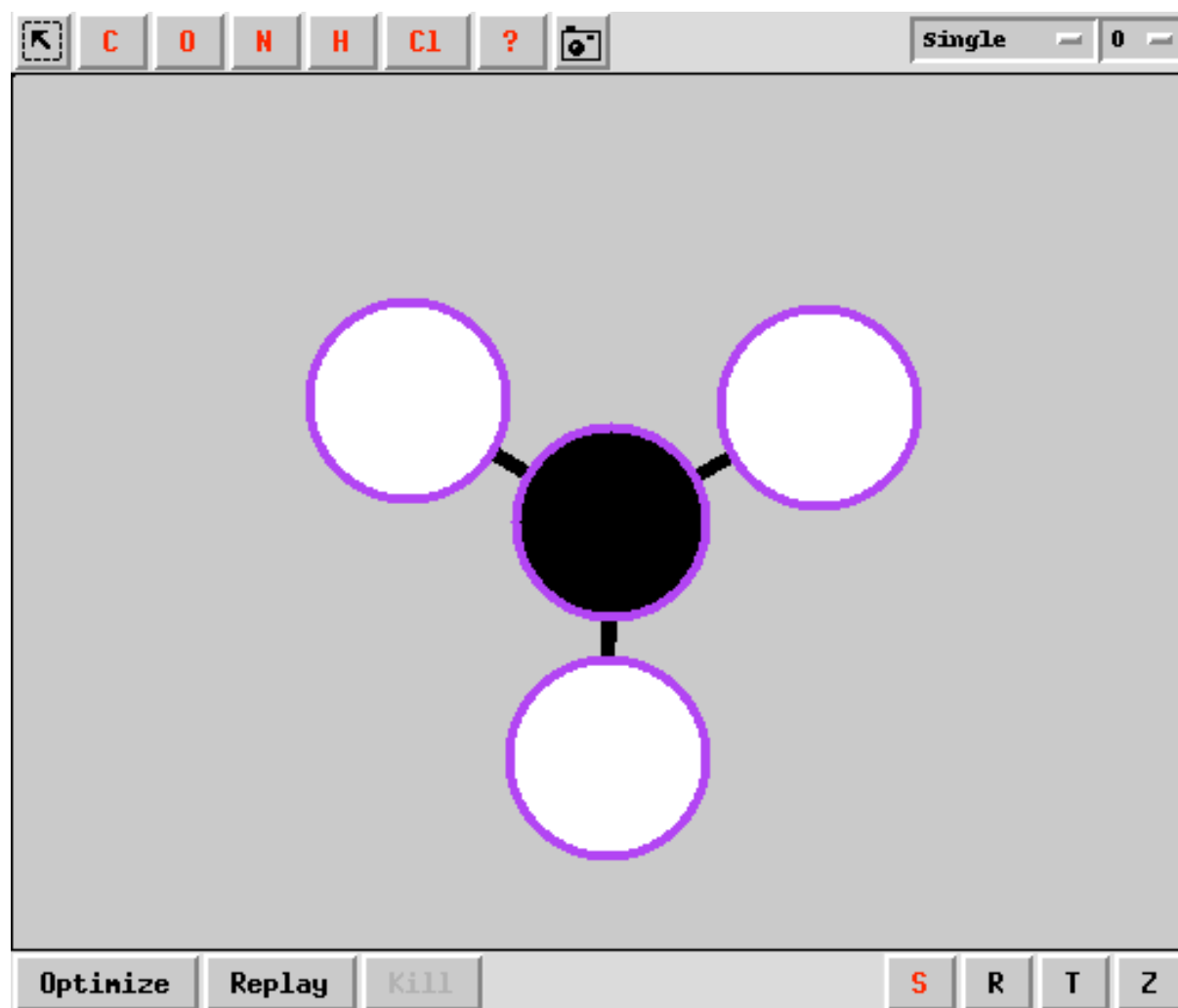
Hold down the shift key, and click once on the top (visible) C atom, and once on each connected H atom.



Rotate the selection

Rotate (with right mouse button). Make sure you move the mouse at the edge of the screen to get a pure rotation. Rotate until the hydrogen atoms are on top of each other.

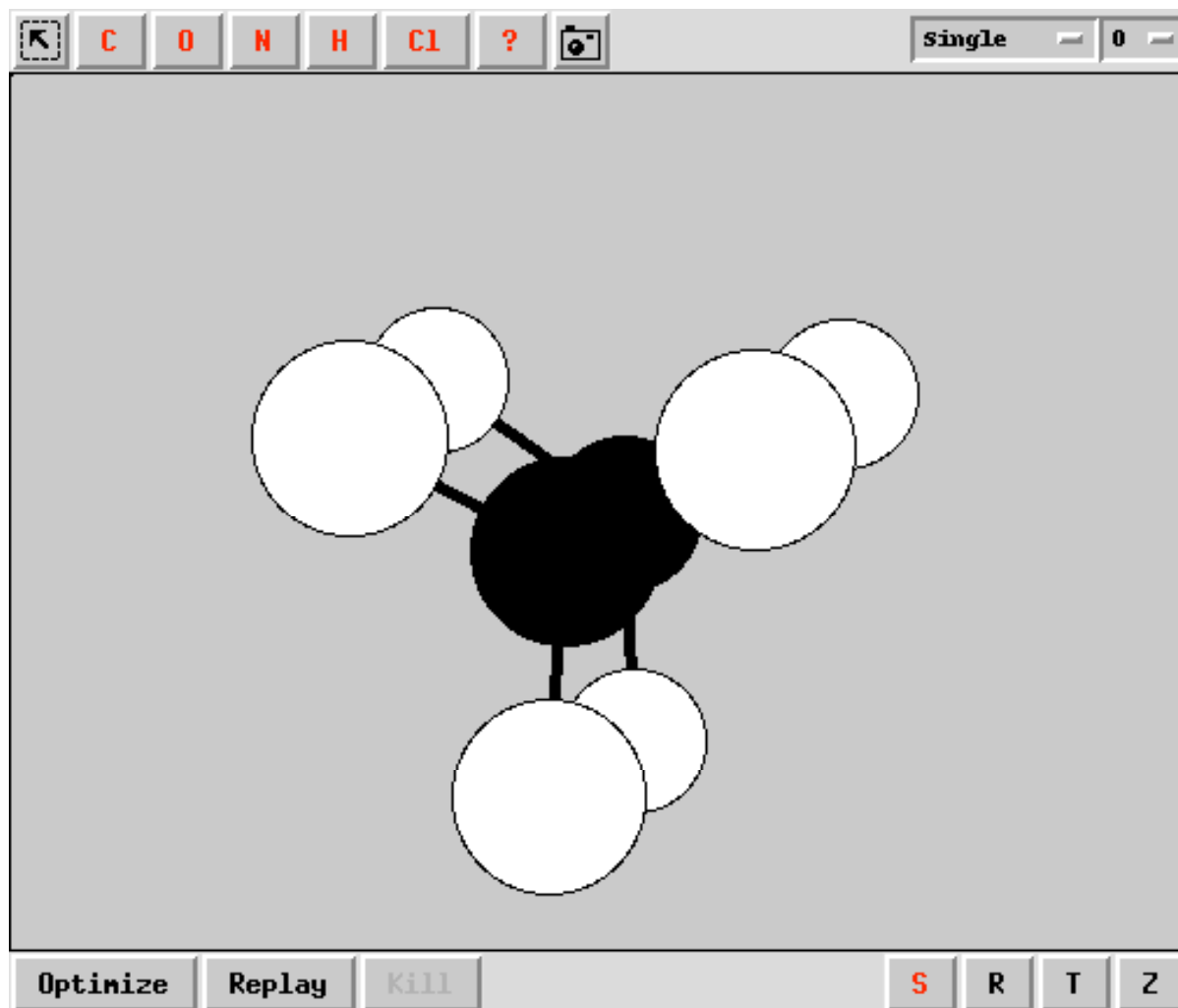
Only the selected atoms will rotate. Your result will look something as the following picture:



Next we rotate the entire molecule a little bit. To do this, you first have to clear the selection (click in empty space):

Click in empty space.

Rotate the molecule slightly.



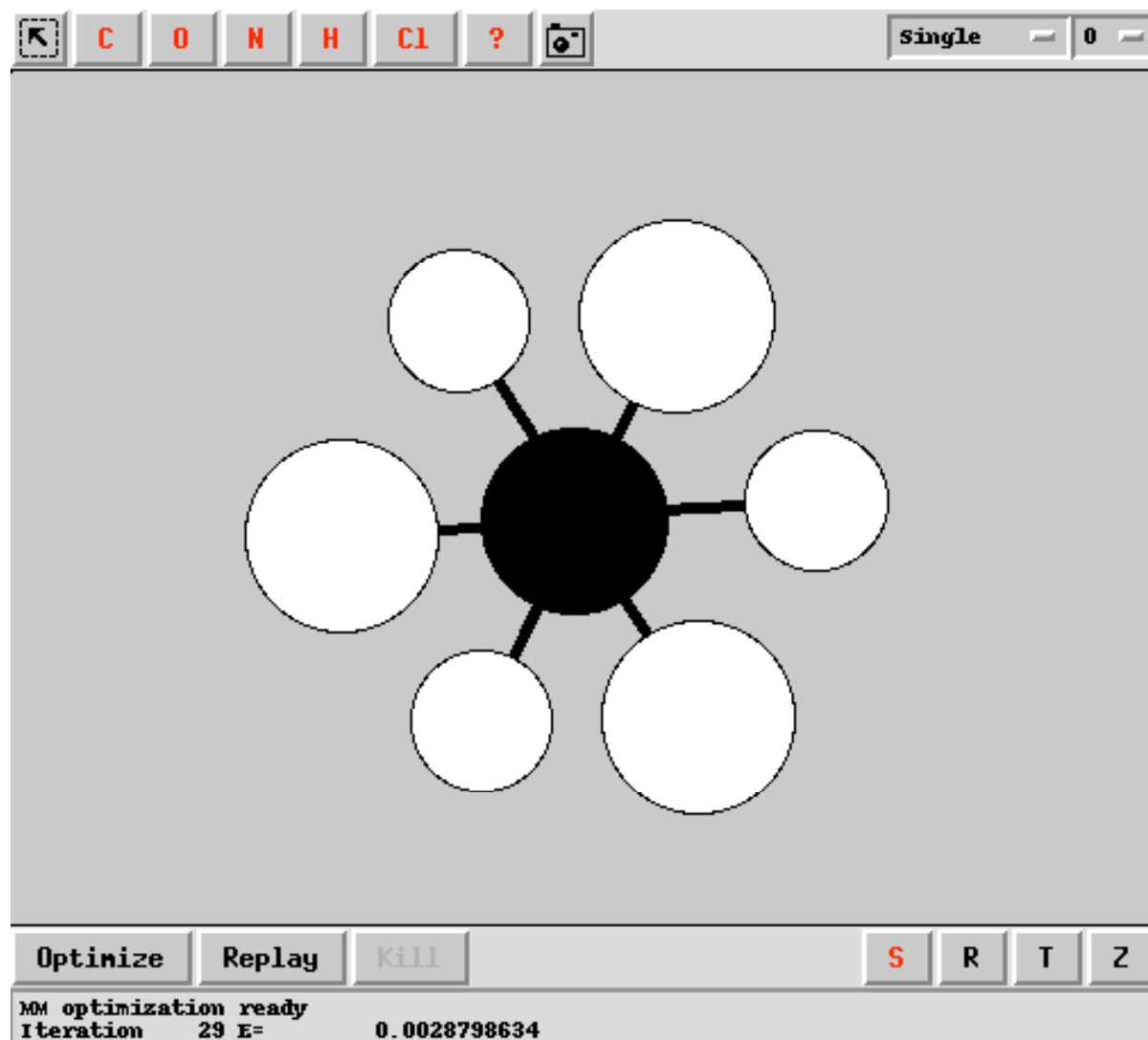
Back to Staggered Geometry

To get back to the staggered geometry, you could do the same trick again. But easier try the following:

Click optimize a few times.

Typically (not always...) the optimizer will bring back your molecule to the staggered geometry. Unless you managed to bring it into the perfect eclipsed geometry in the

previous step, but of course this is not very likely. In that case all forces will balance, and the optimizer will leave the molecule in the perfectly eclipsed geometry.



You need to click optimize more than because the forces in the almost eclipsed geometry are very small, so the optimization algorithm (incorrectly) assumes it is ready too early.

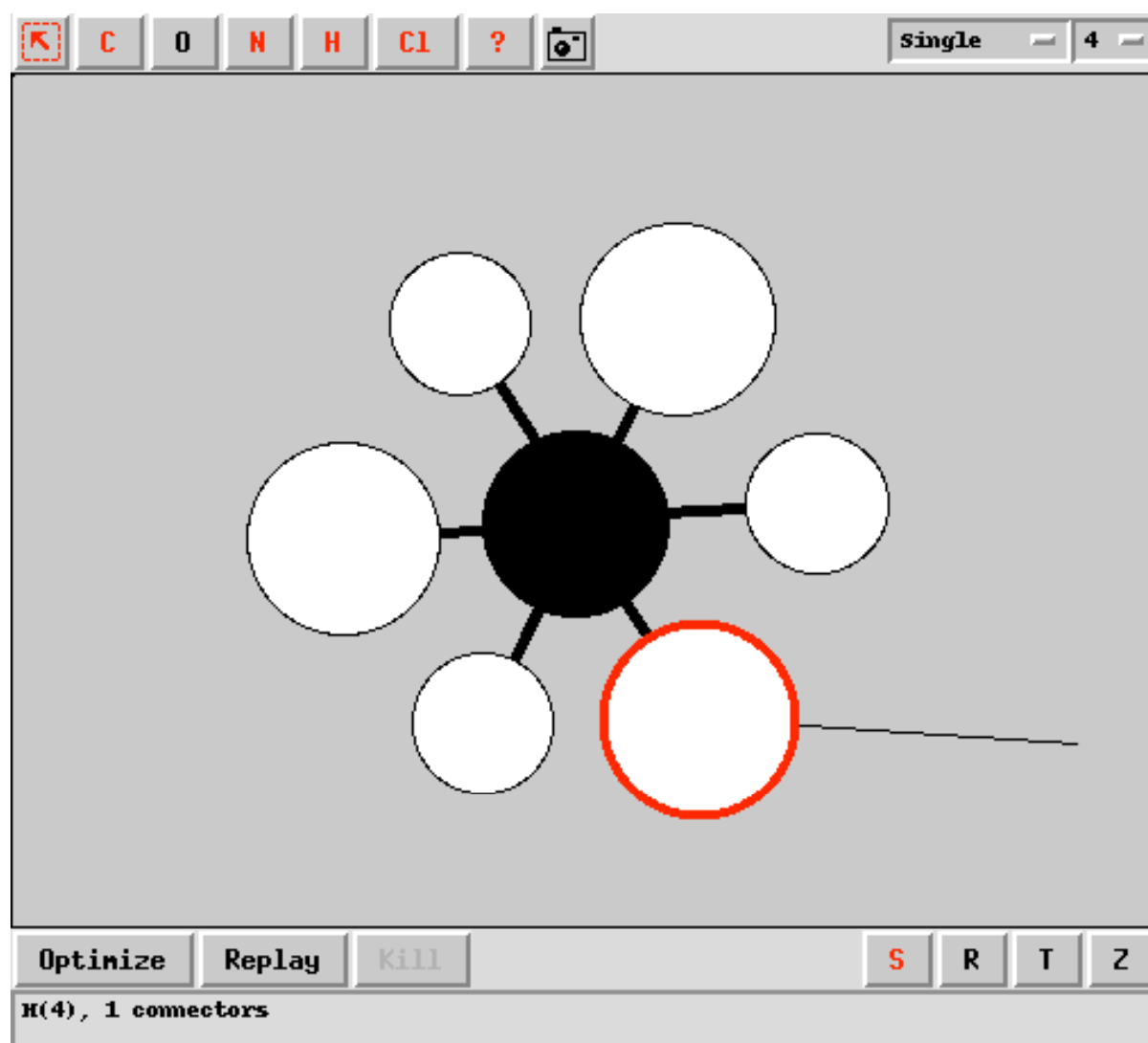
Making Ethanol out of Ethane

Select the O-tool to create an oxygen atom:

Click on the 'O' button.

Change one of the hydrogen atoms into an oxygen atom

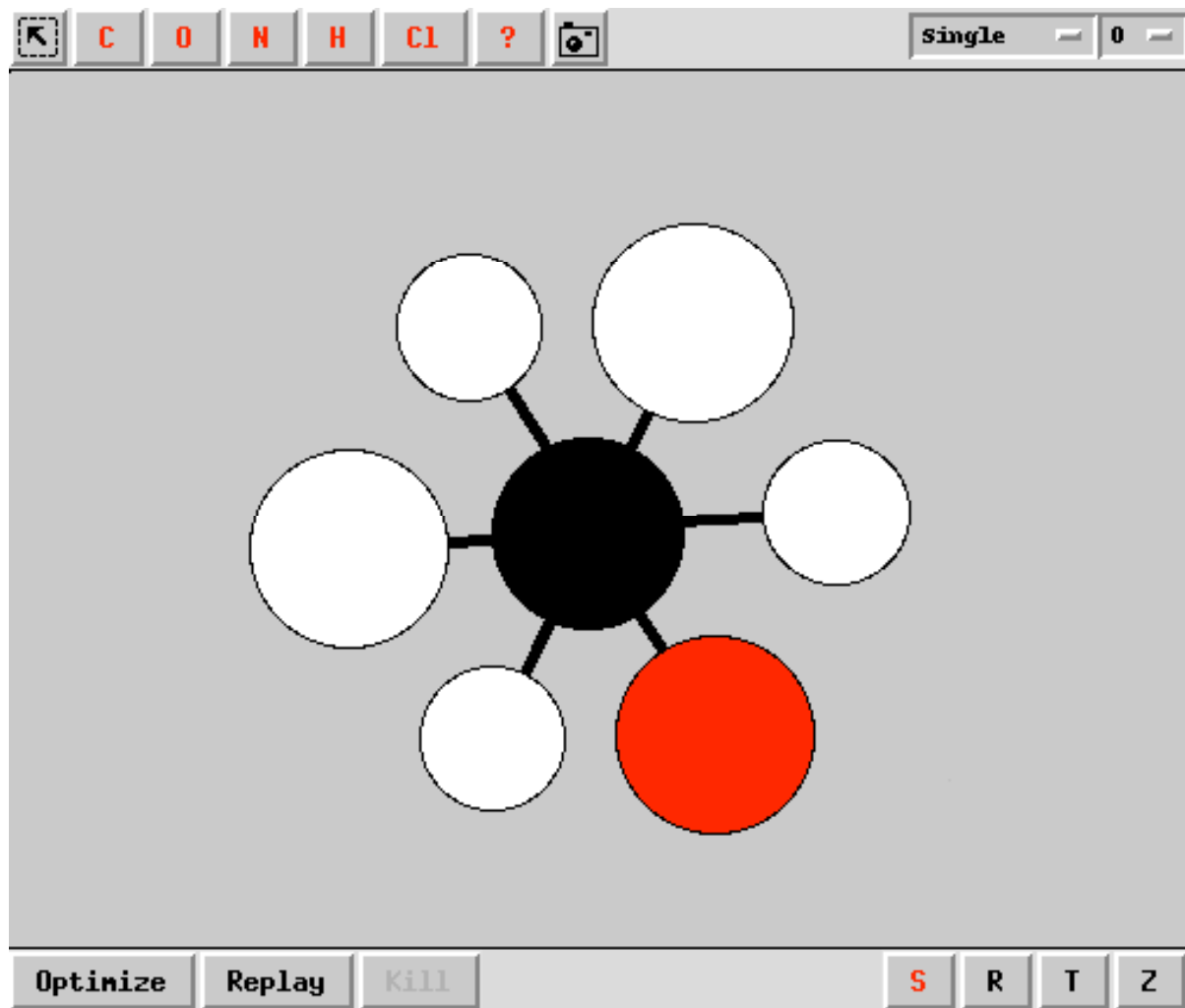
Click once on a hydrogen atom to select it.



Note that the hydrogen atom becomes the selected atom, and that you are in bonding mode.

If you would click in empty space, ADFinput would try to create a new oxygen atom bonded to the hydrogen atom. Since a hydrogen atom can only be connected to one other atom only this would NOT succeed.

Click once more on the same atom to change it into an oxygen atom.

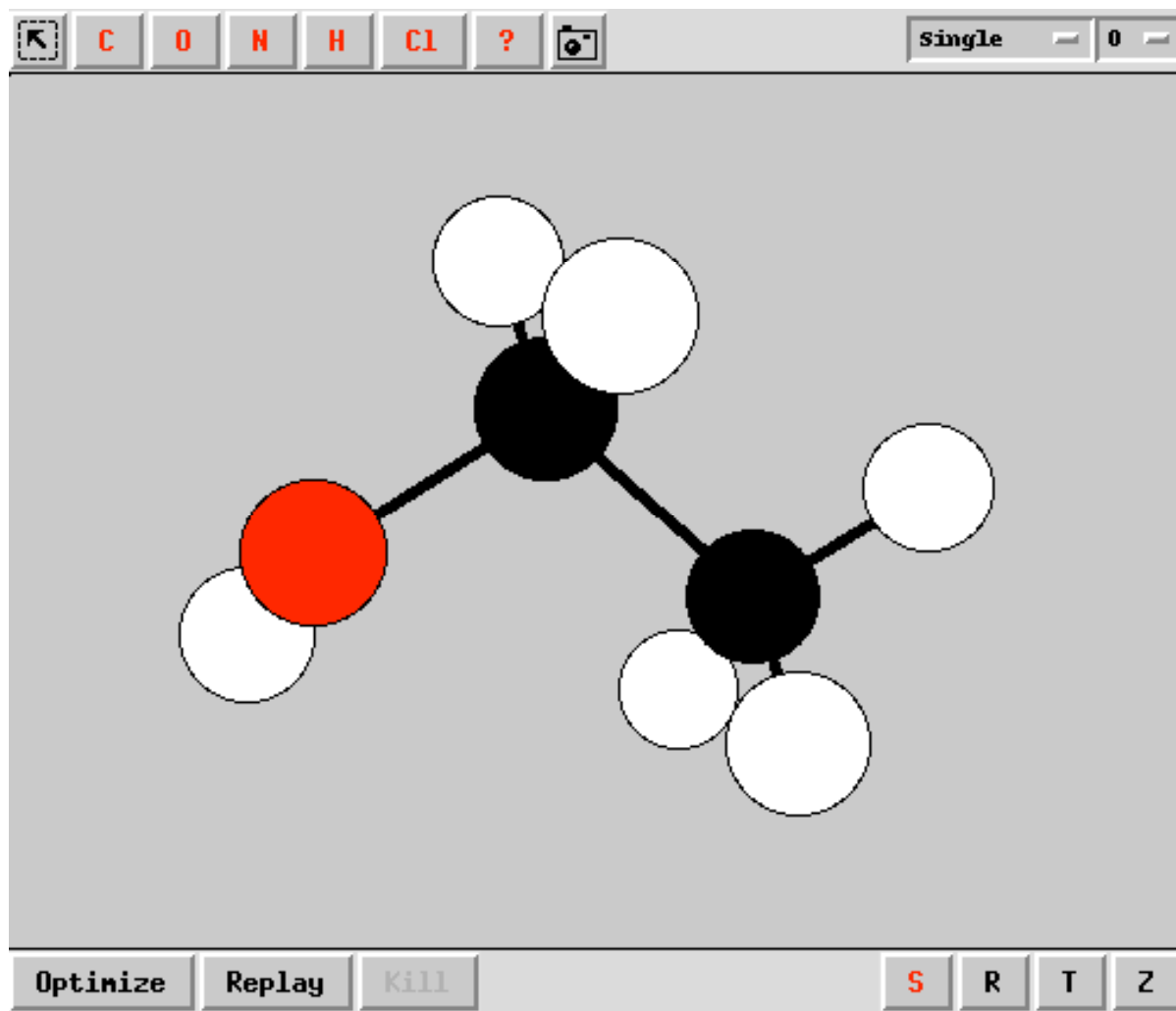


The selected atom will change into an oxygen atom. And since you clicked on the selected atom you will revert to the select tool.

Choose Add Hydrogen from the Molecule command.

Rotate the molecule.

Click on 'Optimize' to optimize the geometry.



Your ethanol is now ready.

STEP 3: SELECT CALCULATION OPTIONS

Template

You should always start by choosing the proper template.

ADF has many different modes of operation. ADFinput presents the correct settings for some common calculations together as 'templates'.

So to optimize the geometry of the ethanol molecule we just choose the proper template:

Select the 'Geometry Optimization' template in the Template menu.

Templates might change any number of input options. In this particular example, only the main Task will change from 'Single Point' to 'Geometry Optimization'.

If you would set the template again later, all input values will revert to the default values and you will loose all your changes!

Title

This field, currently empty, has no special meaning. It will be used as an identifier for your convenience in the result files of the ADF calculation. In this case, lets set the title to the name of the molecule:

Enter 'Ethane' without quotes in the 'Title' field.

Title:	<input type="text" value="Ethane"/>
Template:	<input type="text" value="Geometry Optimization"/>
Task:	<input type="text" value="GeometryOptimization"/>
Basis Set:	<input type="text" value="DZP"/>
Core Type:	<input type="text" value="Large"/>
Integration accuracy:	<input type="text" value="4.0"/>

Note that as soon as you start typing in the title field, the color of the field changes. This indicates that you have made a change with respect to the value stored in the template for this field.

Task

This is the main task the program will perform. In this case it will optimize the geometry of the molecule.

Basis set

With the 'Basis Set' pull-down menu you select the basis set you want to use. The menu gives access to the basis sets regularly used.

For this tutorial we will choose a very small basis set. This will result in poor results, but the calculation runs much faster. Thus:

Select SZ from the Basis Set pull-down menu

Title:	Ethane
Template:	Geometry Optimization
Task:	Geometry Optimization
Basis Set:	SZ
Core Type:	Large
Integration accuracy:	4.0

Core type

With the 'Core Type' pull-down menu you select the kind of core to use. This is really a further specification of the basis set.

For the tutorial a Large core is fine.

Integration

The ADF software package uses a numerical integration scheme for virtually everything it may calculate. The number specified here is roughly the number of significant digits in your results.

Increasing the number makes the results more accurate, but will require substantially more computation time. Similarly, decreasing the number will result in less accurate results, but you will get the results much quicker.

For the tutorial, we will reduce the accuracy in order to speed things up:

Change the integration accuracy to 3.0.

Title:	Ethane
Template:	Geometry Optimization
Task:	GeometryOptimization
Basis Set:	SZ
Core Type:	Large
Integration accuracy:	3.0

Charge and Spin

On the right side of the window you will find many more input fields. They are organized in panels. You select a panel with the pull-down menu showing the title of the panel, along the top side.

Charge and Spin	
Total charge:	0.0
Spin polarization:	0.0
Unrestricted:	<input type="checkbox"/> yes

Alternatively, you can select the panel you are interested in from the main menu (Model, Properties, or Details).

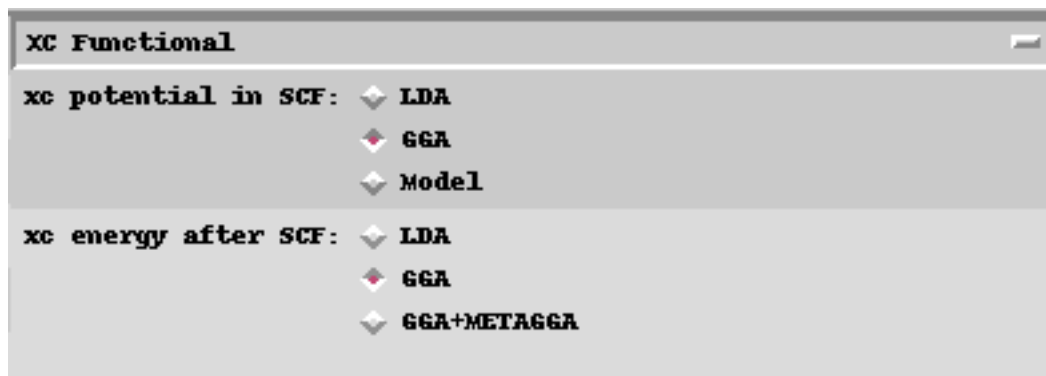
The current panel showing is the 'Charge and Spin' panel. Here you can specify the total charge of your molecule, and the spin polarization.

Since ethanol is a closed-shell neutral molecule the default settings are fine.

XC functional

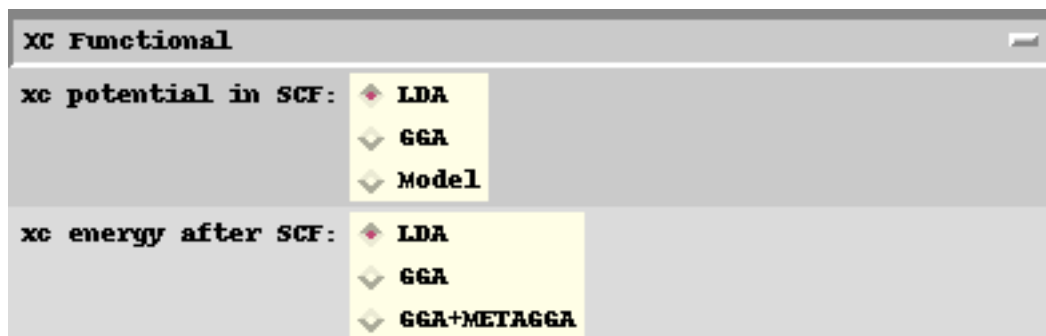
Another important input option is the XC functional to use. To choose the XC functional:

Select the XC functional
(from the drop down menu, or from the main Model menu).



For this tutorial a simple (and faster) LDA potential is sufficient. So:

Change all XC options to LDA.



Again, since you are making changes with respect to the current template, the changes are highlighted.

STEP 4: RUN YOUR CALCULATION

Save your input and create job script

Finally you will want to save your input.

Choose Save from the File menu.

Enter the name 'ethane' in the File name field.



Click on Save

Now you have saved your current options and molecule information.

ADFinput has also created a corresponding script file, which you can use to start the calculation according to your current input options. This script file has the same name, but with an extension '.run'. It also has the execute permission set for the current user.

In your terminal window, check the current files

```
% ls -l
total 24
-rw-r----- 1 visser unknown 4522 Feb 18 16:41 ethane
-rwxr----- 1 visser unknown 2310 Feb 18 16:41 ethane.run
```

Run your calculation

To actually perform the calculation (thus the geometry optimization of the ethane molecule), enter the following command:

```
% ./ethane.run
STOP NORMAL TERMINATION
rm: TAPE*: No such file or directory
STOP NORMAL TERMINATION
rm: TAPE*: No such file or directory
STOP NORMAL TERMINATION
rm: TAPE*: No such file or directory
STOP NORMAL TERMINATION
STOP NORMAL TERMINATION
```

It might take a while before the last line appears, ADF is very busy optimizing the geometry of ethanol ...

STEP 5: RESULTS OF YOUR CALCULATION

Result Files

Now check what has happened:

```
% ls -l
total 4056
-rw-r----- 1 visser unknown 4522 Feb 18 16:41 ethane
-rw-r----- 1 visser unknown 142 Feb 18 16:53 ethane.logfile
-rw-r----- 1 visser unknown 177760 Feb 18 16:53 ethane.out
-rwxr----- 1 visser unknown 2310 Feb 18 16:41 ethane.run
-rw----- 1 visser unknown 69632 Feb 18 16:53 ethane.t13
-rw----- 1 visser unknown 819200 Feb 18 16:53 ethane.t21
-rw----- 1 visser unknown 991232 Feb 18 16:53 ethane.t41
```

The ethane.run script has produced a couple of result files.

Text files (have a look at the contents!):

ethane.**out**: this is the traditional output file with the results of your calculation.

ethane.**logfile**: the logfile, showing a summary of what happened

Binary files:

ethane.**t13**: the 'checkpoint' file, sometimes used for restarts

ethane.**t21**: the TAPE21 result file, containing all relevant results in binary format

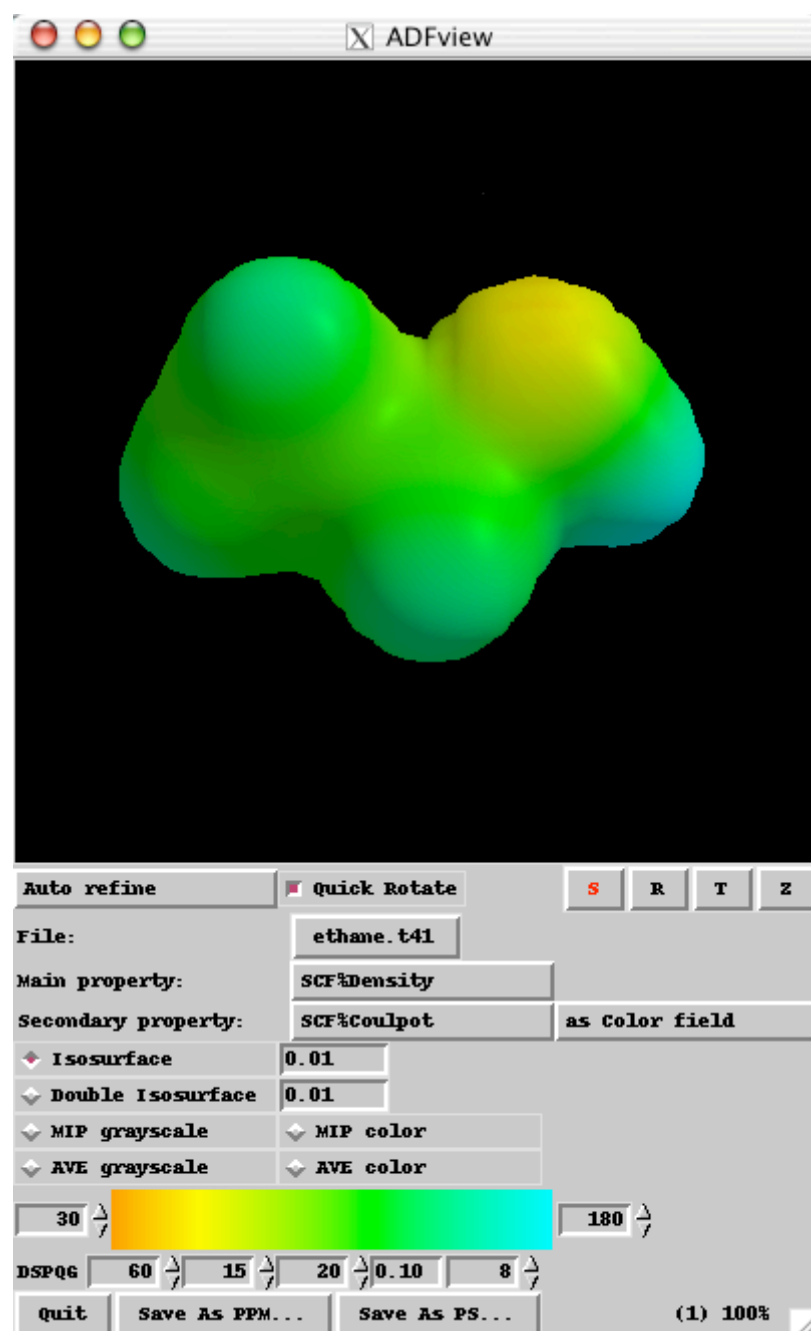
ethane.**t41**: contains grid data for visualization (produced by the DENSF utility).

Visualize Results

The binary files can be used only by ADF or one of its utilities.

For example, you can use the ADFview utility to visualize the final density and electrostatic potential:





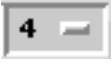


```
adfview ethane.t41
```



The ADFview utility has its own documentation (tutorial and reference manual).

REFERENCE MANUAL

BUTTONS AND TOOLS

Button	Description
	Select Tool: used to select, and to rotate, translate or zoom (with modifier keys or mouse buttons).
	C-tool, O-tool, N-tool, H-tool, Cl-tool: atom-tools used to <ul style="list-style-type: none">• create a C, O, N, H or Cl atom,• change an existing atom,• create bonds between existing atoms. The ?-tool is used with the Element menu.
	Display button: toggle the display between a very simple but fast picture, or a photographic quality picture of your molecule
	Bond Type menu: <ul style="list-style-type: none">• for new bonds• change selected bonds
	Connector menu: number of connectors <ul style="list-style-type: none">• on new atoms• change selected atoms
	Optimizer buttons: use to <ul style="list-style-type: none">• start or stop the optimization• replay the optimization• kill a running optimization
	Mouse-mode buttons: <ul style="list-style-type: none">• S: normal mouse button• R: rotate with left mouse button• T: translate with left mouse button• Z: zoom with left mouse button

TEMPLATES AND DEFAULTS

All input options have default values. However, the default values depend on the main task you have chosen, and on further properties you may select to calculate. ADFinput uses templates that are simply a collection of input values to be used together as defaults.

ADFinput has a couple of templates for typical calculations (currently Single Point, Geometry Optimization, IRC, Frequencies, and Transition State Search). You may also define your own templates.

Use a template

Select the template you want to use from the Template menu, located in the main input options area.

All input values will change to the values specified in the template you select.

Yellow fields: different from template value

After you have selected a template, you can make changes to any input field you like.

The background color of that field turns yellow. This is just feedback for you so you know what fields you changed with respect to the default value specified in the current template.

Red fields: error in template

If you happen to see an input field with a red background, this means that the default value for that field is NOT specified in the current template. If you are using one of the original templates, please notify us so we can fix that template (email to support@scm.com).

Revert to template values

If you want to undo your changes and get back to the default values as specified in the current template, simply select the template again from the Template menu.

Make your own templates

It is very easy to make your own templates, collecting all default values for the typical jobs you like to perform.

If you set the SCM_TPLDIR environment variable, ADFinput will look for additional templates (when starting up) in the directory \$SCM_TPLDIR.

In a terminal window:

- make a directory where you want to store your templates
- set the environment variable SCM_TPLDIR to the complete path to this directory

In ADFinput:

- edit all the fields as you would like them to be stored in a template.
- select 'Save as Template' from the File menu
- select the directory in which you want to store your template
- specify a filename, ending with '.tpl'
- click on Save.

If you now check your Template menu you will find a new entry.

The name of the template is the filename you have chosen, but without the .tpl extension.

MOLECULE EDITOR TRICKS

Selecting

You can select parts of your molecule (atoms and / or bonds) with the mouse, using a combination of the following techniques:

- Click on the item you want to select. If you want to extent the selection with more items, hold the Shift key and click on the item to add. If you want to remove an item from the selection, hold the Shift key and click on the item to be removed.
- Click with the mouse somewhere in the empty space, and drag a selection rectangle by moving the mouse while holding the mouse button down. Release the mouse button when the items to be selected are included within the rectangle.

When extending or reducing the selection by shift clicking, take care not to move the mouse while clicking. Moving in combination with the shift key will rotate the selection.

When selecting does not react as described, make sure you are using the select tool, and that the mouse mode is the normal 'S' mode:



Delete an atom

Select the atom (click on it), and press the Backspace key.

Delete a bond

Select the bond (click on it), and press the Backspace key.

Delete the selection

Make your selection, and press the Backspace key.

Make a bond

Take one of the atom-tools.

Next click once on the first atom you want to connect. You will enter the bonding mode (the line to the mouse position from the atom you just clicked on will be your visual cue for the bonding mode).

Next click on the atom you want to make the bond to.

The bond will be created (if possible), and you will revert to the normal select mode.

Change the bond type

Select the bond or bonds to change.

Chose the required bond type from the Bond-type pull down menu.

The bond type will be visible in the picture by the color used.

Rotate or translate the selection

When you try to rotate or translate while you have some items selected, only the selected items will be rotated or translated.

RUN SCRIPT

Save your input using the Save or Save As ... menu commands.

Your input will be saved in a file with the name you specify, and at the same time a run script will be saved. It has the same name, but with '.run' appended.

To execute your calculation just execute this run script.

In the panel 'Files (Restart)' you can specify what files to save at the end of the run script. By default, TAPE21 (result data), TAPE41 (grid data for visualization) and TAPE13 (checkpoint information) are saved.

If the environment variable SCM_RESULTDIR has been set, the run script will change into that directory. Next it will run from there, and all result files will be stored in that directory.

If the environment variable SCM_RESULTDIR has not been set, the run script will execute in the directory where it is started, and the result files will also be located in that place.

MENU COMMANDS

Print...

The Print command will generate a file containing the picture of the molecule (only). The input options are not printed.

If the simple picture quality is currently in use, a postscript file is generated.

If you have activated the photographic picture mode, a ppm file is generated.

Preferences...

The Preferences... menu command gives access to the 'Preferences' input panel. You may also select this panel from the pull-down menu on top of the input panels.

This panel is used to set a number of preferences for the ADFinput program.

To save the preferences, click on the Save button in the Preferences panel.

Reset View

When you use the 'Reset View' menu command, the translation, zoom and rotation settings will be adjusted such that the entire molecule is visible.

Use it for example when you translate the molecule 'out of view'.

Bond Lengths constrained

When creating new atoms bonded to existing atoms, ADFinput will constrain the bond length to the textbook value.

If you do not wish this to happen, select this menu command to toggle this behaviour.

Add Hydrogen

The 'Add Hydrogen' menu command will add hydrogen atoms to your molecule until every connector is connected. The number of connectors and the number of lone pairs determine the geometry. For example, the Oxygen atom has four connectors and two lone pairs in a tetrahedral arrangement.

Import Molecule...

Use this menu command to import the geometry of your molecule from file.

Currently ADFinput has little knowledge about other formats, it can only read text files, and it assumes to find x, y, z coordinates on a line, and some indication of the atom type (an element name or an atom charge). Most popular formats will work fine, just try with your favorite format.

Bond information is not imported.

Guess Bonds

Roughly guess what atoms are bonded together, depending on the distance between the atoms compared with text book values. The bond type is currently always set to single, so you probably need to make some changes.

Only ADFinput uses the bond information. The ADF program itself does not use any of the bond information.

INPUT OPTIONS REMARKS

Empty fields

Some input fields do not have a value from the template. In those cases ADFinput does not specify the value, but leaves the value to be determined by the ADF program.

Coordinates

The coordinates panel shows the coordinates corresponding to the molecule visible in the molecule display. You may edit the coordinate values here as well.

You may select to use Cartesian or Internal coordinates. For internal coordinates you can currently only edit the values for bond lengths and angles, not the connection information.

If you will optimize the geometry (with ADF), the program will perform this optimization in the coordinate type you have selected here. Thus, the Cartesian or Internal pull-down menu is not only for display purposes, but determines the optimization method used.

By checking the check boxes next to the coordinates you will freeze those coordinates during a geometry optimization.

User Input

You can use the User Input field to specify any kind of text. The text will be appended without any change to the end of the ADF input. This way, you may access some keys that are not (yet) available in ADFinput.

Note that at this point in time you can only add text to the ADF input file, not to the input of any of the property programs.

ENVIRONMENT VARIABLES

Name	Meaning
SCM_ERROR_MAIL	email address for error reports
SCM_GUIRC	location of the preferences file
SCM_TPLDIR	location of the templates directory
SCM_RESULTDIR	location of the results directory
DISPLAY	X-window display to use