

A guide to creating animated 3D Polymers

This guide will explain all there is to know about creating your own interactive structures. There are two routes with several techniques used to make these animations; your chosen route will simply depend on the desired structure you wish to produce.


The guide requires use of the following programs:

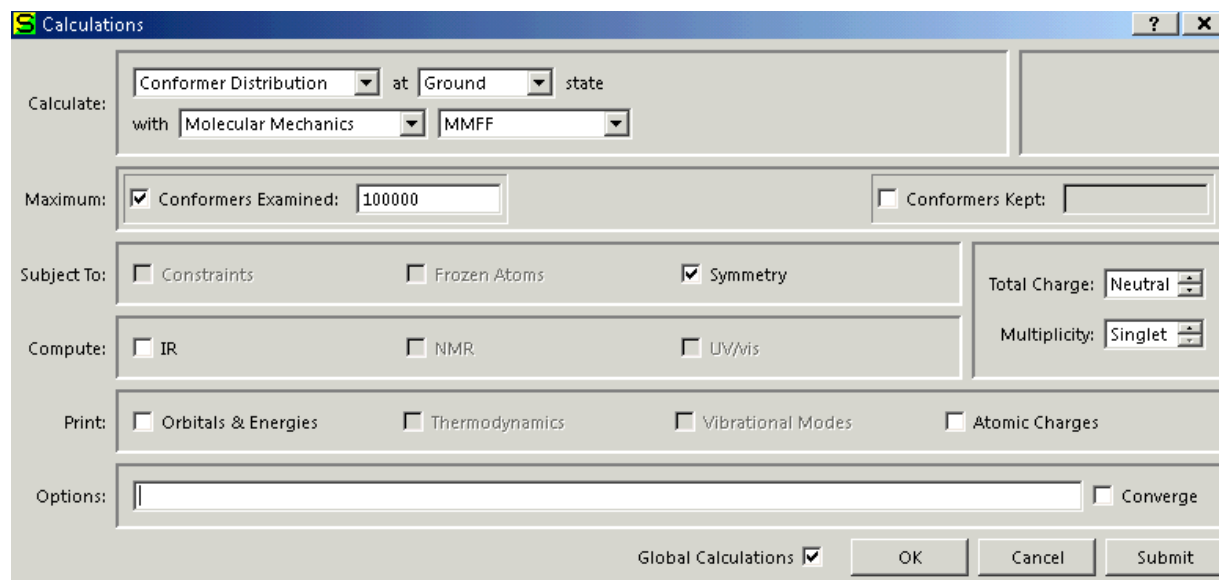
- SPARTAN 08
- Jmol.jar application
- Dreamweaver(CS3/4)

Note: This guide is specific for a PC computer and some of the options may vary from that of a Mac.

Route 1: Using SPARTAN for calculating the minimum conformation energies of short chain polymers.

Short chain polymers can be built directly from SPARTAN.

Open up a blank page in SPARTAN '08 to build the polymer. Once you are happy with the structure select the '**Minimize**' button  located in the tool bar. This will quickly minimize the molecules energy before doing a more precise energy calculation. Under the **setup** menu, select **calculations** and choose **Conformer Distribution, Molecular Mechanics** from the dropdown menus as shown below:



For small molecules this calculation should take a few minutes however, there are ways to shorten this calculation for larger molecules;

In the **Options** box type **KEEPALL SEARCHMETHOD=SYSTEMATIC PRINTLEV=2 SPARSE=100** for a quicker and more random search for the lowest energy conformer.

Once the calculation is complete, SPARTAN will display the lowest energy conformer it has calculated but it is possible to view all calculated conformers. In the **Display** menu, select **Spreadsheet** and an ordered list of conformers will be shown. Click **Add...** followed by **Rel. E** to view each conformers relative energy.

Once you are happy with your calculated structure, go to **file/ save as** and save as a **Brookhaven pdb**.

Interpreting your 3D structures using Jmol

Jmol can highlight important parts of your molecule.

Testing of Jmol commands can be done in jmol.jar or by using Dreamweaver's "Preview in Browser" option. For simplicity, this guide only shows the most important commands.

(In depth explanation of each Jmol command can be found at Bob Hanson's Jmol interactive scripting documentation: <http://chemapps.stolaf.edu/jmol/docs/>)

```
jmolInitialize("./");jmolApplet("400", 'load zSpiralpolystyene.pdb {2 2 2}; moveto 0.0 {-791 -606 -79 16.39} 100.0 0.0 0.0 {-0.052500248 0.16050005 -0.94550014} 9.187463 {0.0 0.0 0.0} 0.62859726 -0.31056595 50.0; boundingbox off; select all; colour cpk; spacefill 90; wireframe 50; connect aromatic auto
```

This command loads pdb file with the applet size of 400*400 pixels.

The moveto command specifies the orientation in which the file is loaded.

The connect aromatic auto will insert all aromatic double bonds however on some occasions it may be necessary to insert double bonds yourself by using the **connect(atomno=n)(atomno=x)Double**.

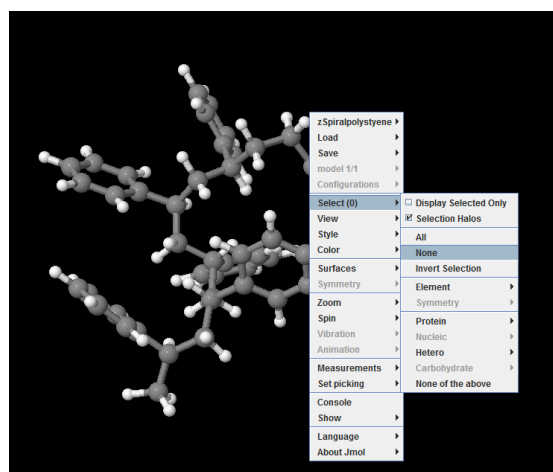
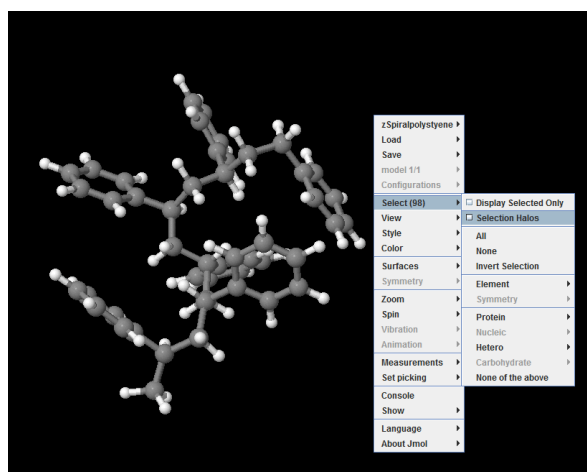
Showing Repeat Units

This is a useful technique when dealing with polymers because it highlights each repeating unit within the polymer. In order to do this, the pdb file must be edited first.

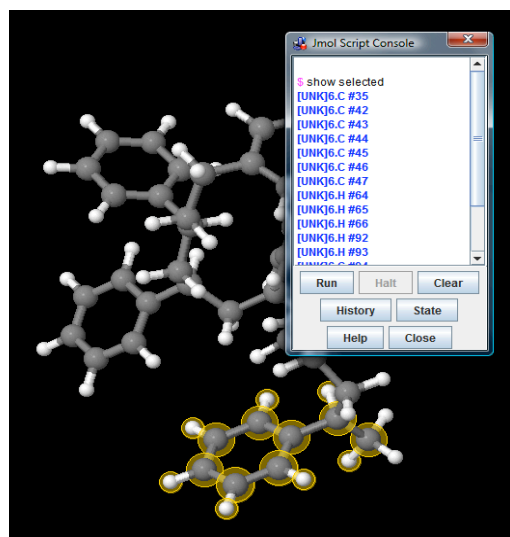
Open up the structure in Jmol, right click and tick **Selection halos on**. Select **none from the**



same menu and select the hand tool in the menu bar above.



Manually select each repeating unit, whilst doing so, type into the console **Show selected** to obtain a list of atom numbers from each group. Make a note of each set of numbers.



Open up the same pdb file in Dreamweaver and change the **UNK 0001** to the desired group number eg. **UNK 0002** for repeat unit/group number 2, **UNK 0003** for repeat unit/group number 3

Assure all the groups are group together in the spreadsheet as shown below.

```

HEADER
REMARK Spartan '08 exported M0001
HETATM 1 C UNK 0001 3.812 2.253 1.263
HETATM 2 C UNK 0001 4.328 1.443 0.098
HETATM 3 C UNK 0001 5.320 -0.042 -2.069
HETATM 4 C UNK 0001 4.506 0.057 0.204
HETATM 5 C UNK 0001 4.661 2.075 -1.108
HETATM 6 C UNK 0001 5.153 1.336 -2.186
HETATM 7 C UNK 0001 4.997 -0.681 -0.874
HETATM 8 C UNK 0001 2.415 1.849 1.758
HETATM 9 C UNK 0002 1.284 2.001 0.711
HETATM 10 C UNK 0002 1.124 3.439 0.238
HETATM 11 C UNK 0002 0.819 6.074 -0.693
HETATM 12 C UNK 0002 1.299 3.746 -1.120
HETATM 13 C UNK 0002 0.790 4.477 1.121
HETATM 14 C UNK 0002 0.639 5.785 0.658
HETATM 15 C UNK 0002 1.148 5.054 -1.582
HETATM 16 C UNK 0002 -0.037 1.435 1.291
HETATM 17 C UNK 0003 -1.173 1.312 0.240
HETATM 18 C UNK 0003 -2.432 2.010 0.751
HETATM 19 C UNK 0003 -4.721 3.357 1.669
HETATM 20 C UNK 0003 -3.223 1.463 1.774
HETATM 21 C UNK 0003 -2.800 3.251 0.209
HETATM 22 C UNK 0003 -3.938 3.918 0.663
HETATM 23 C UNK 0003 -4.363 2.131 2.226
HETATM 24 C UNK 0003 -1.476 -0.162 -0.130
HETATM 25 C UNK 0004 -0.356 -0.887 -0.920
HETATM 26 C UNK 0004 -0.067 -0.263 -2.281
HETATM 27 C UNK 0004 0.548 0.854 -4.789
HETATM 28 C UNK 0004 1.266 -0.080 -2.681

```

Now your file is ready to show repeating units.

Once you have chosen the correct orientation of the molecule using the moveto command, simply use;

Select (group number); colour (chosen colour) to highlight your chosen group/repeat unit.

```

jmolLink('load zSpiralpolystyene.pdb {2 2 2}; moveto 0.0 {-791 -606 -79 16.39} 100.0
0.0 0.0 {-0.052500248 0.16050005 -0.94550014} 9.187463 {0.0 0.0 0.0} 0.62859726 -
0.31056595 50.0; select all; boundingbox off; axes off; select all; colour CPK; spacefill
90; wireframe 50; connect aromatic auto; select 1; colour cadetblue; select 2;
colour cyan; select 3; colour cornflowerblue; select 4; colour yellow tint; select 5;
colour lavender; select 6; colour deeppink; spin 100; delay 3.5; spin off

```

You can add selection halos to this command by using;

```

Selectionhalos true; select 1; delay 1; colour blue; select 2; delay 1; colour red;
selectionhalos false

```

The Hover application

The hover application brings back the original colour of the repeat unit (once coloured) so that the user can see what the repeat unit is made from. Within the "Show repeat unit" syntax (explained above) place;

Hover off; set hoverCallback "jmolscript: script *DocumentName.spt*"

Hover off removes the atom label so that it doesn't get in the way.

Creating a java script file for the Hover application

In Dreamweaver go to **File/New/Blank Page/Java Script/Create** to create a java script document. Within this you need your 'select group and colour' command and a new command that tells the applet to colour the hovered group its original colour, CPK. Eg.

// JavaScript Document

```
select resno=1; colour palegreen; select resno=2; colour yellowgreen; select
resno=3; colour mediumSeaGreen; select resno=4; colour powderblue; select
resno=5; colour dodgerblue; select resno=6; colour mediumslateblue; select
resno=7; colour mediumblue; select resno=8; colour mediumvioletred; select
within(group, atomIndex=_atomHovered); color cpk; centre selected; zoom 500;
delay 4; centre; zoom 115; select resno=1; colour palegreen; select resno=2;
colour yellowgreen; select resno=3; colour mediumSeaGreen; select resno=4;
colour powderblue; select resno=5; colour dodgerblue; select resno=6; colour
mediumslateblue; select resno=7; colour mediumblue; select resno=8; colour
darkviolet; colour mediumvioletred;
```

Here, the pale blue script is the 'colour group command'. The new and important command is shown in red. This tells the molecule to colour the group that is hovered CPK, centre it in the applet box, zoom in to it, delay for four seconds and then return to its original position and colour.

You can change the colours, delay times and how much you want to zoom in to what you please.

Growing Polymers

You can grow your own polymers using Jmol by hiding all groups apart from the group(s) you wish to display. Below is a large polymer.

```
jmolLink('load dendrimerTest2.pdb; spacefill off; connect aromatic auto; hide all;
hide none; hide
1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28; set echo top
centre; echo Core; delay 1; hide none; hide
1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27; echo; echo
Branching Units; delay 1; hide none; hide
1,2,3,4,5,6,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27; delay 1; hide none;
hide 1,2,3,4,5,6,8,9,10,11,12,13,15,16,17,18,19,20,21,22,23,24,25,26,27; delay 1; hide
none; hide 1,2,3,4,5,6,8,9,10,11,12,13,15,16,17,18,19,20,22,23,24,25,26,27; delay 0.7;
```

hide none; hide 1,2,3,4,5,6,8,9,10,11,12,13,15,16,17,18,19,20,22,23,24,25,26,27; delay 0.7;hide none; hide 1,2,3,4,5,6,8,9,10,11,12,13,15,16,17,18,19,20,22,23,24,25,26; delay 0.7; hide none; hide 1,2,3,4,5,6,8,9,10,11,12,13,15,16,17,18,19,20,22,23,25,26; delay 0.7; hide none; hide 1,2,3,4,5,8,9,10,11,12,13,15,16,17,18,19,20,22,23,25,26; delay 0.7; hide none; hide 1,2,4,5,8,9,10,11,12,13,15,16,17,18,19,20,22,23,25,26; delay 0.7; hide none; hide 1,2,4,5,8,9,11,12,13,15,16,17,18,19,20,22,23,25,26; delay 1; hide none; hide 1,2,4,5,8,9,11,12,15,16,17,18,19,20,22,23,25,26; delay 0.7; hide none; hide none; hide 1,2,4,5,8,9,11,12,15,16,18,19,20,22,23,25,26; delay 0.7; hide none; hide 1,2,4,5,8,9,11,12,15,16,18,19,22,23,25,26; delay 0.7; hide none ;hide 1,2,4,5,8,9,11,12,15,16,18,19,22,23,25; echo; echo Terminal Groups; delay 0.5; hide none; hide 1,2,4,5,8,9,11,12,15,16,18,19,22,23; delay 0.5; hide none; hide 1,2,4,5,8,9,11,12,15,16,18,19,22; delay 0.5; hide none; hide 1,2,4,5,8,9,11,12,15,16,18,19; delay 0.5; hide none; hide 1,2,8,9,11,12,15,16,18,19; delay 0.5; hide none; hide 1,8,9,11,12,15,16,18,19; delay 0.5; hide none; hide 8,9,11,12,15,16,18,19; delay 0.5; hide none; hide 9,11,12,15,16,18,19; delay 0.5; hide none; hide 11,12,15,16,18,19; delay 0.5; hide none; hide 12,15,16,18,19; delay 0.5 ;hide none; hide 15,16,18,19; delay 0.5 ; hide none; hide 15,18,19; delay 0.5; hide none; hide 18,19; delay 0.5; hide none; hide 19; delay 0.5; hide none; delay 1; spin y 70; delay 5.3; spin off'

You can see from the syntax that the general command is;

Hide (group numbers); delay (time); Hide none

This is a simple but effective way to grow polymers.



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