Note: The bolded text in the command represents a value that needs to be input. This value may be a word or number depending on the command. Example images correspond to the console commands near them, and the molecule used in the example, when appropriate, will have its location within the *Assets* folder specified. Upload these molecules on the **Virtual Molecular Modeling Kit** (VMMK) via the Load Models > File button.

Getting an atom identifier: Some commands require a specific atom to be selected. The easiest way to do this is to open the Jmol console in the VMMK, click on Compare (since this can't be done in modes like Move), and then click on the atom you want to identify.

C2 #2 1.1298 0.9504 0.26530000000000004
1 atoms selected

You will see something like the above image appear in the console. The number after the hashtag is the atom number. It's used in the change atom color and animated bond rotation examples. The C2 number is an identifier that is specific to carbons, and clicking on a sulfur atom will result in an identifier such as S2. These species-specific identifiers are useful in many of the commands featured on the next page.

Change background color. Basic colors like white, black, blue, pink, grey, and orange can be typed and the resulting color will appear, but hex codes and RGB codes can be used for greater customizability. All commands used in the example result in the same pink color.

background **color**;   background [x**hex-code**];   background [**r**, **g**, **b**];
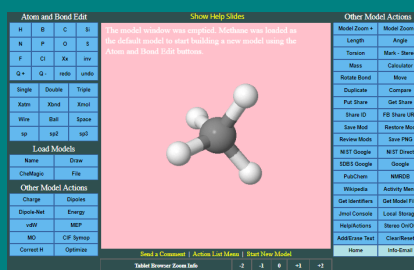
Console: background pink; or background [xFFC1CA]; or background [255, 193, 202];

Change molecule color. Each molecule is numbered starting with 1. So if there are two molecules, one molecule will be 1 and the other will be 2. Typing *getProperty moleculeInfo* gives information on each molecule that can be used to differentiate them. As with the change background color example, it's possible to use hex and RGB codes as a color value. The command colors every bond and atom in the molecule the same color.

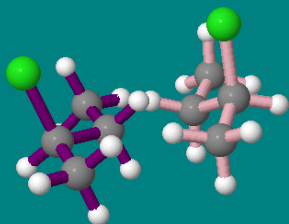select molecule = **molecule-number**; color **color**;
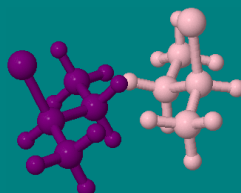
File: Ent_2_chlorobutane   **Console:** select molecule = 2; color purple; select molecule = 1; color pink;

Change molecule bond color. This changes the color only of bonds within a select molecule.

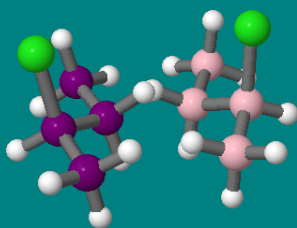select molecule = **molecule-number**; color bond **color**;

File:
Ent_2_chlorobutane

Console:
select molecule = 2; color bond purple; select molecule = 1; color bond pink;

Change the color of a particular element within a molecule. To apply this color change to the element in all molecules, leave "*and molecule=number*" out of the command. Leaving the bond color command out will result in the bonds of that element being colored as well.

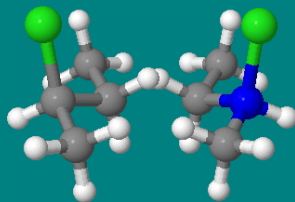Select **element** and molecule = **molecule-number**; color atoms **color**;

File:
Ent_2_chlorobutane.txt
Console:

select molecule = 1; color bonds grey;
select carbon and molecule = 1; color atoms pink;

Change atom color. Alternatively, click on an atom, make sure it's selected via the console dialogue, then type "color" followed by the desired color.

color {atomno=**atom-number**} **color**;

File: Ent_2_chlorobutane   **Console:** color {atomno=2} blue;

spin;	Spins the molecules around a single point.
select molecule = {**molecule-number**}; spin selected;	Spins a specific molecule.
spin false;	Stops the spinning motion. Works for the above command and *animated bond rotation*.
delete;	Deletes everything from the viewing area.

Animated bond rotation. The first atom identified in brackets will remain still while the second atom spins. The number at the end of the command is the degree change per ... second. Negative values change the direction of rotation. This will only spin one atom and its non-specified attachments. "Spin false" stops the spinning. The scripts lower on this page allow the user to spin more than one atom at a time.

spin branch {atomno=**still-atom-number**} {atomno=**rotating-atom-number**} **degrees-per-second**;
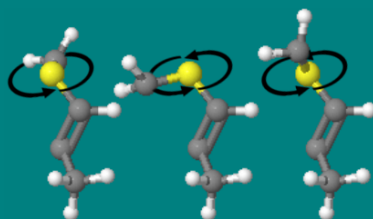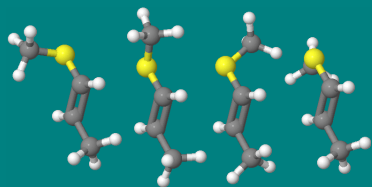

File: methylthiopropene.txt   **Console:** spin branch {atomno=1} {atomno=2} 30;

The following three scripts can be used to display bond rotation animations. To stop the animations, click **clear/reset** in the VMMK. Using frames and anim commands is generally a better way of creating animations.

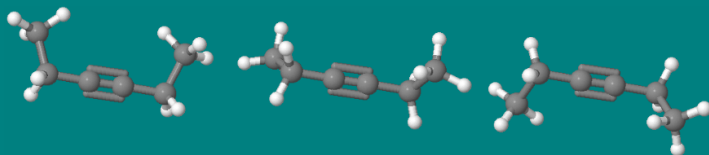### File: methylthiopropene.txt

View GIF


```
bondAnim = true;
function rotateSingleBonds(){
 while (bondAnim = true){
   rotate Branch {atomno=1} {atomno=2} 4 80;
   rotate Branch {atomno=3} {atomno=4} 4 80;
   rotate Branch {atomno=2} {atomno=8} 4 80;
}}
rotateSingleBonds();
```
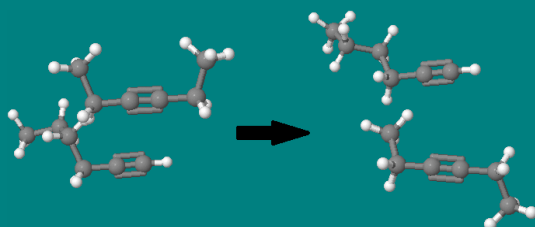
File: hex3yne.txt

View GIF


```
bondAnim = true;
function rotateSingleBonds(){
 while (bondAnim = true){
   rotate Branch {atomno=5} {atomno=6} 4 180;
   rotate Branch {atomno=4} {atomno=5} 4 180;
   rotate Branch {atomno=3} {atomno=2} 4 180;
   rotate Branch {atomno=2} {atomno=1} 4 180;
}}
rotateSingleBonds();
```

File: terminal_internal_alkynes.txt

View GIF


```
bondAnim = true;
function rotateSingleBonds(){
 while (bondAnim = true){
   rotate Branch {atomno=5} {atomno=6} 10 150;
   rotate Branch {atomno=4} {atomno=5} 10 150;
   rotate Branch {atomno=3} {atomno=2} 10 150;
   rotate Branch {atomno=2} {atomno=1} 10 150;
   rotate Branch {atomno=11} {atomno=10} 10 150;
   rotate Branch {atomno=10} {atomno=9} 10 150;
   rotate Branch {atomno=9} {atomno=8} 10 150;
   rotate Branch {atomno=8} {atomno=7} 10 150;
}}
rotateSingleBonds();
```