

Introducing Rasmol

Name:

1. Open Rasmol folder.
2. Open the Raswin icon to start the program. Resize the program and take note of the RasMol Command line in the menu/item bar at the bottom of the computer.

1	<p>Aim : Investigating <i>mouse</i> options</p> <p>Method : From the <i>-ane</i> folder, open <i>pentane</i> or <i>propane</i></p> <p>1) click <i>left mouse</i> anywhere in the <i>rasmol</i> window, hold, and move the mouse about.</p> <p>2) click <i>right mouse</i> anywhere in the <i>rasmol</i> window, hold, and move the mouse about.</p> <p>Now resize the window in the usual way, increasing it to cover about $\frac{3}{4}$ of the screen.</p>	<p>What happens in</p> <p>1)</p> <p>2)</p>
2	<p>Aim : Investigating <i>Display</i> modes</p> <p>Method : Continue using your chosen molecule (<i>pentane</i> or <i>propane</i>)</p> <p>Using the drop down <i>Display</i> menu, investigate each of the alternatives. Note not all alternatives are available for these molecules</p>	<p>What is the initial <i>Display</i> format of molecules when files are first opened?</p> <p>Which of the 8 Display modes can be used to display alkane molecules?</p>
3	<p>Aim : Investigating <i>Colours</i> modes</p> <p>Method : Continue using your chosen molecule (<i>pentane</i> or <i>propane</i>), with <i>Display</i> set to <i>Ball & Stick</i> mode</p> <p>Using the drop down <i>Colours</i> menu, investigate each of the alternatives.</p>	<p>Which of the alternatives enables us to differentiate the atoms as different colours?</p> <p>In the <i>Ball & Stick</i> mode, what colour is Carbon?</p> <p>Hydrogen?</p>
4	<p>Aim : Investigating <i>Options</i> menu</p> <p>Method : Continue using your chosen molecule (<i>pentane</i> or <i>propane</i>), with <i>Display</i> set to <i>Ball & Stick</i> mode, and colour set to CPK</p> <p>Using the drop down <i>Options</i> menu, investigate each of the alternatives.</p>	<p>Which two <i>Options</i> are the default options?</p> <p><i>We won't be using any of the alternative options at this stage. Reset to default.</i></p>
		<p>Continue using your chosen molecule (<i>pentane</i> or <i>propane</i>), with <i>Display</i> set to <i>Ball & Stick</i> mode, and colour set to CPK</p>
5	<p>Aim : Investigating the <i>Rasmol Command line</i></p> <p>Method : Go to the bottom tool bar on your screen, and click to open the <i>Rasmol Command line</i>.</p>	<p>We can use the command line to type in various other commands.</p> <p><i>Click and drag the dialog box to the bottom RHS of the screen, and resize as necessary so that both screens can be viewed simultaneously.</i></p>

5a	<p>Exploring Zoom option: Type zoom 50, then hit <i>Enter</i> Now try zoom 100, <i>enter</i> Zoom 20, <i>enter</i> ZOOM 100, <i>enter</i> ZOMM 80, <i>enter</i></p>	<p>Is the command line case sensitive?</p> <p><i>Note what happens if the command is mistyped. Try again with correct spelling. Note all commands need to be entered</i></p>
5b	<p>Exploring Colour options 1) Type background white Now try background blue And background green Try a few other colours to see if the program recognizes them. <i>Set background to your preferred colour, and continue</i></p> <p>2) Type select carbon Then colour red</p> <p>3) Type select hydrogen This time change spelling to color blue <i>Try a different colour scheme for carbon and hydrogen</i></p>	<p><i>Tip : before printing off any images, switch to background white so as to preserve your coloured ink!</i></p> <p>List 2 or 3 other colours that are recognised</p> <p>How many carbon atoms are there in your molecule?</p> <p>How many hydrogen atoms are there in your molecule?</p> <p>What is the preferred spelling : circle correct alternative Colour or color?</p>
5c	<p>Exploring command sequences Move the molecule down to the bottom left hand quadrant on the screen</p> <p>Now open the file for whichever molecule you didn't use at the start.</p> <p>1) Change display to ball and stick Change the <i>colour</i> of carbon Change the <i>colour</i> of hydrogen Now change display to spacefill</p> <p>Now see if you can work out how to change the <u>carbons</u> to spacefill mode as well!</p> <p>Move the molecule to the top right hand quadrant on the screen. Then open the file for any of the other molecules in the -ane folder</p> <p>2) Change the display and colours for this molecule (your choice for each)</p>	<p><i>Refer back to (1) if necessary.</i></p> <p><i>ie pentane or propane</i></p> <p><i>Note only the hydrogens have been displayed in spacefill mode</i></p> <p>Write down the sequence of commands for how you achieved this:</p>

	<p>With three molecules on the screen, note changes made via the tool bar or via the command line are not affecting all molecules.</p> <p>3) double click on your first molecule and rotate it 90 degrees. Then change the colour of the atoms</p>	<p>Write a general statement to describe what you have discovered about the <i>sequence of commands</i></p> <p><i>To check you have the right molecule!</i></p> <p><i>To verify your answer above</i> <i>If successful, then proceed!</i></p>
5d	<p>Deleting molecules.</p> <p>1) Using the tool bar, try edit delete</p> <p>2) Using the keypad, try control X</p> <p>3) Now type zap into the command line</p> <p>Repeat (3) until all molecules have been deleted</p>	<p>What happens? For (1) For (2) For (3)</p> <p>What did you notice about the order in which molecules were deleted?</p>