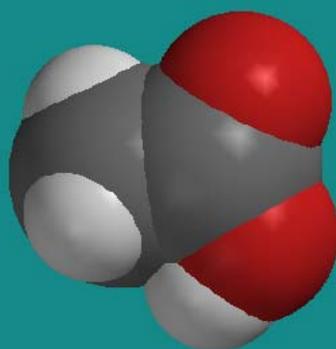# A Student's Guide to Spartan '04^{TM}

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This Guide is an excerpt from "Techniques, Spectra and Reactions, 2d Ed, A Laboratory Manual
for CHM 201, Organic Chemistry I" by Ray A. Gross, Jr.

Table of Contents

Electronic Models

►**Introduction** The advent and use of molecular modeling has revolutionized the science of organic chemistry. In 2004, Spartan was acquired by the Physical Sciences Department of Prince George's Community College and installed on the computers in the Computer Lab, CH 309. Spartan is a program with multiple capabilities. In CHM 201, we are most interested in three basic capabilities of Spartan to *build* models of molecules, *to view* these models in five different formats, and to *measure* distances and angles on a model. The more advanced capabilities will be explored in CHM 204. This experiment consists of three parts, a tutorial in the three basic capabilities of Spartan, a group of practical exercises and a set of 10 questions. The tutorial is designed to be a learning primer and a user's guide. You can refer to it at any time to refresh your memory about specific capabilities of Spartan. The practical exercises are designed to reinforce the knowledge you have acquired in the first three weeks of organic chemistry in a game-like and fun manner. The questions test your understanding of the models and some chemistry. The basic operations of the program are described, including basic mouse commands and certain screen features as well as Menu Bar items and Toolbar icons. Then, we will explore Spartan by following a normal pattern that a typical user follows. We will build models of molecules, explore the various ways of viewing them, and make measurements on them. Thus, we will *build, view, and measure*. The goal is to make you proficient in the use of Spartan, so that you can use it throughout the course as a learning enhancer.
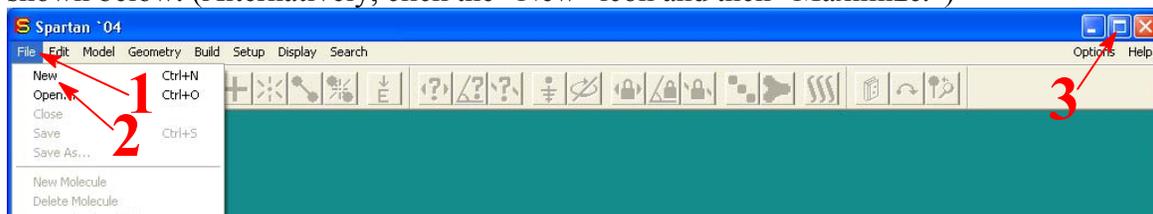
Spartan Tutorial

►**Open Spartan**
Open the Spartan program from the list of academic programs. The Spartan icon is shown below.

Spartan `04 V1.0.0.lnk

The electronic model kit should appear. In turn, click (1) File, (2) New and (3) Maximize, as shown below. (Alternatively, click the "New" icon and then "Maximize.")

The program is now ready to use.

If you cannot open Spartan, ask the instructor for help. With Spartan and the Lab 3 Word file "Electronic Models" open, the two icons for these files should be visible on the bar at the bottom of the screen. To toggle back and forth between the two files simply click on the W

(Word icon for Electronic Models) at the bottom of the screen. Click the W several times to go back and forth from this tutorial to Spartan.

●**General Commands** The command to click means to depress the *left mouse key* (LMK) one time. Double click means to depress the LMK twice in rapid succession. When the right mouse key is required, it will be specifically identified as *RMK* to distinguish it from the LMK. The mouse controls a white arrow or *pointer* on the screen. Move your mouse to see the motion of the pointer. The command to "click on …" means to place the pointer on the specified object and depress the LMK.

►**Screen Features◄** **Spartan initially opens with several visible features. Some of these features will be described briefly here for familiarization and in more detail, as necessary, later. Some advanced features will not be discussed.**
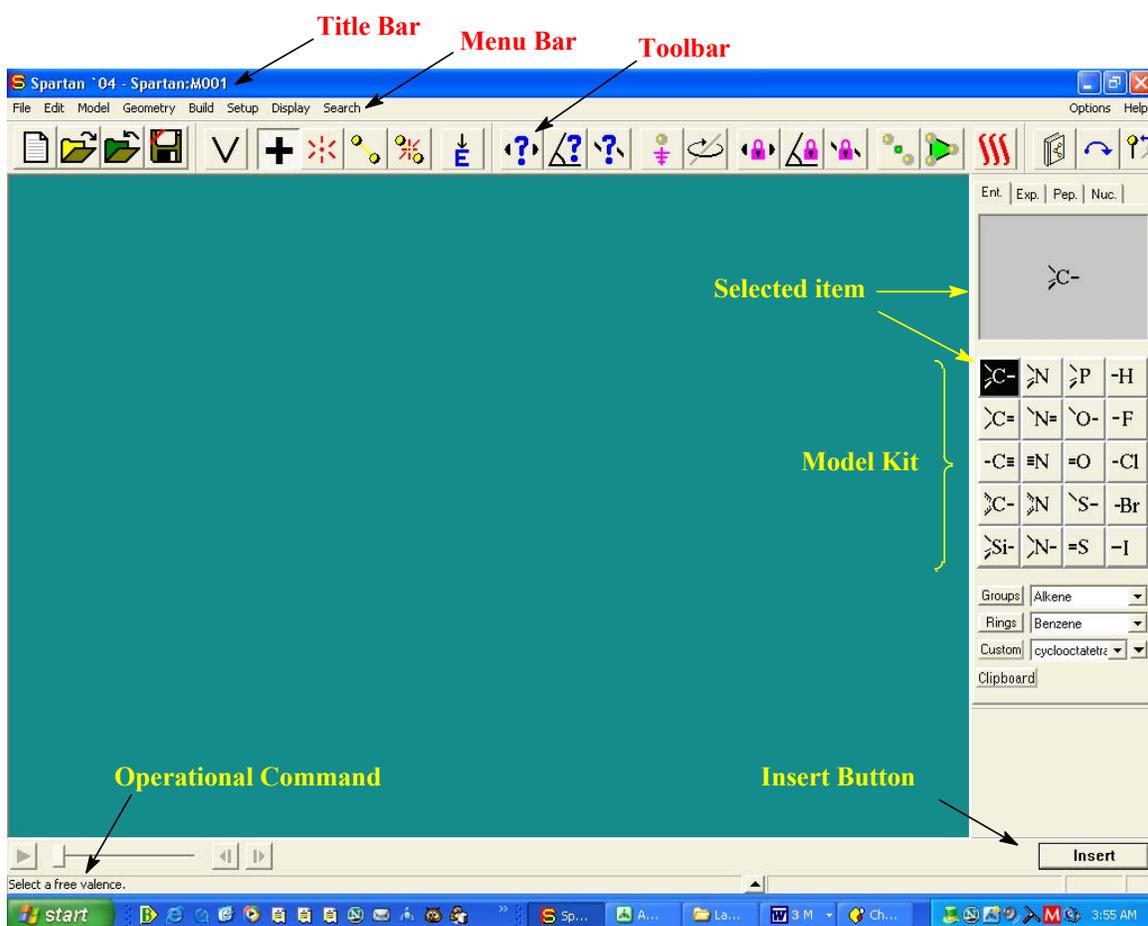

Figure 1. Screen features

●**Title Bar**
The left side of the title bar contains the logo, S, and name of the program (Spartan '04). The right side of the title bar contains three standard command boxes.

◦**Minimize, Maximize, and Close** There are three boxes on the right-hand side of the title bar. Place the pointer over each box until the name of the box appears. The name will

remain visible for approximately five seconds. These are standard commands. When you clicked on the middle box or "Maximize," you opened a full screen. Otherwise, the bottom portion of Spartan is obscured by the Windows data bar at the bottom of the page. Click on File, New and Maximize every time you open Spartan; alternatively, click the File icon and Maximize. Note that the Maximize box becomes "Restore Down" after you have clicked it.

●**Menu Bar** The *Menu Bar* (Figure 1) is the horizontal group of ten names, eight on the left side and two on the right side, starting with File on the left. Click on "File" and the File menu becomes visible. Slowly move the pointer from left to right across the Menu Bar. As the pointer passes each menu item, the contents of that menu item become visible. We will explore these items later. Clicking on any menu item allows you to read the contents of any other menu item by moving the pointer over the menu name
.

●**Toolbar** The *Toolbar* (Figure 1) is the horizontal group of eleven icons, starting with the File icon. The icons are shortcuts to Menu items. Click on each icon in turn, starting with the V icon. Note that a command appears in the lower left corner of the screen each time a new icon is clicked. See "Operational Command" in Figure 1. The command tells the viewer what to do next. For example, clicking the + icon results in the command to "Select a free valence." Click on the "+" icon. Note that the selected icon appears slightly depressed with respect to the other icons. The name of the + icon is Add Fragment. The + icon is more commonly called the build icon, but its name on the Toolbar is Add Fragment, which means build. When you activate Spartan with the clicks noted above, the build icon is active.

●**Model Kit** The *Model Kit* (Figure 1) is on the right side of the screen. It resembles a standard model kit. You can select atoms from the kit and use the atoms to build models of molecules. The kit contains 20 different individual atoms and two sets of bonded atoms in the form of groups or rings from which to choose.

◦**Individual Atoms** In turn, click on several of the individual atoms in the kit. Note that the selected atom changes from black on a white background to white on a black background. A graphic of the selected atom appears in the box just above the 20 symbols.

◦**Groups** What is a group? A *group* is not a complete molecule but a partial structure of two or more atoms joined by covalent bonds. Other atoms must be bonded to a group before it becomes a molecule (i.e., before the molecular model is complete). If you do not complete the model by adding other atoms, the program will automatically complete the molecule for you by adding H atoms when you try to make a measurement on the model or view it in another form. Click on "Groups" then click on the adjacent drop-down menu "▼." A menu of 12 groups opens. Click on "Amide." The structure of an amide group appears in the box above the kit. ***Draw this structure on a piece of paper for practice***.

◦**Rings** What is a ring? A *ring* is group of atoms joined by covalent bonds in a continuous loop. You may start at any atom that is part of the ring and follow bonds from one ring atom to the next until you return to the starting atom. From the Edit menu, click on "Clear" to clear the screen. Click on "Rings" then click on the adjacent "▼." A dropdown menu of eight rings opens. Click on "Cyclopentane" and ***draw the structure of cyclopentane*** as it appears above the kit.

●**Insert** The *Insert button* (Figure 1) is located at the lower right corner of the screen. Two distinct and independent models can be built and viewed on the screen simultaneously. Build the first model, and then click on "Insert" and build the second model. Thereafter, additional models can be built and viewed simultaneously by clicking on Insert before building each model. Each model in the set can be moved or rotated independently of the others on the screen. Before we continue, the screen should be clear. If your screen is not clear, click on "Edit" from the Menu Bar and then click on "Clear."

►**Menu Bar Items** Look at the top of the screen; you see "Spartan." On the next line, you see eight menu items on the left side of the screen and two on the right. On the left side, you see "File, Edit, Model, Geometry, Build, Setup, Display and Search." On the right side, you see "Options and Help." We will explore some of these menu items one at a time but not exactly in the order they appear on the Menu Bar.

●**File** Click on "File" to open the File menu. You see 11 options. Most of these commands are self-evident. The commands "New Molecule, Delete Molecule, and Append Molecule(s)" will become evident in time.

►**Build**◄ **The building of models is associated primarily with the Build Menu.**

●**Build** A Spartan user normally builds, views, and measures in that order. Thus, we'll start with the Build Menu. Likewise, because the Zoom, Rotation, Translation and Spin operations are really part of the build process. We'll consider these functions before we continue with the other Menu Bar items. From the Menu Bar, click on "Build." The Build menu consists of six options. The first option is View. View is not a build tool. View is more appropriately used with the Model Menu and will be discussed there. View is an option in the Build Menu to provide redundancy. The next four options in the Build menu are basic building tools.

◦**Add Fragment** With the screen clear, click on the "Add Fragment" option from the "Build" menu. Note that the + icon on the Toolbar is active. Adding a fragment is the most fundamental operation of "Build." We will build methane, the simplest hydrocarbon. Go to the Model Kit, click on the "C" with four single bonds. The C becomes active (highlighted). Click anywhere in the green area. A carbon atom with four single bonds (methane) appears, but its H atoms are not immediately apparent. Notice that the four bonds coming from the gray carbon atom are yellow. The yellow bonds initially represent either an H atom or a free valence, to which another fragment may be added. When you are finished building your model, the program will automatically add H atoms to any free valence (yellow bond). However, we are still in the build mode. Before continuing with the build options, some useful operations related to building molecules will be introduced.

◦**Minimize** Click on "Minimize" from the "Build" menu. Note that hydrogen atoms automatically appear bonded to all free valences (available bonding sites), and the yellow bonds now appear gray. When the hydrogen atoms appear, the molecule is said to "sprout" hydrogens. The *Minimize* command builds the most stable (lowest energy) model of methane. The model built with the Minimize command is called a ball and spoke model. That is, the atoms are spheres, and the bonds joining atoms are spokes. The carbon atom is gray,

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and the four hydrogen atoms are white. The colors are not pure but slightly off color (i.e., hydrogen is an off-white color).

■Selecting Minimize or the E icon also calculates the energy of the molecule, which is shown at the lower right corner of the screen. ***What is the energy of methane in kcal/mol?***

►**Zoom (Enlarge—Reduce Model)**
Depending on the application, it might be desirable to increase or reduce the size of a molecule. The zoom feature allows us to change the size of the displayed molecule.

● Start with the white arrow (pointer) at the bottom of the screen. Depress and hold the "Shift" key on your keyboard. Simultaneously, depress and hold the RMK. With both keys depressed, move the pointer upward to the top of the screen. This operation increases the size of your methane molecule. Release the mouse key and return the white arrow to the bottom of the screen. Again, hold both keys (Shift + RMK) down and move the white arrow to the top of the screen. You can repeat this operation until you make the molecule the size you desire. Depressing both keys (Shift + RMK) and moving the pointer downward reduces the size of the model.

●The larger the methane molecule appears, the easier it is to see the three dimensional aspects of the model. You may increase or decrease the size of models during the remainder of this tutorial to suit your needs.

►**Rotation of Whole Molecule** A molecule rotates when it tumbles in any direction (three-dimensions) about a stationary point. Rotation does not imply movement through space.

●Move the white arrow (pointer) until it is just above your methane molecule. Depress and hold the LMK. Simultaneously move the mouse so that the white arrow makes circles around your methane molecule. Notice what happens when you simultaneously hold the LMK and swirl the mouse. With a combination of up or down and clockwise or anticlockwise swirls with the mouse, you can orient the molecule in any manner you please.

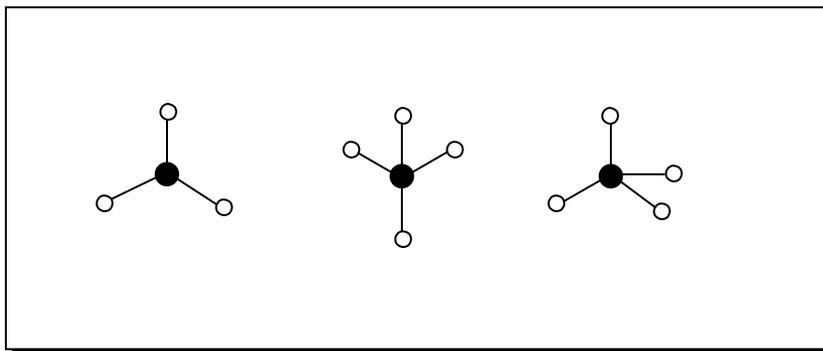●For practice, orient your methane molecule three different ways, as shown in Figure 2.

Figure 2. Orientations of methane.

►**Translation** When a molecule moves through space by changing its three-dimensional or x, y, z coordinates, the molecule is undergoing translational motion. Translation does not imply spinning.

●Depress and hold the RMK, then move the pointer up and down and right and left in the green area of the screen. These operations allow you to position the molecule any place on the screen you desire. The model moves from one location to another by translation.

●For practice, move your methane molecule, in turn, to each corner of the screen. From the Edit menu, click on "Center." The model moves to the center of the screen.

■ *Can a real molecule undergo rotation and translation at the same time? Can a molecule in Spartan undergo rotation and translation at the same time? Explain the difference between rotation and translation of a molecule.*

◦**Add Fragment (Continued from above)** Click the + (Add Fragment) icon to return to the build mode. The model on the screen can now be modified. The four bonds of carbon are yellow. The tips of the yellow bonds are free valences or available bonding sites. Note that the command line at the bottom left of the screen reads, "Select a free valence." A free valence is a yellow tip. Click at the very end of any one of the yellow tips. An ethane model is built, because the C atom in the Model Kit with four single bonds is still active. You can add as many fragments as you please. Click on another free valence and propane is built. Click on an end-carbon's free valence twice more, and pentane is built. Click on "E" the Minimize icon and the molecule appears in its most stable conformation with its hydrogen atoms visible.

►**Rotation About a Selected Bond (Spin)** Two common properties of organic molecules are the rotation about carbon—carbon single bonds and the restricted rotation about multiple bonds.

●With pentane on the screen, depress the "Alt" key on the keyboard. Depress and hold the LMK and move the mouse up and down. This action causes rotation (spinning) about the last-made single bond, which is indicated by a red ribbon around the bond. Click in the middle of one of the other carbon—carbon bonds. This changes the red ribbon to the desired bond. Then repeat the "Alt + LMK" procedure to rotate about the new bond with the red ribbon.

►**Changing a Bond Length** A bond highlighted by a red ribbon may be elongated or shortened. You might want to do this to get a better view of a portion of a molecule.

●With pentane on the screen, depress the "Alt" key on the keyboard and the RMK. Move the mouse up and down while depressing the "Alt" key. The bond is lengthened when the mouse is moved upward and shortened when the mouse is moved downward. The operation works only on the highlighted bond.

►**Spinning a Molecule** Spinning differs from rotation in that spinning is two-dimensional and rotation is three-dimensional.

●With pentane on the screen, simultaneously depress "Shift + Ctrl" on the keyboard. Depress the LMK and move the cursor upward. The model makes a clockwise spin. Move the cursor downward and the model makes a counterclockwise spin.

◦**Delete** Click on "Delete" from the "Build" menu. The command line (lower left corner) reads, "Select object to delete." Do not click on a free valence, but click on the center of a terminal carbon atom. A methyl group is deleted, leaving butane.

◦**Make Bond** Click on "Make Bond" from the "Build" menu. You are going to make cyclobutane by joining the end carbon atoms of butane. The command line reads, "Select two free valences." What are free valences? They are the yellow ends of bonds. Do not click carbon atoms, they are not free valences. Click on two yellow tips in succession. First, click on a free valence at one end of your butane model. Then, click on a free valence at the other end of the molecule. By selecting two free valences, you created a bond joining their carbon atoms (i.e., cyclobutane.). Click the "E" icon and, if necessary, rotate the model to get a better view of it. You should have a nice model of cyclobutane.

◦**Break Bond** Click on "Break Bond" from the "Build" menu. With Break Bond selected from the Build menu, click on the center of any carbon—carbon bond. Yellow tips appear where the bond breaks, creating two free valences. Although the yellow color between the two carbon atoms indicates that a bond has broken, it is sometimes difficult to see the new bonds. Click on the "E" icon. When the model adjusts to its most stable conformation, the new bonds of butane become clearly visible.

●**Edit** Click on "Edit" to open the edit menu. You see several options, including "Undo, Copy, and Clear." The "Undo" and "Copy" commands work just like they do in Word. Clicking "Undo" deletes the last command you made. Clicking "Copy" copies the structure to a clipboard from which it may be pasted to another file.

◦**Clear** This command clears the screen. Unlike the Exit command in the File menu, Clear allows you to continue building models. Click on "Clear." The butane model disappears, and you are back in the build mode. Click anywhere in the green space and methane reappears (the C atom with four bonds is still highlighted in the Model Kit). Click on the very end of one of the yellow tips (free valence). A methyl group (the highlighted fragment in the kit) is now bonded where you clicked, making ethane. Click on "Undo" from the "Edit" menu. The methyl group added by your last command is deleted, leaving methane. Click on "E". Methane appears as a "Ball and Spoke" structure.

●**Building Multi-atomic and Multiple Molecules**

●**Multi-atomic Molecules**

●**Alkanes** Building complex molecules involves adding fragments. Build methane and click the + icon. Highlight the tetrahedral carbon in the kit. Click on one of the yellow tips and ethane appears. Click on an end carbon's yellow tip again and you get propane. Continue until you have made pentane. Click on "E" then "V." Zoom the molecule and note the clarity of the apparent three-dimensional structure.

●**Alkenes** From the Edit menu, clear the screen. The Add Fragment (+) icon is active. Highlight a double-bond carbon in the Model Kit. Click on the screen. Click on the end of the double yellow lines and a double bond between two carbon atoms appears. Clear

the screen. Click on the screen, and a double bond fragment appears. This time click on one of the single yellow lines. A single bond is formed between the two carbon atoms, making two double bonds available. An important feature of the build mode is that like valences must bond to like valences.

●**Alkynes** Clear the screen. Highlight the triple bond carbon in the Model Kit. Click on the screen. Click on the three-line bond and you get a triple bond. Click on the one line bond and you get a single bond. Like valences bond to like valences.

●**Oxygen** There are two choices for oxygen atoms, one with two single bonds and one with a double bond. Clear the screen and build a methane model. Highlight the double bond oxygen and click on a yellow tip. You get an audible no-no, meaning that you have tried to join unlike valences. To add a double-bond oxygen to an existing fragment, the fragment must have a double bond site open. Clear the screen, click on a double bond carbon in the kit, then on the screen. Highlight the double bond oxygen and click on the double bond on the screen. A carbon—oxygen double bond appears. You have a carbonyl (carbon + oxygen) group. This is an important group in organic chemistry. Highlight the single bond oxygen in the Model Kit and click on a yellow single bond on the screen. You have a carboxyl (carbonyl + hydroxyl) group, another important group in organic chemistry.

●**Other Heteroatoms** The other atoms in the kit are manipulated exactly as oxygen is manipulated. There are five options for nitrogen. Take care to bond like valences. You will get a no-no signal if you try to join unlike valences (i.e., a single bond to a double bond).

●**Groups** Clear the screen. Click on "Groups" and select "Carboxylic Acid" from the dropdown menu. Click on the screen and the carboxyl group appears. Add a methyl group to the free valence from carbon and click "E". Acetic acid appears. The other six groups work similarly.

●**Rings** Clear the screen. Click on "Rings" and select "Cyclohexane" from the dropdown menu. Click on the screen and on "E" and cyclohexane appears. The other seven ring commands work similarly.

●**Multiple Molecules on the Screen** Multiple models are made by clicking "Insert." Build the first model as usual, then click "Insert" and build the next model, etc. Build a model of methane, click "Insert" and build a model of ethane. The models can be moved or rotated individually or as a group. The rotation and translation commands, given above, move the entire set of molecules on the screen. To rotate or translate individual molecules, the program must be in the build mode. Highlight one of the molecules by clicking on it. Depress "Ctrl" and use the LMK to rotate the highlighted molecule. Depress "Ctrl" and use the RHK to translate the highlighted molecule. Move the model around and then clear the screen.

Note that the five basic commands available in the Build Menu are also available on the Build Toolbar, as shown in the graphic below.

Build Toolbar

►View◄ The viewing of models is associated primarily with the Model menu.

●**Model** Build a methane molecule. Click on "Model" to open the model menu. The first five options provide five different ways to view a molecular model in Spartan. These five options are "Wire, Ball and Wire, Tube, Ball and Spoke, and Space Filling." Two additional options we shall use are "Hydrogens and Labels." They allow us to remove hydrogen atoms from a model if we wish, or to label all of the atoms or defined planes in the molecule. Note that the "Ball and Spoke" model and "Hydrogens" commands are already selected. The selected items in the "Model" menu define the picture on the screen. Thus far, we have been in the build mode. We cannot change the model from "Ball and Spoke" until we are in the view mode. Click on the "V" icon on the toolbar to change the mode from build to view.

◦With the V icon active, click on "Wire" from the "Model" menu. The methane molecule now appears as a wire model.

◦With the V icon active, click in turn on "Ball and Wire," "Tube," "Ball and Spoke," and "Space Filling" from the "Model" menu. These names describe the models shown on the screen. These options allow you to view a molecule in the way that best allows you to gain the information you seek.

◦With the V icon active, click on "Ball and Wire" to return to that model of methane, and then click on "Hydrogens" from the "Model" menu. Clicking on "Hydrogens" removes the check from the menu and also removes the hydrogens from the screen, leaving only the carbon atom of methane visible. Click on "Hydrogens" to restore the H atoms to the model. The default condition is for the H atoms to be visible.

◦With the H atoms visible and methane as a ball and wire model, click on "Labels" from the "Model" menu. Each atom is labeled. With each atom labeled, two or more people can view the model and have a common frame of reference. Click on "Labels" to remove the labels from the model. The numbering system in "Labels" is not the same as the IUPAC system and is not consistent from one molecule to the next. Therefore, labels are normally used for the limited purpose of identifying atoms for a specific molecule that is visible on the screen.

►Measure◄ The making of measurements on models is associated primarily with the Geometry menu.

●**Geometry** Click on "Geometry" to open the geometry menu. You see three command options at the top of the menu. These three options are commands that allow us to

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measure various aspects of a molecule. The measurement commands are "Measure Distance, Measure Angle, and Measure Dihedral." The "Measure Distance" command allows us to find the distance between any two atoms in a model in Angstrom units (Å); the two atoms need not be bonded to each other. The "Measure Angle" command allows us to measure any angle in degrees (º) made by three atoms. The "Measure Dihedral" command allows us to measure a dihedral angle in degrees (º). A *dihedral angle* is an apparent angle made by four atoms. Two additional command options in the Geometry menu are "Define Point and Define Plane." These commands are not for making measurements but for helping the viewer see symmetry aspects of a molecule or to clarify the structure in some way. The "Define Point" command allows us to highlight any atom or multiple atoms as points for reference. Defined points are visible on models when the point lies on an atom. From plane geometry, three points define a plane. The "Define Plane" command allows us to visualize a plane that is common to any three atoms by selecting those atoms. This tool can be very useful in helping a beginner visualize organic molecules. The five options for making measurements or defining points or planes in the geometry menu are also accessible by five icons on the toolbar. Collectively, these five icons along with six others that we shall use next semester are known as the Geometry Toolbar.
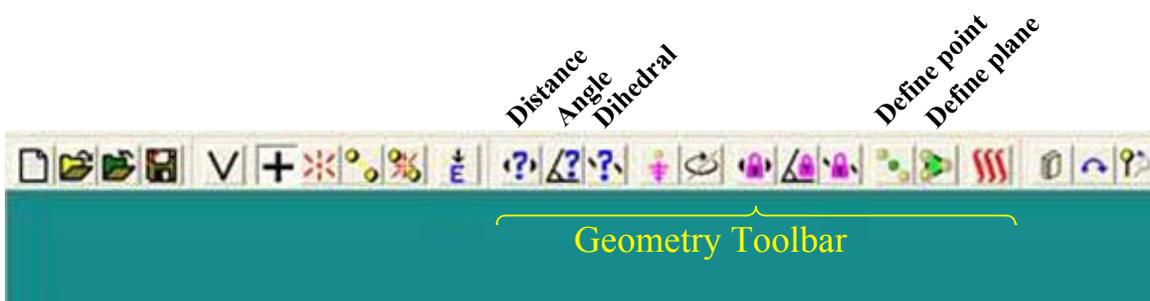
◦**Measure Distance** With methane on the screen in a ball and wire model, click "Measure Distance" from the "Geometry" menu or click the "Distance" icon. Enlarge the model if necessary. Click on any H and then the C atom. What is the H—C bond length? _____Å Find the bond length in the lower right corner of the screen. Find the bond length of any other H—C bond._____ Å Note: After you measure one distance by clicking two atoms, you can continue directly to the next measurement without clearing the last operation. How does the first H—C bond length compare to the second H—C bond length in methane? _____ From your measurements, what is the carbon—hydrogen bond length, rounded to one decimal place, when carbon is sp^3 hybridized? _____ Å Alternatively, you can click on the midpoint of a bond to find the distance between two bonded atoms. Click on any C—H bond where the gray and white halves meet. Read the bond distance at the bottom right corner of the screen. Note that the selected atoms are highlighted by the appearance of a larger circle around the atom. A selected bond changes from half gray-half white to a solid metallic color.

◦**Measure Angle** With methane on the screen, click "Measure Angle" from the Geometry menu or click the "Angle" icon. Click on any H, the C, and another H in that order. Rounded to one decimal place, what is the H—C—H angle? _____ Verify that all H-C-H bond angles in methane are identical.

◦**Measure Dihedral** Build a model of ethane and click "E" and "V." Click "Measure Dihedral" from the Geometry menu or click the "Dihedral" icon. Click in turn on bonded atoms H-C-C-H. Rotate the molecule so that one C atom completely obscures the other C atom. The angle made by these three highlighted atoms is called the dihedral angle.
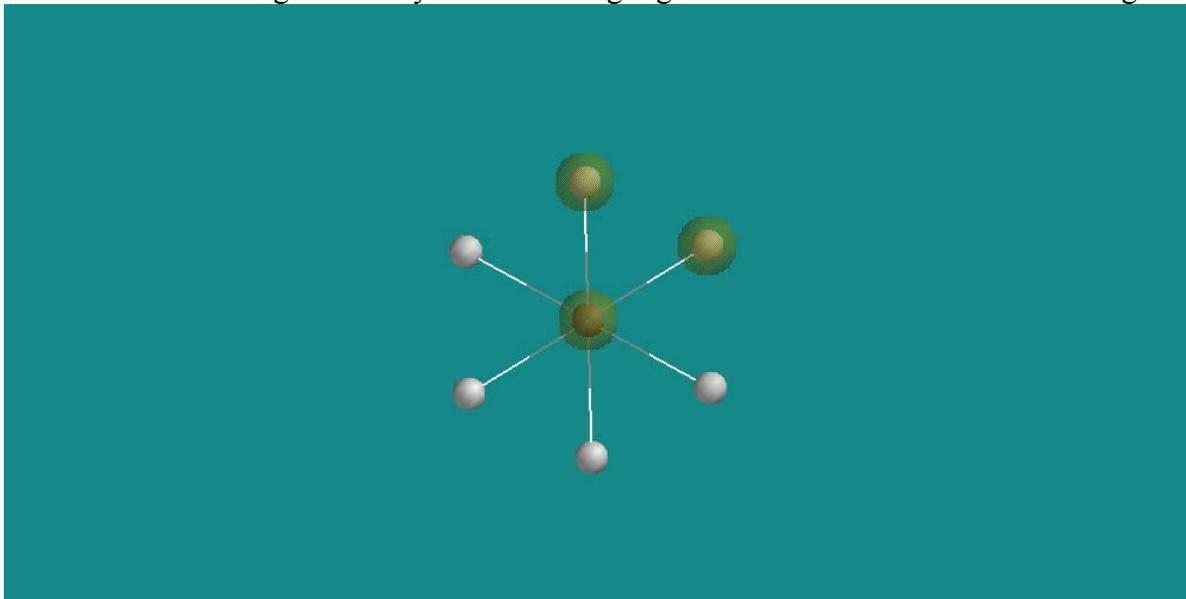
A *dihedral angle* is an apparent angle made by four atoms, one of which is obscured. The value is found in the box at the bottom right of the screen. The program measures the angle from the near bond to the rear bond. If the angle generated by going from the near bond to the rear bond is clockwise, the angle is a positive or (+) angle. A corresponding counterclockwise angle is negative. We are generally more interested in the magnitude than we are of the sign of a dihedral angle. Make another dihedral measurement by clicking on one different H atom but re-clicking on three atoms selected before.

◦**Define Point** Build a model of methane, open the Model menu and ensure that the Ball and Wire and Hydrogens options are checked. Click "Define Point" from the "Geometry" menu or click on the "Define point" icon. Click on the carbon atom. The carbon atom is highlighted. In turn, click on each of the H atoms. Each H atom is highlighted as you click it. When every atom in your model has been highlighted, click any of the highlighted atoms. The model reverts to a ball and wire model with no highlighted atoms. With the define point command active, take care to click in the center of the carbon atom. The carbon atom is highlighted. Click in the center of the C atom again. The highlight is removed and the model appears to be the same as is was before. Click on the "V" icon, and then select "Wire" from the "Model" menu. You see that the carbon atom is now the "defined point." Thus, double clicking an atom when the Define Point command is active creates a visible marker on wire models. The defined point is invisible in the other models. Clear the model from the screen, and build a new ball and wire model of methane. Click "Define Point" from the "Geometry" menu. Click on carbon, then any hydrogen, then on carbon again. A point is created midway between the two atoms. This point is visible on the ball and wire model because the point does not coincide with an atom. Three clicks are required to make a point between two atoms; whereas, only two clicks are required to make an atom a point. Points

can be made at the midpoint of any bond in the model and on any atom. All points are visible on the wire model. Clear the screen.

◦**Define Plane** With a new ball and wire model of methane on the screen, click "Define Plane" from the "Geometry" menu or click the "Define plane" icon. Click on the carbon and on two hydrogen atoms. A plane, connecting the three atoms, appears. Click on carbon and on the other two hydrogen atoms. A new plane appears. Select both "Hydrogens" and "Labels" from the "Model" menu. The hydrogen atoms disappear, and the planes are labeled Plane 1 and Plane 2. Select "Wire" from the "Model" menu. ***What is the relationship between Plane 1 and Plane 2?***

_____
Hint: rotate the molecule so that neither plane is visible. The above examples show how the point and plane options can be helpful in the visualization of models.

►User Options◄ Most user options are associated with the Options menu.

●**Options** On the right side of the Menu Bar, click on "Options" to open the options menu. You see six options above a line, five in the middle and three options below the bottom line. The five options already checked are active or visible on your screen. The six options above the line are "About …, Preferences …, Colors, Fonts, Monitor, and Calculator."

◦**About Spartan…..** Click "About …" from the "Options" menu. A window opens that provides information on how to contact Wavefunction, the company that makes Spartan software.

◦**Preferences** With methane on the screen in a ball and spoke model, click on "Preferences" from the "Options" menu. A new window labeled Preferences opens. The preferences window contains four sub-menus, "Miscellaneous, Molecule, VDW Radii, and Paths." The Miscellaneous sub-menu is active. Select "large icons" from the dropdown menu called Toolbar Style. Then click the box labeled "Apply." Click the Molecule sub-menu and select "Ball and Spoke" from the dropdown menu called Model. Then click "Apply" and "OK." If the preferences window obscures your model, move one or both of them in the usual manner so that methane is visible on your screen. The preferences window can be moved by depressing and holding the LMK with the pointer in the blue field in which the word Preferences appears, and then dragging the window to the desired location on the screen with the LMK depressed.

◦**Colors** Click on "Colors" from the "Options" menu. A new window called Set Color appears. This window controls the background color you see on the screen. The default color is a green background. The Set Color window contains three scrollable options made up of the three primary colors, Red, Green, and Blue. Depress and hold the LMK on the scrollbar under "Blue." With the LMK depressed, scroll the bar upward and notice that the screen turns blue. With the three scrollable keys, you can adjust the background color on the screen to any color you please. Make several color adjustments, then click the "Default" option. The original green background color returns. Adjust the background color to the color of your choice. There are two red boxes on your screen with an X. Take care to be in the Set Color box and click the X in the upper right corner of the active window. The new

background color remains active until changed. If you accidentally click the wrong red box, you must reload Spartan.

 ◦**Model Kit, File Toolbar, Build Toolbar, Geometry Toolbar, Search Toolbar** Click on "Options" to open the options menu. Five items are already checked. Checked items are visible on your screen. When you click on a checked item, the check disappears and the Kit or Toolbar disappears. Checking the item causes it to reappear on the screen.

Before going on to the next section, make sure the Model Kit, Build Toolbar, and Geometry Toolbar are checked in the Options menu. Likewise, make sure that a Toolbar Style (i.e., small, medium or large icons) is selected in the Preferences window of the Options menu.

►Keystrokes◄

►**Keystrokes for Manipulating Molecules in Spartan** The keystrokes for the fundamental manipulations possible in Spartan are given in Table 1.

Table 1. Keystrokes for Spartan

Operation	Mode	Keystrokes
Translation Single Molecule All Molecules One of Multiple Molecules	 (+) highlighted	 RMK RMK Ctrl + RMK
Rotation (three-dimensional) Single Molecule All Molecules One of Multiple Molecules	 (+) highlighted	 LMK LMK Ctrl + LMK
Spin (two-dimensional) Single Molecule All Molecules One of Multiple Molecules About single bond	 (+) highlighted (+) select bond (dashed)	 Shift + LMK Shift + LMK Ctrl + Shift + LMK Alt + LMK
Zoom Enlarge Molecule Reduce Molecule		 Shift + RMK (mouse ↑) Shift + RMK (mouse ↓)
Change Bond Length Lengthen Shorten	 (+) select bond (dashed) (+) select bond (dashed)	 Alt + RMK (mouse ↑) Alt + RMK (mouse ↓)

Molecular Modeling Exercises

The following exercises are designed to allow you to collect useful information about organic molecules while exploring the build, view, and measure features of Spartan. The 10 questions at the conclusion of this lab require you to use your data. Therefore, answer the questions as you go along and keep them for the follow-on problems that must be turned in for a grade.

Functional Groups: *Functional groups* are unique partial structures that allow us to classify organic compounds into families. Because each member of the family contains the same functional group, each member of the family reacts similarly. There are many organic families, which we can sub-divide into three major categories. These categories are (1) hydrocarbons, (2) compounds that contain a heteroatom, and (3) compounds that contain a carbonyl group. It is important to be able to identify functional groups, because they define the reactivity of the families to which they belong. **Structure begets reactivity!**

Hydrocarbons: *Hydrocarbons* are compounds that contain only carbon and hydrogen. They may contain rings (i.e., be *cyclic*) or they may not contain any rings (i.e., be *acyclic*). The hydrocarbons are sub-divided into several families, depending on their structures. We shall consider the various hydrocarbon families.

Though hydrocarbons contain no heteroatoms, they may contain any combination of π bonds and rings. The number of π bonds and their locations within a given structure determines the family to which a given hydrocarbon is assigned. Hydrocarbons may have no multiple bonds or a double bond, a triple bond, or alternating single and double bonds in a six-membered ring. The families are alkanes, alkenes, alkynes, and arenes, respectively. Figure 3 shows examples of these families. The next several exercises relate to these four compounds.
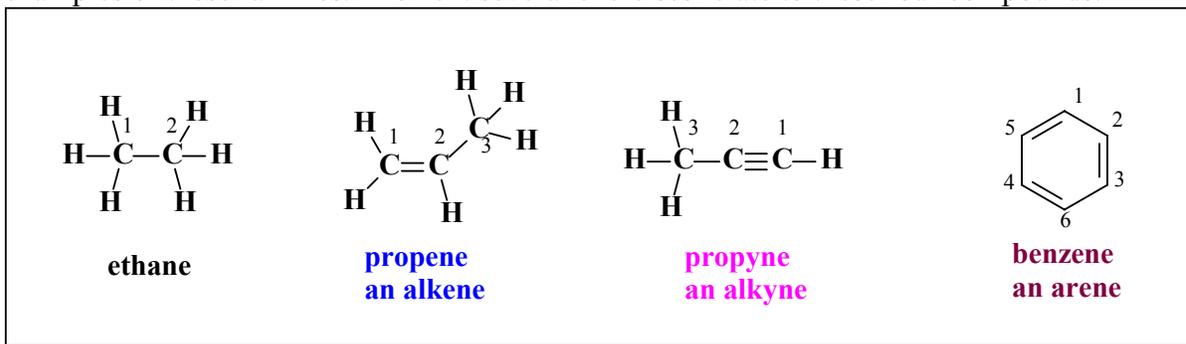

Figure 3. Hydrocarbon Families

●**Alkanes:** *Alkanes* are hydrocarbons that contain no π bonds, only σ bonds. Alkanes may be cyclic or acyclic. Cyclic alkanes are called *cycloalkanes*. Alkanes are unique, because they do not contain an identifiable functional group.

Note: Refer to Figure 3 for the numbering systems when answering the questions about hydrocarbons. The ball and wire model is recommended for the following exercises.

►Ethane: From your studies, what is the hybridization of an alkane carbon atom? _____
Build and minimize a model of ethane. Make and record the following measurements for a

typical alkane. C-H bond length _____ C-C bond length _____ H-C-H bond angle
_____

●**Alkenes:** *Alkenes* contain one double bond that is made up of one σ bond and one π bond. A compound that contains two double bonds is called a diene, and one with three double bonds a triene, etc. Alkenes react primarily at the double bond or functional group.

► From your studies, what is the hybridization of an alkene carbon atom? _____ Build and minimize a model of propene. See Figure 3 for numbering. What is the shape of the molecule around the double bond? _____ (Shapes are visible but not specified by the program, you must identify the shape.) What is the C1 to H1 bond length? _____ What is the C1 to C2 (alkene) bond length? _____ What is the H1 to C1 to C2 (alkene) bond angle? _____

●**Alkynes:** *Alkynes* contain one triple bond that is made up of one σ bond and two π bonds. A compound that contains two triple bonds is called a diyne, and one that contains three is a triyne, etc. Alkynes typically react at the triple bond or functional group.

►Build, minimize, and label a model of propyne. See Figure 3 for numbering; what is the hybridization of C1? _____ What is the shape of the molecule around the triple bond? _____ What is the C1 to H bond length? _____ What is the C1 to C2 (alkyne) bond length? _____ What is the C1 to C2 to C3 (alkyne) bond angle? _____

●**Arenes:** *Arenes* contain an aromatic ring, a six-membered ring with alternating single and double bonds. Benzene is the first or simplest member of the arene family.

► Build a model of benzene, using the Rings command, and minimize the structure. What is the hybridization of all of the C atoms? _____ What is shape of the whole molecule (hint: rotate it, if necessary)? _____ What is the C1 to H1 bond length? _____ What is the C1 to C2 (arene) bond length (Note, see Figure 3 for numbering)? _____ What is the C1 to C5 bond length? _____ What is the C1 to C2 to C3 (arene) bond angle? _____

Isomers: *Isomers* have the same formula (i.e., the same numbers and kinds of atoms) but differ in structure. There are several different kinds of isomerism. Two of the most important kinds are constitutional isomerism and cis—trans isomerism.

●**Constitutional Isomers:** *Constitutional isomers* differ in the way their atoms are connected to each other (i.e., their connectivity). Figure 4 shows three alkanes that each contains five carbon atoms.
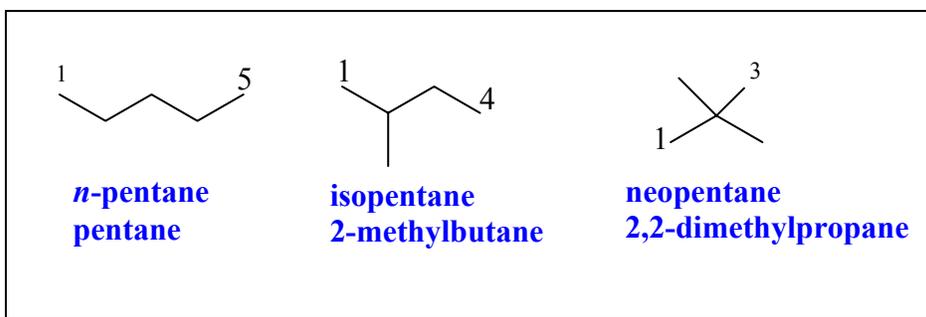
Figure 4. Five-carbon alkanes

►Build models of pentane, 2-methylbutane, and 2,2-dimethylpropane on the same screen, and scale them to fit on the screen so that all of them are visible. Minimize but do not label the structures. What is the molecular formula of pentane? _____, of 2-methylbutane? _____, and 2,2-dimethylpropane? _____ Are these compounds isomers? _____ What kind of isomers? _____
Measure the distance between the terminal carbon atoms (IUPAC numbering) in each compound. C-1 to C-5 in pentane _____ C-1 to C-4 in 2-methylbutane _____ and C-1 to C-3 in 2,2-dimethylbutane _____ Change the models to space-filled models. If they overlap, go to build (+), and move and or scale the molecules so that each is observable. Which compound is most compact (most closely resembles a ball)? _____Which compound is least compact? _____

●**cis—trans Isomerism:** Cis is a term that means two groups are on the same side of a molecule, and trans means that two groups are across from each other in a molecule. In order to have cis—trans isomers, the molecule must clearly have two identifiable "sides." The necessary condition for cis—trans isomerism is afforded by carbon—carbon double bonds and rings (i.e., alkenes and cyclic compounds). Figure 5 shows how the two "sides" are identified.
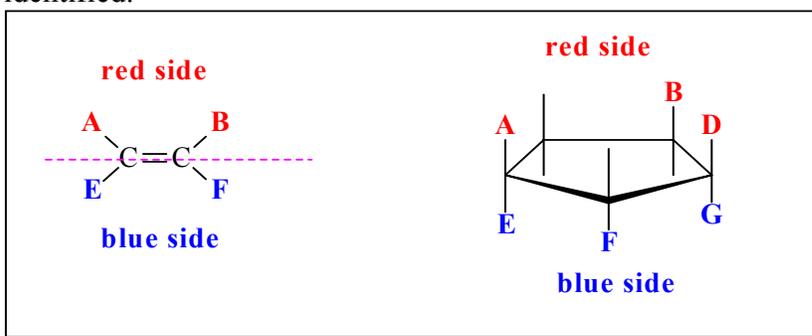

Figure 5. Cis-trans Isomerism

The double bond of an alkene determines the "sides." The double bond is extended as shown by the dashed magenta line in Figure 5, and the sides lie on either side of the magenta line. For a cycloalkane, the ring determines the sides. Though most rings are not planar, once a structure is drawn, we can clearly identify whether a group is one side or the other as shown in red and blue in Figure 5. In general, we compare only two groups at a time. Cis means the two groups we mention are on the same side (either red or blue in Figure 5). Trans means the two groups we mention are on opposite sides of the ring and across the ring; two groups that

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are trans are not bonded to the same atom. Thus, A and E are not trans in either structure of Figure 5. For the alkene, A and B and E and F are cis; A and F and B and E are trans. For the cylcoalkane, A is cis to B and to D; A is trans to F and to G but not to E. Note that A and B are on the same side of the ring but not next to each other. Cis only means "same side." Cis—trans isomers do not differ in connectivity. Exactly the same atoms are bonded to each other in both compounds. Cis—trans isomers differ in their three-dimensional geometry. They are one example of stereoisomers. We shall cover other examples of stereoisomers later in the course.

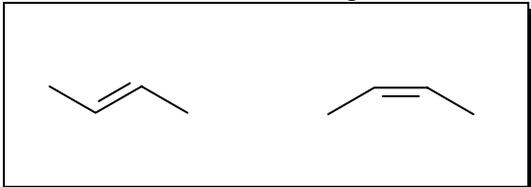►Build models of the compounds shown in Figure 6 on the same screen and minimize.

Figure 6. Two 2-Butenes

In one of the molecules, the two methyl groups are on the same side and in the other they are across from each other. Give complete names for these compounds, including the stereochemical prefixes cis and trans. _____
and _____ The prefix precedes the rest of the name. When cis or trans becomes part of a name, it is italicized. For example, *cis*-1,3-dimethylcyclopentane. In the future, when you see cis as an italicized prefix, be aware that there is a corresponding trans stereoisomer! Change the view to space filling. Which of the space-filled molecules seems to be more compact?_____

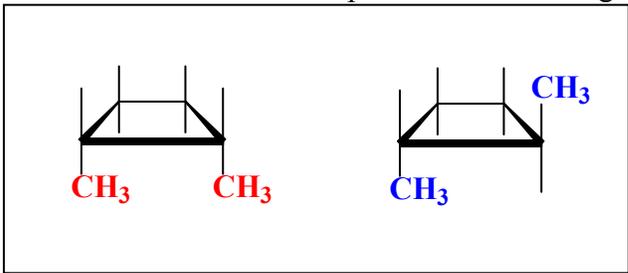►Build models of the compounds shown in Figure 7 on the same screen of and minimize.

Figure 7. Two dimethylcyclobutanes

Name these compounds, _____
and _____.
According to your models, does either of the compounds have a perfectly planar ring? _____ Explain any differences you observe in the Spartan models vs the structures as they appear in Figure 6.

_____

_____

Measure the angle made by any three of the ring carbon atoms. _____ Subtract your answer from the tetrahedral angle of 109.5°? _____ The difference is a measure of the **angle strain** in the molecule. Angle strain is the number of degrees the normal tetrahedral angle is compressed from its normal value of 109.5°. Start with either red carbon atom of

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Figure 6 in the cis-isomer and measure the dihedral angle made by the four carbon atoms, red-ring-ring-red. _____ The smaller the dihedral angle, the greater is the ***torsional strain***. In the trans-isomer, measure the dihedral angle made by the four carbon atoms blue-ring-ring-blue. _____ Which isomer has the greater torsional strain?_____ View the molecules as space-filled models. Locate the two methyl groups in each model. When adjacent groups are closer together than the sum of their van der Waals radii, both groups try to occupy the same space. When two groups touch each other, we call it a steric (spacial) interaction. The stain that a spacial interaction places on a molecule is called ***steric strain***. Which isomer has the greater steric strain?

_____

Organic Families Containing a Single-bonded Heteroatom: *Heteroatoms* are any atoms other than carbon or hydrogen. For most purposes, heteroatoms are nitrogen, oxygen, sulfur, or a halogen (fluorine, chlorine, bromine, or iodine). Although nitrogen, oxygen, and sulfur can form multiple bonds, this group of families contains a heteroatom and no multiple bonds. Examples of families in this group are alkyl halides, alcohols, ethers, amines, thiols, and sulfides. Ethers and sulfides are derivatives of alcohols and thiols, respectively. They will be covered later in the course. Figure 8 shows an example of an amine, an alcohol, a thiol, and four alkyl halides.
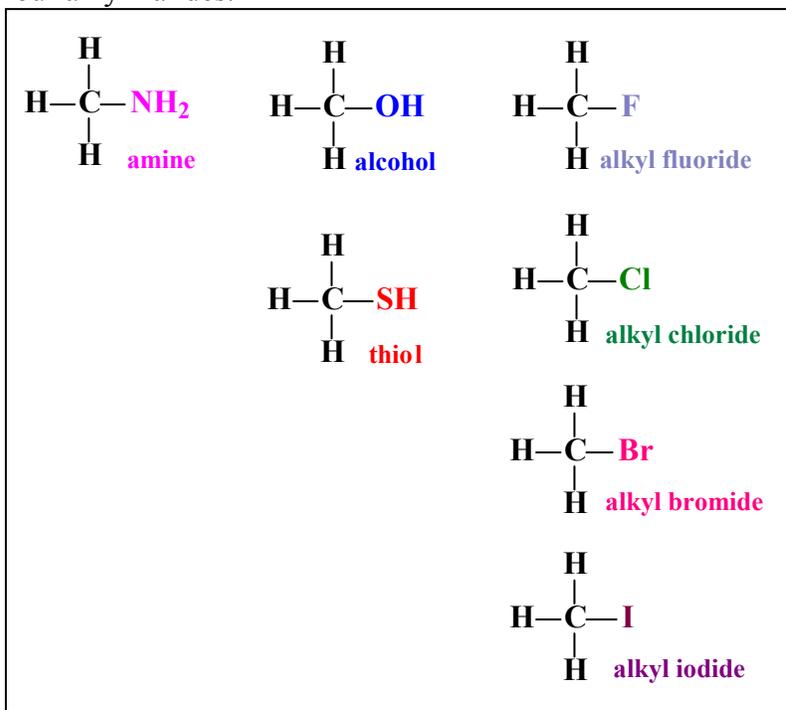

Figure 8. Families with Single-bond Heteroatoms

The families are arranged in Figure 8 according to the location of the heteroatom in the periodic table. Note that nitrogen has three bonds, oxygen and sulfur two bonds each, and fluorine, chlorine, bromine, and iodine one bond each, a reflection of the periodic groups of these atoms. The methyl group in each of the structures is the organic part, the colored part of each molecule is the functional group that defines the family. Reactions involving these molecules generally occur at the functional group. The four alkyl halides are considered to be one family with four sub-families. The names of the specific compounds in Figure 8 are

methylamine, methanol, methanethiol, and methyl fluoride, methyl chloride, methyl bromide, and methyl iodide.

●**Alkyl Halides:** *Alkyl groups* are alkanes with one H atom missing. When the missing H is replaced by a halogen, F, Cl, Br, or I, the compound is an ***alkyl halide***.

►Build models of methyl fluoride, methyl chloride, methyl bromide and methyl iodide and minimize them. While still in the build mode, rotate each model so that the halogen atom completely obscures the carbon atom. Arrange the molecules left to right, fluoride, chloride, bromide, and iodide. View the models as space-filled models. What is the order of increasing size of the halogen atoms? _____

●**Alcohols:** *Alcohols* contain an alkyl group and a hydroxyl group (-OH), the functional group. The hydroxyl group (-OH) replaces the missing H atom. If you start with water (H-O-H) and replace one of the H atoms with an alkyl group, you make an alcohol. Alcohols generally react at the OH group.

►Build two models of methyl alcohol on the same screen. The second model is active (has yellow tips). Move it so that the yellow tip from the red oxygen touches the red oxygen of the first molecule, and the alkyl part of the second alcohol is as far away from the first alkyl group as possible. Build a third model of methyl alcohol. Move it so that its H from OH just touches the red O of the second model, while ensuring that the alkyl groups are as far from each other as possible. Click E to minimize. You have an array of three molecules. There is an endless array of methyl alcohol molecules in a sample of methyl alcohol. ***Hydrogen bonding*** exists in organic compounds when an H atom is bonded to either an N or O atom and is attracted through space to another N or O atom. Hydrogen bonds are strong dipole—dipole forces of attraction. When hydrogen bonding is present in liquids, the boiling point of the liquid is higher than that of non-hydrogen bonded compounds of comparable mass. Does your array of molecules depict hydrogen bonding? _____ Describe hydrogen bonding in alcohols. _____

_____

●**Amines:** *Amines* contain an alkyl group and an amino (-NH$_2$) group, the functional group. Amines generally react at the –NH$_2$ group.

►Build a model of methylamine and minimize the structure. Can you distinguish the carbon atom from the nitrogen atom by color? _____ By number of H atoms bonded to the N atom? _____ Make the model as large as possible but still on the screen. Now, can you distinguish N from C in the model? _____ What color is the C atom? _____ The N atom? _____ In a Lewis structure of methyl amine, the N atom has a lone pair of electrons. Where is the lone pair in the model?

●**Thiols:** *Thiols* contain an alkyl group and a mecapto group (-SH), the functional group. The prefix thio means sulfur, so thiols are –ols (alcohols) that contain sulfur instead of oxygen. Indeed, thiols can be considered compounds in which the O of an alcohol has been replaced by S. Thiols are important in certain biochemical processes. Thiols generally undergo reactions in which the mercapto group participates.

►Build a model of methanethiol and minimize it. What color is the sulfur atom in the model? _____

Organic Families Containing a Carbonyl Group: A carbonyl group is a carbon and oxygen atom joined by a double bond. The carbon atom of the carbonyl group has two open or free valences.
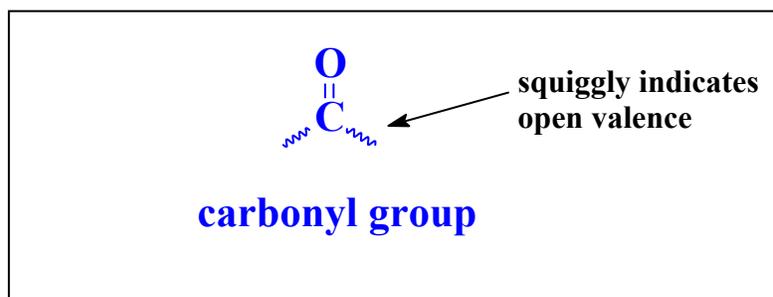
carbonyl group

Several different kinds of groups or atoms can be bonded to these two valences, giving rise to a number of families that contain the carbonyl group as a central structural feature. Examples of families in this group are aldehydes, ketones, carboxylic acids, esters, amides, and acid chlorides. For convenience, this group can be broken into two sub-groups. One group is aldehydes and ketones. The other group is carboxylic acids and the derivatives of carboxylic acids.

●**Aldehydes and Ketones:** *Aldehydes and ketones* contain a carbonyl group but no additional heteroatoms. *Aldehydes* must contain one H atom bonded directly to the carbonyl carbon atom. If both of the free valences of the carbonyl group are bonded to H atoms, the compound is the aldehyde called methanal or formaldehyde. *Ketones* must contain two carbon atoms bonded to the carbonyl carbon atom. Figure 9 shows examples of aldehydes and ketones. The carbonyl group is shown in blue.
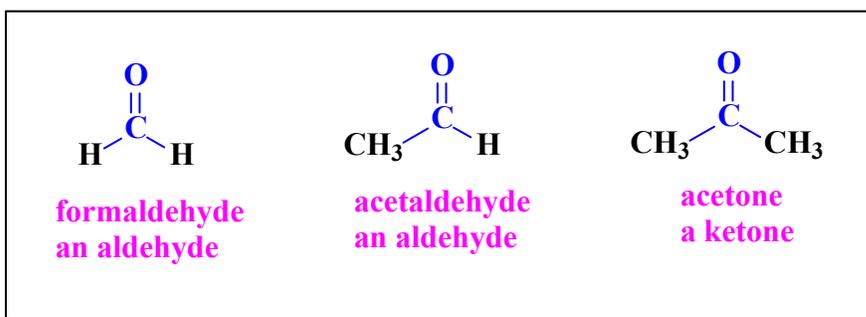

Figure 9. Aldehydes and Ketones

►Build models of formaldehyde, acetaldehyde and acetone on the same screen and click E. Measure and record the oxygen to carbon double (carbonyl) bond length in each. _____ _____ and _____ Measure and record one angle in each compound in which the carbonyl carbon is the middle atom. _____ _____ _____ View the molecules as tubes. What is the geometry around the carbonyl group? _____ What structural feature is necessary for a pure sample of a given compound to form intermolecular

hydrogen bonds? _____From the structures in
Figure 9, can a pure aldehyde form intermolecular hydrogen bonds? _____

●**Acids and Acid Derivatives:** *Carboxylic acids* contain a hydroxyl group bonded directly to
the carbonyl carbon. Esters, amides, and acid chlorides are derivatives of carboxylic acids in
which the H or OH of the acid's hydroxyl group has been replaced. Acids and acid
derivatives are characterized by a heteroatom bonded to the carbonyl carbon. Figure 10
shows examples of these families. The carbonyl group is shown in blue. The heteroatom
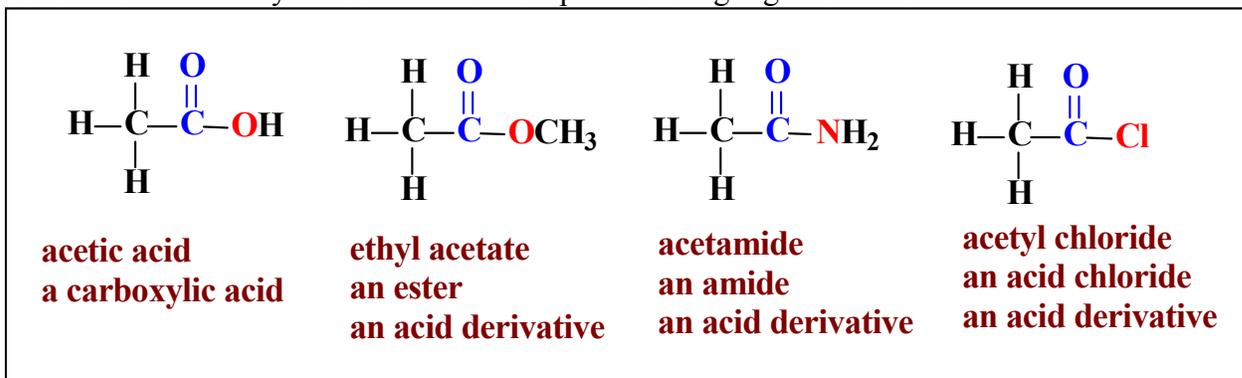bonded to the carbonyl carbon in these compounds is highlighted in red.

Figure 10. Acetic Acid and its Acid Derivatives

►Build and minimize a model of acetic acid. View the molecule as a ball and spoke model.
Change the model, in turn, into ethyl acetate, acetamide, and acetyl chloride. Change acetyl
chloride into acetyl bromide. What is the structure of the acetyl group?_____

Questions Electronic Models

1. What angle strain did you find in the cyclobutane ring? _____

2. Why isn't the cyclobutane ring planar?

3. From your lab results, which stereoisomer, *cis*-1,2-dimethylcyclobutane or *trans*-1,2-dimethylcyclobutane, has the higher overall strain (i.e., sum of angle, torsional, and steric strains)?

4. From your lab results, what is the relationship between branching in alkane constitutional isomers and the compactness of the molecules?

When a compound boils, the molecules of the compound are separated (pushed apart) by the application of heat. In a series of isomeric compounds, the most heat is required to separate the molecules of the isomer with the strongest intermolecular forces. Thus, that isomer has the highest boiling point of the group. Likewise, the least amount of heat is required to separate the molecules of the isomer with the weakest intermolecular forces. Thus, that isomer has the lowest boiling point of the group. In the alkane family, what is the relationship between compactness and intermolecular forces?

Finally, for the alkane family, what is the relationship between compactness and boiling point?

From your analysis, rank pentane, 2-methylbutane, and 2,2-dimethylpropane in order of increasing boiling point.

 (Use the Internet to verify your conclusion. If your initial conclusion is incorrect, go back through this question until you understand: small diameter space-filled model = compact molecule = weak intermolecular forces = low bp.)

5. From your lab results, what is the bond length of the double bond in a carbonyl group, rounded to two significant figures?

6. Does methanol or methanal (formaldehyde) have the higher boiling point?
Explain why your answer is correct.

7. What is the hybridization of a carbonyl carbon atom?

8. Write the family name beneath each of the structures.

$$\begin{array}{ccc} O & O & O \\ || & || & || \\ CH_3CH_2COH & CH_3CH_2CH & CH_3CH_2COCH_2CH_3 \end{array}$$
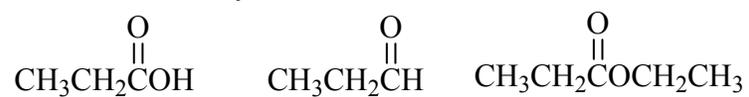
9. Explain how torsional strain is a function of dihedral angle.

10. From your experimental results, complete the following table.

Kind of Bond	Structure	Bond Length (rounded to 0.1 Å)
sp^3 carbon-hydrogen	C-H	1.1
sp^2 carbon-hydrogen		
sp carbon-hydrogen		
sp^3 carbon- sp^3 carbon		
sp^2 carbon- sp^2 carbon		
sp carbon- sp carbon		
arene carbon-arene carbon		

.