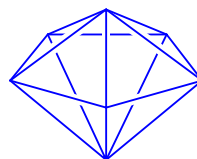
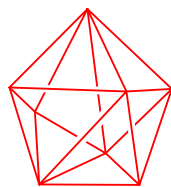
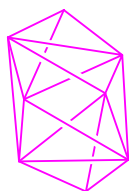


A Student's Guide to SpartanBuild[®]

Ray A. Gross, Jr., Ph.D.

**Department of Physical Sciences
Prince George's Community College**



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by Ray A. Gross, Jr.

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Electronic Models

► **Introduction** The advent and use of molecular modeling has revolutionized the science of organic chemistry. You may be familiar with SpartanView, which allows a viewer to look at pre-made models and modify them on the screen. SpartanBuild is a companion software program that provides viewers with three primary capabilities: to *build* molecules, to *view* these molecules in five different model formats, and to *measure* distances and angles on a model. This guide consists of two parts, a tutorial on the use of SpartanBuild and a set of practical exercises, which require SpartanBuild. The tutorial is designed to be both a learning primer and a user's guide. You can refer to it at any time to refresh your memory about specific capabilities of SpartanBuild. The practical exercises are designed to reinforce the knowledge you have acquired thus far in your study of chemistry in a game-like and fun manner. First, the basics of the program will be described, including basic mouse commands, certain screen features, Menu Bar items, and Toolbar icons. Then, we shall explore SpartanBuild by following a normal pattern that a typical user would follow. We shall build models of molecules and explore the various ways of viewing and making measurements on them. That is, we shall execute the three principle functions of SpartanBuild (i.e., *build*, *view*, and *measure*). The goal is to make you proficient in the use of SpartanBuild, so that you can use it as a learning enhancer.

SpartanBuild Tutorial

► Setup SpartanBuild

Insert your CD (ISBN: 0-534-37364-X) into the computer and open the disc. Double click on WFKIT (press the left mouse key twice with the arrow pointed at WFKIT, the colored icon with a B on it). The electronic model kit appears.

• **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 "click on" means to place the pointer on the specified object and depress the LMK.

► **Screen Features** ◀ **SpartanBuild initially opens with several visible features. Each of these features will be described briefly here for familiarization and in more detail, as necessary, later.**

• **Title Bar** The left side of the title bar contains the logo, B, and name of the program (SpartanBuild), and 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. Click on the middle box or "Maximize". This brings up a full screen. Otherwise, the bottom portion of SpartanBuild is obscured by the windows data bar at the bottom of the page. **Click on**

Maximize every time you open SpartanBuild. Note that the Maximize box changes to “Restore Down” after you have clicked the maximize box. That is, Maximize and Restore Down are reversible operations.

• **Menu Bar** The *Menu Bar* is the horizontal group of seven items (five to the left and two to the right) at the top of the screen, starting with File. 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 become visible. We shall explore these items later. By clicking on any menu item, you can read the contents of any other menu item by moving the pointer as described above.

• **Toolbar** The *Toolbar* is the horizontal group of eleven icons, starting with the V icon. 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. The command tells the viewer what to do after that particular icon is active (has been clicked). For example, clicking the + icon results in the command to “Select an open 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 open SpartanBuild, the build icon is active.**

• **Model Kit** The *Model Kit* 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 black on a white 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 “▼.” A menu of six 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. Click on “Rings” then click on the adjacent “▼.” A menu of eight rings opens. Click on “Cyclopentane” and draw the structure of cyclopentane as it appears above the kit.

• **Insert** The *Insert button* 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 where you see “SpartanBuild.” On the next line, you see five menu items on the left side of the screen and two on the right. On the left side, you see “File, Edit, Model, Geometry, and Build.” On the right side, you see “Options and Help.” We will explore these menu items one at a time, but not in the exact order as they appear on the Menu Bar.

• **File** Click on “File” to open the File menu. You see only three options, “Print, Print Setup, and Exit.” These commands are self-evident.

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

• **Build** A SpartanBuild 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 items on the Menu Bar. From the Menu Bar, click on “Build.” The Build menu consists of six options. The first option is View. View is really 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 simply 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 is active. Adding a fragment is the most fundamental operation of SpartanBuild. We shall build methane, the simplest hydrocarbon. Go to the Model Kit, click on the “C” with four single bonds. The C become 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. Look closely and you will see that the four bonds coming from the gray carbon atom turn yellow at the mid-point of the bond. The yellow half of each bond represents an H atom or an open valence. When you are finished building your model, the program will automatically add H atoms to any open valence (yellow tip). 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 bonding sites (valences), and the half of the bond that was yellow now appears white. 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 wire model. That is, the C and H atoms are **balls**, and the bonds joining atoms are **wires**. The carbon atom is gray, and the four hydrogen atoms are white. The colors are not pure but slightly off (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 a user to change the size of the displayed molecule.

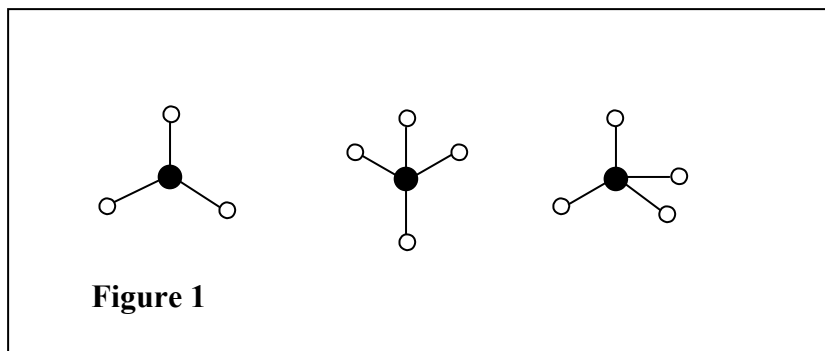
- Start with the white arrow (pointer) at the bottom of the screen. Depress and hold the “Shift” key on your keyboard. Simultaneously, depress and hold the RMK. With both keys depressed, move the pointer upward to the top of the screen. This operation increases the size of your methane molecule. Release the mouse key and return the white arrow to the bottom of the screen. Again, simultaneously depress both keys (Shift + RMK) 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 personal style or to keep the models on the screen.

► **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 and down and clockwise/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 1.



► **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.

- Can a real molecule undergo rotation and translation at the same time? Can a molecule in SpartanBuild 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 be modified. The four bonds of carbon are again half gray and half yellow. The yellow tips are open or available bonding sites called open valences. Note that the command line at the bottom left of the screen reads, “Select an open valence.” An open valence is a yellow tip. Click at the very end of any one of the yellow tips. Ethane is built, because the tetrahedral C atom with four single bonds is still the active atom in the 20-atom model kit. You can add as many fragments as you please. Click on another open valence and propane is built. Click on an open valence that originates from the middle carbon of propane and isobutane (2-methylpropane) is built. Click on “E” the Minimize icon and the molecule appears as a ball and wire model, showing the most stable conformation of isobutane 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 isobutane 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. The last-made bond is dashed (connected to the residual molecule by a dashed bond). To rotate about another bond (or if spinning did not occur on you model) go back to the build mode by clicking the “+” icon. Click in the middle of a carbon—carbon bond. This action changes the bond from a solid line into a dashed line. The dashed line is the “active” bond about which rotation will occur. Then repeat the “Alt + LMK” procedure to rotate about the newly dashed bond. With “+” active, click at the gray-yellow mid-point of a free carbon valence and repeat the “Alt + LMK” procedure. This action causes rotation about the dashed carbon—hydrogen bond.

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

- With isobutane on the screen, depress the “Alt” key on the keyboard and the RMK. Move the mouse up and down. The dashed bond is lengthened when the mouse is moved upward and shortened when the mouse is moved downward. The operation works only on a dashed line. The last-made bond will be dashed in the ball and wire model. Another bond can

be made to be the dashed bond in the model by going to the build mode and clicking on the mid-point of the bond.

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

- With isobutane 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 an open valence, but click on any of the three equivalent carbon atoms. A methyl group is deleted, leaving propane.

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

- **Break Bond** Click on “Break Bond” from the “Build” menu. Before continuing, note that the carbon—carbon bonds are solid gray, whereas the carbon—hydrogen bonds are half gray and half white. Also note that the last bond formed in the build mode appears as a dashed line (C----C) instead of a solid line (C—C). 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 open 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 become clearly visible.

- **Edit** Click on “Edit” to open the edit menu. You see three options, “Undo, Copy, and Clear.” The “Undo” and “Copy” commands work as they do in the Word program. 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 (e.g., to a PowerPoint slide).

- **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 propane model disappears, and you are back in the build mode. Click anywhere in the green space and methane reappears, providing the tetrahedral C atom 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 again. 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 Wire” 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 E. Zoom the molecule and note the clarity of the apparent three-dimensional structure.

● **Alkenes** From the Edit menu, clear the screen. Click the + icon. Highlight a double-bond carbon. Click on the screen. Click on the end of the two 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.** Thus, clicking the double bond yellow tip produces a double bond, and clicking the single bond yellow tip produces a single bond.

● **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 three oxygen atom choices, one with two single bonds, one with a double bond, and one with three single bonds and a positive formal charge. 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 (i.e., a yellow tip with two lines). 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. This is a carbonyl group, an important group in organic chemistry. Highlight the single bond oxygen in the Model Kit and click on a carbon single bond on the screen. You have a carboxyl (**carbonyl + hydroxyl**) group.

● **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.

● **Groups** Clear the screen. Click on “Groups” and select “Carboxylic acids” 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 are built in the same way the carboxyl group was built.

● **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 above-described rotation and translation commands

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 RMK to translate the highlighted molecule. Move the model around and then clear the screen.

► **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. You see five options above a line and two below the line. The five options above the line 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.” The two options below the line are “Hydrogens and Labels.” These two options 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 Wire” and “Hydrogens” commands already have a check mark. The checked 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 Wire” until we are in the view mode. Click on the “V” icon (directly below “File” 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. Labels are only visible on wire and ball and wire models.** Click on “Labels” to remove the labels from the model. The numbering system in “Labels” is not the same as the IUPAC system, and the label numbers depend on the order of formation of the partial structures.

► **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 above a line, and two command options below the line. The three options above the line are commands that allow a user to measure various aspects of a molecule. The measurement commands are “Measure Distance, Measure Angle, and Measure Dihedral.”

The “Measure Distance” command allows the user 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 a user to measure any angle in degrees (°) made by three atoms. The “Measure Dihedral” command allows a user to measure dihedral angles in degrees (°). A *dihedral angle* is an apparent angle made by four atoms. The two command options below the line 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 clarify the structure in some way. The “Define Point” command allows a user to highlight any atom or multiple atoms as points for reference or to create or define a point on an atom in the molecule or on a bond between two atoms. **The “Define Point” command is active only on a ball and wire model.** Highlighted atoms are visible on ball and wire models only. Defined points are visible on ball and wire models when the point is midway between two atoms. Defined points are visible on wire 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 in the geometry menu are also accessible by five icons on the toolbar. Collectively, these five icons 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. Label the atoms by clicking on “Labels” from the “Model” menu. Enlarge the model if necessary. Click on H1 and then C1. What is the H1—C1 bond length? _____ (Look in the lower right corner of the screen.) Find the H2—C1 bond length. _____ 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 H2—C1 bond length compare to the H1—C1 bond length?

_____ From your measurements, what is the carbon—hydrogen bond length, rounded to one decimal place, when carbon is sp^3 hybridized? _____ Alternatively, you may 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 bond or two selected atoms turn into a golden color when they are highlighted.

◦ **Measure Angle** With methane on the screen with labeled atoms, click “Measure Angle” from the Geometry menu. Click on H1, C1, and H2 in that order. Rounded to one decimal place, what is the H1—C1—H2 angle? _____ What is the H1—H2—H3 angle? _____ How does the H3-C1-H4 angle compare to the H1—C1—H2 angle? _____ Note that it is unnecessary for the three atoms to be bonded; an angle can be found for any three atoms in the structure.

◦ **Measure Dihedral** Clear the screen, build a model of ethane and click “E.” Click “Measure Dihedral” from the Geometry menu. Enlarge the model if desired. If the label option is not active, click on “Labels” from the Model menu. Click on an H bonded to C1 and it will turn a gold color. Click on C1 and it turns golden. Then click on C2 and on an H atom bonded to C2. You have clicked on four atoms in all, and they are all golden. Rotate the molecule so that C1 completely obscures (eclipses) C2. You will see a V shape, made by the three visible highlighted (golden) atoms. The angle made by these three highlighted atoms is called the dihedral angle. A *dihedral angle* is an apparent angle made by four atoms,

three of which are visible and one of which is obscured. Look to the bottom right of the screen and see the dihedral angle is either $+60^\circ$ or -60° . 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 (-). These conventions are specific to SpartanBuild. Click on the appropriate atoms to change your dihedral angle from -60° to $+60^\circ$ or visa versa. We are generally more interested in the magnitude than we are of the sign of a dihedral angle.

◦**Define Point** Clear the screen and build a model of methane. Open the Model menu and ensure that only the Ball and Wire and Hydrogens options are checked. With methane on the screen, click “Define Point” from the “Geometry” menu. The model now appears as a ball and wire model, regardless of what kind of model was previously on the screen. Click on the carbon atom. The carbon atom is highlighted by turning a golden color. 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 by turning golden. Click in the center of the C atom again. The highlight is removed and the model appears to be the same as it was before. Click on the “V” icon, then select “Wire” from the “Model” menu. You see that the carbon atom has been made the “defined point.” Thus, double clicking an atom when the Define Point command is active creates a visible ball on wire models. The defined point is invisible in the other models. Clear the model from the screen, and build a new methane molecule. 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 between any and all bonds in the model and at any or all atoms. All points are visible on the wire model. Clear the screen.

◦**Define Plane** With a new methane on the screen, click “Define Plane” from the “Geometry” menu. The model now appears as a ball and wire model, regardless of what kind of model was previously on the screen. 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. Clear the screen.

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** Click on “Options” to open the options menu. You see three options above a line and three options below the line. The three options below the line are already checked,

meaning they are active or visible on your screen. The three options above the line are “About SpartanBuild...”, “Preferences ...”, and “Colors...” This top option gives us information about the company that developed Spartan and the other five options give us alternative ways to setup or modify what we see on the screen.

◦ **About SpartanBuild.....** Click “About SpartanBuild” from the “Options” menu. A window opens that provides information on how to contact Wavefunction, the company that makes Spartan software. Note, the WFKIT icon you clicked to open the model kit stands for Wavefunction kit. Click on “OK” and the window disappears.

◦ **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 offers the viewer three basic options, “View, Stereo, and Toolbar Style.” 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. The View and Stereo options determine how the molecule appears on the screen. The Toolbar options give the viewer three different ways to display the Toolbar.

◦ **Stereo** The default View selection is titled “Orthogonal.” With “Orthogonal” selected, check “Stereo” then click “OK” in the “Preferences” window. The window disappears and the methane model is now viewable in stereo. That is, when viewed through the red and blue stereo glasses, the model appears to be in three dimensions. If you have stereo glasses, view the methane model through these glasses. Reopen “Preferences” from the “Options” menu. Select “Perspective” from the View menu. Note that one of the two choices, Orthogonal or Perspective, will always be active. With “Stereo” still checked, click on “OK.” The methane model now appears even better when viewed through the 3d glasses. Thus, we will generally use the Orthogonal selection without Stereo and the Perspective selection with Stereo. Reopen the “Preferences” window and click on “Orthogonal” and “Stereo,” then click “OK.” The window disappears, and the methane model returns to a standard ball and spoke model.

◦ **Toolbar Style** We shall examine the use of the toolbar icons in the next segment. For now, we will learn three different ways to display the toolbar. The default toolbar style is “Small Icons”. Open the “Preferences” window from the “Options” menu. In turn, click on “Text and OK”, “Large Icons and OK”, and “Small Icons and OK.” The Preferences window must be reopened each time. Note how the toolbar changes on your screen. The last-selected style remains active until the user changes it.

◦ **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 SpartanBuild.

◦ **Model Kit, Build Toolbar, Geometry Toolbar** Click on “Options” to open the options menu. The three choices below the line are already checked. Checked items are visible on your screen.

· **Model Kit** Click on “Model Kit.” The model (atom selection) kit disappears. Click on “Model Kit,” again from the Options menu and the atom selection kit reappears. Thus, you have a choice of viewing the kit or not viewing the kit. Obviously, when you are building a model, you’ll want to view the kit.

· **Build Toolbar** Click on “Build Toolbar.” The Build Toolbar consists of the first six icons on the toolbar at the top of the screen. These six icons disappear when the Build Toolbar is unchecked in the Options menu. Click on “Build Toolbar” again from the Options menu and the six icons reappear. Selecting one of the six icons in this group is the same as selecting that option from the Build menu as discussed above.

· **Geometry Toolbar** Click on the “Geometry Toolbar.” The Geometry Toolbar consists of the last five icons on the toolbar at the top of the screen. These five icons disappear when the Geometry Toolbar is unchecked in the Options menu. Click on “Geometry Toolbar” again from the Options menu and the five icons reappear. Selecting one of the five icons in this group is the same as selecting that option from the Geometry menu as discussed above.

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 either Small Icons or Large Icons is selected in the Preferences window of the Options menu.

► **Shortcuts** ◀ **Most shortcuts are associated with the Toolbar icons.**

► **Toolbar Icons** The eleven icons displayed at the top of the screen just below the menu items are shortcuts to the six options in the Build menu and five options in the Geometry menu, which we have already discussed. The title of an icon is revealed when the cursor is placed over the icon without clicking the mouse. The title of an icon disappears in about five seconds. Slowly move the pointer over each of the first six icons, starting with the “V” icon, until the title of each icon appears. You will note that the first six icons have the same names as the six options in the Build menu. Thus, these six icons are collectively known as the Build Toolbar. Likewise, the final five icons have the same names as the five options in the Geometry menu. Hence, these five icons are collectively known as the Geometry Toolbar. Clicking on any one of the eleven icons is the same as selecting the corresponding name from the Build or Geometry menu. Thus, you save a mouse click each time you use the toolbar instead of the Build or Geometry menus.

• **Distance** With a methane molecule on the screen, click on the “Distance” icon. The icon is active when it appears slightly depressed. Next, click on the midpoint of any C—H bond and read the bond length at the bottom right of the screen. Note, this operation gives the

same result you found above. Like the Distance icon, the other 10 icons are shortcuts to menu selections. Two clicks are necessary to open a menu item, whereas the same operation is performed by a single click on the corresponding icon from the Toolbar.

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

Table 1. Keystrokes for SpartanBuild

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 explore the build, view, and measure features of SpartanBuild, while collecting useful data about organic compounds. The 10 questions at the end of the exercises require the data you acquire from these exercises. Therefore, answer the questions as you go along and keep them for the follow-on problems.

Functional Groups: *Functional groups* are unique partial structures that allow organic compounds to be classified into families. Because each member of a 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.

● **Alkanes:** *Alkanes* are hydrocarbons that contain σ bonds only. Alkanes may be cyclic or acyclic. Cyclic alkanes are called *cycloalkanes*. Alkanes are unique, because they do not contain a functional group.

Note: The following exercises require the use of IUPAC numbering for the molecules, because the “Labels” option in the Model menu gives unpredictable numbers.

► Ethane: Build and minimize a model of ethane (CH_3CH_3). Make and record the following measurements. C-H bond length _____ C-C bond length _____ H-C-H bond angle _____ What is the hybridization of an alkane carbon atom? _____

Hydrocarbons do not contain heteroatoms, and alkanes do not contain π bonds. However, other kinds of hydrocarbons do contain π bonds. The number of π bonds and their locations within a given structure determines the family to which a given hydrocarbon is assigned. The functional groups that may be present in hydrocarbons are a double bond, triple bond, and alternating single and double bonds in a six-membered ring. The families are alkenes, alkynes, and arenes, respectively. Figure 2 shows examples of these families. The next several exercises relate to these compounds.

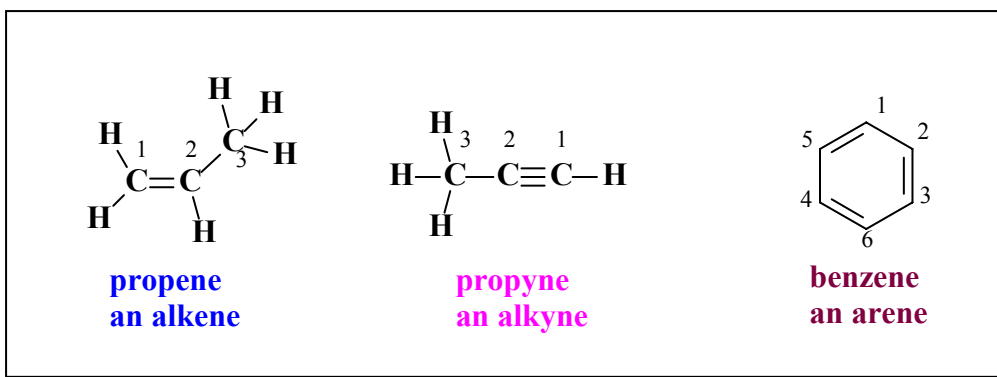


Figure 2. Hydrocarbon Families

● **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.

► Build and minimize a model of propene. What is the hybridization of C1? _____ (Hybridization is not shown on the screen, you are supposed to know it!!!) 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 bond length? _____ What is the angle made by the two hydrogen atoms and C1? _____

● **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. A compound that contains both a double and triple bond is an enyne (i.e., it contains three π bonds). Alkynes typically react at the triple bond or functional group.

► Build and minimize a model of propyne. What is the hybridization of C1? _____ What is the shape of the molecule around the triple bond? _____ What is the C1 to H1 bond length? _____ What is the C1 to C2 bond length? _____ What is the C1 to C2 to C3 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, minimize the structure and label it. What is the hybridization of C1? _____ What is shape of the molecule? _____ What is the C1 to H1 bond length? _____ What is the C1 to C2 bond length? _____ What is the C2 to C3 bond length? _____ What is the C1 to C2 to C3 bond angle? _____

Isomers: *Isomers* have the same molecular 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 3 shows three alkanes that each contains five carbon atoms.

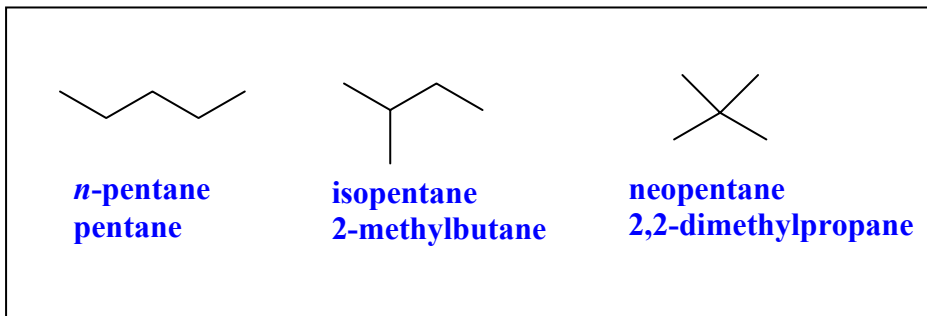


Figure 3. Five-carbon alkanes

► 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 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-dimethylpropane _____. Convert all of the models into space-filled models. If they overlap, go to build (+), and move and or scale the molecules so that each is observable as a space-filled model. 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 by rings (i.e., alkenes and cycloalkanes). Figure 4 shows how the two “sides” are identified.

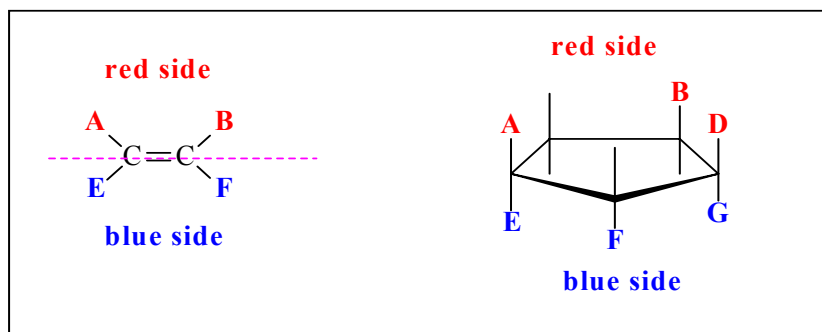


Figure 4. Cis-trans Isomerism

The double bond of an alkene determines the “sides.” The double bond is extended as shown by the dashed magenta line in Figure 4, 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 4. In general, we compare only two groups at a time. Cis means the two groups that we mention are on the same side (either the red side or blue side in Figure 4). Trans means that the two groups we mention are on opposite sides of the ring and across the ring; two groups that are trans are not bonded to the same atom. Thus, A and E are not trans in either structure of Figure 4. For the alkene, A and B and E and F are cis; A and F and B and E are trans. For the cycloalkane, 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 an example of stereoisomers. There are other examples of stereoisomers not covered here.

► Build models of the compounds shown in Figure 5 on the same screen of SpartanBuild and minimize.

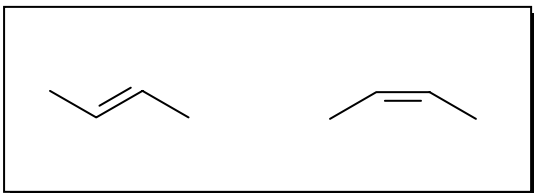


Figure 5 Alkenes

In one of the molecules, the two methyl groups are on the same side and in the other they are across from each other. Use the stereochemical prefixes cis and trans to name these compounds. _____ 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 (or trans) as an italicized prefix, be aware that there is a trans (or cis) 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 6 on the same screen of SpartanBuild and minimize.

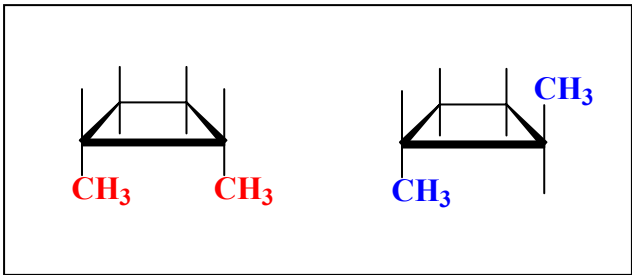


Figure 6. Cycloalkanes

Name these compounds, _____ and _____.

Do either of the compounds have a perfectly planar ring? _____ Explain any differences you observe in the SpartanBuild 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 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 strain 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 these atoms only with single 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 are covered elsewhere. Figure 7 shows an example of an amine, an alcohol, a thiol, and four alkyl halides.

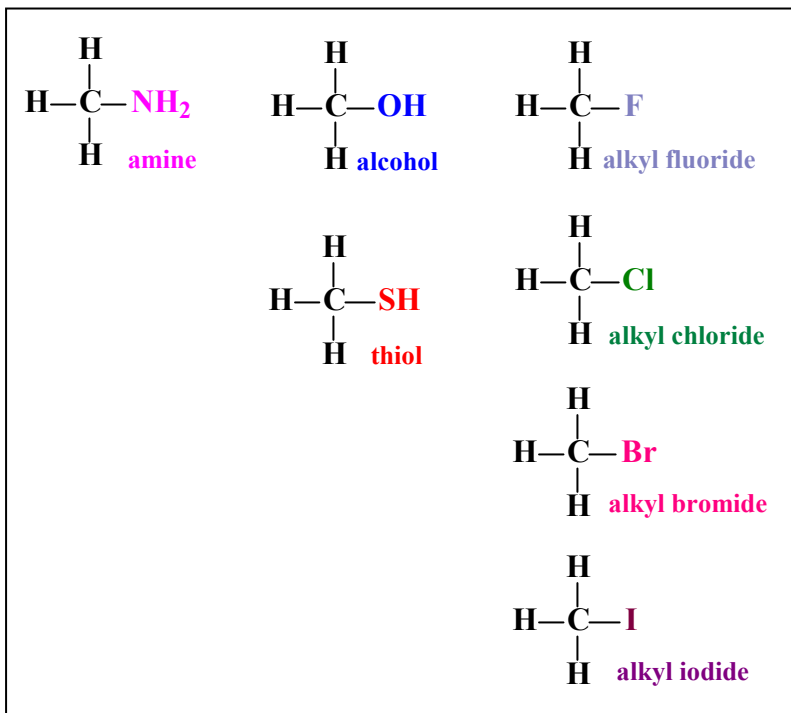


Figure 7. Families with Single-bond Heteroatoms

The families are arranged in Figure 7 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 will generally occur at the functional group. The four alkyl halides are considered to be one family with four sub-families. The names of the compounds in Figure 7 are methanamine, methanol, methanethiol, and fluoromethane, chloromethane, bromomethane, and iodomethane.

● **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 fluoromethane, chloromethane, bromomethane and iodomethane and minimize them. While still in the build mode, rotate the molecules so that the halogen atom completely obscures the carbon atom. Arrange the molecules left to right, fluoride, chloride, bromide, and iodide. View all of the molecules as space-filled models. What is the order of increasing size of the halogen atoms? _____ Delete all of the models except the bromide. Click the “Define Plane” icon. Make a plane on the model by clicking the three H atoms. Rotate the molecule until only the plane and the three H atoms are visible. Build a separate hydroxide ion on the screen (“Insert → “-O-” → “Delete” → click on one yellow tip of —O— to make -O). Move the -O to the center of the green plane, and then minimize. What angle in degrees is made by the Br-C-O atoms (rotate the pair until you can clearly see the angle)? _____ When hydroxide reacts with an alkyl halide it bonds to the back side of the carbon as the halide leaves from the front side.

● **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 (methanol) 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 they are present in liquids, the boiling point of the liquid is higher than that of similar compounds, which do not possess hydrogen bonding. Does your array of molecules depict hydrogen bonding? _____ Describe hydrogen bonding in alcohols.

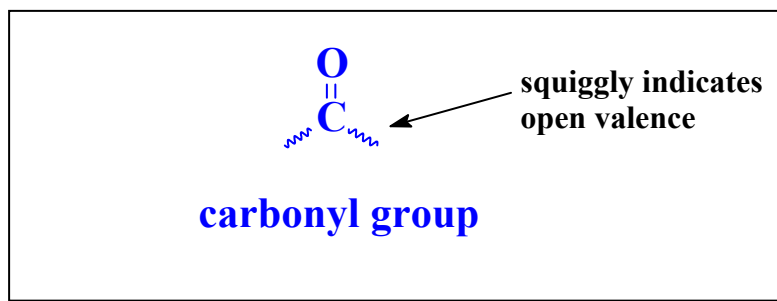
● **Amines:** *Amines* contain an alkyl group and an amino (-NH₂) group, which is the functional group. Amines generally react at the -NH₂ group.

► Build a model of methylamine (methanamine) and minimize the structure. Can you distinguish the carbon atom from the nitrogen atom by color? _____ Can you distinguish C from N by number of H atoms bonded to them? _____ Make the model as large as possible but still on the screen. Now, can you distinguish N from C in the model by color? _____ What color is the C atom? _____ The N atom? _____ In a Lewis structure of methylamine, 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 mercapto group (-SH), which is 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?

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 valences.



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 comprised of aldehydes and ketones, and the other group is comprised of carboxylic acids and derivatives of them.

● **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 open 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 8 shows examples of aldehydes and ketones. The carbonyl group, shown in blue, is always present in aldehydes and ketones.

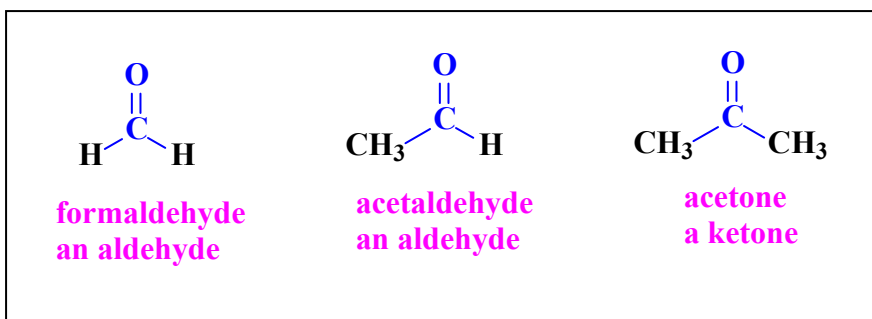


Figure 8. Aldehydes and Ketones

► Build models of formaldehyde, acetaldehyde and acetone on the same screen and click E. Measure and record the oxygen to carbon double 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 8, 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 9 shows examples of these families. The carbonyl group, which is always present in carboxylic acids and acid derivatives, is shown in blue. The heteroatom bonded to the carbonyl carbon in these compounds is highlighted in red.

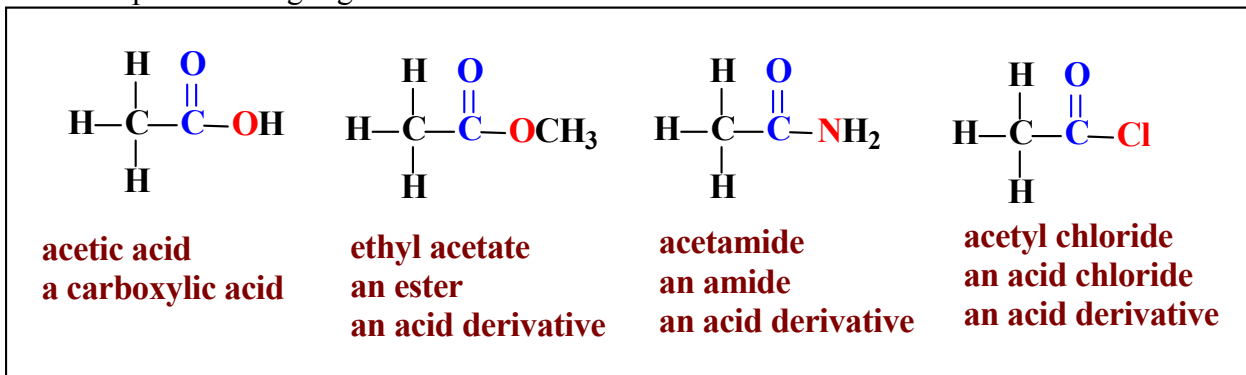


Figure 9. Acetic Acid and its Acid Derivatives

► 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? _____

© This completes the tutorial. Ten questions that review SpartanBuild are provided on the next page.

Questions Electronic Models

1. What angle strain did you find in the cyclobutane ring? _____ Find the angle strain in cyclopentane. The angle strain in cyclopentane is _____ .
2. Build a model of cyclohexane in SpartanBuild and minimize it. Is the ring planar? _____ Delete the hydrogen atoms (“Model” → “Hydrogens”). Describe the shape of the carbon ring system. _____
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 model building 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?

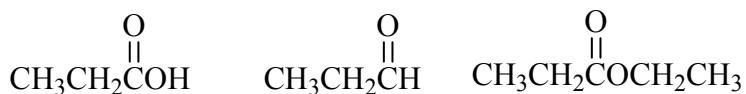
Finally, for the alkane family, what is the relationship between compactness and boiling point?

From your analysis, rank order 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 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 following structures.



9. Build models of cyclopropane and cyclohexane in SpartanBuild. Measure the dihedral angle between adjacent cis hydrogen atoms in each structure. Which molecule has the larger torsional strain?

Explain how torsional strain is a function of dihedral angle.

10. From data you collected during the exercises, 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		