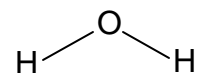


Molecules in Motion

How would you describe the motion of the water molecule to the right?

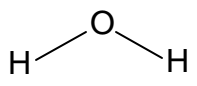
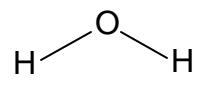
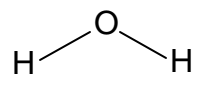


How would a group of gaseous water molecules behave in a closed container? Illustrate and explain.

Circle the correct choice for the three states of matter:

state of matter	translational	rotational	vibrational
gas	yes or no	yes or no	yes or no
liquid	yes or no	yes or no	yes or no
solid	yes or no	yes or no	yes or no

Vibrational Modes in the Water Molecule

symmetrical	asymmetrical	bending
		

Using the right click on the mouse, turn the animation on for the three water molecules. (If a check mark is there at animation, click it off and then on.) Sketch the results above.

Which vibrational modes influence the bond length?

Which vibrational mode influences the bond angle?

Are bond lengths and bond angles constant in a molecule? Explain.

Turn on the animation of the ethane molecule, C_2H_6 , shown below. What is occurring along the carbon-carbon single bond?

Would this type of motion occur around a double or triple bond? Explain.

Translational and rotational modes are important in gases and liquids, where particles are not bound to a fixed position. A molecular vibration is any movement that changes the size and shape of a molecule (bond lengths and angles). A vibration may change the dipole of a molecule. The vibrational mode occurs in all states of matter; however, in solids it is the only mode due to particles being bound in a crystalline structure. Bond rotation as in ethane is a type of vibration. Only single bonds have the ability to undergo internal rotation. [Click here](#) to view the nine vibrations of dichloromethane, CH_2Cl_2 . Vibrations are induced by infrared radiation (IR) in the energy range from 400 to 4000 cm^{-1} .

Decide which relationship holds for the order of energy (wave number, cm^{-1}). Circle the correct order.

bending > stretching bending = stretching bending < stretching

What influences the molecular motion?

Click on the link to go to an [Excel interactive spreadsheet](#) to address the next set of questions. The white boxes can have their values varied, press the ENTER key after typing in a number.

How does the molar mass influence the velocity of a gaseous atom or molecule? What do you predict will be the outcome? Sketch a graph of your prediction. Then see the graph - click on the molar mass tab at the bottom left of the screen.

How does temperature influence the velocity of a gaseous atom or molecule?

In a container with one mole of pure gas (constant molar mass) at a constant temperature of 298 K, will all the atoms or molecules have the same velocity? Explain.

Now click on the distribution tab, and set up the distribution of velocities on molecules in one mole of gas. Set the temperature of gas 1 to 298 K and select a molar mass of a gas, leave gas 2 set at zero.

How would you describe the velocities or energies of the molecules in a gas at a specific temperature?

How does the distribution change when the temperature is increased?
Set up gas 2 as the same gas as gas 1 at a higher temperature. Sketch and label a low and high temperature graph of the distributions.



How does the molar mass of the gas influence the distribution when temperature is held constant?

As you saw on the plots, there is a distribution of velocities for any gas at a specific temperature. As temperature increases, the distribution shifts to the right (higher temperature) while flattening (wider variation in velocities). Lowering the molar mass does the same thing. Why?

What happens when the molecule gets more complicated in its structure?

Now observe the motion of the cyclohexane molecule, C_6H_{12} , given below. Turn on the animation of the center image and describe what is happening to the molecule. The two conformations (forms) of cyclohexane are shown to the left (chair) and right (boat). Wooden models are available!

This illustrates the natural conversion of the chair form to the boat form of cyclohexane due to the molecular motion in the molecule. The chair form is the lower energy state of the two conformations.

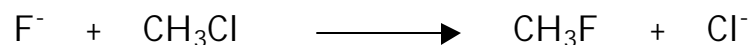
Some final thoughts:

Write a description outlining the behavior of a group of gaseous formaldehyde molecules, CH_2O . How about liquid formaldehyde molecules? Are there any differences between the gaseous and liquid states?

Write a description outlining the behavior of the molecules in solid carbon dioxide, dry ice. How would the motion be influenced by a decrease in temperature?

Is there a possible temperature where molecular motion could stop? Explain.

Observe the attack of the F^- ion on the CH_3Cl molecule given below.



Start the animation to see the attack. This is an example of the classical S_N2 reaction of organic chemistry.

Does there appear to be a preferred direction of attack? Explain. If so, what happens when the F^- ion approaches in a different direction?

Watch the reaction and then see if you can draw the structure of the transition state or activated complex. How does it compare to the reactant and product structures?

Watch the hydrogens as the reaction proceeds. Describe what happens to them.