

## Molecular Modeling Activity for Solutions

Time required: one 50-minute period

### Introduction



Imagine a tall glass of Kool-Aid on a warm summer day. Water and Kool-Aid powder were mixed to make the solution. We define a solution as a homogeneous mixture of a solute, the Kool-Aid powder, in a solvent like water. In this model-based activity, you will learn the main concepts behind the process of dissolving.

### Materials

The Solutions Set

### Procedure

Both solid-liquid solutions and liquid-liquid solutions are important in chemistry. A solid that dissolves in a solvent is soluble while a solid that does not dissolve is said to be insoluble. When the solvent and solute are both liquids, we say that the two liquids are miscible. If liquids do not dissolve in each other, they are said to be immiscible

"**Like dissolves like**" is an expression chemists use when discussing the solubility of substances. The "like dissolves like" rule, in general, means that nonpolar substances dissolve in nonpolar solvents and polar substances dissolve in polar solvents. By definition, polar molecules have a partially positive side and a partially negative side, or a dipole. Water is a polar molecule.

The central atom in the water molecule is oxygen, represented by the red atomic model. A neodymium magnet represents the lone pairs of electrons on the oxygen atom. Oxygen is bonded to two hydrogen atoms, represented by white plastic atomic models with magnetic centers.

Water molecules in the liquid and solid states tend to stick together. The oxygen atom attracts the electrons within the covalent bonds leaving the hydrogen atoms with a slightly positive charge. The oxygen atom has a partial negative charge. Water is a **dipole** (or **polar molecule**) because it has partial positive and partial negative charges separated by a distance.

A **hydrogen bond** is formed when the slightly positive hydrogen atom of one water molecule is attracted to the oxygen atom of another water molecule.

1. How can you form a hydrogen bond between two water molecules? \_\_\_\_\_

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If you have ever played with magnets, you have noticed the attraction between magnets. As the hydrogen atom of one water molecule approaches the oxygen atom of another water molecule, the attraction can be quite strong. Molecules are not magnets, but the electrical attractions similarly increase as the water molecules approach each other. The attraction between the molecules is called a hydrogen bond. Hydrogen bonds are much weaker than covalent bonds; they break and easily form again.

Table salt (NaCl) is a crystal, held together by strong ionic bonds. An ionic bond is formed from the electrostatic attraction between oppositely charged ions. In ions, electrons of one atom are transferred to another atom. The atom that loses the electrons becomes a positively charged ion, or a **cation**, while the one that gains electrons becomes a negatively charged ion, or an **anion**.

In the model of sodium chloride, the silver model represents the sodium ion while the green model represents the chloride ion. Complete the model of sodium chloride by adding the six white ionic bonds. The sodium ions should be bonded to chloride ions.

Move the hydrogen end of the water molecule near to the green chloride ion.

2. Is the partial charge of the hydrogen end of the water molecule positive or negative?

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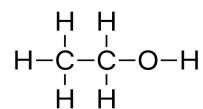
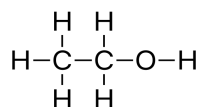
3. Since oppositely charged particles attract, what is the charge of the chloride ion?

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**Work with the models to see how the water molecules attract to the ions in the crystal.**

Sodium chloride is soluble in water. When we try to dissolve an ionic compound by stirring it in water, the positive poles of the water molecules are attracted to the anions, while the negative poles of other water molecules are attracted to the cations. Eventually the ionic bonds break and ions are released into the water. When the salt dissolves, each ion becomes surrounded by water molecules. This process is called **hydration**.

Assemble two molecular models for ethanol,  $C_2H_5OH$ . The hydrogen atom that is attached to the red oxygen atom is polar and has a magnet. The other five hydrogen atoms are nonpolar and do not have magnets.



4. Look at your models for water and ethanol.

How are they alike? \_\_\_\_\_

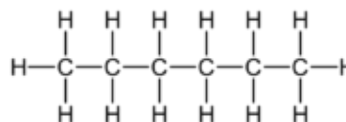
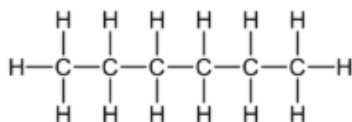
How are they different? \_\_\_\_\_

Will the two ethanol molecules attract? \_\_\_\_\_

Will the ethanol and water models attract? \_\_\_\_\_

Ethanol and water are miscible. Ethanol has a molecular structure that includes the polar -OH group. The OH atoms on the ethanol molecule are linked with a polar covalent bond. The shared pair of electrons in the covalent bond gets "shifted" towards the oxygen atom, giving the oxygen a localized negative charge. The hydrogen atom from which an electron was shifted, becomes positively charged. Compared to ions, polar molecules carry much weaker localized charges. The ethanol molecule shows an intermediate polarity because it has both a polar OH group and a nonpolar CH<sub>3</sub>CH<sub>2</sub> section.

Build the two molecular models for hexane, C<sub>6</sub>H<sub>14</sub>.



The hydrogen atoms in hexane are nonpolar and therefore do not have magnets. It may seem like there is no attraction between the hexane molecular models. However, hexane exists in the condensed state as a liquid at room temperature. Therefore, attractions between the molecules, although weak, must exist to cause them to cling together.

5. Look at your models for water and hexane.

How are they alike? \_\_\_\_\_

How are they different? \_\_\_\_\_

Quite a different situation occurs when hexane and water are mixed. Hexane and water are immiscible. The layer of hexane floats on top of the water. Hexane molecules have no -OH group and are nonpolar. Water molecules stick tightly together. Hexane molecules are not strongly attracted to the water molecules and are immiscible in water. We call the hexane molecules "hydrophobic" (water-fearing) because polar water molecules, being attracted to each other, push the hydrophobic molecules away, usually to the surface.

### You're the Chemist

Chemists use the "like dissolves like" rule: when two liquid molecules are alike in polarity, they tend to be miscible and form a solution. The rule allows chemists to use the chemical composition and molecular structure to predict the likelihood of two substances dissolving in each other.