CHEMICAL FORMULAS

FORMULAS

There are many ways to represent a chemical substance on paper and it is important to understand what each type of representation indicates and does not indicate.

EMPIRICAL FORMULA

- **The empirical formula is the reduced, whole-number formula giving the smallest whole-number ratio of each atom to each of the others.**
- H_2O_2 can be reduced to HO: a ratio of one atom of oxygen to every atom of hydrogen.
- H_2O cannot be reduced and has a ratio of two hydrogen atoms to every oxygen atom.
- Only integers are used in empirical formulas so $H0_{0.5}$ would not be correct.

MOLECULAR FORMULA

- A molecular formula is the unreduced, full formula of the compound representing the actual composition found by an experiment.
- **It gives the exact number of each atom of an element in the molecule**
- In an experiment, data would indicate the ratio of hydrogen atoms to oxygen atoms in hydrogen peroxide is one to one or H0.
- The molecular formula is always a whole—number multiple of the empirical formula.
- In the case of hydrogen peroxide, the empirical formula H0 is multiplied by 2 to give the molecular formula of H_2O_2.
- While this type of formula fully describes the constituent parts and is used in many calculations, it does not give any idea of the actual geometry or of the arrangement of the atoms in the compound.

STRUCTURAL FORMULA

- **A structural formula shows how atoms are arranged in the molecule and how they are connected with bonds (represented by lines), providing the position of covalent bonds.**
- If two lines are between two atoms, they are sharing four electrons and the connecting bond is called a double bond
- If there are three lines, the bond is a triple bond and they are sharing six electrons.
- A triple bond is the highest order bond between two atoms.
- There are no quadruple bonds, and so on.
- While the structural formula tells us more about the connectivity and orders of bonding within the molecule, it still does not tell us anything about the geometry of the molecule.

BALL-AND-STICK MOLECULAR MODEL

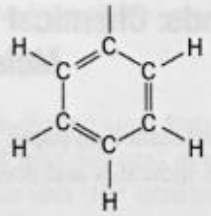
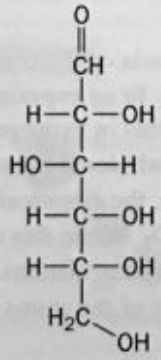
- The ball-and-stick molecular model represents atoms as balls and bonds as sticks.
- This model is a good representation of the connectivity of the atoms in a molecule, and of the three dimensional structure and bond angles.
- At the same time, however, it is much less convenient in many cases, particularly where calculations are being performed.

SPACE-FILLING MOLECULAR MODEL

- The space-filling molecular model represents how the model would look scaled to size with the electron orbitals included from the outside of the molecule. It is a fair approximation to how the molecule would look, should we be able to see something that small.

EXAMPLES

The diagram below shows several compounds with how it would be represented using each of the methods listed above.

Name of Compound	Empirical Formula	Molecular Formula	Structural Formula	Ball-and-Stick Model	Space-Filling Model
Benzene	CH	C_6H_6			
Acetylene	CH	C_2H_2	H—C≡C—H		
Glucose	CH_2O	$C_6H_{12}O_6$			
Ammonia	NH_3	NH_3