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**Dipole Moment**

**Learning Objective**

* Predict which molecules will have low and high dipole moments.

**Key Points**

* + A dipole exists when a molecule has areas of asymmetrical positive and negative charge.
  + A molecule’s polarity (its dipole) can be experimentally determined by measuring the dielectric constant.
  + Molecular geometry is crucial when working with dipoles.

**Terms**

* debyea CGS unit of an electrical dipole moment equivalent to 3.33564 x 10-30 coulomb meter; used for measurements at the molecular scale
* dipoleany molecule or radical that has delocalized positive and negative charges

A dipole exists when there are areas of asymmetrical positive and negative charges in a molecule. Dipole moments increase with ionic bond character and decrease with covalent bond character.

### Dipole Moment

A dipole moment is a quantity that describes two opposite charges separated by a distance.  It is a quantity that we can measure for a molecule in the lab and thereby determine the size of the partial charges on the molecule (if we know the bond length).  By definition the dipole moment, μ, is the product of the magnitude of the separated charge and the distance of the separation:

where qq is the magnitude of the separated charge and rr is the distance between them.

If we were to use SI units, charge would be in Coulombs and distances in meters.  However, the charges were are talking about in molecules are very small (partial electron charges) and the distances are tiny as well (less than 1 nm).  So this would lead to dipoles that are very, very small.  So instead we use another historical unit, the Debye.  1 Debye is approximately 3.33 x 10-30 C\*m.  Molecules typically have dipole moments around 1 D.

If a molecule has a dipole moment, then we call it "polar."  However, how big does the dipole have to be?  Can it be 0.0001 D?  That is ten thousand times less than a molecule with a dipole of 1 D.  There is no strict cutoff.  Nonetheless, molecules with atoms with very small electronegativities differences typically will have bonds that are only very slightly polar.  This will lead to overall dipole moments for the molecule that are very, very small and would be considered non-polar. The most important example of this is hydrocarbons, molecules that contain hydrogen and carbon.  While H and C don't have identical electronegativities, they are very close.  So the C-H bond is very, very weakly polar.  Overall, chemists (and biologists) would consider hydrocarbons to be non-polar (even though technically they might have very tiny dipole moments).

Most important when determining if a molecule has a dipole moment are two factors. One it must have polar covalent bonds. Two, it must have a shape in which all the dipoles don't cancel.  Thus, our great interest in the shapes of different molecules.

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**Bond dipole moment**

The bond dipole moment uses the idea of the electric dipole moment to measure a chemical bond’s polarity within a molecule. This occurs whenever there is a separation of positive and negative charges due to the unequal attraction that the two atoms have for the bonded electrons. The atom with larger electronegativity will have more pull for the bonded electrons than will the atom with smaller electronegativity; the greater the difference in the two electronegativities, the larger the dipole. This is the case with polar compounds like hydrogen fluoride (HF), where the atoms unequally share electron density.

Physical chemist Peter J. W. Debye was the first to extensively study molecular dipoles. Bond dipole moments are commonly measured in debyes, represented by the symbol D.

Molecules with only two atoms contain only one (single or multiple) bond, so the bond dipole moment is the molecular dipole moment. They range in value from 0 to 11 D. At one extreme, a symmetrical molecule such as chlorine, Cl2, has 0 dipole moment. This is the case when both atoms’ electronegativity is the same. At the other extreme, the highly ionic gas phase potassium bromide, KBr, has a dipole moment of 10.5 D.

**Bond Symmetry**

Symmetry is another factor in determining if a molecule has a dipole moment. For example, a molecule of carbon dioxide has two carbon—oxygen bonds that are polar due to the electronegativity difference between the carbon and oxygen atoms. However, the bonds are on exact opposite sides of the central atom, the charges cancel out. As a result, carbon dioxide is a nonpolar molecule.

**The linear structure of carbon dioxide.**The two carbon to oxygen bonds are polar, but they are 180° apart from each other and will cancel.

**Molecular Dipole Moment**

When a molecule consists of more than two atoms, more than one bond is holding the molecule together. To calculate the dipole for the entire molecule, add all the individual dipoles of the individual bonds as their vector. Dipole moment values can be experimentally obtained by measuring the dielectric constant. Some typical gas phase values in debye units include:

* carbon dioxide: 0 (despite having two polar C=O bonds, the two are pointed in geometrically opposite directions, canceling each other out and resulting in a molecule with no net dipole moment)
* carbon monoxide: 0.112 D
* ozone: 0.53 D

phosgene: 1.17 D

* water vapor: 1.85 D
* hydrogen cyanide: 2.98 D
* cyanamide: 4.27 D
* potassium bromide: 10.41 D

KBr has one of the highest dipole moments because of the significant difference in electronegativity between potassium and bromine.