MULTIPOLE FORCES

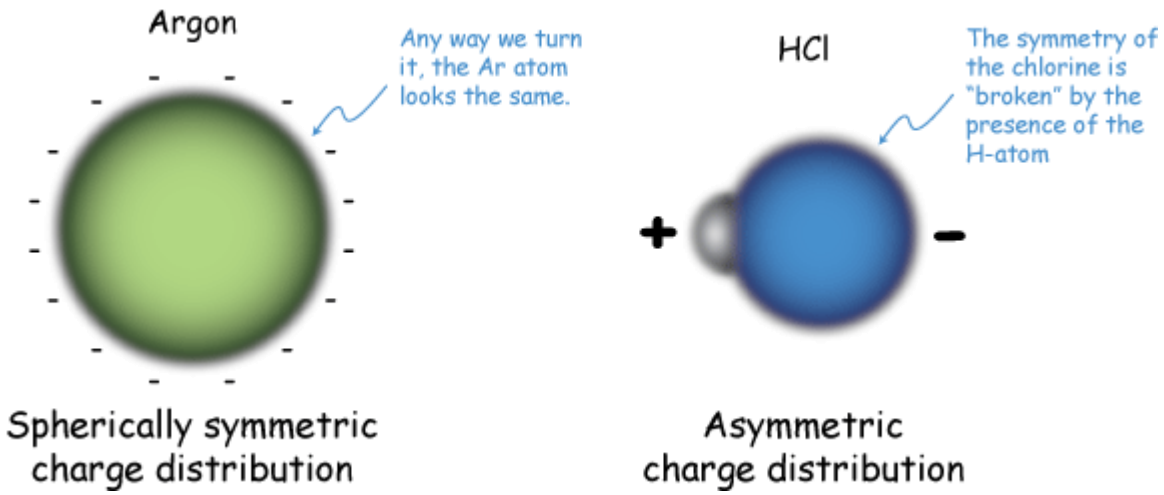
Think for a moment about an atom like an inert gas atom, say Argon (Ar). Although we know that the electrons aren't arranged in a strictly spherical cloud around the nucleus (p-orbitals and all that), because the atom is free to rotate, the distribution of electrons is more-or-less **spherical**.

Because an atom is **spherically symmetric**, we can't identify any one "side" or portion of its electron cloud that is any more or less positive or negative than any other.

Now think of a molecule like hydrogen chloride (HCl). It doesn't have that spherical symmetry. It's a sphere with a "bump".

In fact, because the chlorine atom is quite electronegative, it pulls the single H-atom electron mostly away from the hydrogen, leaving a mostly bare proton. HCl has two different "ends", one clearly more positive than the other.

The H-atom side is more positive than the Cl-atom side. Here's a picture:

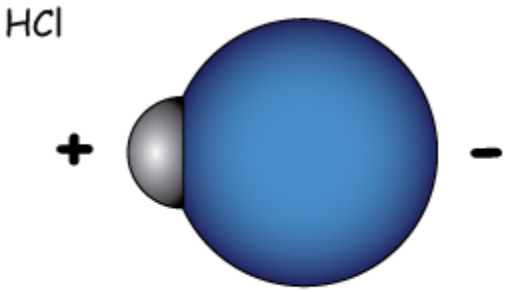


This situation is sometimes described with this language: An atom is **isotropic**. It looks the same viewed from any direction. The HCl molecule is **anisotropic** (*not* isotropic) because as we approach it from different directions, we get a different view. Space is anisotropic. It has no special direction. We only define "up" as north on our globe out of long-standing convention, not because space has an up or down.

Dipoles

You can see how the symmetry of a molecule, or we often say the "breaking" of some underlying symmetry, can lead to an asymmetric distribution of the electrons around it.

This makes one part of the molecule "less negative" (and therefore more positive) than another. A molecule that clearly has two sides or ends, one more negative than the other, is called a **dipole** (two poles, like a battery, + and -), and has interesting properties because of it.



Any molecule with one end more negative than the other is a **dipole**

Non-linear molecules can be dipoles, too. In the top row of the table below are some molecules for which are highly symmetric and are not dipoles.

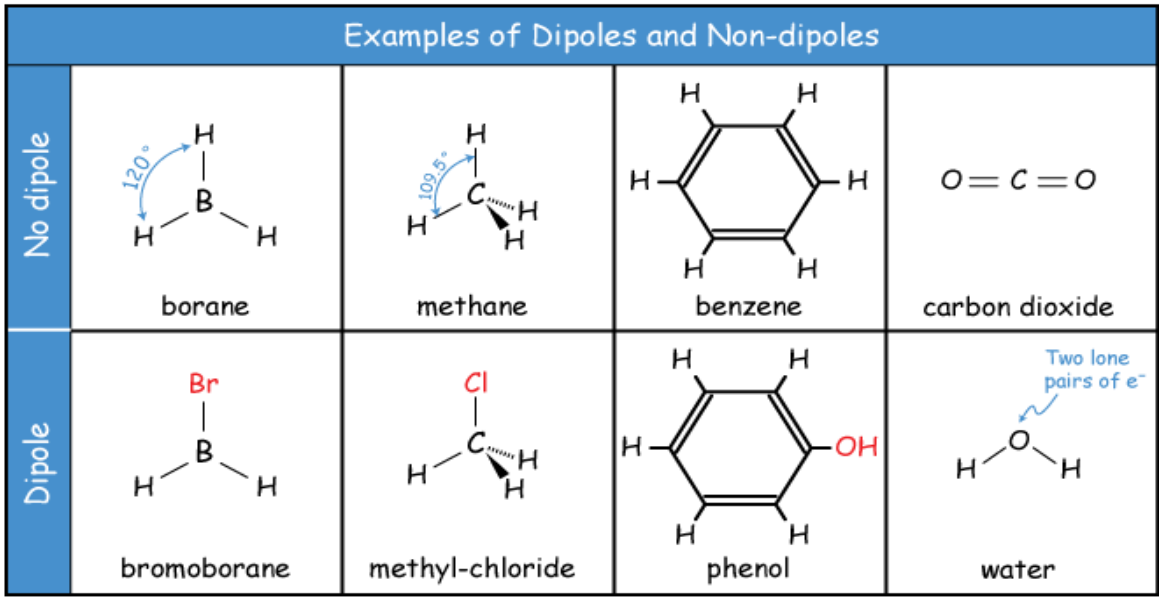
- Borane is a flat (planar) molecule with three equivalent bond angles. It's not possible to find a unique "end". If we substitute a bromine for one of the hydrogens to make bromo borane ($BrBH_2$), we break the symmetry to form a dipole.

- Methane as a 3-D analog of borane. It's tetrahedral structure, with four equivalent bond angles gives it too much symmetry to be a dipole. But if we substitute a chlorine for one of the hydrogens to make methyl chloride, that

symmetry is broken and the Cl end is more negative than the rest of the molecule.

- The benzene molecule (C_6H_6) has six-fold symmetry and is planar. If we put an OH onto one of the carbons, we form polar phenol (C_6H_5OH).
- Finally, carbon dioxide (CO_2) is a linear molecule with identical ends. Water has identical "ends" but it's bent, with lots of negative electron density near the oxygen. Water is actually very polar.

Breaking of the underlying symmetry of a molecule leads to formation of a permanent dipole.



Dipole moments of selected molecules

(D)

Water (H_2O)	1.85 D
Bromine chloride (BrCl)	0.6 D
Hydrogen iodide (HI)	0.44 D
Hydrogen fluoride (HF)	1.82 D
Ammonia (NH_3)	1.42
Chloromethane (CH_3Cl)	1.8 D
Ethanol (C_2H_5OH)	2.69 D
Carbon dioxide (CO_2)	0

Dipole strength: The dipole moment

We need a way to measure the relative **strengths** of dipoles, because a dipole can exert a force on another atom or molecule, and the amount of force exerted will depend on the strength or magnitude of the dipole.

The strength of a dipole depends on how much charge difference exists between one "end" of a molecule and another, and the separation of those ends.

We call the measure of dipole strength the **dipole moment**. In mathematics, a moment is a (vague) measure of shape.

← this table lists the dipole moments of some commonly encountered substances. The unit of measurement of dipole moment is the Debye (D).

How Dipoles Interact

The figures on the right show how two or more dipoles interact when they are close. First, we introduce a shorthand notation, the crossed-arrow symbol; the plus goes on the positive side of the dipole and the arrow on the negative side.

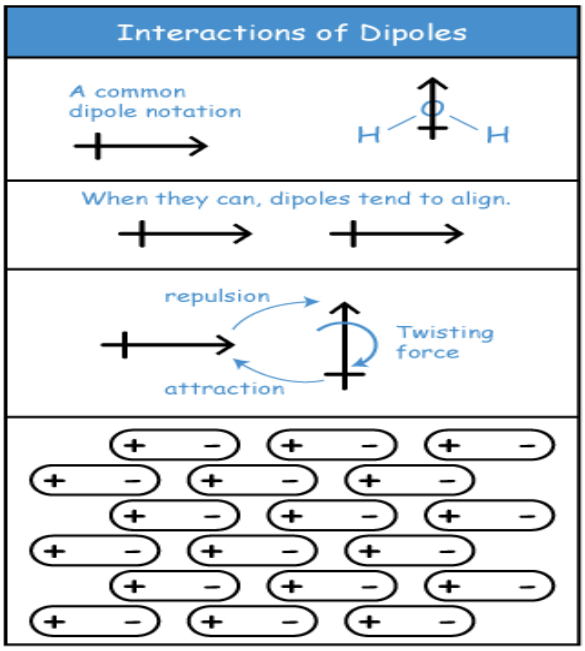
When dipoles are free to rotate, they tend to align, as shown. This happens because of the twisting force shown. That twisting force is simply due to the electrostatic force: A region of high negative charge will repel the more negative end of a dipole and (relatively speaking) attract the more positive end.

When many dipoles collect, e.g. in a solid, they tend to align as shown in the bottom panel. Note the each + and - charge is surrounded by opposite charges.

A note on + and - : δ+ and δ-

When designating the + and - ends of a molecular dipole, we generally use the symbols δ+ and δ- rather than + and -.

We use the Greek letter δ (delta) to indicate that we're not talking about a full positive or negative charge, just a **partial charge**. δ+ means "a little more positive."



In the absence of any other forces, dipoles tend to align, δ+ to δ- .

Higher multipole moments

It turns out that the dipole moment is not the only kind of charge moment a molecule can have. CO_2has no dipole moment, but it does have a **quadrupole moment**. While these higher moments must be considered in some weak interactions, they are of less importance than the dipole.

Source: http://www.drcruzan.com/IntermolecularForces.html