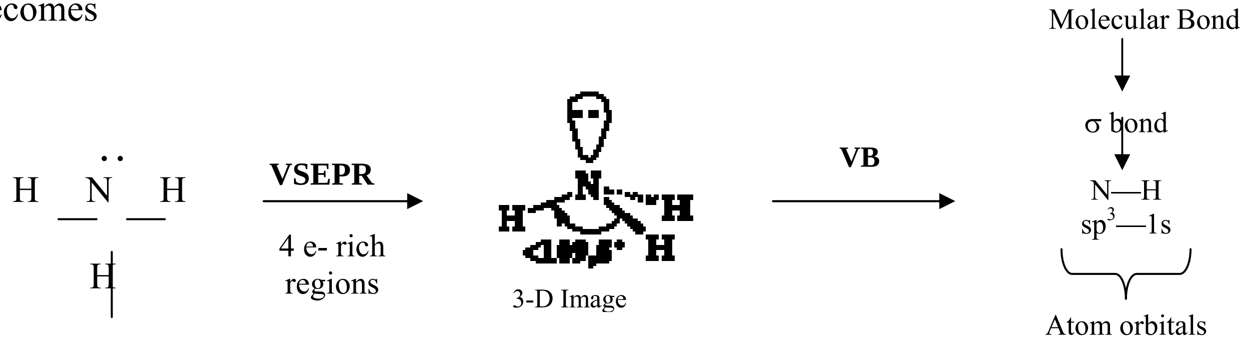
LECTURE 10. TURNING 2D STRUCTURES INTO 3D VSEPR MODELS TO INVESTIGATE POLARITY

The Really Big Picture

In our first lectures on bonding, we dealt in two-dimensions with our chemical structures as well developed ionic and covalent 2D structures based upon simple concepts like ΔEN and the stability of Lewis structures in octet electronic configurations.

Now we become more sophisticated as we develop three-dimensional structures of covalently bonded compounds. We will use electron pair repulsion theory (VSEPR) and devise more satisfactory bonding orbitals based on valence bond (VB) theory. Then we learn about a sophisticated mathematical model for bonding called molecular orbital (MO) theory.

Example 1: NH_3 with an octet rule Lewis structure becomes



In VSEPR theory, the first thing you look for is the number of regions of electron density. Regions of e- density are made by either nonbonding e- pair or bonding e-pair around an atom. Note that NH_3 has four regions, three are bonding and one is nonbonding.

What do the regions of e- density tell you?

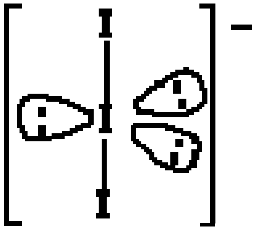
Answer: three important structural features.

- Electronic Geometry—NH_3 with 4 electron rich regions is tetrahedral
- Bond Angle—NH_3 with 4 electron rich regions is 109.5^o
- Hybridization—NH_3 with 4 electron rich regions is sp^3

Two electron rich regions: Example CO_2

O=C=O is linear, 180˚, sp

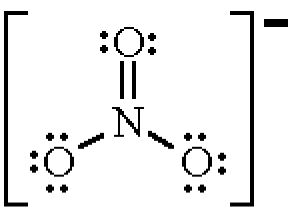
Five electron rich regions: Example I^-_3



90˚
is Trigonal Pyramidal > 120˚ > dsp^3
180˚

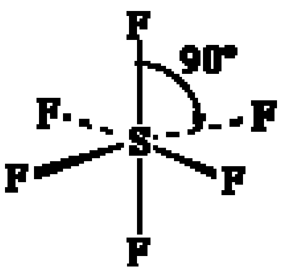
Three electron rich regions Example NO^-_3

Trigonal Planar, 120˚, sp^2



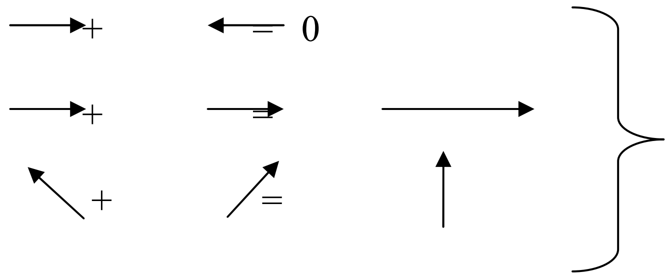
Six electron rich regions: Example SF_6

Octahedral, 90˚, 180˚, sp^3d^2



Identifying polar and non-polar compounds using vector algebra.

And now a time-out for a bit of vector math so we can learn about another layer of chemical information, whether a compound is polar or nonpolar.



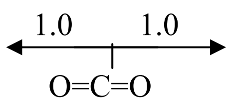
This bit of high school math will be used to add ΔEN vectors together. Why?

So by Definition:

$\Sigma\ \Delta EN = 0$ non-polar molecule

$\Sigma\ \Delta EN \neq 0$ polar molecule

For example: CO_2

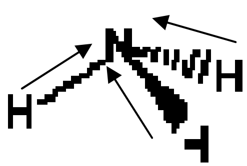


Summing two ΔEN vectors = 3.5-2.5 = 1.0

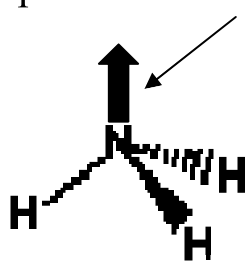
So add together $\Sigma\ \Delta EN = -1.0 + 1.0 = 0$

So CO_2 is non-polar

For example: NH_3



$\Sigma\ \Delta EN \rightarrow$

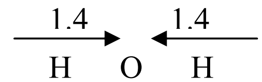


$\Sigma\ \Delta EN \neq 0$ So NH_3 is polar

And now a famous example of why VSEPR explains that H_2O is polar

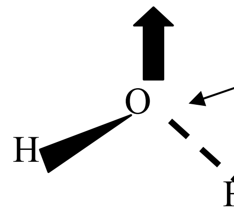
Lewis structure of H_2O in 2 dimensions. H:Ö:H So $\Sigma\Delta EN = 0$ which would suggest that H_2O is non-polar.

Add ΔEN



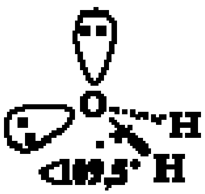
But VSEPR creates an H_2O structure in 3 dimensions

Now ΣΔEN →



$\Sigma\Delta EN \neq 0$

so H_20 is polar



We will see that this result has profound consequences on the chemistry of water solutions.

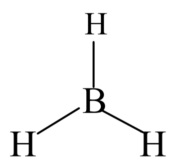
So let's do some more examples using the simple summation of ΔEN vectors.

Polar: $\Sigma\Delta EN = 0$ or not symmetrical Non-polar: $\Sigma\Delta EN \neq 0$ or symmetrical

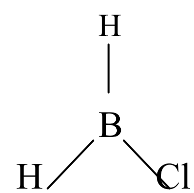
Assign these molecules as polar or non-polar based strictly on symmetry. Answer. They are all symmetrical and therefore nonpolar.

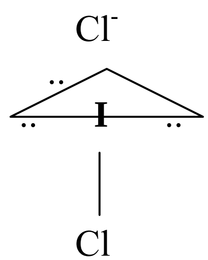
Examples:

N ≡ N



O=C=O





Polar, not symmetrical

BH_2Cl

Non-polar symmetry

N_2, CO_2, BH_3, ICl^-_2