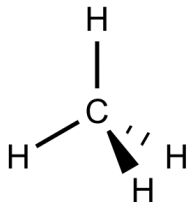
Understand Why Molecules Adopt Their Shapes

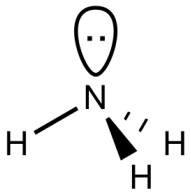
What factors lead to molecular geometry?

- The shapes of molecules depend upon the number of valence pairs that are present in sigma bonds and lone pairs. Shape has nothing to do with pi bonds. Sigma bonds and lone pairs will arrange themselves to be as far apart as possible from each other (since negative electrons repel). This gives **tetrahedral**, **trigonal planar**, and **linear** shapes.
- Starting with Carbon, the molecule methane (C bonded to 4 hydrogens) has only sigma bonds, which repel each other. The **tetrahedral** shape is simply the furthest away these four bond pairs can get from each other. When pi bonds are introduced it is still the single bonds that dictate shape; **trigonal** (3) **planar** for 3 sigma and **linear** for 2.

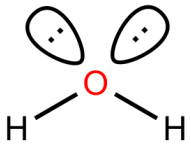
Tetrahedral



109.5°

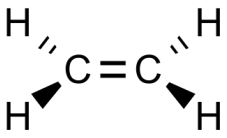


107°

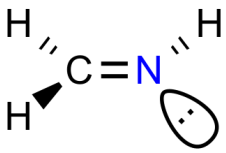


104.5°

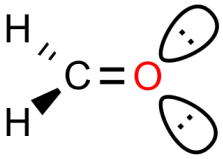
Trigonal Planar



120°



H-N-C 110.5°

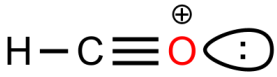


H-C-H 120°

Linear

180°

180°



180°

- Moving to Nitrogen and Oxygen we recognize the introduction of lone pair(s) which are known to take up more volume that bond pairs and so change these shapes slightly. For ammonia (N bonded to 3 hydrogens) and water (O bonded to 2 hydrogens) the **tetrahedral** shape still applies but with slightly different bond angles. Similarly, for N and O in double bonds the shape is roughly **trigonal planar** but the associated lone pairs distort the angles away from 120. The molecules will, however, still be flat overall. For the **linear** molecules the N equivalent (nitriles) has the lone pair opposite to the alkyl group attached with the molecule still being linear overall.