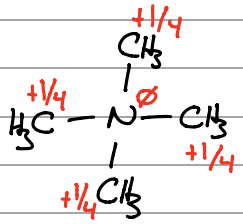
Reality of Formal Charge

Reading:
- MPOC Ch 1
- CS Ch 1

- For an atom with an octet in its neutral state:

1 fewer bond	neutral	1 more bond
(-1)	∅	(+1)

$\oplus N(CH_3)_4$ Calculations Show

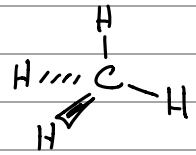


N is more e⁻neg than C so it doesn't want the ⊕ charge

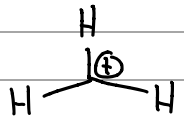
VSEPR

- Groups on an atom will space out as far as possible

Ideal Systems



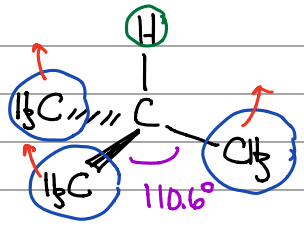
tetrahedral - 109.5°



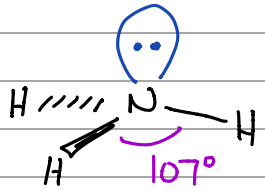
trigonal planar - 120°

linear - 180°

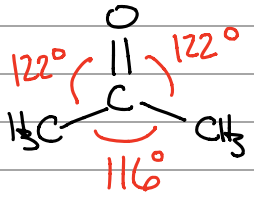
Most molecules deviate from the ideal

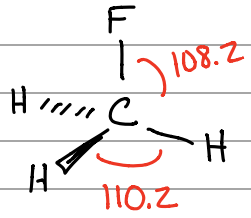


Steric repulsion



lone pair behaves as if it is larger than a bonded e⁻ pair





Explain

Hybridization provides an explanation for deviation from ideal bond angles.

$sp \longrightarrow sp^2 \longrightarrow sp^3 \longrightarrow p$

180° 120° 109.5° 90°

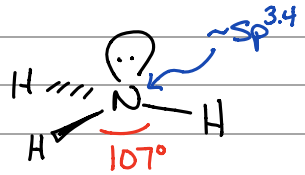
More e⁻neg — less e⁻neg

* As s-character ↓ bond angle ↓

Hybridization Index

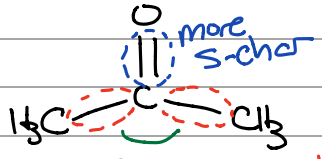
$\boxed{sp^i}$ $1 + i\cos\Theta = 0$

↑ bond angle



N has lost s-character

- N-H bonds have more p-character
- lone pair takes on extra s-character



More p-character

↑ smaller bond angle

* N lone pair is not shared by another atom. The e⁻neg N prefers to put more s-character in it so as to keep the e⁻ to itself. Effect even larger in a more e⁻ neg atom

The C places more p-character in the C-F bond which makes it easier for the F to withdraw e⁻

= larger bond angle

Electronegativity

↗ F lowest energy orbital that can accept e⁻

↓ Atoms get larger + valence orbitals get higher in E

→ Valence orbitals become lower E

H 2.1	F 4.0
C 2.5	Cl 3.0
O 3.5	Br 2.8
	I 2.5

The unequal distribution of electron density in covalent bonds produces a bond dipole.

Explain: H_3C-F H_3C-Br

Both have a molecular dipole of 1.8 D

C-Br bond is longer and $\mu = q \times r$ (q: charge, r: distance)

Explain:

Polarizability is also important.

↳ the ability of an e⁻ cloud to distort in response to an external field. This distortion induces a dipole, adding to the permanent dipole.

Electronegative atoms hold their e⁻ tightly and are not polarizable

As $Nu^{\ominus}$ approaches H_3C-I, changes in the electronic structure develop.

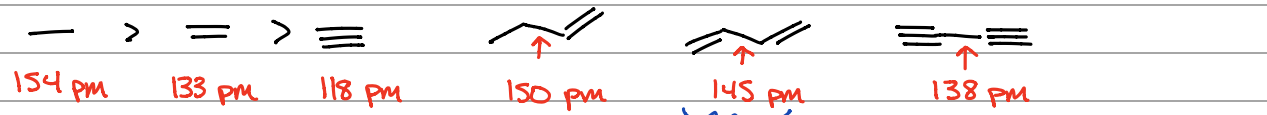
Group Electronegativities

- Can be applied to a functional group
- Can be used in comparison w/ Pauling scale

An Aside: C vs H e⁻neg

More e⁻neg $C_{sp^2} > H \approx C_{sp^3}$ less e⁻neg

Bond Length



a hybridization (not resonance) effect