12/3/2018

Molecular polarity

$\sum$ bond dipoles = molecular/overall dipole

$= 0$ → Non-polar

$\neq 0$ → Polar

CO_2

- non-polar

VSEPR: $O=C=O$

linear, 180°

overall dipole = 0

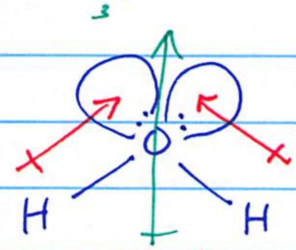
non-polar

H_2O

- polar

Lewis: $H - \ddot{O} - H$

VSEPR:



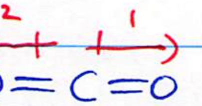
mol. geom = bent

overall dipole $\neq 0$ ⇒ Polar

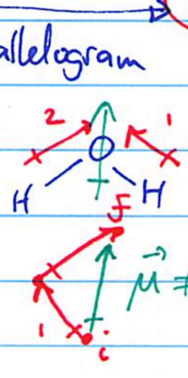
we can add these dipole moment vectors

- intuitively
- vectors addition → add component / head-to-tail / parallelogram

CO_2: $O=C=O$

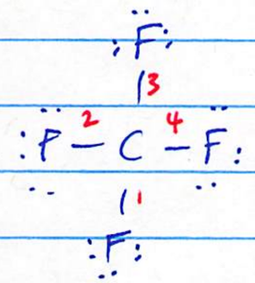


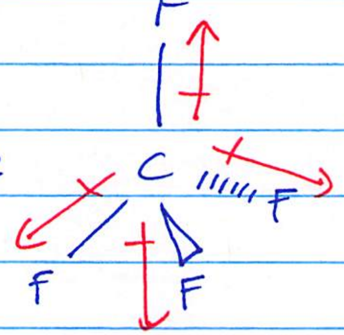
$\vec{\mu} = 0$



$\vec{\mu} \neq 0$ ⇒ Polar.

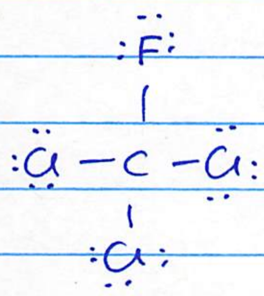
ex: CF_4

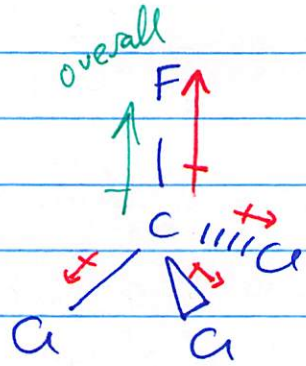
Lewis 

VSEPR: 

$\vec{\mu}_{molecule} = \emptyset$ Non-polar

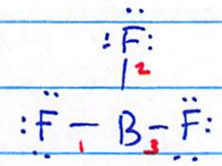
ex: $CFCl_3$

Lewis: 

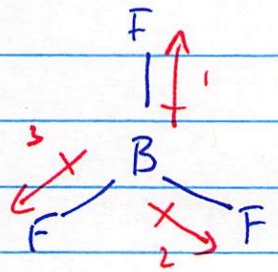
VSEPR: 

polar.

BF_3

Lewis 

polar/non-polar ?

VSEPR 

$\vec{\mu}_{overall} = \emptyset$ ⇒ Non-polar!

trigonal-planar
120°

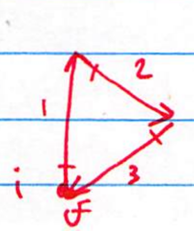


TABLE 10.2 Common Cases of Adding Dipole Moments to Determine Whether a Molecule Is Polar

Linear

Nonpolar

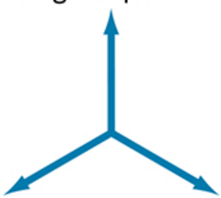
The dipole moments of two identical polar bonds pointing in opposite directions cancel. The molecule is nonpolar.

Bent

Polar

The dipole moments of two polar bonds with an angle of less than 180° between them do not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.

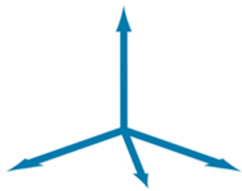
Trigonal planar



Nonpolar

The dipole moments of three identical polar bonds at 120° from each other cancel. The molecule is nonpolar.

Tetrahedral



Nonpolar

The dipole moments of four identical polar bonds in a tetrahedral arrangement (109.5° from each other) cancel. The molecule is nonpolar.

Trigonal pyramidal

Polar

The dipole moments of three polar bonds in a trigonal pyramidal arrangement do not cancel. The resultant dipole moment vector is shown in red. The molecule is polar.

Note: In all cases in which the dipoles of two or more polar bonds cancel, the bonds are assumed to be identical. If one or more of the bonds are different from the other(s), the dipoles will not cancel and the molecule will be polar.

<u>Valence-bond theory (VB)</u>

QM model of bonding.

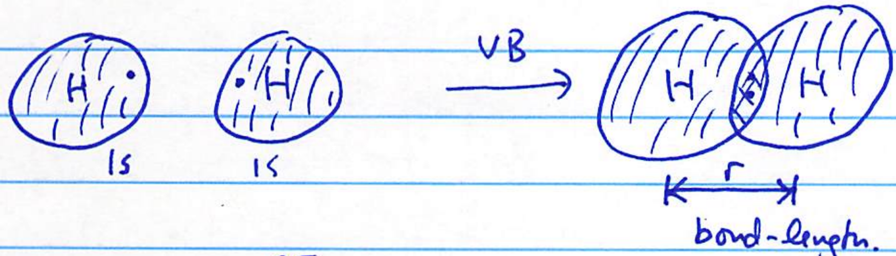
Bond = overlap a pair of orbitals (1 from each atom)
w/ $2e^-$ max (typically 1 from each atom)

ex: H_2

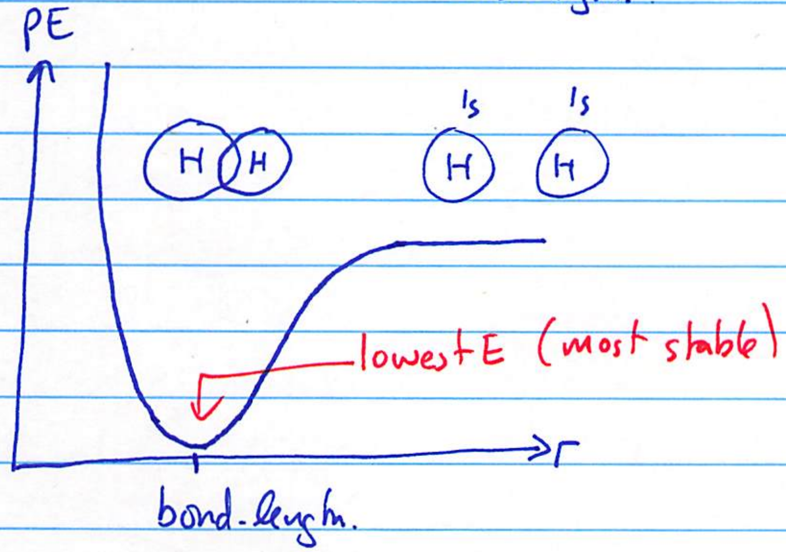
covalent bond

H• •H $\xrightarrow{\text{Lewis}}$ H:H H—H

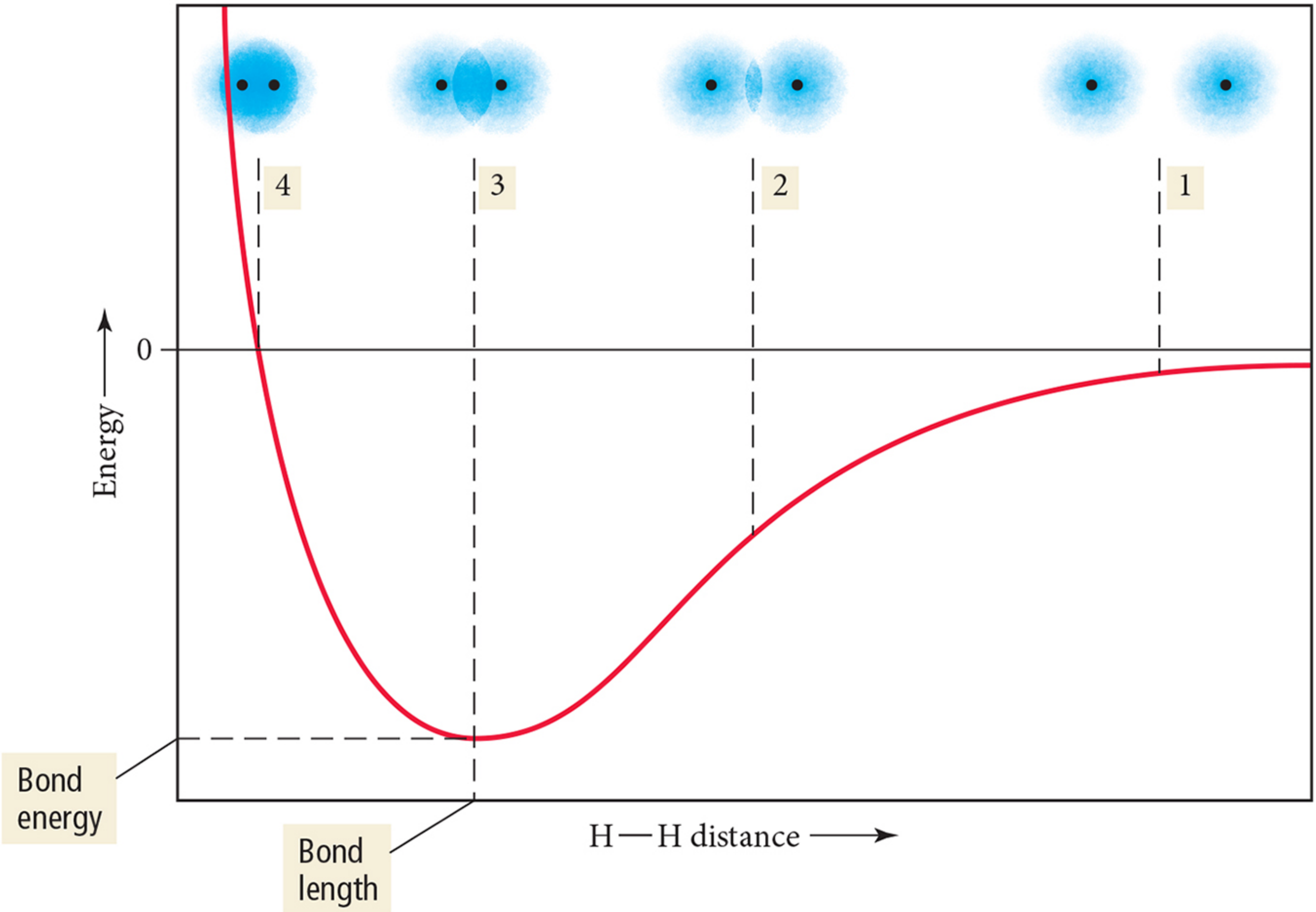
1s' 1s'



QM
- calculate E
from overlap:



Interaction Energy of Two Hydrogen Atoms

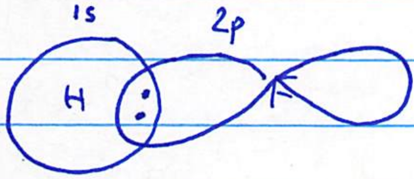


HF

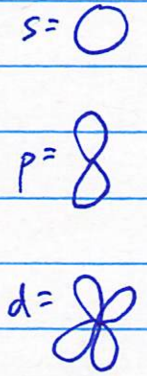
Lewis $H:\ddot{\underset{..}{F}}:$ or $H-\ddot{\underset{..}{F}}:$

VB: $H\cdot$ $\boxed{\uparrow}$ $\qquad \cdot\ddot{\underset{..}{F}}:$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow|\uparrow\downarrow|\uparrow}$

$1s^1$ 1s $\qquad 1s^2 2s^2 2p^5$ 1s 2s 2p



- head-on bonding



What about CH_4?

Problem: Lewis

$$\begin{array}{ccc} & H & \\ H & :\ddot{\underset{..}{C}}: & H \\ & H & \end{array} \quad \text{or} \quad \begin{array}{ccc} & H & \\ & | & \\ H- & C & -H \\ & | & \\ & H & \end{array}$$

according to VSEPR bond ∠'s are 109.5° (tetrahedral)

H $\boxed{\uparrow}$

$1s^1$ 1s

C $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow|\uparrow|\ }$

$1s^2 2s^2 2p^2$ 1s 2s 2p

Linus Pauling ... here's how we do it!

Step 1: Promotion

problem: @90°

$\boxed{\uparrow\downarrow}$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow|\uparrow|\ }$ $\xrightarrow{\text{promote}}$ $\boxed{\uparrow\downarrow}$ $\boxed{\uparrow}$ $\underbrace{\boxed{\uparrow|\uparrow|\uparrow}}$

C 1s 2s 2p $\qquad$ 1s 2s 2p

(2) Hybridize the 1x 2s and the 3x 2p $\}$ → 4x sp^3 hybrid orbitals

@ 109.5°

$\boxed{\uparrow\downarrow}$ 1s $\quad$ $\boxed{\uparrow}$ 2s $\quad$ $\boxed{\uparrow|\uparrow|\uparrow}$ 2p → $\boxed{\uparrow\downarrow}$ $\quad$ $\boxed{\uparrow|\uparrow|\uparrow|\uparrow}$ sp^3

hybridize

1s : 3p

Formation of sp^3 Hybrid Orbitals