12/4/2019

Bonding theory (QM)

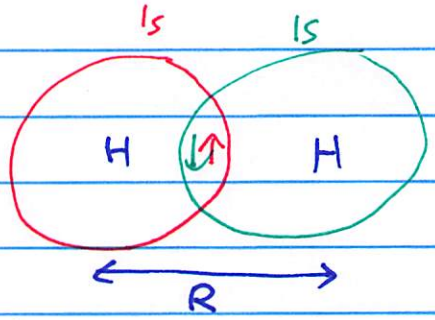
Valence-bond theory:

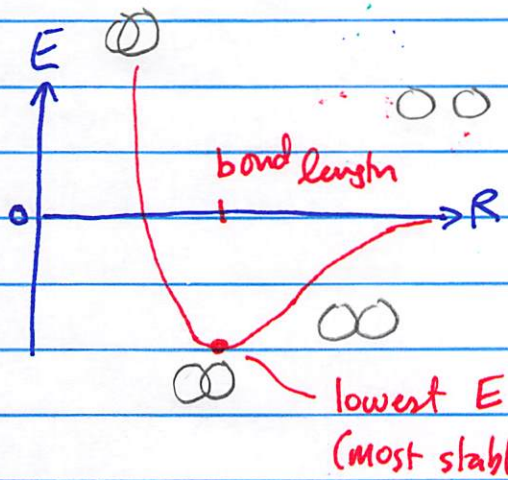
bond = overlap of 2 orbitals w/ 2 e^- (max)

ex: H_2

H: $1s^1$ — e^- config

orb. diag



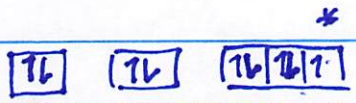


If we look @ overlapping orbitals side-on.

F_2

Lewis: :F–F:

$_9F$: $1s^2 2s^2 2p^5$

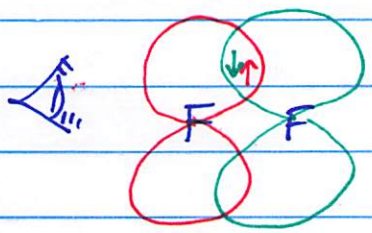


side-on view

2 possible overlaps:

sigma, σ

OR



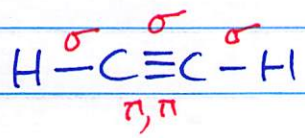
pi, π

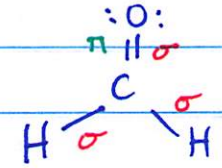
Strongest bond / Lowest E: σ-bond

- In general, the first bond we form is always σ!

- The 2nd, 3rd bonds are always π.

or: acetylene

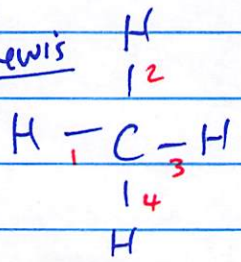




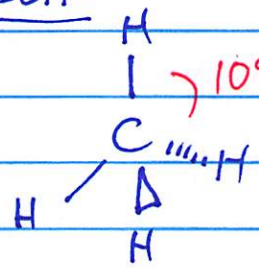
Problem

CH_4

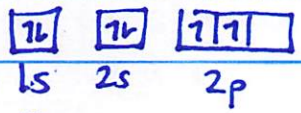
Lewis



VSEPR



C: $1s^2 2s^2 2p^2$



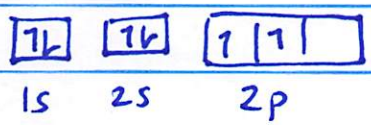
→ 2 bonds???

H: $1s^1$

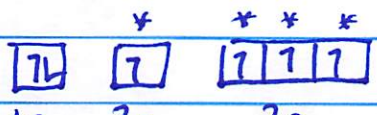
Soln:

only 2 bonds? need 4!

C:



① promote e^- from $2s \rightarrow 2p$

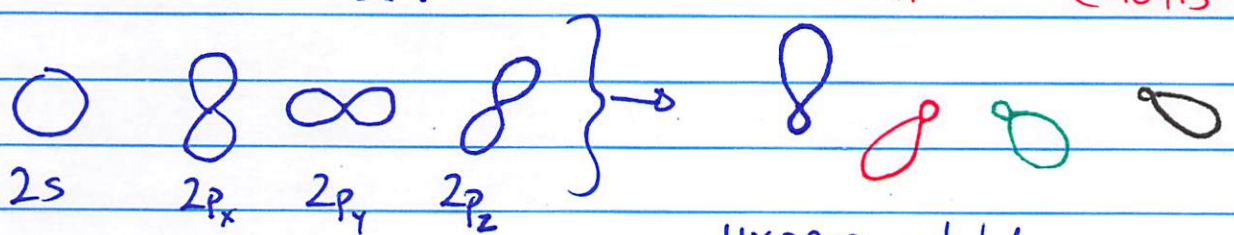


$2p_x, 2p_y, 2p_z$ @90°

problem: bonds are supposed to be @109.5°

② Hybridize our orbitals

...

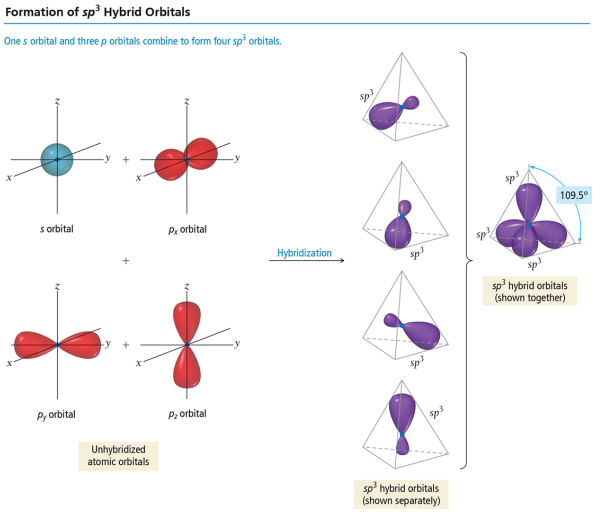


HYBRID orbitals

1 part s : 3 parts p

4 × sp^3 @109.5°

Formation of sp^3 Hybrid Orbitals



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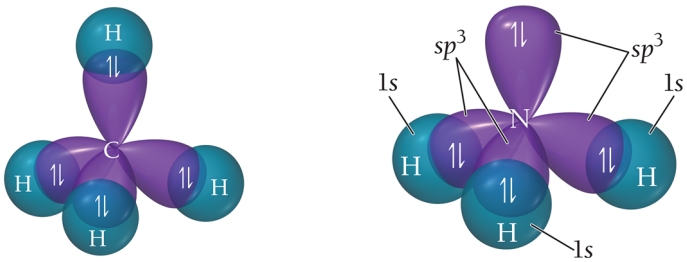
sp^3 Hybridization

- Atom with four electron groups around it
  - Tetrahedral geometry
  - 109.5° angles between hybrid orbitals
- Atom uses hybrid orbitals for all bonds and lone pairs.



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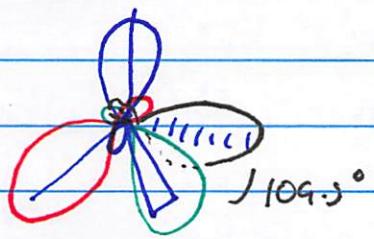
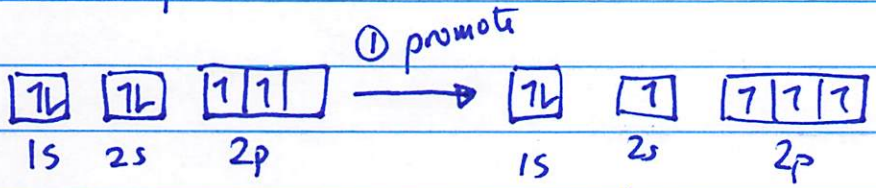
$4 \times sp^3$ 109.5°



CH_4:

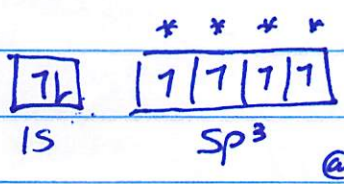
H: $1s^1$ 

C: $1s^2 2s^2 2p^2$

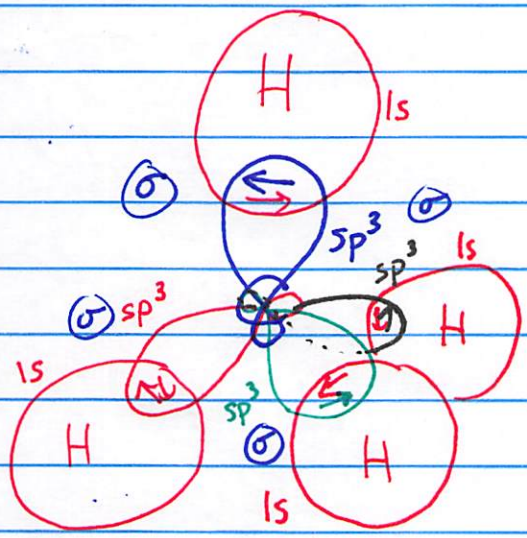


② Hybridize

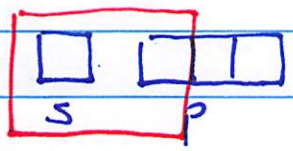
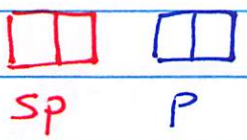
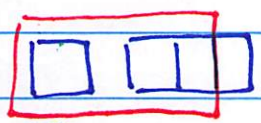
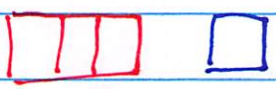
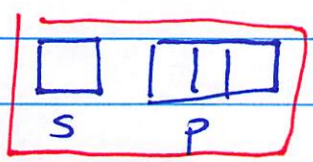
s : p : p : p → sp^3



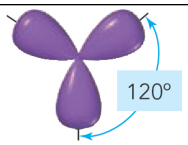
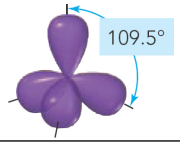
@ 109.5°


H
1s
σ
σ
sp3
sp3
1s
σ
sp3
H
1s
sp3
H
σ
H
1s

Other hybridizations

# rep (VSEPR)	geom (VSEPR)	Atomic orbitals	Hybridize
2	linear 180°		 ↖ unhybridized orbitals
3	trigonal planar 120°		 ↙
4	tetrahedral 109.5°		

Hybridization Scheme for Electron Geometry (1 of 2)

Number of Electron Groups	Electron Geometry (from VSEPR Theory)		Hybridization Scheme
2	Linear	*sp*	
3	Trigonal planar	sp^2	
4	Tetrahedral	sp^3	

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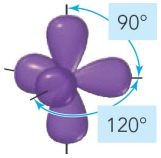
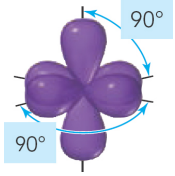
Hybridization Scheme for Electron Geometry (2 of 2)

Number of Electron Groups	Electron Geometry (from VSEPR Theory)		Hybridization Scheme
5	Trigonal bipyramidal	sp^3d	
6	Octahedral	sp^3d^2	

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