Announcements – 11/15/00

- **Exam #3**: tonight at 7:00 pm
- No quiz Friday!

Questions?

- How can we relate this *molecular orbital* model to the bonding and molecular geometries of some real molecules?

Example: **CH_4**

-tetrahedral structure (109.5° bond angles)

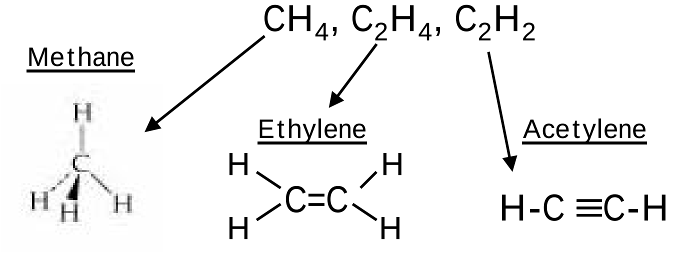
-all four C-H bonds identical

-all nicely predicted using VSEPR model

***BUT:** how do we combine the 2p orbitals of Carbon with the 1s orbitals of Hydrogen to obtain this structure?

More Questions!

- Look at the structures of some simple hydrocarbons:



tetrahedral

trigonal planar

linear

How can this be done with carbon's $2s^2 2p^2$ config?

Hybrid Orbitals

- We can combine *atomic orbital wavefunctions* to make a **new** set of ***hybrid orbitals*** that better represent the bonding properties observed
- For carbon, in CH_4, we need ***four equivalent orbitals*** which are oriented towards the corners of a tetrahedron:

$$\psi_{hybrid} = C_s \psi_{2s} + C_p \psi_{2p}$$

NOTE: it's really more complicated than this (as we are combining FOUR orbitals: 2s plus the three 2p orbitals of carbon).

Example

- Let's look first at a simpler example: **BeF_2**

Be: $1s^2 2s^2$ ← filled orbitals, ***no e^- to share***

F: $1s^2 2s^2 2p^5$ ← has e^- in a 2p orbital to share

Solution: put the 2 Be valence e^- in *new* orbitals (unpaired)

How? First, promote 1 e^- to a 2p orbital:

$$2s^2 \rightarrow 2s^1 2p^1$$

Then, *mix and combine* the 2s and 2p orbitals, to make ***two NEW equivalent orbitals:***

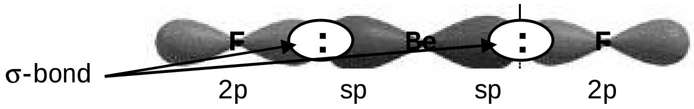
$$2s^1 2p^1 \rightarrow \underline{\uparrow}\ \underline{\uparrow}$$

sp *hybrid* orbitals

sp Hybrid Orbitals

- This is what they look like:

Now, Be has unpaired electrons to share with F:



sp^2 Hybrid Orbitals

- If we need *three* equivalent orbitals, we can mix the s-orbital with *two* p-orbitals:

Example:

BF_3

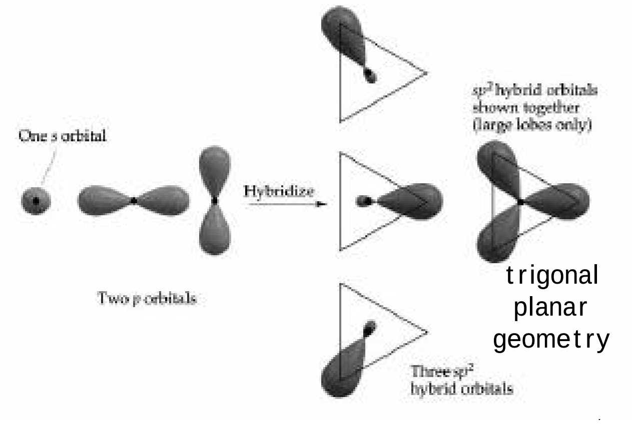
B: $1s^2 2s^2 2p^1$

promote ↓

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

hybridize ↓

$1s^2 (sp^2)^3$



trigonal planar geometry

sp^3 Hybrid Orbitals

- If we need *four* equivalent orbitals, we can mix the s-orbital with *all three* p-orbitals:

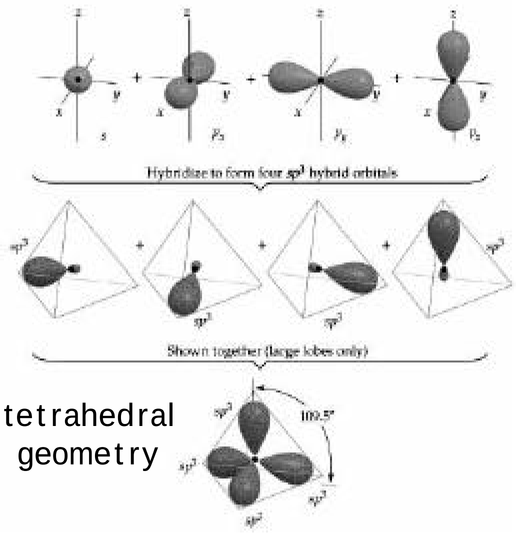
Example:

CH_4

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

↓ *hybridize*

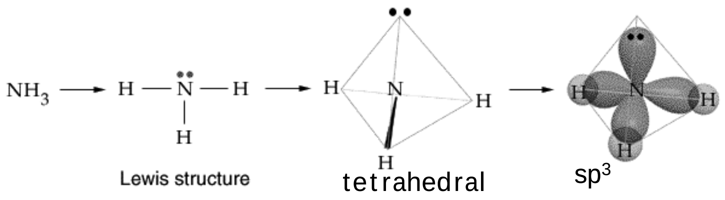
$1s^2 (sp^3)^4$



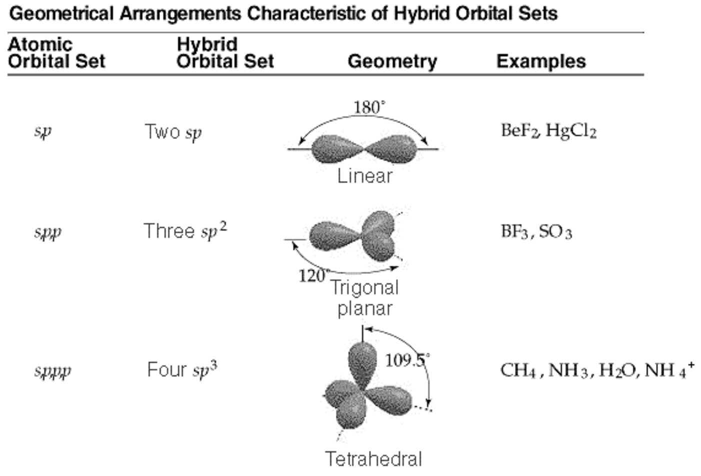
tetrahedral geometry

How do we know which hybrid orbitals to use?

- **Three step process:**
  1. Draw the *Lewis structure*
  2. Determine the *electron-domain geometry* (VSEPR)
  3. Select the *hybrid orbitals* needed to obtain the determined geometry



Hybrid Orbitals and Electron-Domain Geometry



Geometrical Arrangements Characteristic of Hybrid Orbital Sets

Atomic Orbital Set	Hybrid Orbital Set	Geometry	Examples
s,p	Two *sp*	180° Linear	BeF_2, $HgCl_2$
s,p,p	Three sp^2	120° Trigonal planar	BF_3, SO_3
s,p,p,p	Four sp^3	109.5° Tetrahedral	CH_4, NH_3, H_2O, NH_4^+

What about “Expanded Octets”?

- Need to include some of the *d-orbitals* in our hybridization scheme:

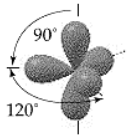
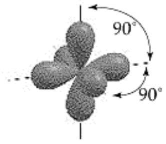
s + ppp + d = *FIVE* **sp³d** hybrid orbitals
in a **trigonal bipyramidal**
orientation

s + ppp + dd = *SIX* **sp³d²** hybrid orbitals
in an **octahedral** orientation

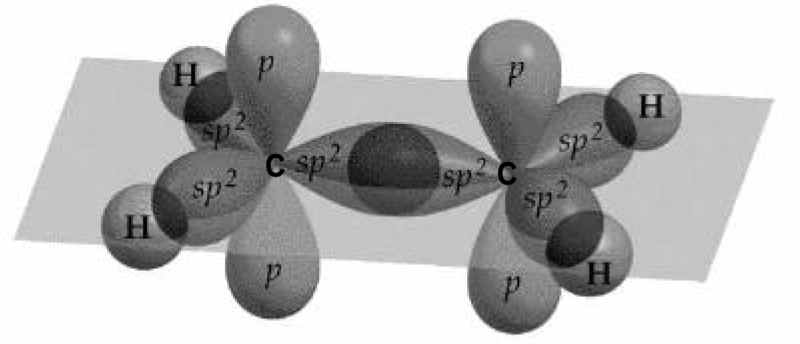
So *that's* why P and S can accommodate “expanded octets” but N and O cannot . . . there are no “2d” orbitals!

More Hybrid Orbitals and Electron-Domain Geometry

Geometrical Arrangements Characteristic of Hybrid Orbital Sets

Atomic Orbital Set	Hybrid Orbital Set	Geometry	Examples
spppd	Five sp^3d	 Trigonal bipyramidal	PF_5, SF_4, BrF_3, $SbCl_5^{2-}$
spppd , d	Six sp^3d^2		SF_6, ClF_5, XeF_4, PF_6^-

Ethylene (C_2H_4) Orbitals



Carbon: sp^2 hybridized (trigonal planar)