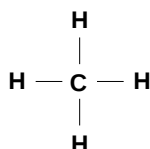


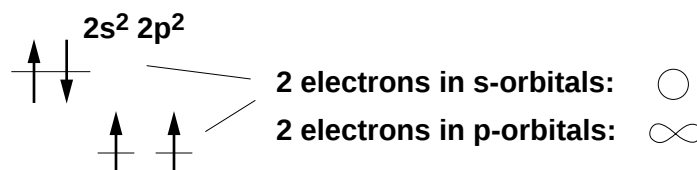
Hybridization

- Okay, you know the atomic picture of electronic structure around the nucleus (spdf, etc.), and you know how to draw Lewis diagrams that represent covalent bonds between atoms in the molecules. Now, the problem with these two pictures is that they contradict one another, and this is where orbital hybridization comes in.
- For example look at methane CH₄:

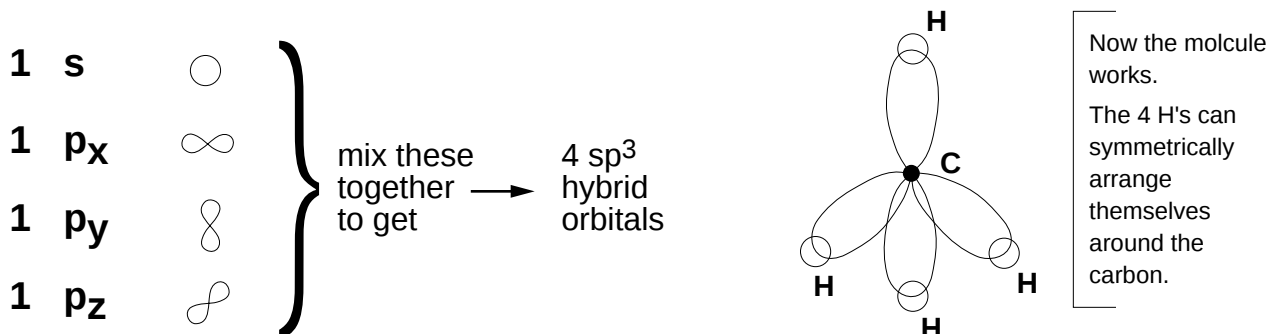
We know the Lewis picture



We know about atomic carbons valence shell



- So the quandary is how do you get four symmetric covalent bonds from these s and p atomic orbitals.
- What you do is mix them all up in a soup and come out with four symmetric molecular orbitals.

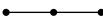
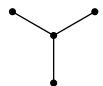
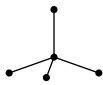
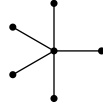
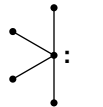
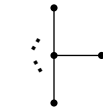
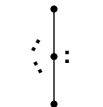
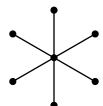
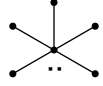
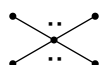


- For any bonded atom, the # of hybrid orbitals = the # of σ bonds + the # of nonbonding pairs
- The # of hybrid orbitals = # of molecular orbitals you combine to form them.

# of hybrid orbitals required	Atomic orbital soup	Hybrid name	Base geometry that results
2	s+p	sp	linear
3	s+p+p	sp ²	trigonal planar
4	s+p+p+p	sp ³	tetrahedral
5	s+p+p+p+d	sp ³ d	trigonal bipyramidal
6	s+p+p+p+d+d	sp ³ d ²	octahedral

Hybrid vs. atomic orbitals in bonding

- Bonds formed by hybrid orbitals are always internuclear sigma (σ) bonds.**
- Pi (π) bonds (which are not on the path between nuclei) are formed by the overlap of atomic p-orbitals.**

Hybridization	# of σ Bonds	# of Non-Bonding Pairs	Molecular Shape	Bond Angles	Example
sp	2	0	 Linear	180°	BeH ₂ , CO ₂
sp ²	3	0	 Trigonal planar	120°	SO ₃ , BF ₃
sp ²	2	1	 Angular	<120°	SO ₂ , O ₃
sp ³	4	0	 Tetrahedral	109.5°	CH ₄ , CF ₄ , SO ₄ ²⁻
sp ³	3	1	 Trigonal pyramidal	<109.5°	NH ₃ , PF ₃ , AsCl ₃
sp ³	2	2	 Angular	<109.5°	H ₂ O, H ₂ S, SF ₂
sp ³ d	5	0	 Trigonal bipyramidal	120°, 90°	PF ₅ , PCl ₅ , AsF ₅
sp ³ d	4	1	 Sawhorse (irregular tetrahedron)	<120°, <90°	SF ₄
sp ³ d	3	2	 T-shaped	<90°	ClF ₃
sp ³ d	2	3	 Linear	180°	XeF ₂ , I ₃ ⁻ , IF ₂
sp ³ d ²	6	0	 Octahedron	90°	SF ₆ , PF ₆ ⁻ , SiF ₆ ²⁻
sp ³ d ²	5	1	 Square pyramidal	<90°	IF ₅ , BrF ₅
sp ³ d ²	4	2	 Square planar	90°	XeF ₄ , IF ₄ ⁻

Student Packet: 2.3: Molecular Structure: AssessMe questions

- 1) Which molecule has a triangular bipyramid geometry?
- A) PF_5 B) H_2O C) SF_6 D) ClF_3 E) I'm clueless
- 2) The approximate OSO angle in the SO_2 molecule is:
- A) 90° B) 109° C) 120° D) 180° E) I'm clueless
- 3) Which geometries are possible for compounds whose central atoms are sp^3 hybridized?
- A) Trigonal planar or bent.
B) Tetrahedral, bent, or trigonal pyramidal.
C) Square planar, tetrahedral, or trigonal planar.
D) Trigonal bipyramidal or seesaw.
E) I'm clueless
- 4) The geometries of the molecules BF_3 and NF_3 are trigonal planar and trigonal pyramidal respectively. Which statement best accounts for the difference?
- A) N is more electronegative than B.
B) BF_3 is ionic, while NF_3 is covalent.
C) B utilizes sp hybridization, while N does not.
D) N has a non-bonding pair of valence electrons, while B does not.
E) I'm clueless
- 5) Which molecule exhibits sp^3d^2 hybridization?
- A) SO_2 B) SF_6 C) CH_4 D) PCl_5 E) I'm clueless
- 6) In which of the following molecules or ions would the hybridization be sp^3d ?
- A) CoCl_6^{3-} B) PCl_5 C) PCl_6^- D) CO_2 E) I'm clueless

Student Packet: 2.3: Molecular Structure: ShowMe questions

- 1) What is the molecular geometry of CCl_4 ?

- 2) What is the molecular geometry of OF_2 ?

- 3) Describe XeF_6 according to valence bond theory. Assume the molecular geometry is the same as given by the VESPR model.

- 4) What is the geometry for SnCl_5^- ?

Student Packet: 2.3: Molecular Structure: TestMe questions

- 1) What is the molecular geometry of PH_3 ?
- tetrahedral
 - trigonal pyramidal
 - trigonal planar
 - trigonal bipyramidal
 - None of the above
- 2) Which of the following molecules has the bent or angular shape?
- I. ClO_2^- ; II. H_2O ; III. CO_2 ; IV. SO_2
- I, II, III
 - II, III
 - I, II, III, IV
 - I, II, IV
 - III, IV
- 3) The hybrid orbitals around the sulfur in SF_6 can be described as sp^3d^2 . Which geometry matches this?
- tetrahedral
 - square pyramidal
 - octahedral
 - T-shaped
 - trigonal bipyramidal
- 4) What are the bond angles in CH_4 ?
- 180
 - 90
 - 109.5
 - 120
 - 50
- 5) CaCl_2 is known to be linear. Which diagram of hybrid orbitals accounts for its bonding?
- | | | |
|---|-------|-------|
| A) $[\text{Ar}] \underline{\neq \emptyset} \underline{\neq \emptyset}$ | _____ | _____ |
| 4 sp | 4p | |
| B) $[\text{Ar}] \underline{\neq \emptyset} \underline{\neq \emptyset}$ | _____ | _____ |
| 5 sp | 5p | |
| C) $[\text{Ar}] \underline{\neq \emptyset} \underline{\neq \emptyset} \underline{\neq \emptyset}$ | _____ | _____ |
| 4 sp | 4p | |
| D) $[\text{Ar}] \underline{\neq \emptyset} \underline{\neq \emptyset} \underline{\neq \emptyset}$ | _____ | _____ |
| 5 sp^2 | 5p | |
| E) None of the above | | |