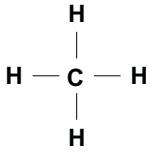
Molecules: Valence Bond Theory: Student Review Notes

Orbital Hybridization

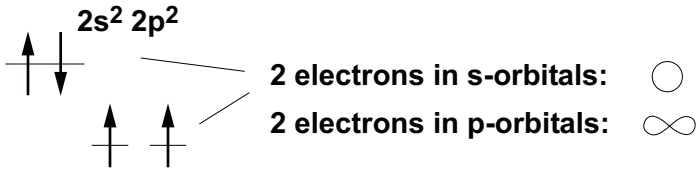
Okay, you know the atomic picture of electronic structure around the nucleus (spdf, etc.), and you know how to draw Lewis diagrams that represent covalent bonds between atoms in the molecules. You can also get basic geometries from VSEPR. Now, the problem is that atomic orbitals and VSEPR contradict one another, and this is where orbital hybridization comes in.

For example look at methane CH_4

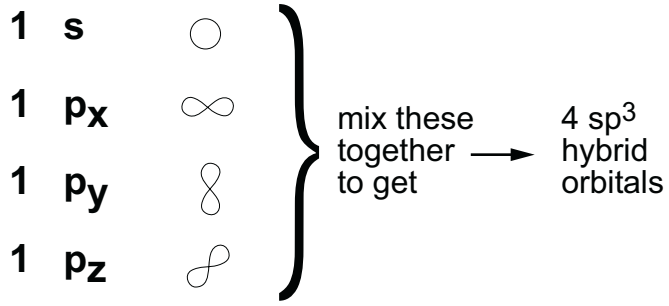
We know the Lewis picture

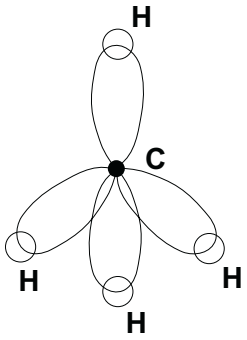


We know about atomic carbon's valence shell



So the quandary is how do you get four symmetric covalent bonds from these s and p atomic orbitals. VB Theory says to mix together the atomic orbitals and come out with four symmetric molecular orbitals.





Now the molecule works.

The 4 H's can symmetrically arrange themselves around the carbon.

For any bonded atom, the No. of hybrid orbitals = the # of σ bonds + the # of nonbonding pairs
The No. of hybrid orbitals = No. of molecular orbitals you combine to form them.

No. 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^3d	trigonal bipyramidal
6	s+p+p+p+d+d	sp^3d^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.

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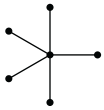
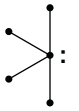
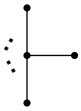
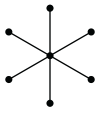
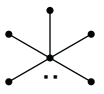
Hybdridization	# of σ Bonds	# of Non-Bonding Pairs	Molecular Shape		Bond Angles	Example
sp	2	0		Linear	180°	BeH_2, CO_2
sp^2	3	0		Trigonal planar	120°	SO_3, BF_3
sp^2	2	1		Angular	<120°	SO_2, O_3
sp^3	4	0		Tetrahedral	109.5°	CH_4, CF_4, SO_4^{2-}
sp^3	3	1		Trigonal pyramidal	<109.5°	NH_3, PF_3, $AsCl_3$
sp^3	2	2		Angular	<109.5°H	H_2O, H_2S, SF_2
sp^3d	5	0		Trigonal bipyramidal	120°, 90°	PF_5, PCl_5, AsF_5
sp^3d	4	1		Seesaw (irregular tetrahedron)	<120°, <90°	SF_4
sp^3d	3	2		T-shaped	<90°	ClF_3
sp^3d	2	3		Linear	180°	XeF_2, I_3^-, IF_2
sp^3d^2	6	0		Octahedron	90°	SF_6, PF_6^-, SiF_6^{2-}
sp^3d^2	5	1		Square pyramidal	<90°	IF_5, BrF_5
sp^3d^2	4	2		Square planar	90°	XeF_4, IF_4^-