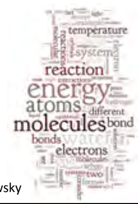
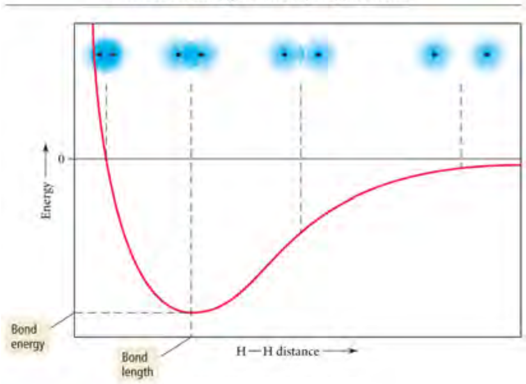
Covalent Bonding



Chemistry, Life, the Universe & Everything – Cooper & Klymkowsky

Interaction Energy of Two Hydrogen Atoms



Covalent Bonds

- Valence electrons of one atom attracted to nucleus of other atom
- Electrons are located between nuclei
- Nuclei attract both electrons in the bond

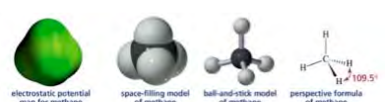
Bonding in carbon compounds

- Carbon forms four bonds!
- It forms bonds to C, H, O, N, S, P, and lots of others
- The properties of compounds are emergent (not just the sum of the elements involved)

Bonding in carbon compounds

- Why are the four bonds usually arranged so that they point towards the corners of a tetrahedron? (what other arrangements are possible)
- If bond formation is stabilizing, why doesn't carbon form six bonds, since it has six electrons?
- Why doesn't helium bond with carbon?
- What would be the consequences if carbon bonds with other atoms were very weak?
- What would be the consequences if carbon bonds with other atoms were very strong?

Representing Structures



All these structures show different information about CH_4 methane

Make a model of CH_4

- Draw a picture of it – try to include all the aspects of the model –**show its 3D structure**, and bond angles. Compare your picture with others around you – do they look the same?

Make a model of C_2H_6

- Draw a picture of it – try to include all the aspects of the model –**show its 3D structure**, and bond angles. Compare your picture with others around you – do they look the same? Are they easily recognizable as the same thing?

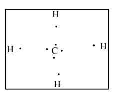
What if you wanted to draw a "quick" picture of the structure. What would that look like? (draw it)

Drawing Lewis Structures (intuitively)

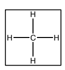
(this works for most compounds using H or second row elements)

- Things you need to know:
  - How many valence electrons each atom has
    - H = 1, B = 3, C = 4, N = 5, O = 6, F = 7.
  - How many bonds the atom **normally** forms (the valence)
    - H = 1, B = 3, C = 4, N = 3, O = 2, F = 1. (note that the # bonds + # valence electrons usually = 8)

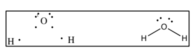
Write out the atoms in the order you think they are connected eg CH4



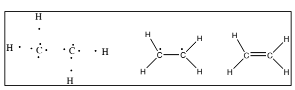
Attach the atoms using 2 electrons for each bond



Leftover electrons are lone pairs



Not enough electrons? Form Mulitiple bonds!



Drawing Lewis Structures (rules)- these will work for anything – but its hard to see how the bonds form

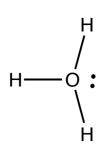
1. Calculate total valence electrons for + ions remove electrons, and – ions add electrons
2. Write the skeleton structure (this is the hard part – it takes practice, the way the structure is written may give you a clue
3. Use 2 electrons for each bond.
4. Make sure each atom (except H) has 8 electrons by adding lone pairs
5. If there are not enough electrons form multiple bonds.

In practice

- Use one method to draw structures
- Use the other method to check whether structures are "correct"
- If the number of bonds and electrons is not the "usual" you may need to add a formal charge

Formal Charge

- Formal charge = (# electrons the atom can use for bonding) – (# electrons the atom "has" when bonded)
- OR: FC = (valence electrons – ½ bonding electrons + electrons in lone pairs)



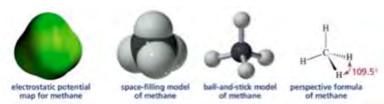
FC on O = 6 (# valence electrons) – (1/2 x 6) (bonding electrons) + 2 (lone pair electrons)

= 6 –5 = +1

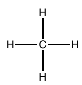
What is the formal charge on each atom for:

- NH_4^+
- O_3
- OH^-
- CN^-

Representing Structures



All these structures show different information about CH_4 methane



Lewis Structures give information – but YOU have to translate to 3D

Valence Shell Electron Pair Repulsion VSEPR

- Helps figure out shape of molecules
- Assume all centers of electron density repel each other
- There is a minimum energy arrangement that the atom will naturally take up.

VSEPR

Centers of electron density (around atom)	Electron geometry	Bond Angle	Example
2	Linear	180°	CO_2
3	Trigonal planar	120°	BF_3
4	Tetrahedral	109°	CH_4
5	Trigonal bipyramid	90°, and 120°	PCl_5
6	Octahedral	90°	SF_6

Note: single bonds, double bonds, triple bonds, and lone pairs all count as 1 center

Compounds with lone pairs (only up to 4 centers of electron density)

Centers of e density	Example	E pair geometry	Molecular shape	Bond angle
4	CH4	Tetrahedral	Tetrahedral	109
4	NH3	Tetrahedral	Trigonal pyramid	< 109
4	H2O	Tetrahedral	Bent	< 109
3	BF3	Trigonal planar	Trigonal planar	120
3	SO2	Trigonal planar	Bent	120

Question: Why are all the bonds in CH_4 the same?

- They are the same (from experiment)
- But electron configuration [He] $2s^2$ $2p^2$
- If s and p orbitals are used for bonding why aren't the bonds different?
- Two models of bonding – used to explain
- Valence Bond Theory
- Molecular Orbital theory
- (we use the theory that works to explain what we see)

Valence bond Theory

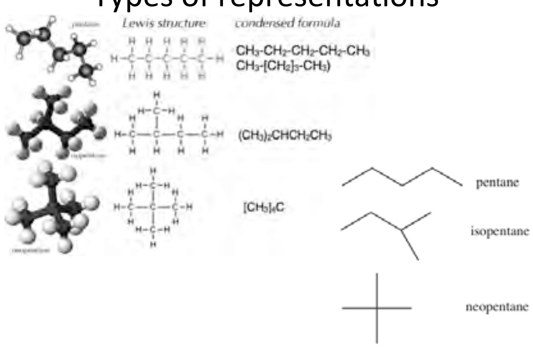
- Orbitals overlap to form bonds – located between two nuclei
- Easy to understand for H–H (a σ 1s – 1s bond) or H–F a σ 1s - 2p bond).
- But CH4?
- Answer is hybridized orbitals
- Hybridize (mix) orbitals to produce enough centers of electron density

VSEPR

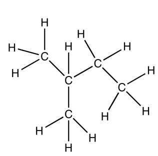
Centers of electron density (around atom)	Electron geometry	Bond Angle	Example	Hybridization
2	Linear	180°	CO_2	sp
3	Trigonal planar	120°	BF_3	sp^2
4	Tetrahedral	109°	CH_4	sp^3
5	Trigonal bipyramid	90°, and 180°	PCl_5	sp^3d
6	Octahedral	90°	SF_6	sp^3d^2

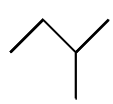
Note: single bonds, double bonds, triple bonds, and lone pairs all count as 1 center

Types of representations

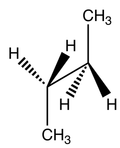


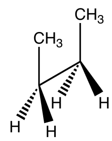
Same or different?





Same or Different

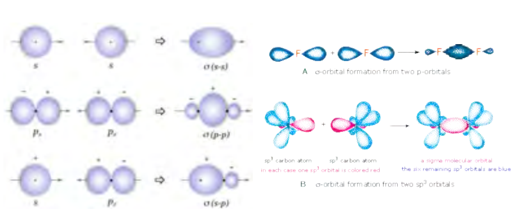




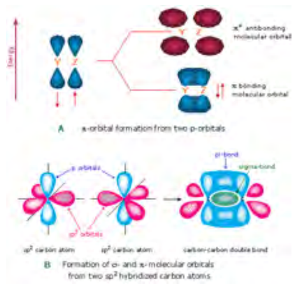
Multiple bonds – sigma and pi

- A single bond is always a sigma bond
- All the rest are always pi bonds
- Sigma bonds allow for rotation around the bond
- Pi bonds do not (it would break the pi bond)

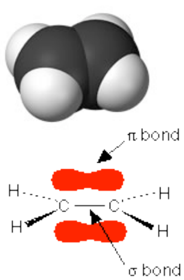
Sigma bonds



Sigma and pi bonds

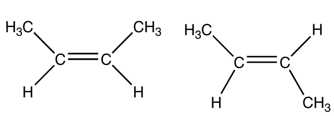


Alkenes



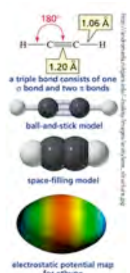
- C sp2 hybridized
- One sigma bond
- One pi bond
- Restricted rotation around the double bond

Same or different?



Vision

Triple bonds



- C - sp hybridized
- One sigma bond
- Two pi bonds

Questions

Question to answer:
• Why are the melting and boiling points of methane higher than the melting and boiling points of H2?
• How many different compounds can you draw for the formula C5H12?
• Is there a generic formula for an alkane containing "n" carbon atoms?
• How would this generic formula change if you joined the ends of a carbon chain and made a ring? (for example cyclohexane has six carbons in a ring - how many hydrogens would it have?)
• Which has the higher boiling point, a spherical alkane or a linear alkane?
• How will boiling points and melting points change as molecular weight increases?
• Make a prediction as to the melting and boiling points of ethane, compared to methane; what assumptions are you making?
Question to ponder:
• How would you design an investigation to test your hypothesis (hint - what information should you look up?) What evidence did you use? How does it support your hypothesis?
• Why does the shape of a molecule influence its behavior?

More questions

- Given a particular hydrocarbon, what factors would influence your prediction of its melting and boiling points?
- Can you generate some tentative rules?
- How does the presence of a double bond influence the structure of a hydrocarbon?
- How about a triple bond?
- Why, do you think, there is no tetra-bonded from of C (that is C four bonds C).
- **Questions to ponder:**
- What limits the size and shape of a hydrocarbon?