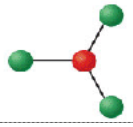
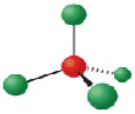
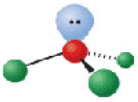
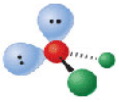
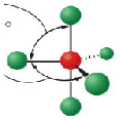
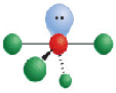
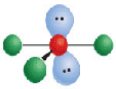
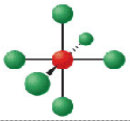
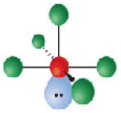
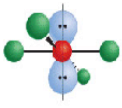
Molecular Geometry

Formula: AB_ne_m A = central atom, B = directly bonded atoms to A, and e = nonbonding (unshared) pairs of electrons

*Note that a molecule formed by joining only **two (2) atoms together is linear** regardless of the number of unshared pairs of electrons (AB, ABe, ABe_3, etc).

AB_ne_m	# of Electron Regions	Electron Geometry	# of Bonding Regions	# of Nonbonding Regions	Molecular Geometry	Structural representation	Hybrid Orbitals	Examples
AB_2	2	Linear	2	0	Linear		sp	$HgCl_2$, CO_2, HCN
AB_3	3	Trigonal Planar	3	0	Trigonal Planar		sp^2	BF_3, BCl_3, SO_3, CO_3^{-2}
AB_2e	3		2	1	Bent		sp^2	SO_2, NO_2^-
AB_4	4	Tetrahedral	4	0	Tetrahedral		sp^3	CH_4, $SiCl_4$, $POCl_3$
AB_3e	4		3	1	Trigonal pyramidal		sp^3	NH_3, PF_3
AB_2e	4		2	2	Bent		sp^3	H_2O, H_2S, BrO_2^-
AB_5	5	Trigonal Bipyramidal	5	0	Trigonal Bipyramidal		dsp^3	PH_5, PCl_5, SbF_5, $IO_3F_2^-$
AB_4e	5		4	1	Distorted tetrahedron (“See-Saw”)		dsp^3	SF_4, IF_4^+
AB_3e_2	5		3	2	T-Shape		dsp^3	ClF_3, BrF_3
AB_2e_3	5		2	3	Linear		dsp^3	I_3^-, ICl_2^-, XeF_2
AB_6	6	Octahedral	6	0	Octahedral		d^2sp^3	SF_6, PF_6^-
AB_5e	6		5	1	Square Pyramidal		d^2sp^3	IF_5, $XeOF_4$
AB_4e_2	6		4	2	Square Planar		d^2sp^3	XeF_4, BrF_4^-

Lewis Structures

CAUTION: Different course/instructors may ask for more or less.
***Make sure you are clear on your instructor's expectations*.**

Lewis originally sold his idea based on a cubic shape because it has eight points (origin of the octet rule). This has since mutated to formatting a beginning Lewis structure off of a square with the center atom being the center of that square.

Electrons are considered more "stable" as pairs, so "always" try to keep them paired.

1. Total the **valence** electrons from each atom AND **count "charges"** as extra or lost electrons.
2. Choose a central atom to act as a **connector or bridge**. This is usually the least electronegative (or most metallic). *(Exception: anything that cannot "bridge").* Place remaining atoms on face of square around center atom.
3. Add the electrons in pairs to the MOST electronegative atom (or least metallic) first to satisfy the octet rule *(noble rule)*: eight electrons around every atom except hydrogen (no more than two electrons).
4. Continue adding electrons to the rest of the atoms until the **total electrons** (from Step 1) are accounted for.
5. Convert pairs of electrons **between** atoms into a "line" to represent a bond.
6. Move non-bonding pairs of electrons between atoms that have not satisfied "*their*" octet.
   - **RESONANCE**: If there is more than one atom that has non-bonding electrons, then you MUST draw all possible structures.
7. **CHM130**: Assign all non-zero Formal Charges in the upper right corner outside a bracket set: [ ]^{charge}.
   Other CHM: Assign non-zero Formal Charges to *each atom*
   Formal Charge = # valence electrons - # non-bonding electrons - # bonds
8. **For ADVANCED classes/instructors**: Choose the best structure according to the following priority:
   1. All atoms satisfy octets. 2. Minimize charge even at cost of *exceeding* octet

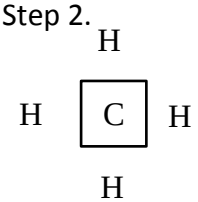
Electron regions: Count the *faces of the square* that have electrons present
Bonding regions: Count the *faces of the square* that have at least one bond
Nonbonding regions: Count the *faces of the square* that have a non-bonding pair of electrons.

Examples:

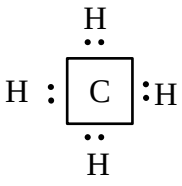
Methane: CH_4

Step 1. Valence electrons Found on Periodic Table as column title
C: 4 e^-
\+ H: 1 e^- x4 atoms
8 electrons

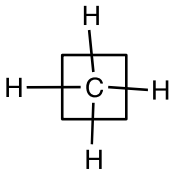
Step 2.



Step 3-4



Step 5-done.

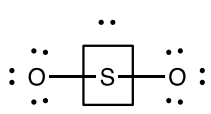


Electron regions: 4 Bonding regions: 4 Nonbonding regions: 0

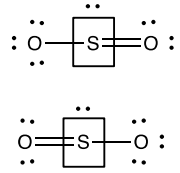
Sulfur Dioxide: SO_2

Step 1. Valence electrons Found on Periodic Table as column title
S: 6 e^-
\+ O: 6 e^- x2 atoms
18 electrons

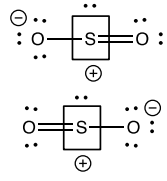
Step 2-5



Step 6.



Step 7.



Formal Charge O:
6 - 6 - 1 = -1
and
6 - 4 - 2 = 0
Formal Charge S:
6 - 2 – 3 = +1

Electron regions: 3 Bonding regions: 2 Nonbonding regions: 1