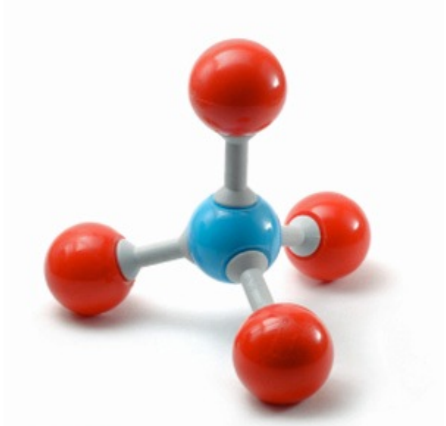
Ch10

VSEPR

Valence Shell Electron Pair Repulsion theory allows you to predict molecular shape.

Lewis Dot theory extended to 3 dimensions.



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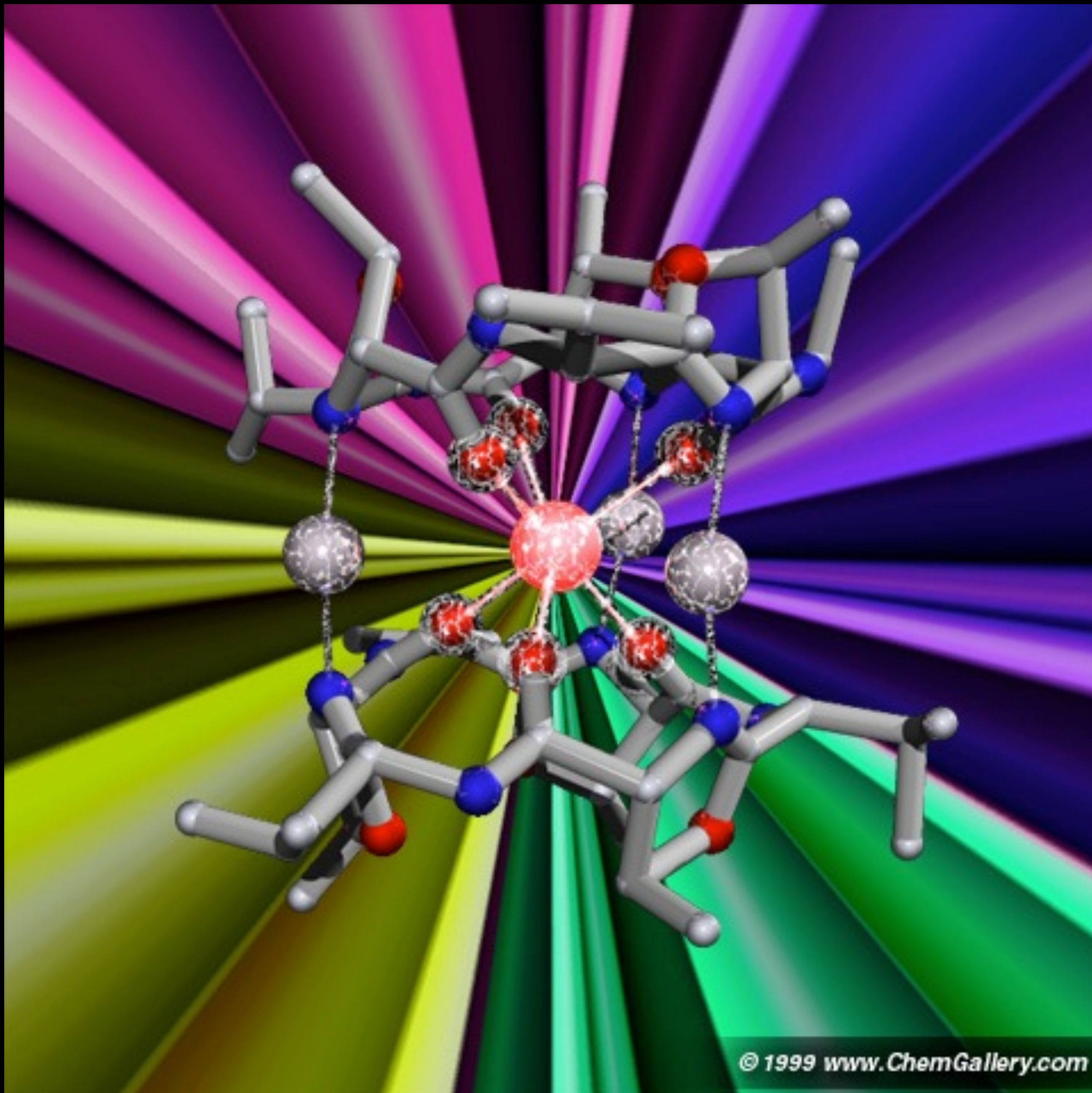
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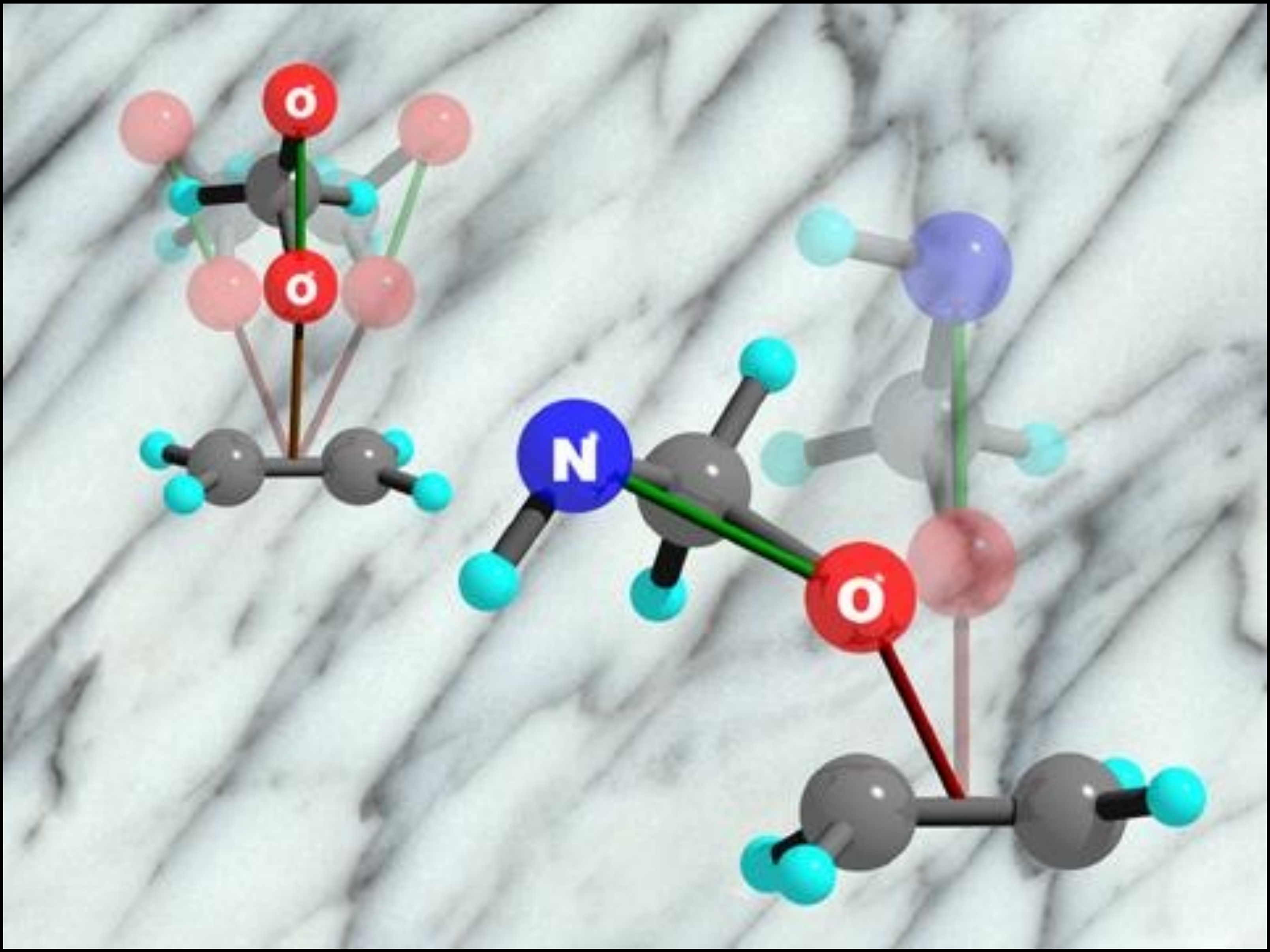

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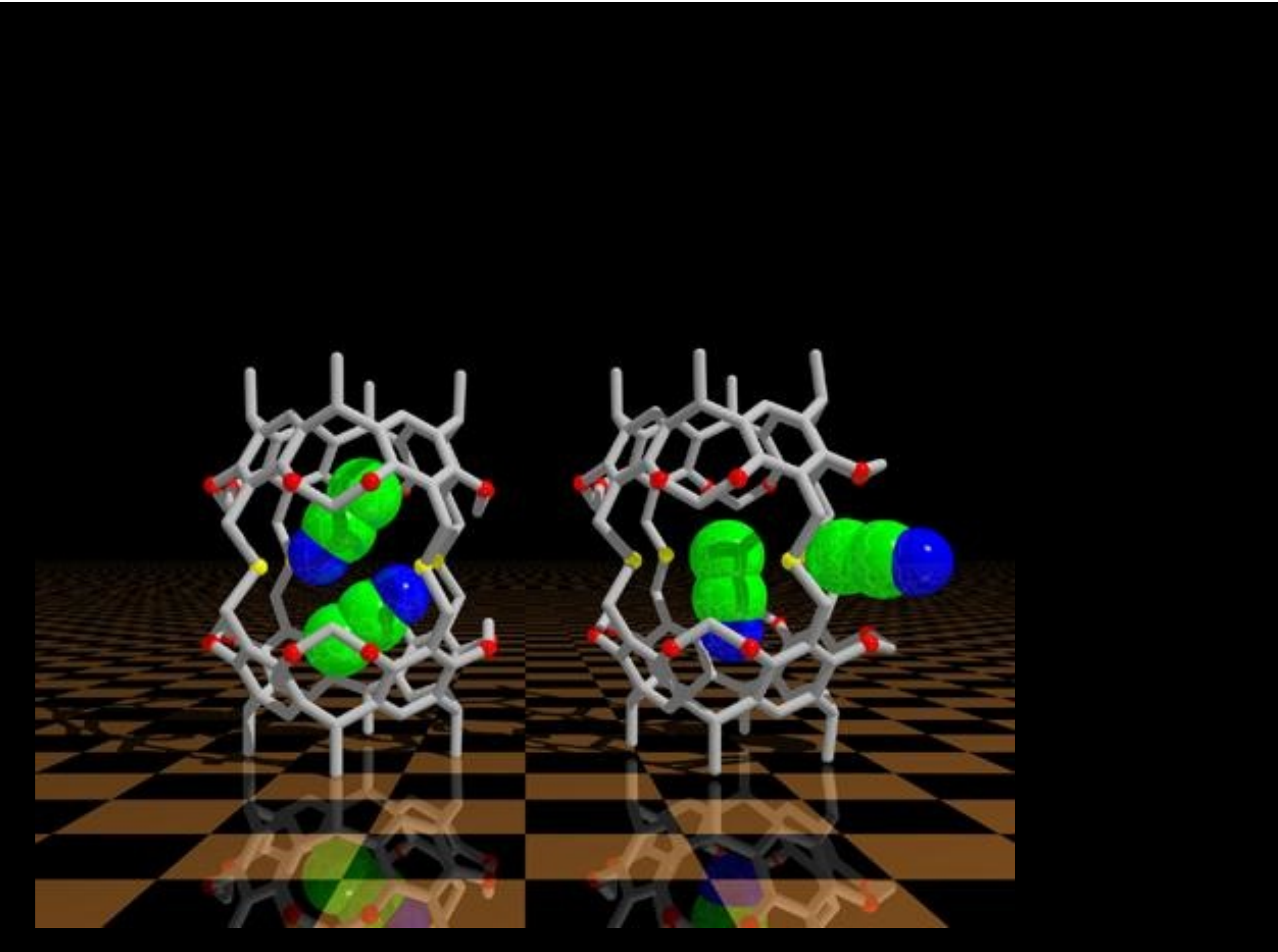
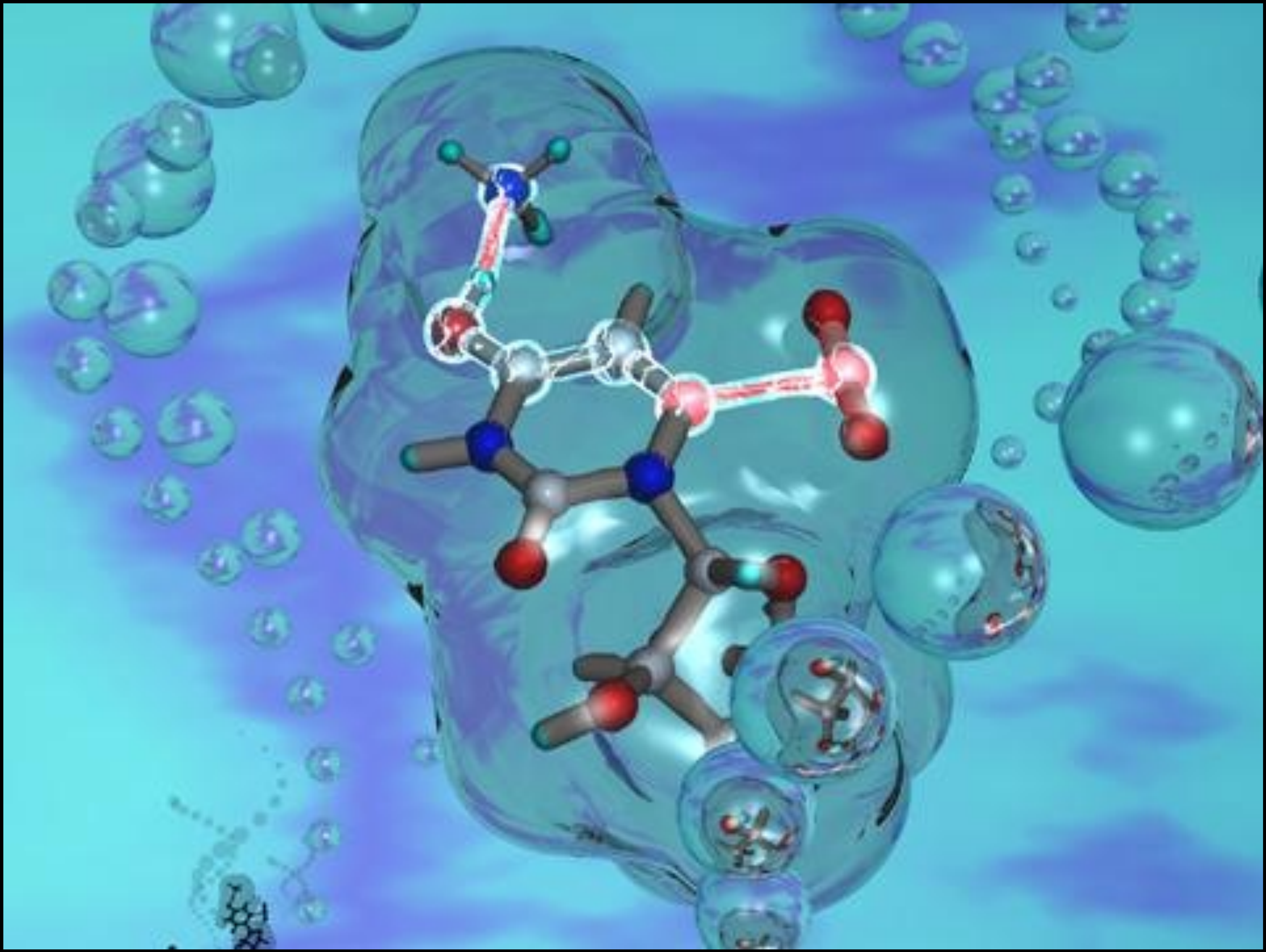
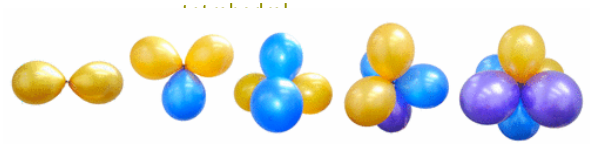


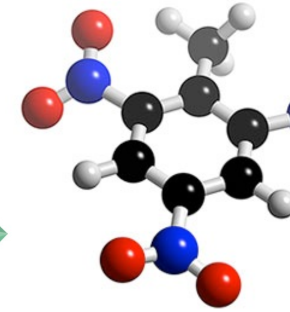


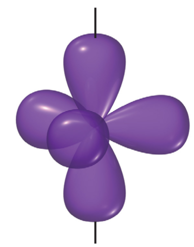
Valence Shell Electron Pair Repulsion

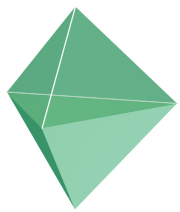
- Microscopic properties
  - Composition, Connectivity & Shape
  - Molecular Shape
    - eg: sense of taste; active sites
- VSEPR Theory: Electronic Geometry
  - Kinds of Electron Groups
  - Electron Domains
  - Electron Pair Repulsion
  - Basic shapes (geometry)
    - linear
      - two electron groups, eg: $BeCl_2$, CO_2
    - trigonal planar
      - three electron groups, eg: BF_3, H_2CO
    - tetrahedral
      - four electron groups, eg: CH_4
    - trigonal bipyramidal
      - five electron groups, eg: PCl_5
    - octahedral
      - six electron groups, eg: SF_6
- VSEPR Theory: Molecular Geometry
  - Difference between electron and molecular geometries
  - Four electron groups with lone pairs
    - trigonal pyramidal
      - one lone pair; smaller bond angle than tetrahedral

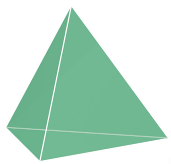


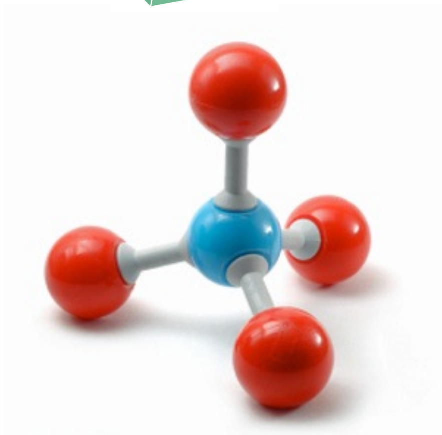
    - bent
      - two lone pairs; smaller bond angle than tetrahedral or trigonal bipyramidal
      - example: H_2O
  - Five electron groups with lone pairs
    - seesaw
      - one lone pair; goes in trigonal plane
      - example: SF_4^+
    - T-shaped
      - two lone pairs, both in trigonal plane
      - example: BrF_3
    - linear
      - three lone pairs, all in trigonal plane
      - example: XeF_2
  - Six electron groups with lone pairs
    - square pyramidal
      - example: BrF_5
    - square planar
      - lone pairs 180o apart; example: XeF_4
- VSEPR Theory: Predicting Geometries
  - Procedure
    - Draw the Lewis structure.
    - Find the number of domains
      - Which gives you the electronic geometry.
      - Divide the domains into bonding and non-bonding groups.
    - Draw the molecular geometry.
    - Write the name of the name of that geometry.
  - Shapes of molecules with more than one central atom.



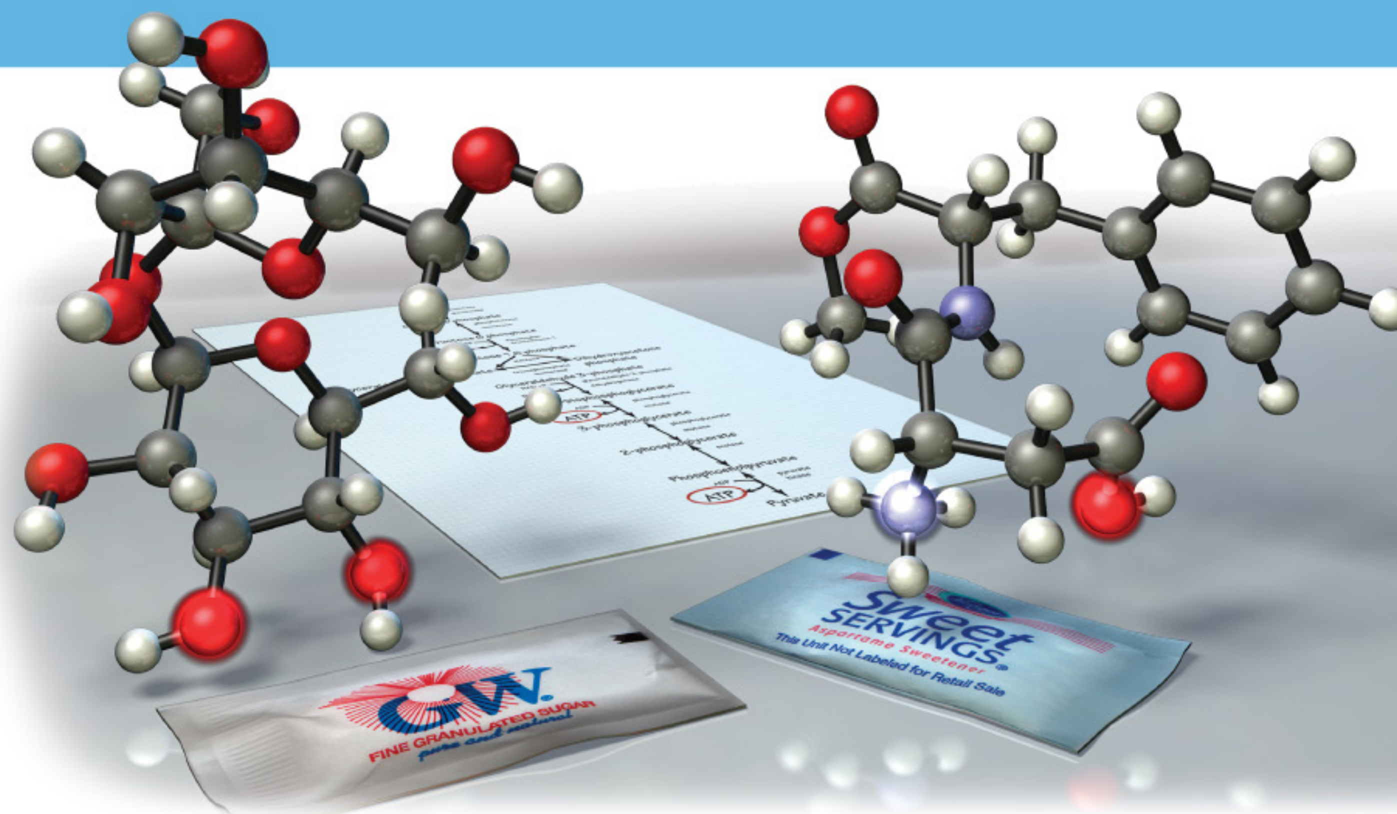




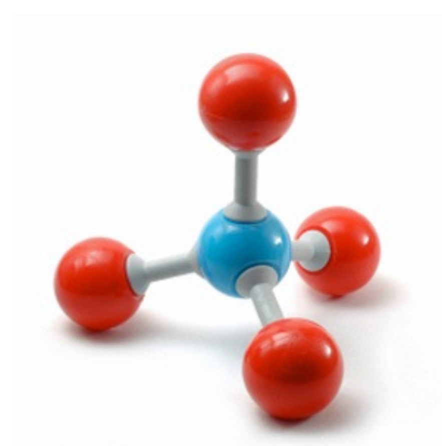




Sweetness is a function of molecular shape.



- The taste of a food depends on the interaction between the food molecules and taste cells on your tongue.
- The main factors that affect this interaction are the shape of the molecule and charge distribution within the molecule.
- The food molecule must fit snugly into the active site of specialized proteins on the surface of taste cells.
- When this happens, changes in the protein structure cause a nerve signal to transmit.
- Sugar molecules fit into the active site of taste cell receptors called Tlr3 receptor proteins.
- When the sugar molecule (the key) enters the active site (the lock), the different subunits of the T1r3 protein split apart.
- This split causes ion channels in the cell membrane to open, resulting in nerve signal transmission.
- Artificial sweeteners also fit into the Tlr3 receptor, sometimes binding to it even stronger than sugar, making them “sweeter” than sugar.



Molecular Shape

- Properties of molecular substances depend on the structure of the molecule.
- The structure includes many factors:
  - The atoms that make up the molecule (composition).
  - The skeletal arrangement of the atoms and the kind of bonding between the atoms (connectivity).
    - Ionic, polar covalent, or covalent
  - The 3D form of the molecule (shape).
- Bonding theory should allow you to predict the shapes of molecules.
- Molecules are three-dimensional objects.
- We often describe the shape of a molecule with terms that relate to geometric figures.
- These geometric figures have characteristic "corners" that indicate the positions of the surrounding atoms around a central atom in the center of the geometric figure.
- The geometric figures also have characteristic angles that we call bond angles.

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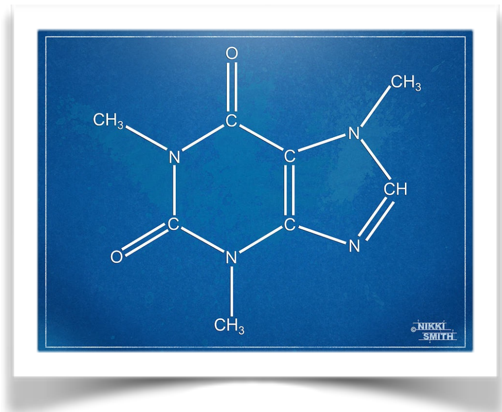
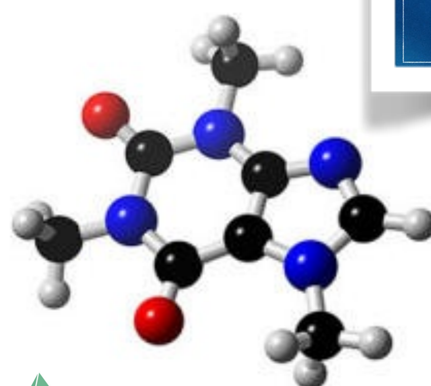
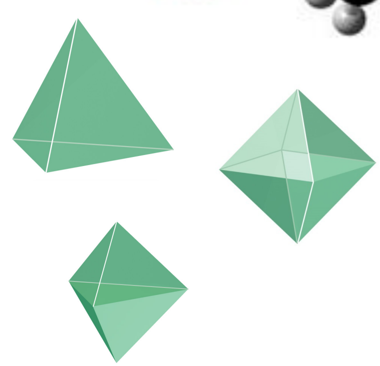
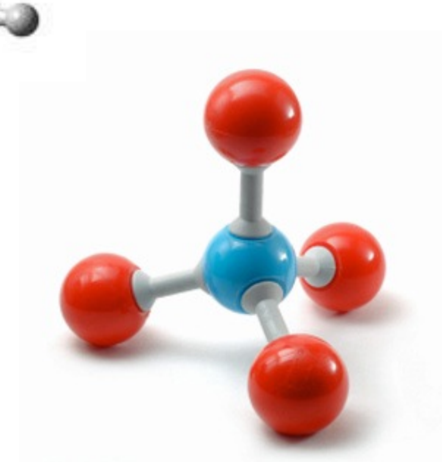
$C_8H_{10}N_4O_2$



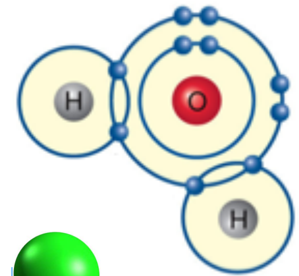


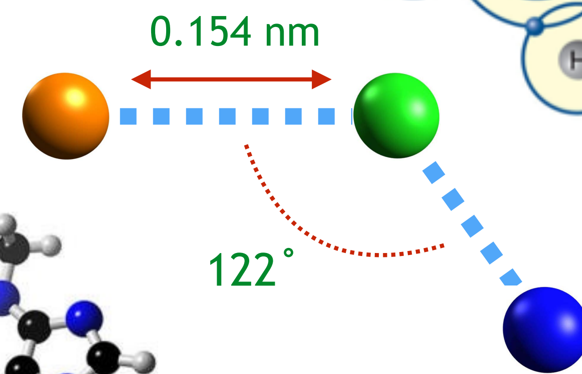


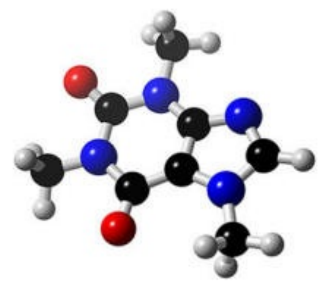


Defining Molecular Shape

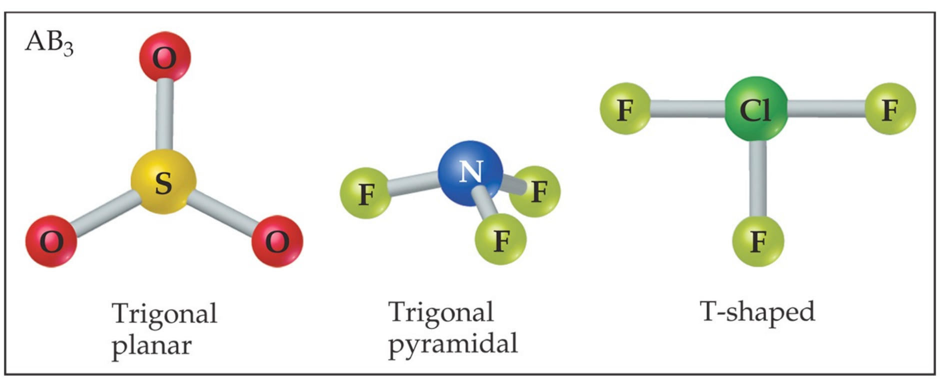
- Covalent bonds lock electrons into positions between atoms.
- Multiple covalent bonds can connect to a central atom in different geometries.
- Geometries are defined by:
  - bond angles: the angle between two bonds
  - bond distances: the distance between two bonded atoms
- Molecules can have the same composition, same connectivity — but different shapes.
  - A central atom with two valence atoms can be:
    - Bent
    - Linear
  - A central atom with three valence atoms can be:
    - Planar
    - Pyramidal
    - T-Shaped
- Overall molecular shape is the sum of shape around each atom.
- The shape of a molecule plays an important role in its reactivity.
- We need a tool to predict valence atom shapes.







3 Valence Atom Shapes



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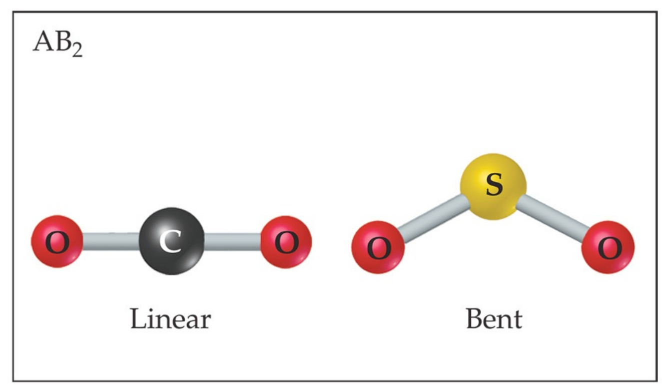


A model for predicting shape.

Composition

(What's in it.)

CCl_4

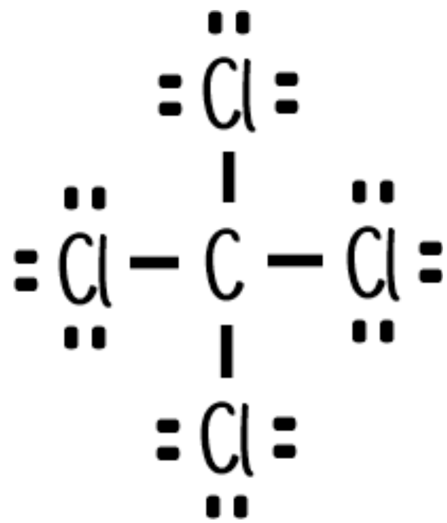
1 Carbon
4 Chlorine

Chemical Symbols

Molecular Formula

Connectivity

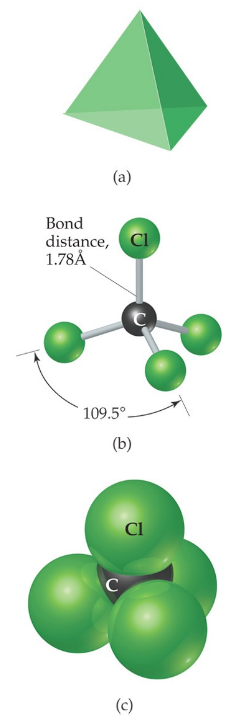
(What's connected to what.)



Lewis Dot Structure

Shape

(Bond Angles & Distances)



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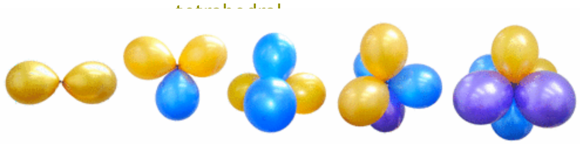

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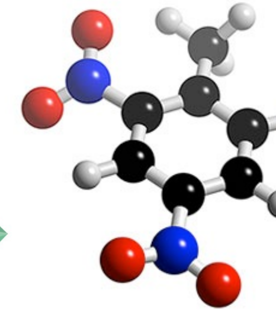
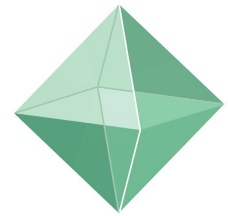
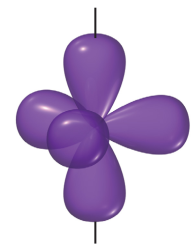
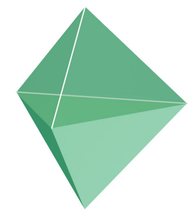
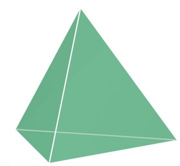
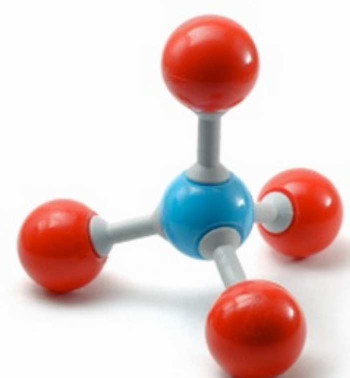






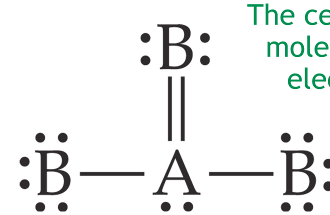




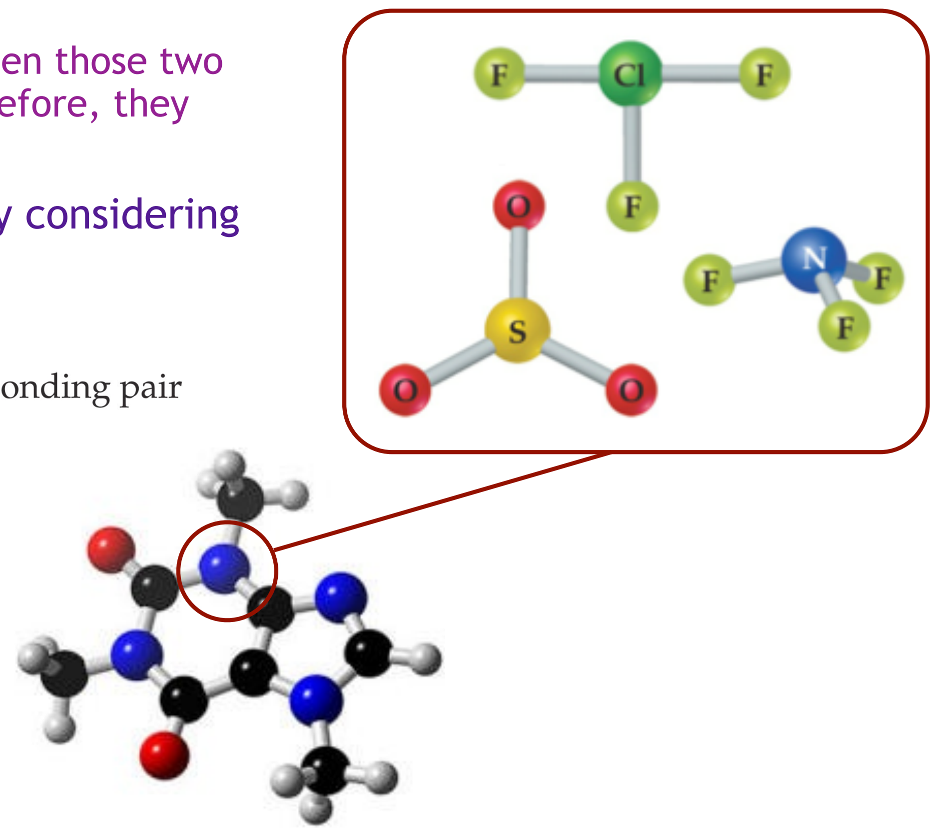


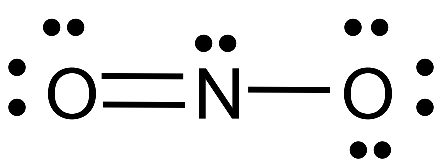
Electron Domains

- To identify the shape around atoms in a molecule, we need to understand the shape formed by the electron pairs around that atom.
- By noting the number of bonding and nonbonding electron pairs we can predict bond angles and distances.
- We refer to the electron pairs as electron domains.
  - In a double or triple bond, all electrons shared between those two atoms are on the same side of the central atom; therefore, they count as one electron domain.
- This allows us to predict the shape of a molecule, by considering electron repulsion…

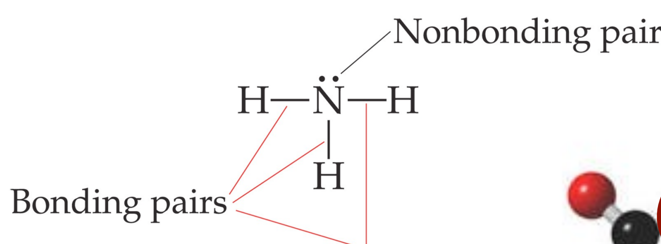


The central atom in this molecule, A, has four electron domains.

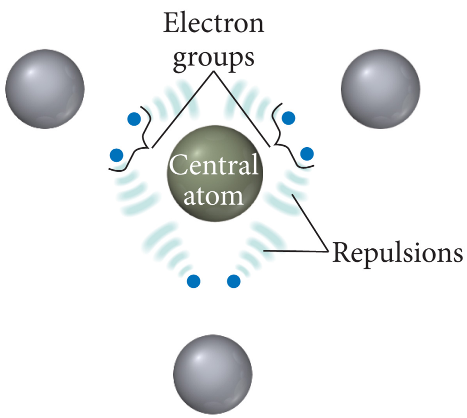




There are three electron groups on N:
- One lone pair
- One single bond
- One double bond



Electron Repulsion

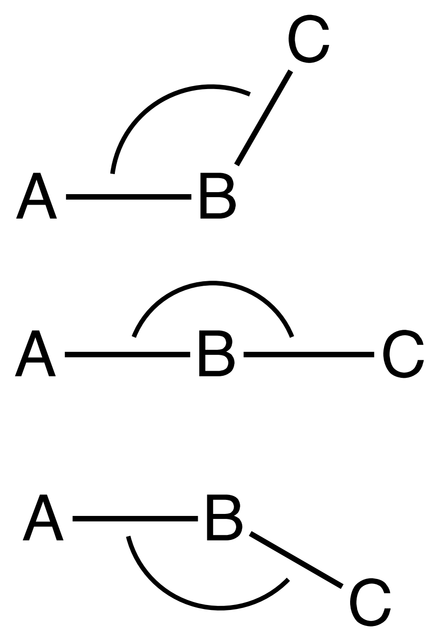


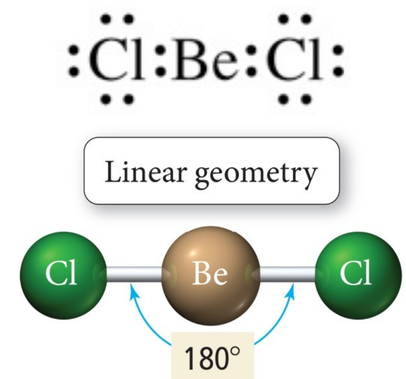
- Electron pairs, whether they be bonding or nonbonding, repel each other.
- By assuming the electron pairs are placed as far as possible from each other, we can predict the shape of the molecule.
- There are five basic arrangements of electron groups around a central atom.
  - That's based on a maximum of six bonding electron groups around an atom.

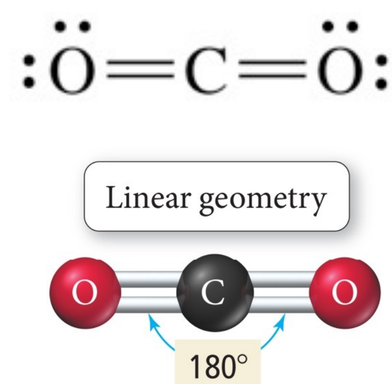
    (There may be more than six on very large atoms, it is very rare. — We won't worry about those)
- Each of these five basic arrangements results in five different basic electron geometries.
  - In order for the molecular shape and bond angles to be a "perfect" geometric figure, all the electron groups must be bonds and all the bonds must be equivalent.
    - We'll tweak the model later to account for differences.
  - For molecules that exhibit resonance, it doesn't matter which resonance form you use as the underlying electron geometry will be the same.
- All atoms that have 2-6 Electron Domains will have their electron pairs arranged in one of these five basic geometries.

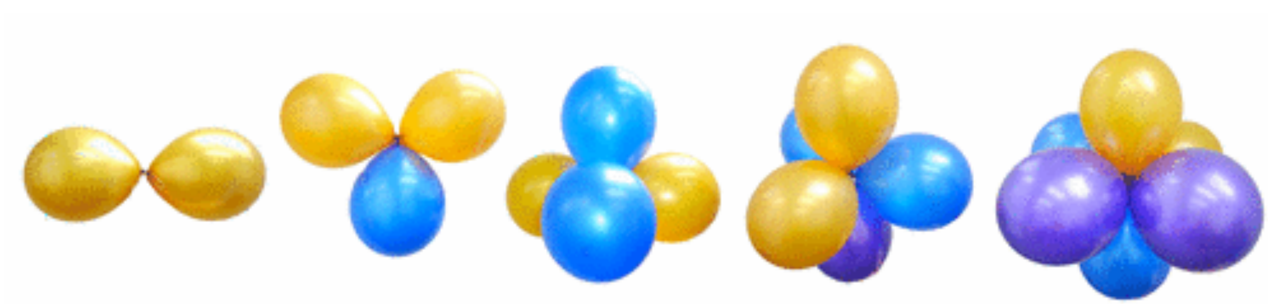
2 Electron Domains — Linear

- The best arrangement of two electron domains around a central atom is linear.
- A pushes C away until the ABC bond angle is 180˚
- Pushing any farther than 180˚ brings C closer to A — on the other side.



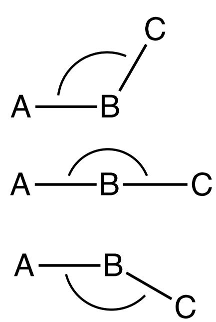


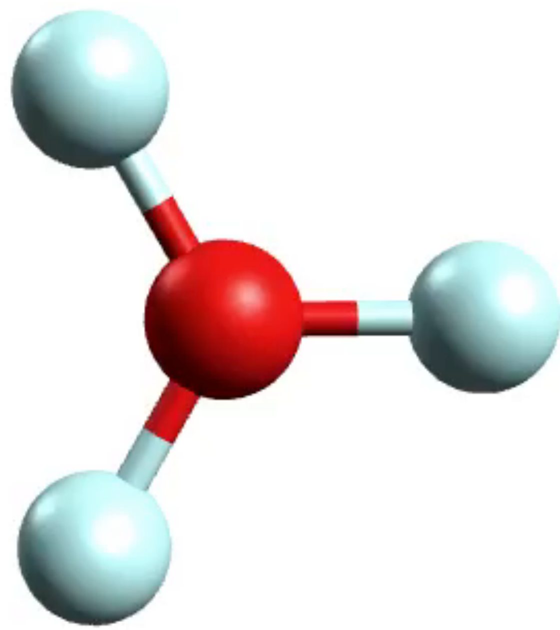


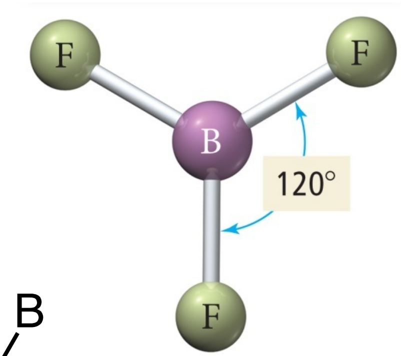


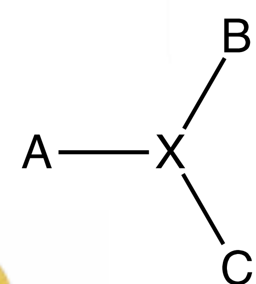
3 Electron Domains – Trigonal Planar

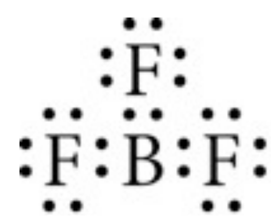
- Three electron domains around a central atom form a trigonal planar arrangement.
- The bond angle between each atom is 120˚
- The three domains remain in the same plane for the same reason they remain linear when there are two domains.





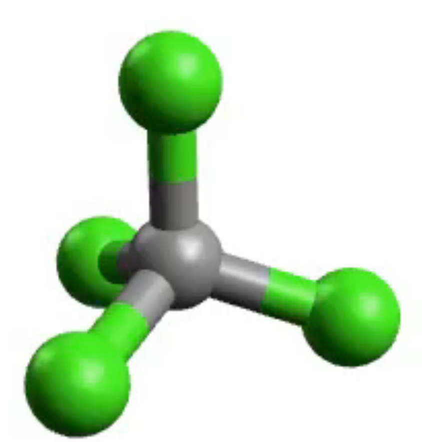


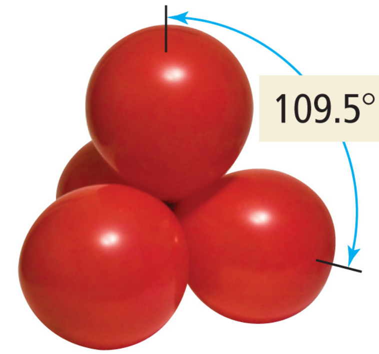


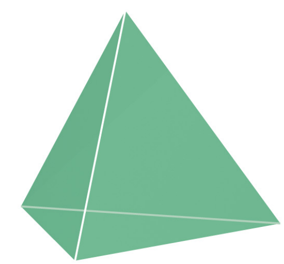


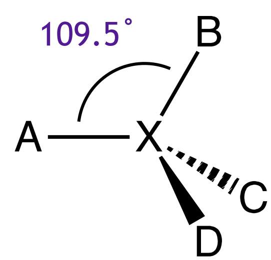
4 Electron Domains – Tetrahedral

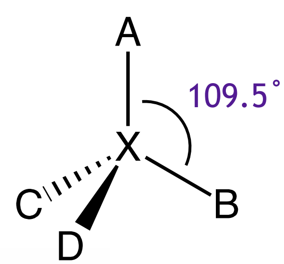
- Four electron domains form a tetrahedral arrangement around the central atom.
- A tetrahedron, a pyramid with a triangular base, defines the position of each domain.
- All domains are equidistant from each other.
- The bond angle between any two domains is 109.5˚
- To draw a tetrahedral atom, draw three atoms in the plane and then use a dotted line to show one behind and a triangle to show one in front.

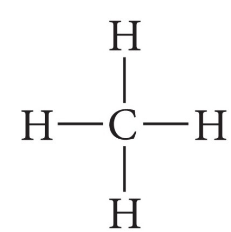


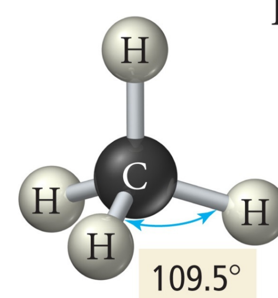


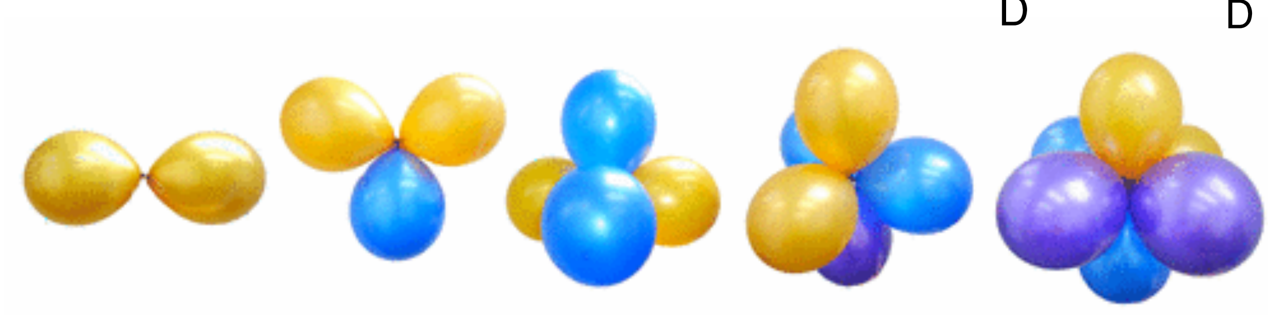






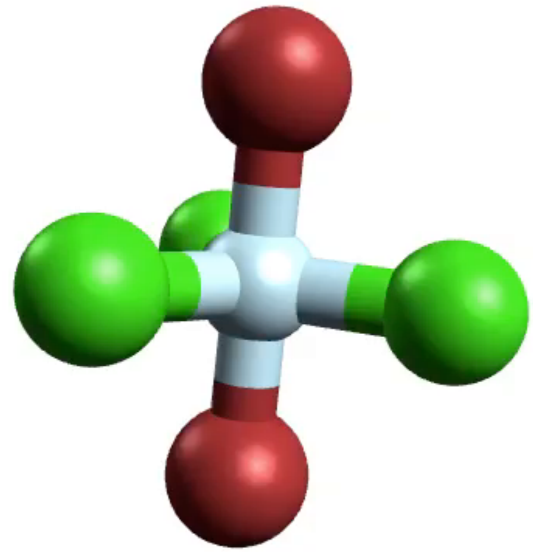


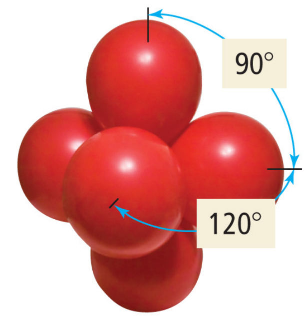


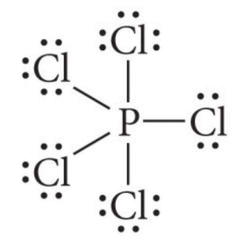


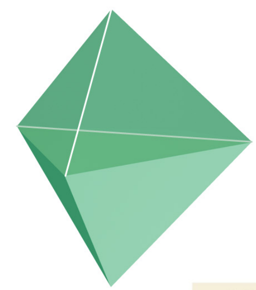
5 Electron Domains – Trigonal Bipyramidal

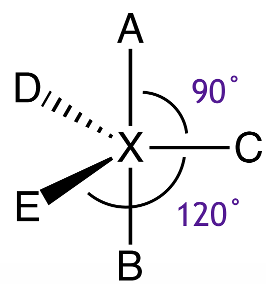
- Five electron domains form a trigonal bipyramidal arrangement around the central atom.
- This optimal arrangement has two types of positions:
  - Equatorial
  - Axial
- Equatorial positions are 120˚ apart.
- Axial positions are above and below the equatorial plane.
- Axial positions are 90˚ from the equatorial plane.

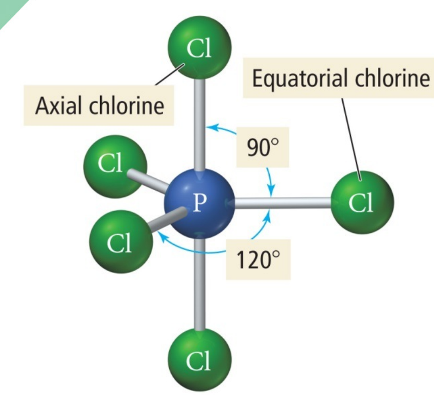


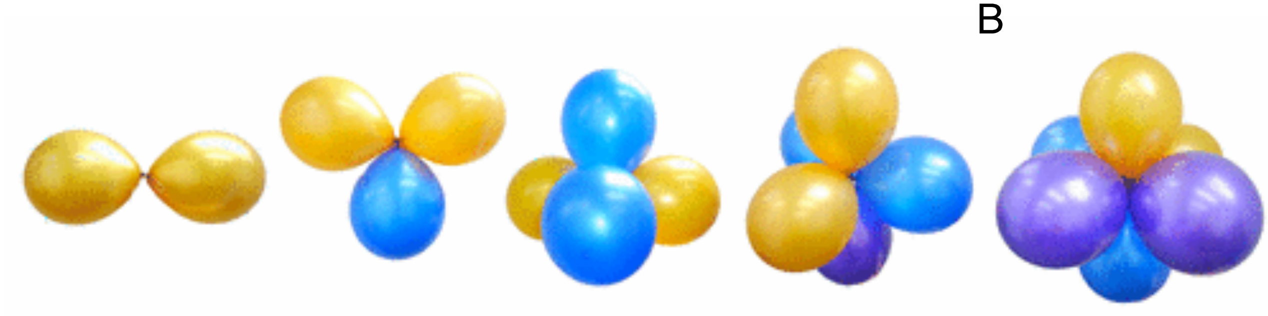








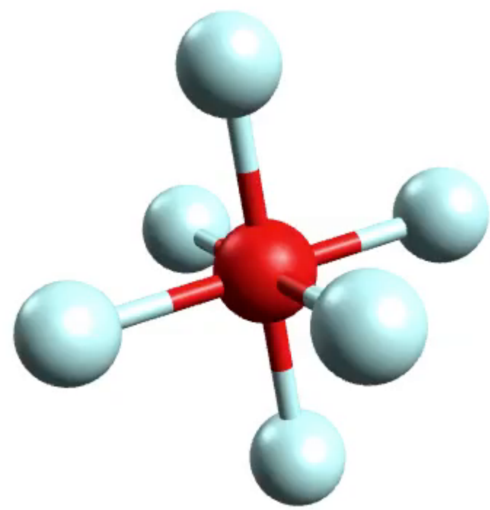


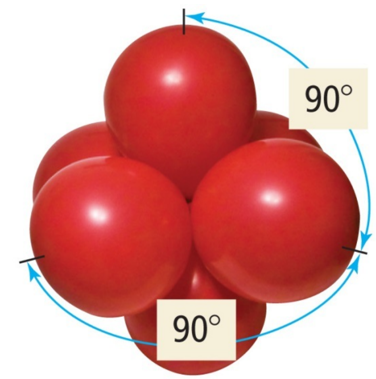


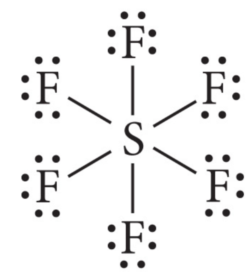
6 Electron Domains — Octahedral

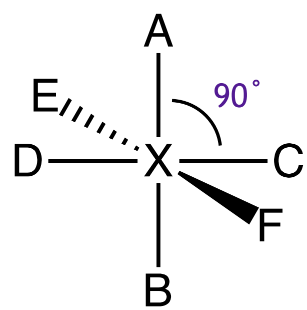
- Six electron domains form an octahedral arrangement around the central atom.
- The points of an octahedron geometric shape defines the positions of domains in an octahedral arrangement.

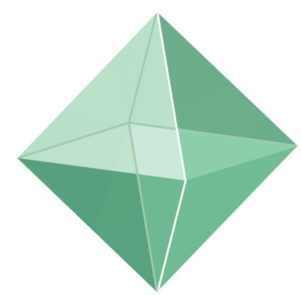
  (Played D&D? Think 8 sided dice!)
- All six positions are equivalent.
- Each position is equidistant from 4 other positions and forms a 90˚ angle with each.
- It is also opposite the last position and has 180˚angle with it.

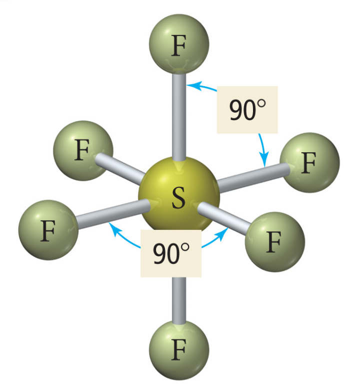




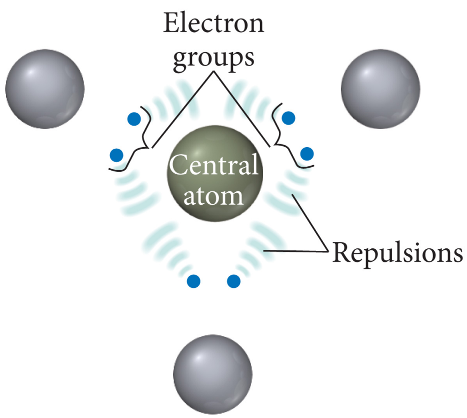


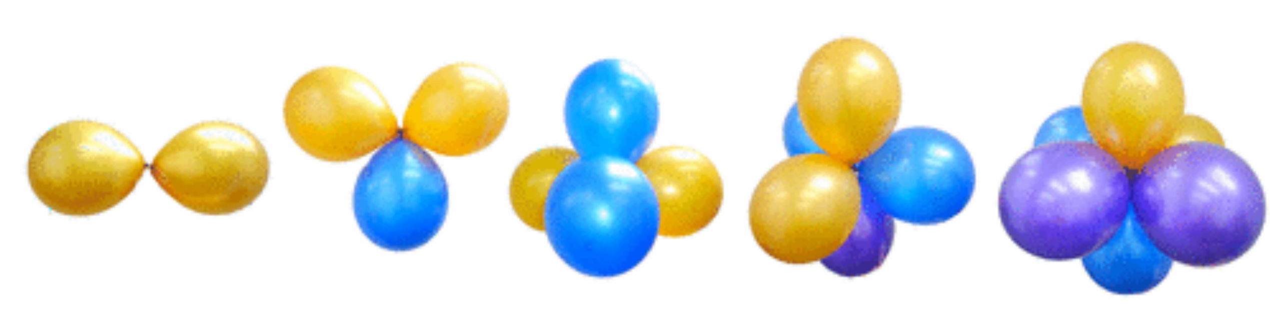






Electron Repulsion





- Electron pairs, whether they be bonding or nonbonding, repel each other.
- By assuming the electron pairs are placed as far as possible from each other, we can predict the shape of the molecule.
- There are five basic arrangements of electron groups around a central atom.
  - That's based on a maximum of six bonding electron groups around an atom.

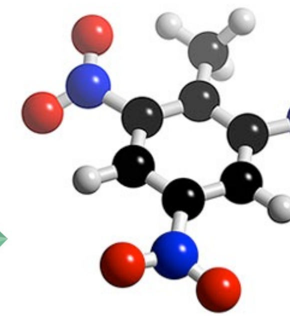
    (There may be more than six on very large atoms, it is very rare. – We won't worry about those)
- Each of these five basic arrangements results in five different basic electron geometries.
  - In order for the molecular shape and bond angles to be a "perfect" geometric figure, all the electron groups must be bonds and all the bonds must be equivalent.
    - We'll tweak the model later to account for differences.
  - For molecules that exhibit resonance, it doesn't matter which resonance form you use as the underlying electron geometry will be the same.
- All atoms that have 2-6 Electron Domains will have their electron pairs arranged in one of these five basic geometries.

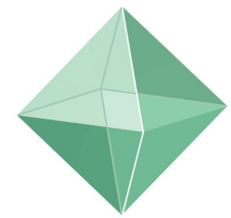
	Electronic Geometry	Bond Angles
1 e pair	Linear	180˚
2 e pair	Linear 	180˚
3 e pair	Trigonal Planar 	120˚
4 e pair	Tetrahedral 	109.5˚
5 e pair	Trigonal Bipyramidal 	90˚ and 120˚
6 e pair	Octahedral 	90˚

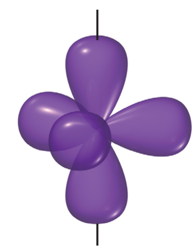
Valence Shell Electron Pair Repulsion

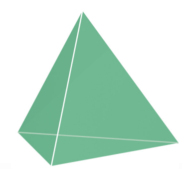
- Microscopic properties
  - Composition, Connectivity & Shape
  - Molecular Shape
    - eg: sense of taste; active sites
- VSEPR Theory: Electronic Geometry
  - Kinds of Electron Groups
  - Electron Domains
  - Electron Pair Repulsion
  - Basic shapes (geometry)
    - linear
      - two electron groups, eg: $BeCl_2$, CO_2
    - trigonal planar
      - three electron groups, eg: BF_3, H_2CO
    - tetrahedral
      - four electron groups, eg: CH_4
    - trigonal bipyramidal
      - five electron groups, eg: PCl_5
    - octahedral
      - six electron groups, eg: SF_6
- VSEPR Theory: Molecular Geometry
  - Difference between electron and molecular geometries
  - Four electron groups with lone pairs
    - trigonal pyramidal
      - one lone pair; smaller bond angle than

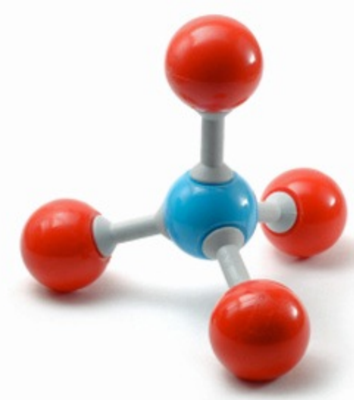
    - bent
      - two lone pairs; smaller bond angle than tetrahedral or trigonal bipyramidal
      - example: H_2O
  - Five electron groups with lone pairs
    - seesaw
      - one lone pair; goes in trigonal plane
      - example: SF_4^+
    - T-shaped
      - two lone pairs, both in trigonal plane
      - example: BrF_3
    - linear
      - three lone pairs, all in trigonal plane
      - example: XeF_2
  - Six electron groups with lone pairs
    - square pyramidal
      - example: BrF_5
    - square planar
      - lone pairs 180^o apart; example: XeF_4
- VSEPR Theory: Predicting Geometries
  - Procedure
    - Draw the Lewis structure.
    - Find the number of domains
      - Which gives you the electronic geometry.
      - Divide the domains into bonding and non-bonding groups.
    - Draw the molecular geometry.
    - Write the name of the name of that geometry.
  - Shapes of molecules with more than one central atom.



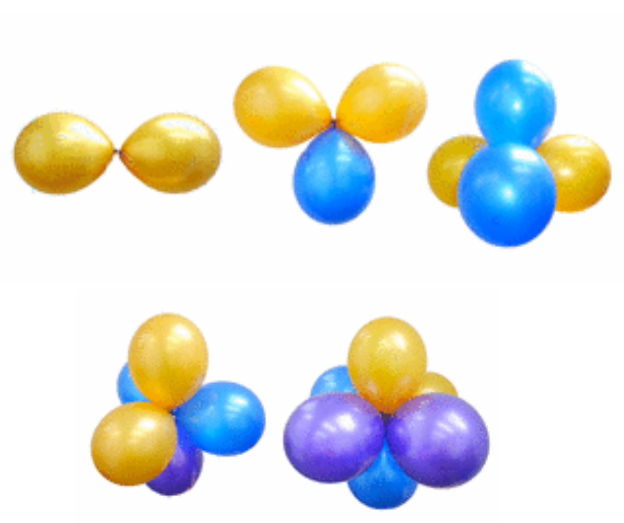




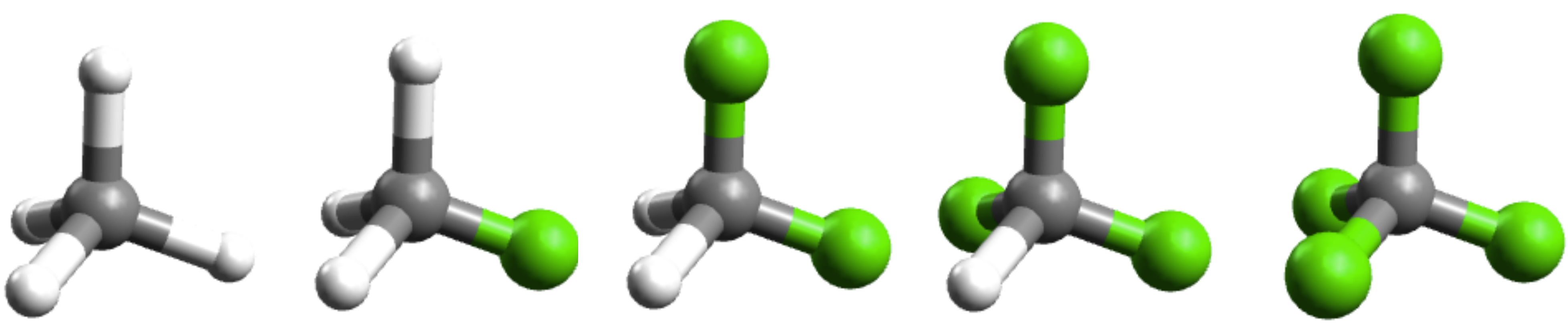




Electronic vs Molecular Geometry

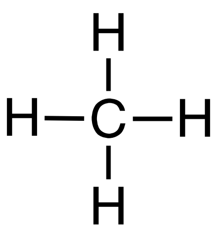


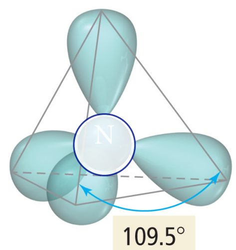
- Electronic geometry is the shape defined by the electron domains.
- Molecular geometry is the shape defined by atoms which *may* be attached to those domains.
- Don't confuse the two!
- There are only five electronic geometries.
- The question "what is the electronic geometry of an atom?" will only have one of these five answers:
  - Linear (two domains)
  - Trigonal Planar (three domains)
  - Tetrahedral (four domains)
  - Trigonal Bipyramidal (five domains)
  - Octahedral (six domains
- If there are 4 electron domains, the electronic structure is tetrahedral.
- With a tetrahedral electronic geometry we could have one atom, two atoms, three atoms, or four atoms stuck onto the central atom.
- A tetrahedral electronic geometry could produce 4 different molecular geometries.

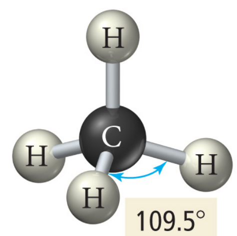


Tetrahedral Electronic Geometry

- There are only five electronic geometries, but each can result in many molecular geometries.
- Only one electronic geometry occurs when there are 4 electron domains.
- But there are multiple molecular geometries that can be built on a tetrahedral electronic geometry.

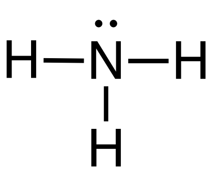


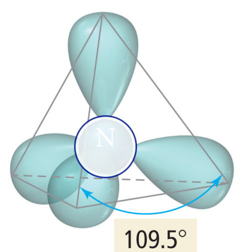


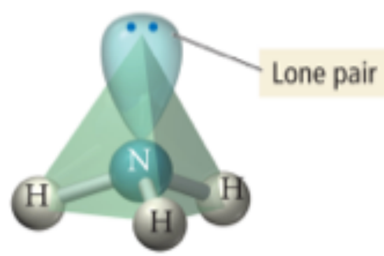


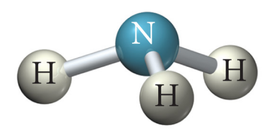
Electronic Geometry: Tetrahedral

Molecular Geometry: Tetrahedral



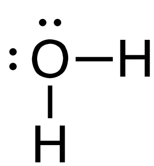


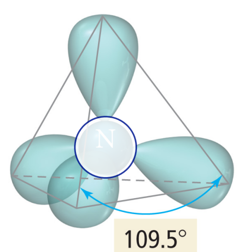


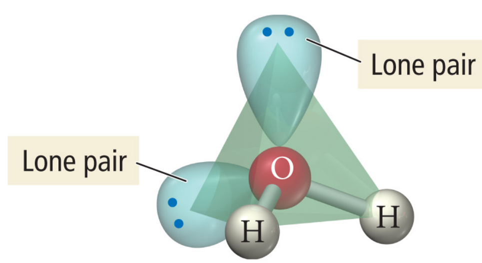


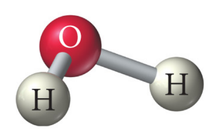
Electronic Geometry: Tetrahedral

Molecular Geometry: Trigonal Pyramidal







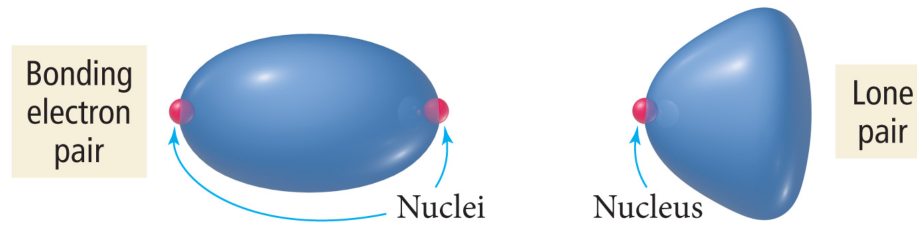


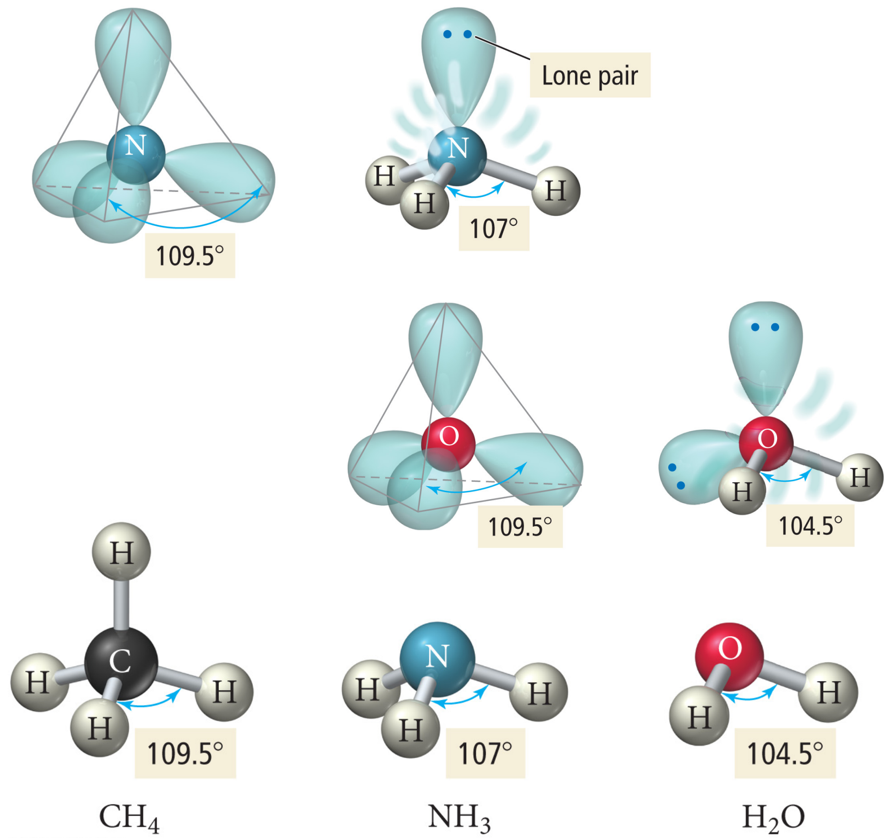
Electronic Geometry: Tetrahedral

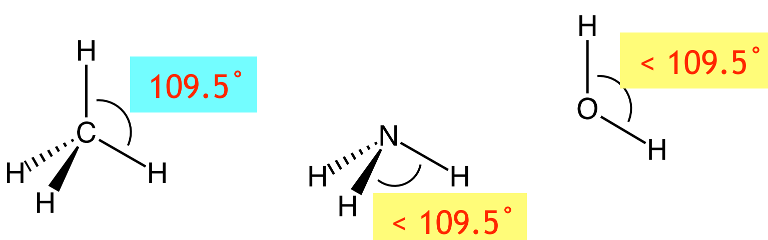
Molecular Geometry: Bent

Bond Angle Compression

- Two electrons, a lone pair, in an electronic domain spread out.
- When those same electrons are in a covalent bond, the nuclei of the two atoms pull them into a smaller area.
- Lone pairs occupy more space than covalent bonds.
- Lone pairs press on adjacent covalent bonds and compress the bond angles between covalent bonds.
- You are responsible for knowing the ideal bond angle of a tetrahedral geometry is 109.5˚
- You are responsible for knowing when bond angle compression produces an angle less than 109.5˚
  - Write " < 109.5" when asked to label compressed bond angles.
- You are not responsible for knowing the exact angle of a compressed bond.



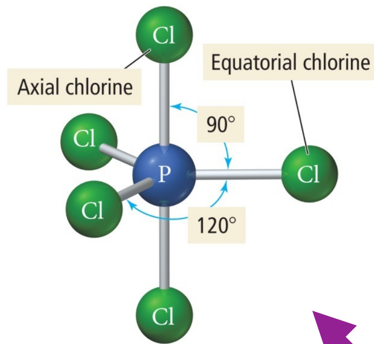




Trigonal Bipyramidal Electronic Geometry

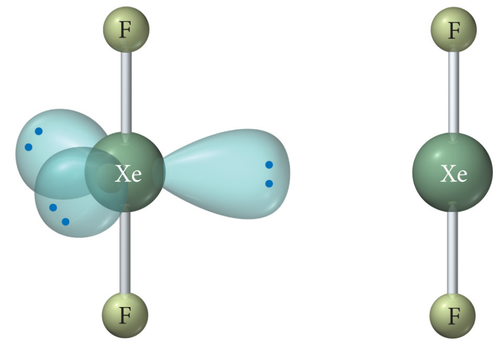
Electronic Geometry:
Trigonal Bipyramidal

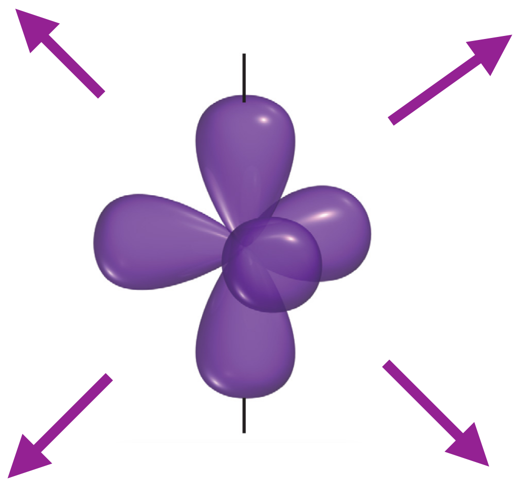
Molecular Geometry:
Trigonal Bipyramidal



Electronic Geometry:
Trigonal Bipyramidal

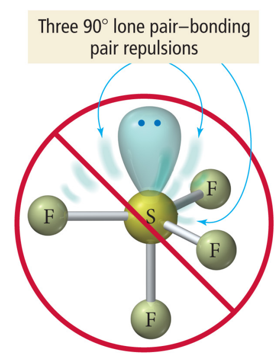
Molecular Geometry:
Linear





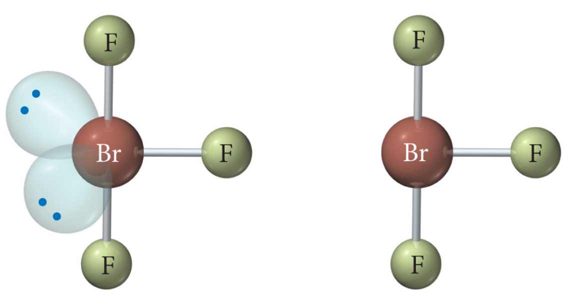
Electronic Geometry:
Trigonal Bipyramidal

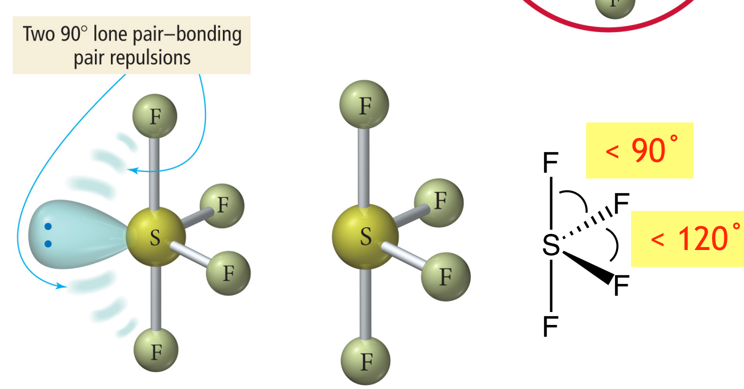
Molecular Geometry:
Seesaw



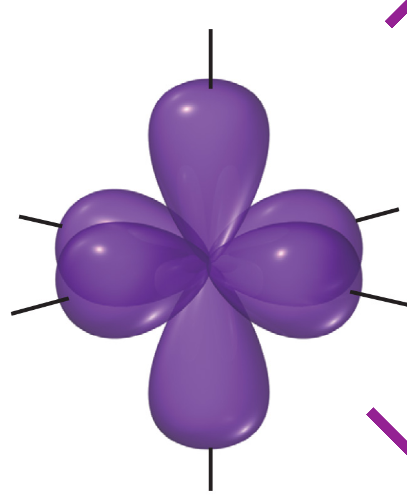
Electronic Geometry:
Trigonal Bipyramidal

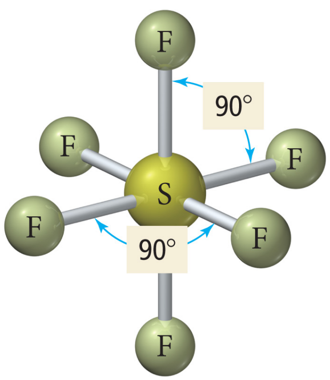
Molecular Geometry:
T-Shaped





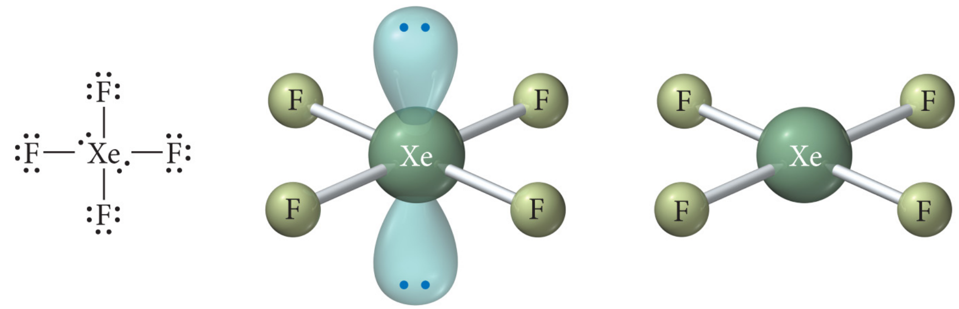
Octahedral Electronic Geometry





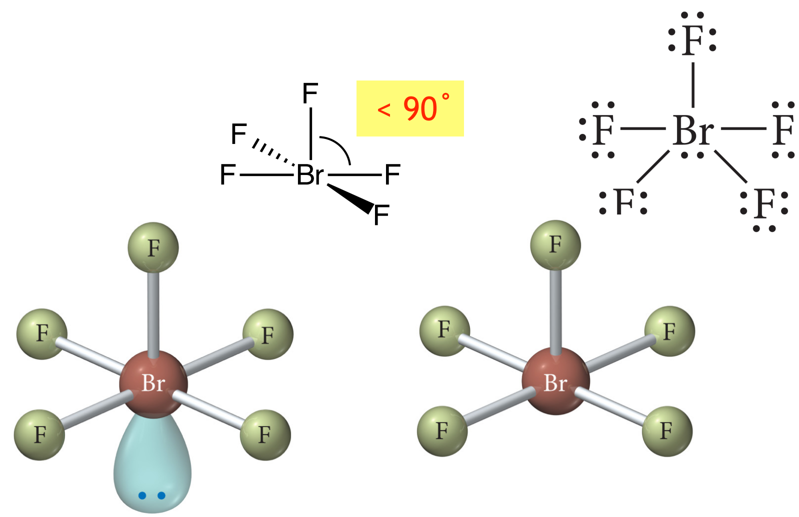
Electronic Geometry:
Octahedral

Molecular Geometry:
Octahedral



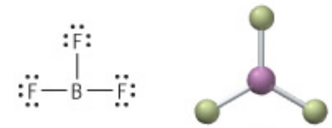
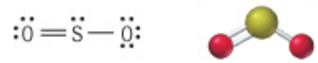
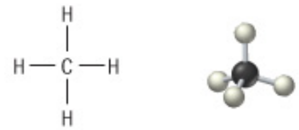
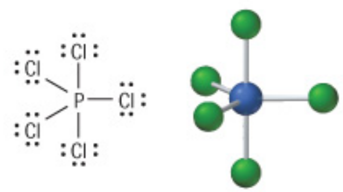
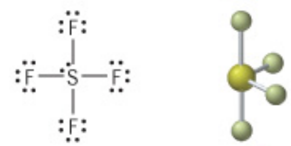
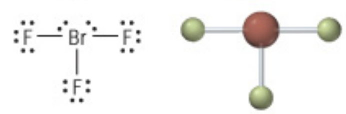
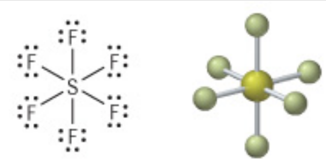
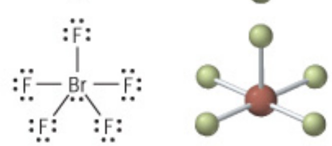
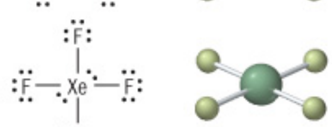
Electronic Geometry:
Octahedral

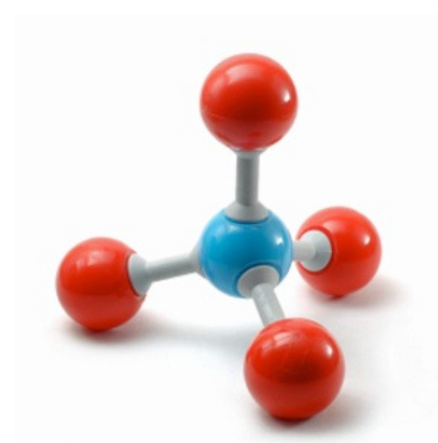
Molecular Geometry:
Square Planar



Electronic Geometry:
Octahedral

Molecular Geometry:
Square Pyramidal

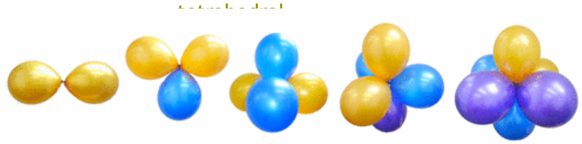
Electron Groups*	Bonding Groups	Lone Pairs	Electron Geometry	Molecular Geometry	Approximate Bond Angles	Example
2	2	0	Linear	Linear	180°	
3	3	0	Trigonal planar	Trigonal planar	120°	
3	2	1	Trigonal planar	Bent	<120°	
4	4	0	Tetrahedral	Tetrahedral	109.5°	
4	3	1	Tetrahedral	Trigonal pyramidal	<109.5°	
4	2	2	Tetrahedral	Bent	<109.5°	
5	5	0	Trigonal bipyramidal	Trigonal bipyramidal	120° (equatorial) 90° (axial)	
5	4	1	Trigonal bipyramidal	Seesaw	<120° (equatorial) <90° (axial)	
5	3	2	Trigonal bipyramidal	T-shaped	<90°	
5	2	3	Trigonal bipyramidal	Linear	180°	
6	6	0	Octahedral	Octahedral	90°	
6	5	1	Octahedral	Square pyramidal	<90°	
6	4	2	Octahedral	Square planar	90°	



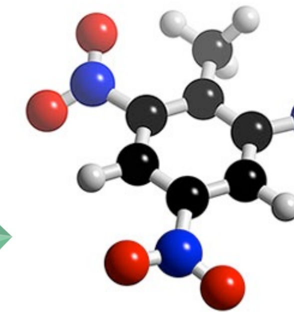
	Electronic Geometry	Molecular Geometry	Bond Angles
1 e pair	Linear	Linear	180˚
2 e pair	Linear 	Linear	180˚
		Linear	
3 e pair	Trigonal Planar 	Trigonal Planar	120˚
		Bent	
		Linear	
4 e pair	Tetrahedral 	Tetrahedral	109.5˚
		Trigonal Pyramidal	
		Bent	
		Linear	
5 e pair	Trigonal Bipyramidal 	Trigonal Bipyramidal	90˚ and 120˚
		See-saw	
		T-Shaped	
		Linear	
		Linear	
6 e pair	Octahedral 	Octahedral	90˚
		Square Pyramidal	
		Square Planar	
		T-Shaped	
		Linear	
		Linear	

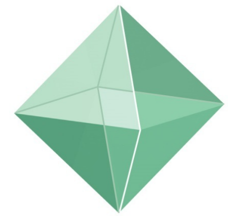
Valence Shell Electron Pair Repulsion

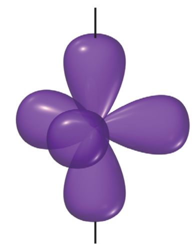
- Microscopic properties
  - Composition, Connectivity & Shape
  - Molecular Shape
    - eg: sense of taste; active sites
- VSEPR Theory: Electronic Geometry
  - Kinds of Electron Groups
  - Electron Domains
  - Electron Pair Repulsion
  - Basic shapes (geometry)
    - linear
      - two electron groups, eg: $BeCl_2$, CO_2
    - trigonal planar
      - three electron groups, eg: BF_3, H_2CO
    - tetrahedral
      - four electron groups, eg: CH_4
    - trigonal bipyramidal
      - five electron groups, eg: PCl_5
    - octahedral
      - six electron groups, eg: SF_6
- VSEPR Theory: Molecular Geometry
  - Difference between electron and molecular geometries
  - Four electron groups with lone pairs
    - trigonal pyramidal
      - one lone pair; smaller bond angle than

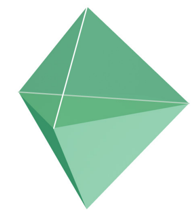


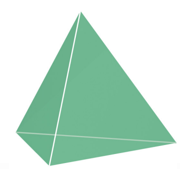
    - bent
      - two lone pairs; smaller bond angle than tetrahedral or trigonal bipyramidal
      - example: H_2O
  - Five electron groups with lone pairs
    - seesaw
      - one lone pair; goes in trigonal plane
      - example: SF_4^+
    - T-shaped
      - two lone pairs, both in trigonal plane
      - example: BrF_3
    - linear
      - three lone pairs, all in trigonal plane
      - example: XeF_2
  - Six electron groups with lone pairs
    - square pyramidal
      - example: BrF_5
    - square planar
      - lone pairs 180o apart; example: XeF_4
- VSEPR Theory: Predicting Geometries
  - Procedure
    - Draw the Lewis structure.
    - Find the number of domains
      - Which gives you the electronic geometry.
      - Divide the domains into bonding and non-bonding groups.
    - Draw the molecular geometry.
    - Write the name of the name of that geometry.
  - Shapes of molecules with more than one central atom.

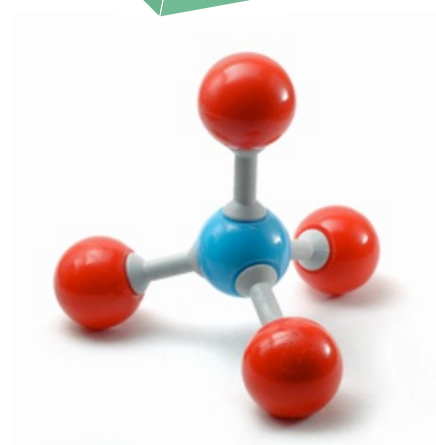








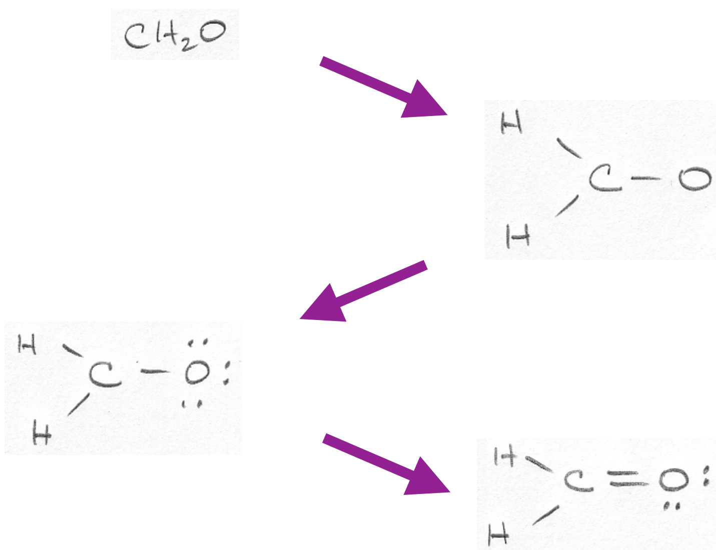




VSEPR Process

- What is the molecular geometry of carbon in CH_2O?

- To find the molecular geometry of an atom:
  - Draw the Lewis structure.
  - Find the number of domains
    - Which gives you the electronic geometry.
  - Divide the domains into bonding and non-bonding groups.
    - Draw the molecular geometry.
    - Write the name of the name of that geometry.



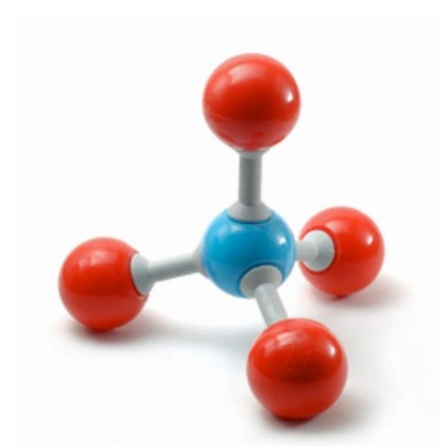
C $4e^-$
2x H $2e^-$
O $6e^-$
$12e^-$

3 bonds $6e^-$
$6e^-$

$6e^-$
0

Carbon has 3 domains.
(0 nonbonding; 3 bonding)

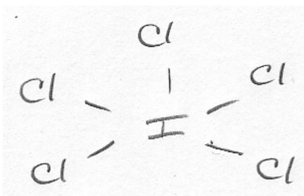
Electronic → Trigonal Planar
Molecular → Trigonal Planar

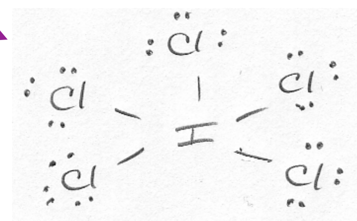


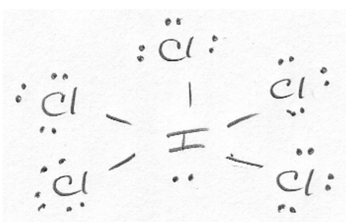
VSEPR Process

- What is the molecular geometry of iodine in ICl_5?

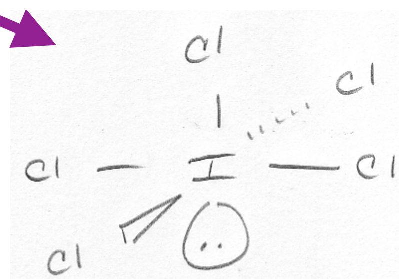
- To find the molecular geometry of an atom:
  - Draw the Lewis structure.
  - Find the number of domains
    - Which gives you the electronic geometry.
  - Divide the domains into bonding and non-bonding groups.
    - Draw the molecular geometry.
    - Write the name of the name of that geometry.





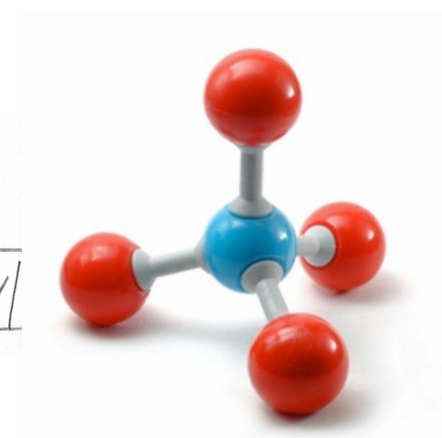


Iodine has 6 domains
(1 non bonding 5 bonding).



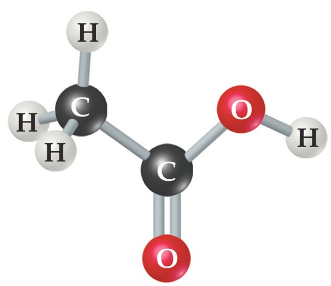
I	7
5x Cl	35
	$42e^-$
	$10e^-$
	$32e^-$
	$30e^-$
	$2e^-$

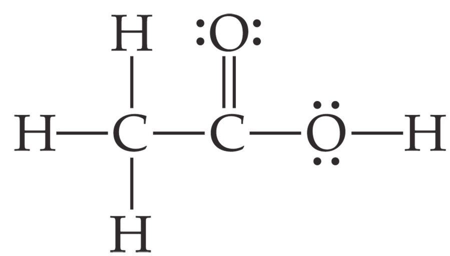
Electronic:
6 domains → Octahedral
Molecular
5 bonds → Square Pyramidal

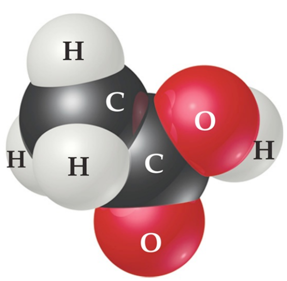


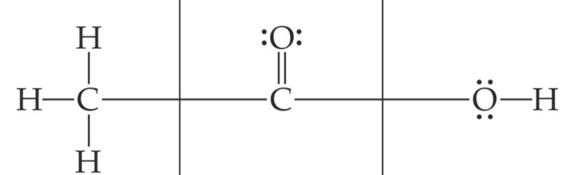
Larger Molecules

- VSEPR is a tool for understanding the geometry around each atom.
- For larger molecules, sketch out the structure using the Lewis model, and then apply VSEPR separately to each central atom.

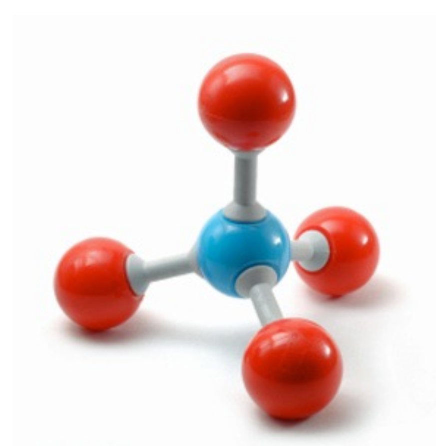








Number of electron domains	4	3	4
Electron-domain geometry	Tetrahedral	Trigonal planar	Tetrahedral
Predicted bond angles	109.5°	120°	109.5°



Valence Shell Electron Pair Repulsion

- Microscopic properties
  - Composition, Connectivity & Shape
  - Molecular Shape
    - eg: sense of taste; active sites
- VSEPR Theory: Electronic Geometry
  - Kinds of Electron Groups
  - Electron Domains
  - Electron Pair Repulsion
  - Basic shapes (geometry)
    - linear
      - two electron groups, eg: $BeCl_2$, CO_2
    - trigonal planar
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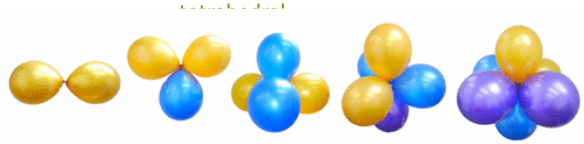

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      - example: H_2O
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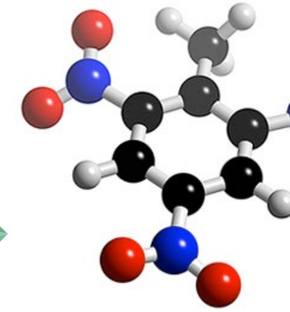

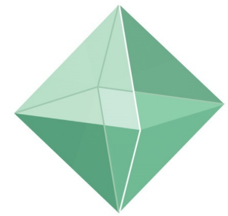

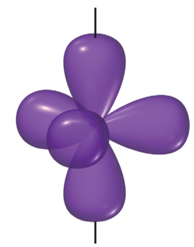

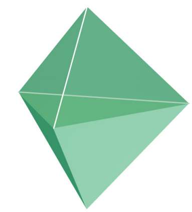

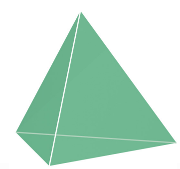

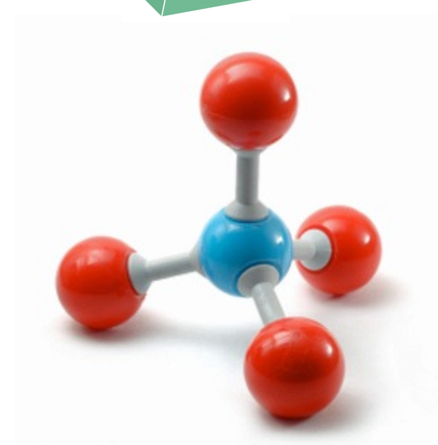

Questions?