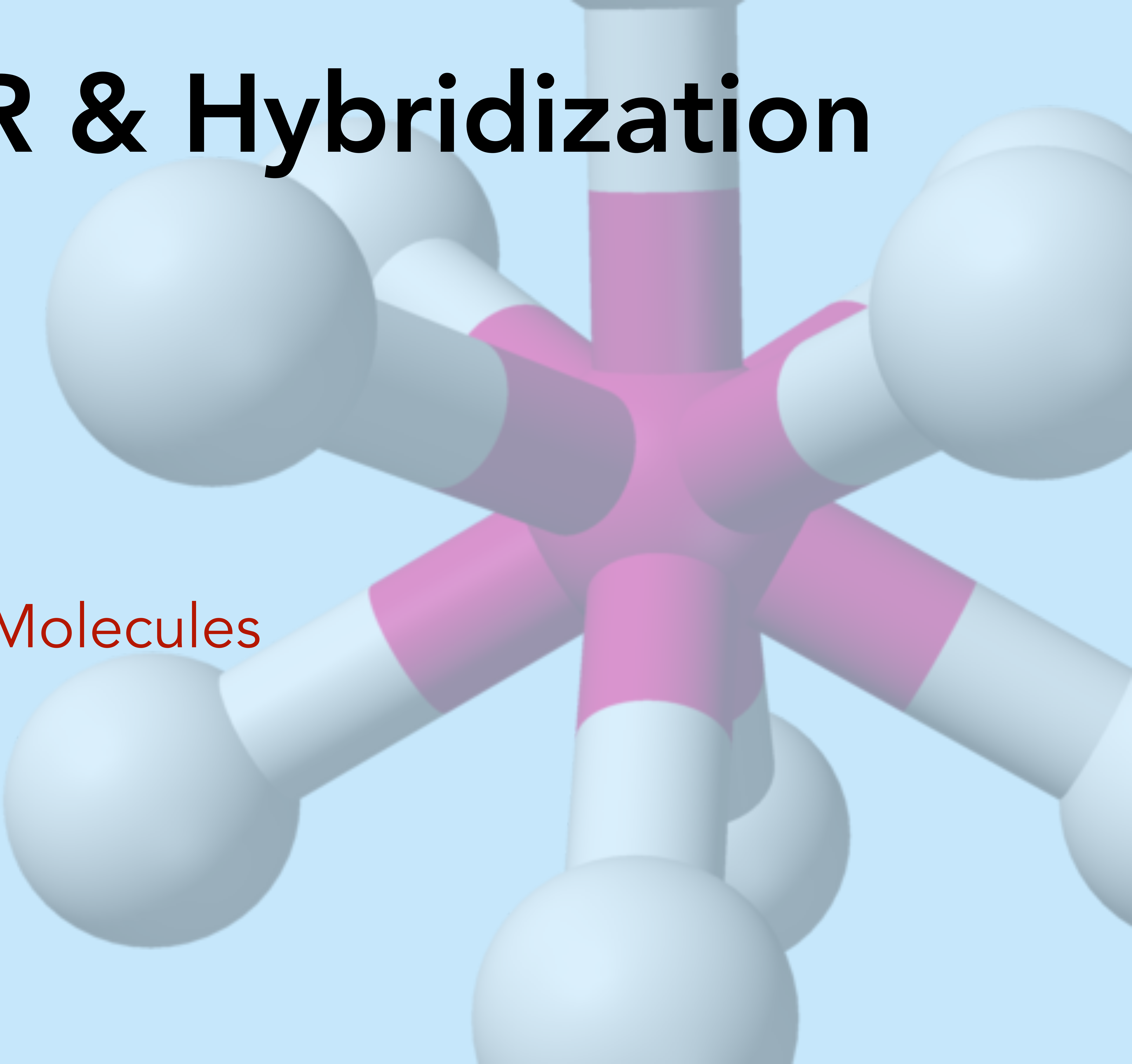
2.7 VSEPR & Hybridization

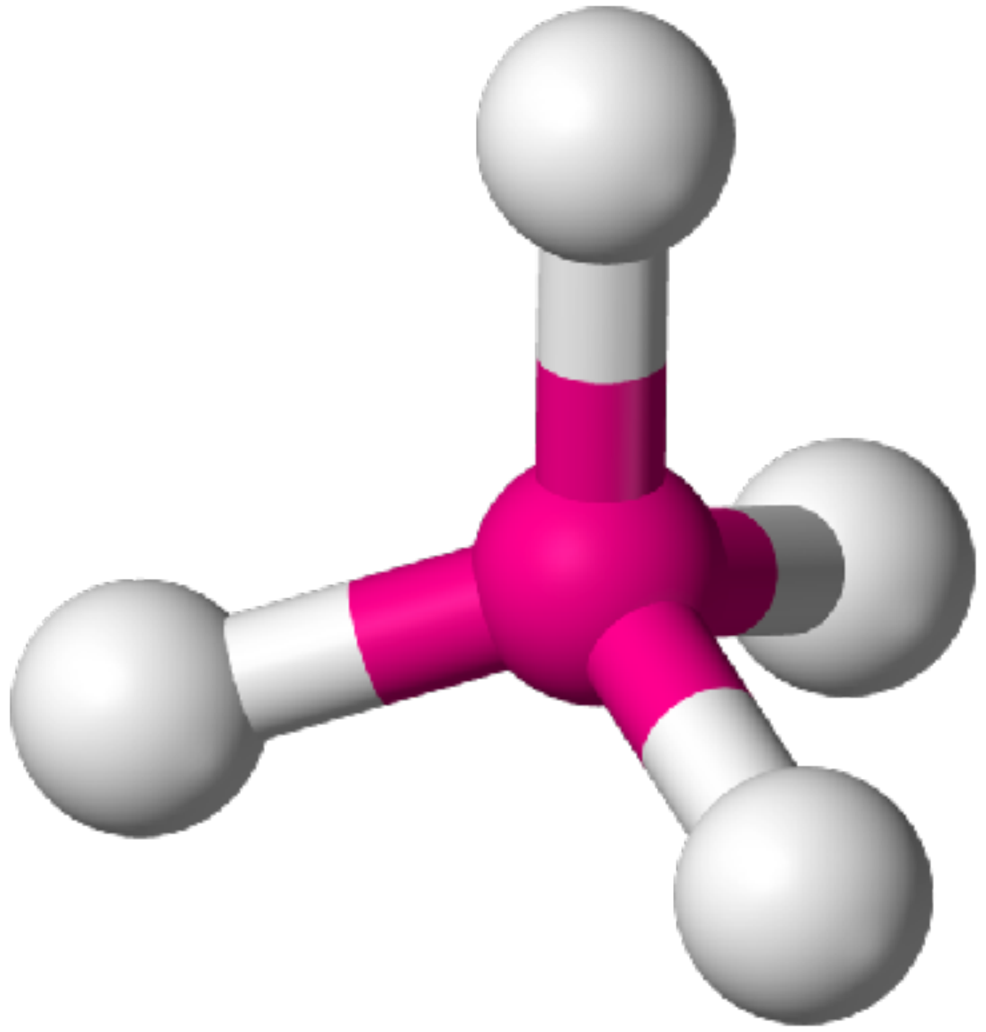
- VSEPR Theory
- Molecular Shape
- Polar and Non-polar Molecules
- Hybrid Orbitals

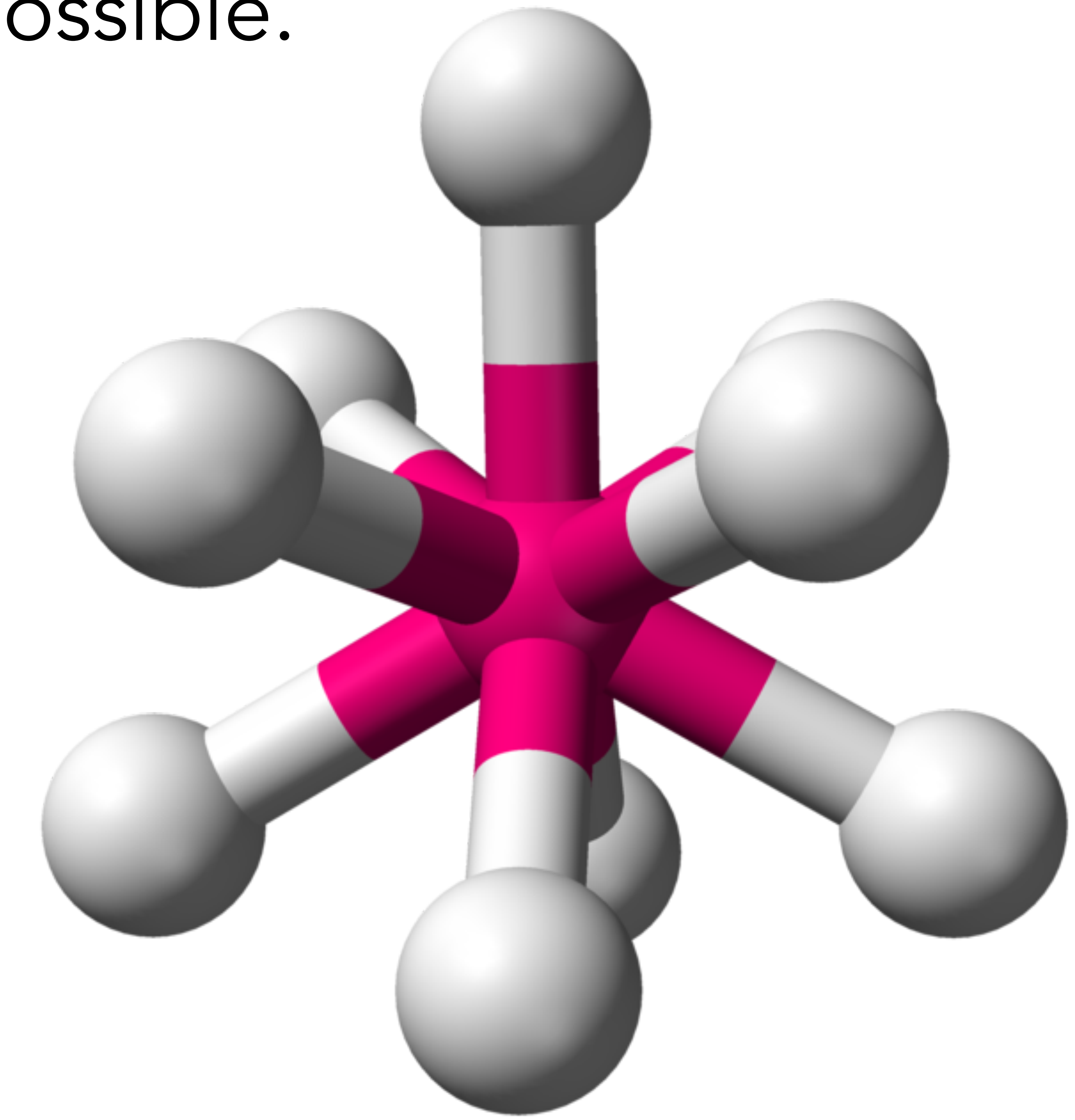


VSEPR Theory

Valence **S**hell **E**lectron **P**air **R**epulsion Theory

- Charge clouds (centers) repel each other due to Coulombic forces.
- Terminal atoms move as far away from one another as possible.
- Distinctive geometric shapes result.





VSEPR Theory

Two Step Process

1. Count the number of charge clouds, bonds and lone pairs around the **central atom**.
2. Predict the shape.
    a. 13 shapes which you must know by name and the bond angles (FLASH CARDS)

VSEPR Theory

Charge Clouds (Centers)

- One single bond (2 electrons)
- One double bond (4 electrons)
- One triple bond (6 electrons)
- One lone pair (2 electrons)
- One single unpaired electron

One Bond

- single bond (2 electrons)
- double bond (4 electrons)
- triple bond (6 electrons)

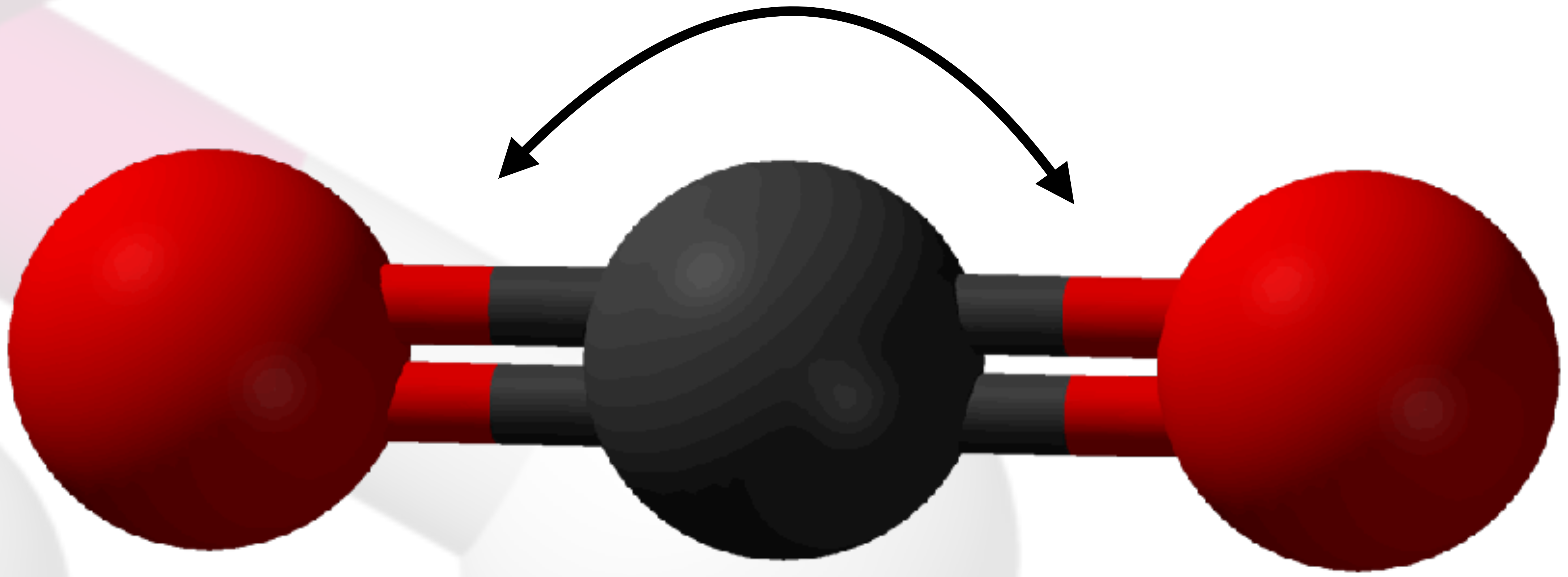
Lone Pairs

- 1 lone pair = 2 electrons
- 1 single unpaired electron

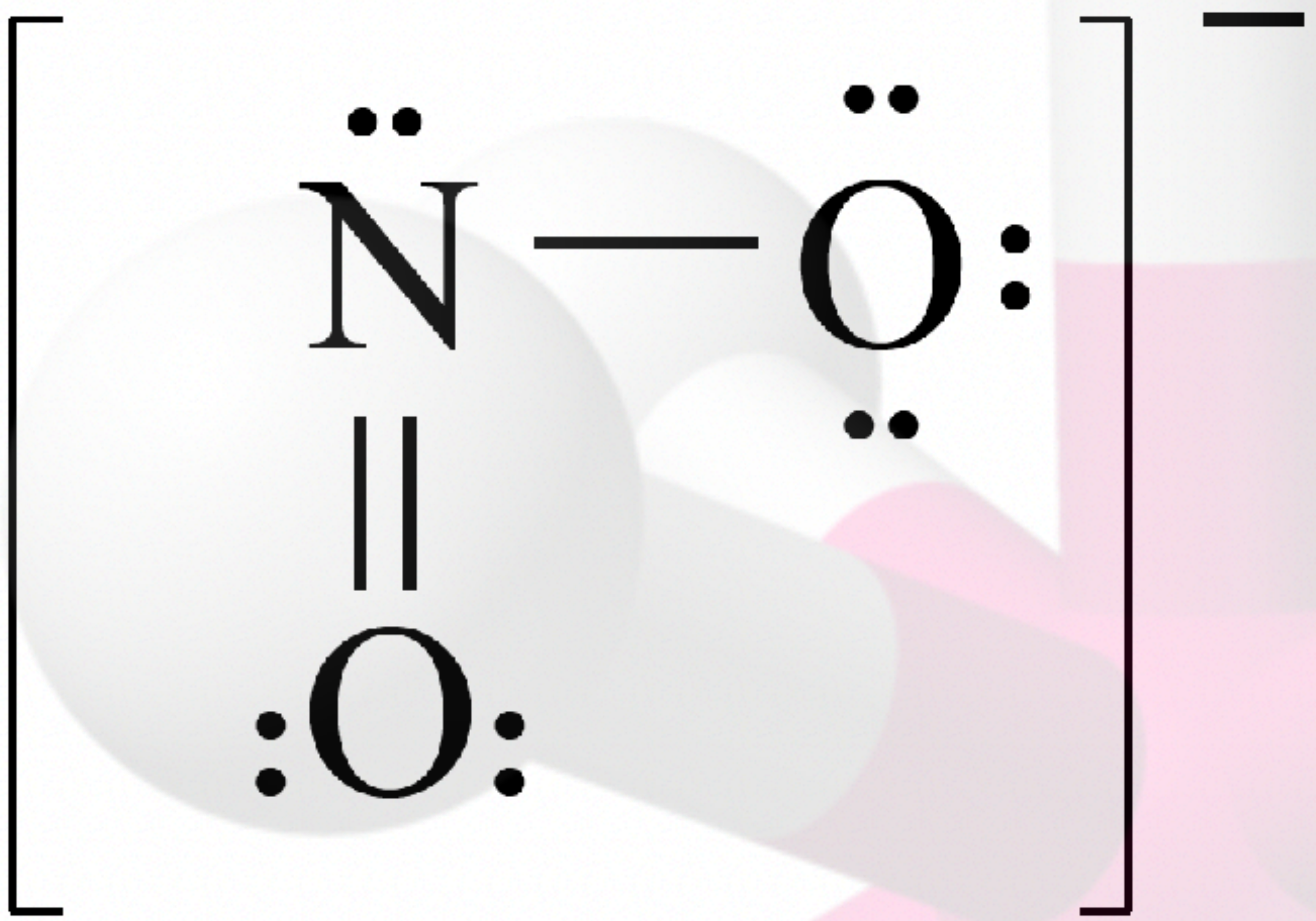
2 Charge Clouds (CO_2)

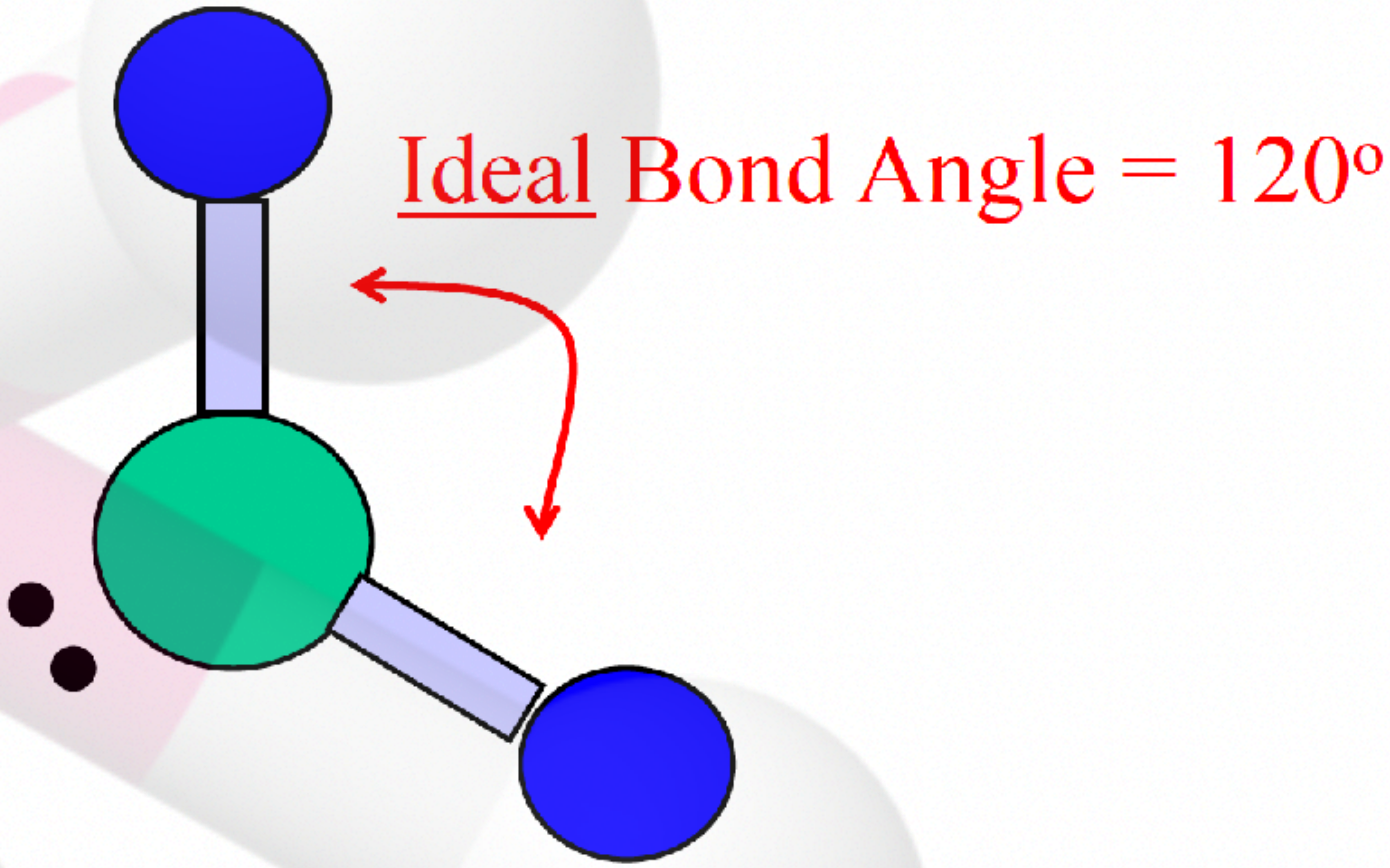
Charge Clouds	Bonds	Lone Pairs	Shape
2	2	0	Linear

Bond Angle = 180°



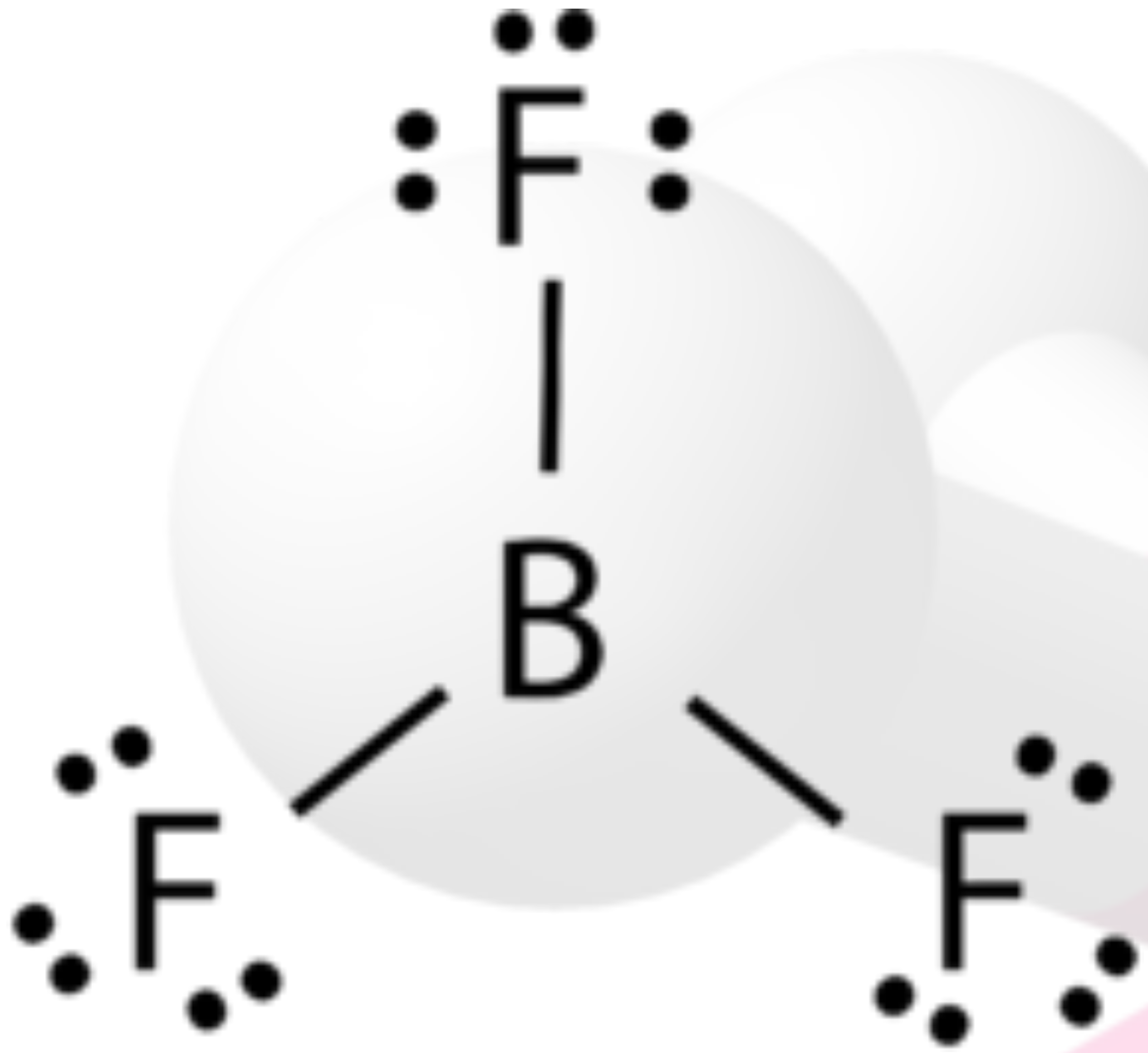
3 Charge Clouds (NO_2^-)

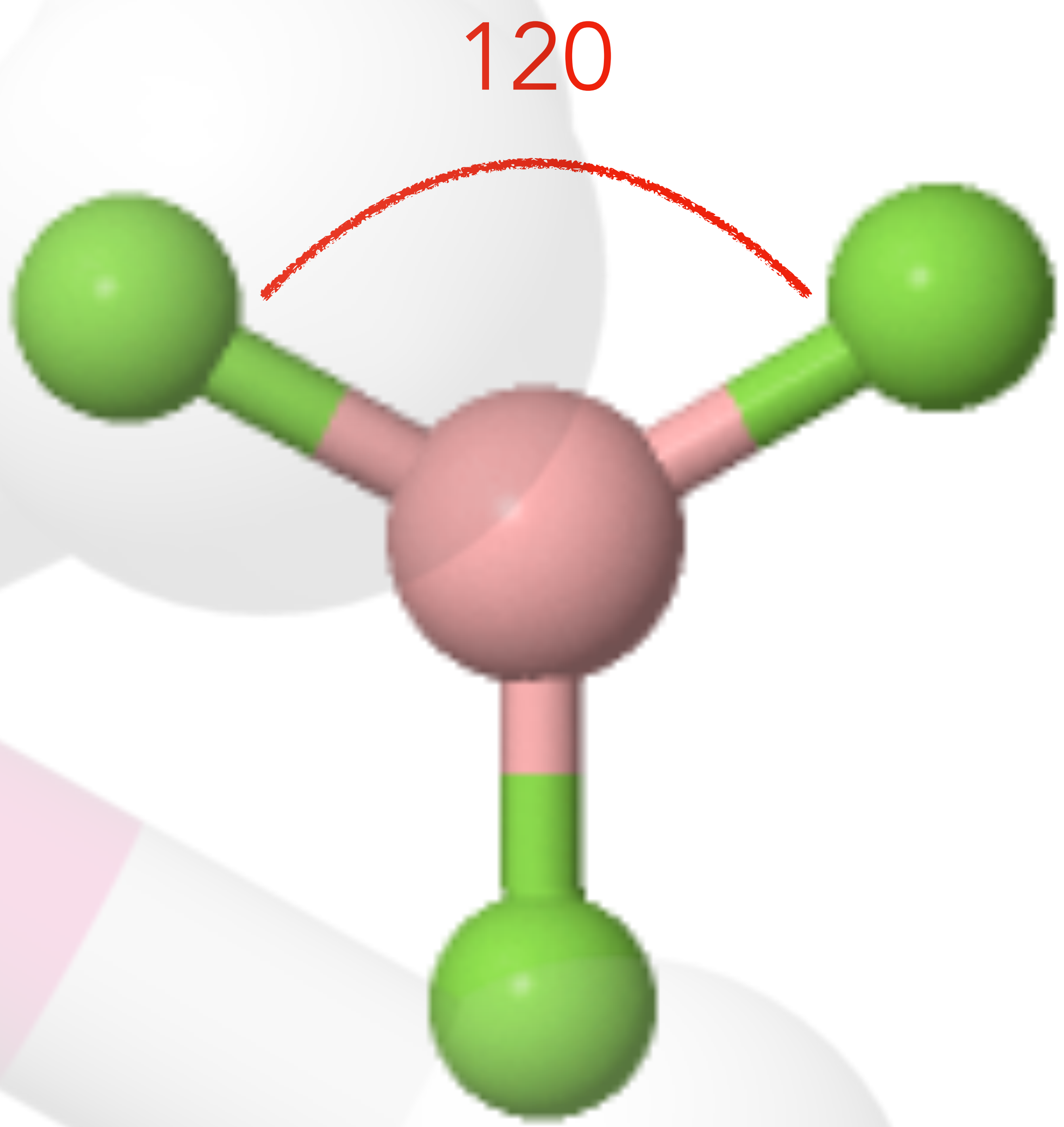




Charge Clouds	Bonds	Lone Pairs	Shape
3	2	1	Bent

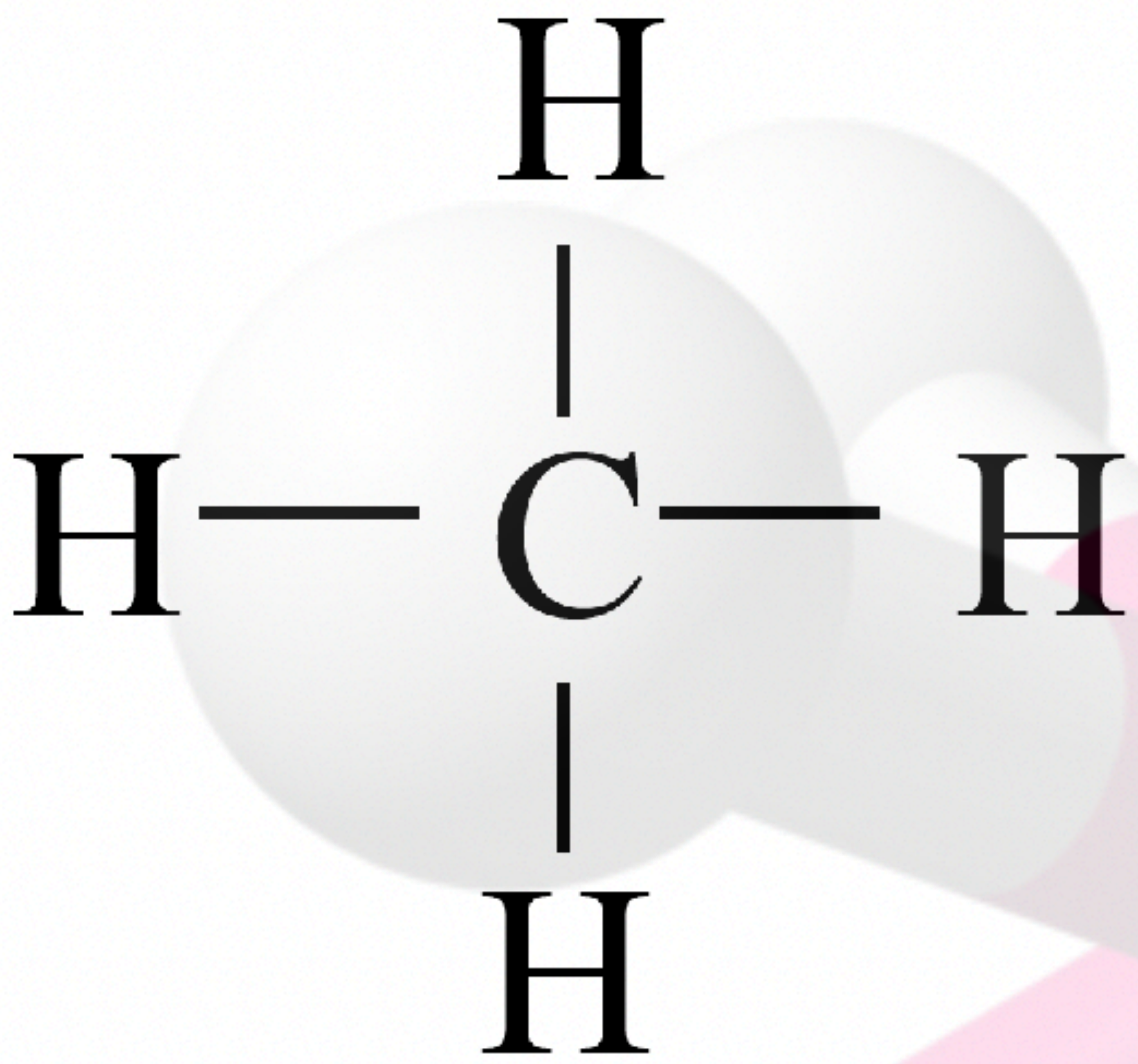
3 Charge Clouds (BF_3)

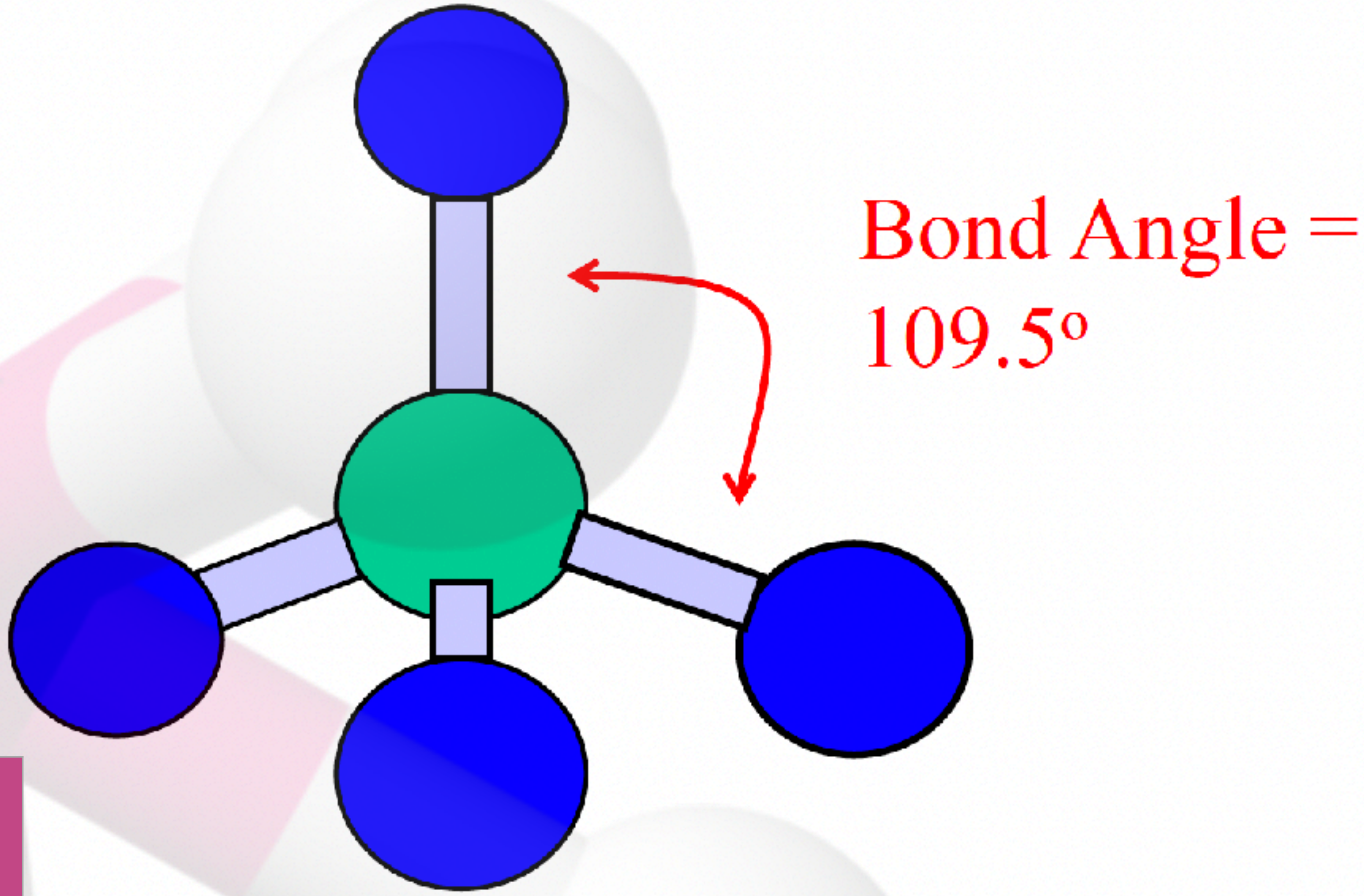




Charge Clouds	Bonds	Lone Pairs	Shape
3	3	0	Trigonal Planar

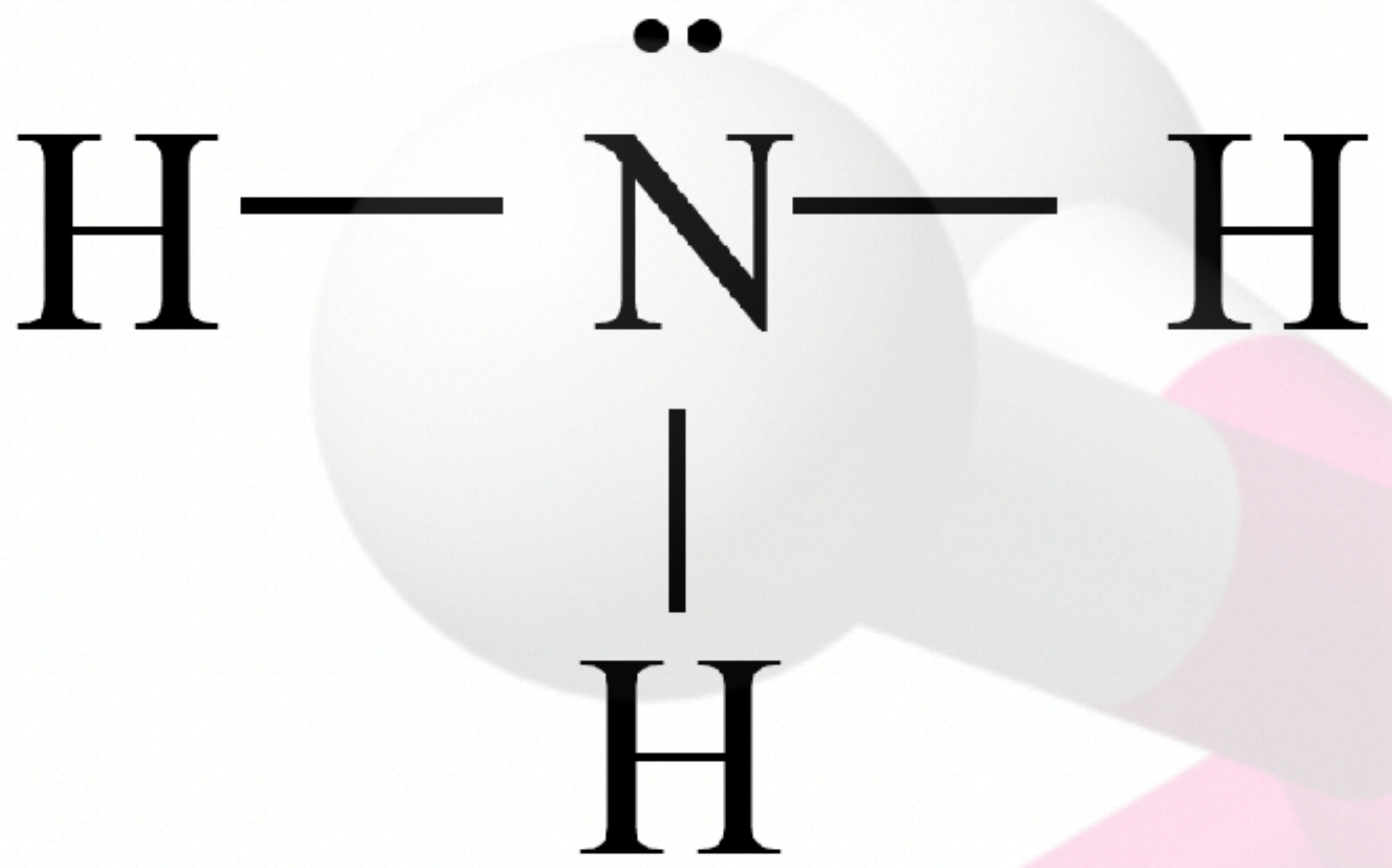
4 Charge Clouds (CH_4)

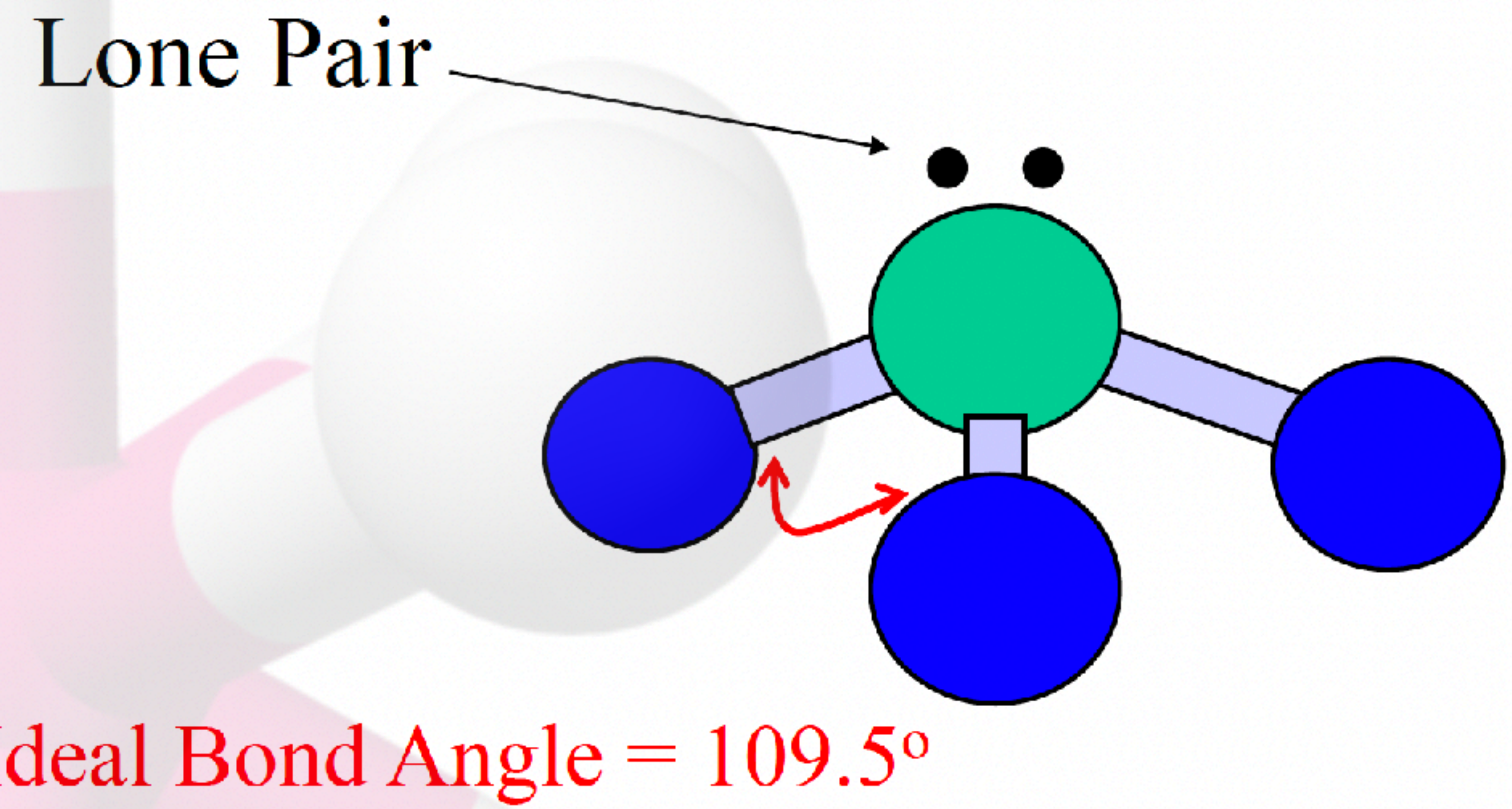




Charge Clouds	Bonds	Lone Pairs	Shape
4	4	0	Tetrahedral

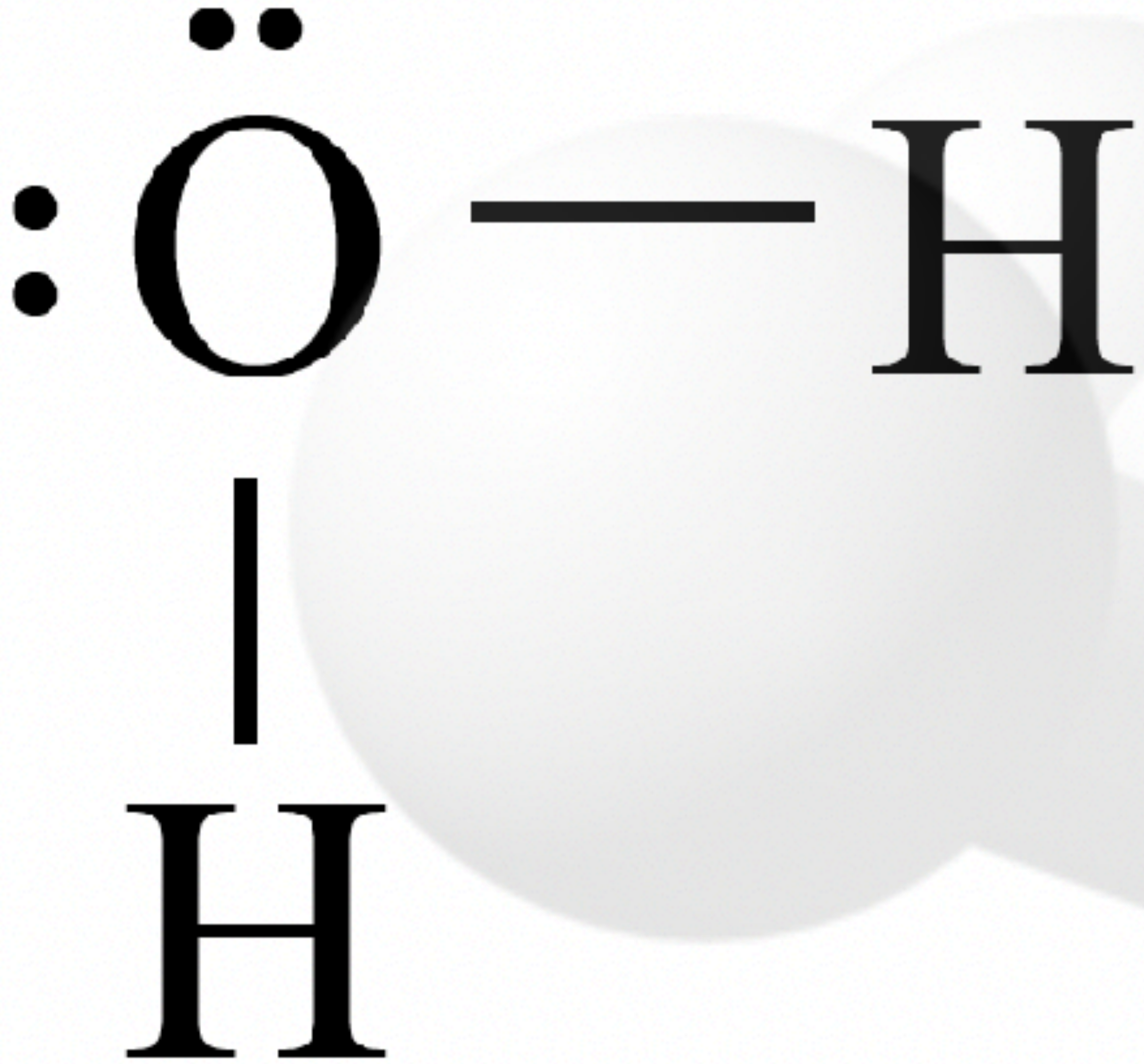
4 Charge Clouds (NH_3)

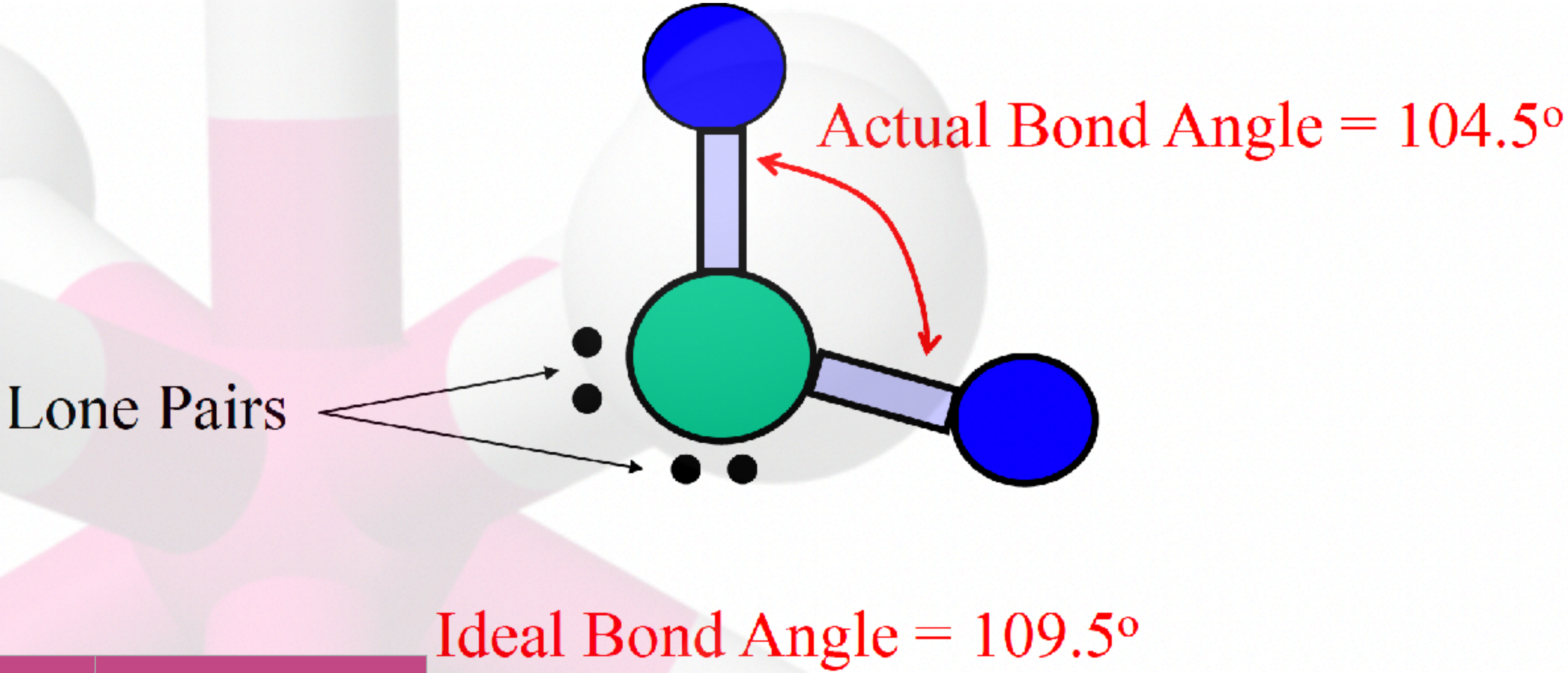




Charge Clouds	Bonds	Lone Pairs	Shape
4	3	1	Trigonal Pyramidal

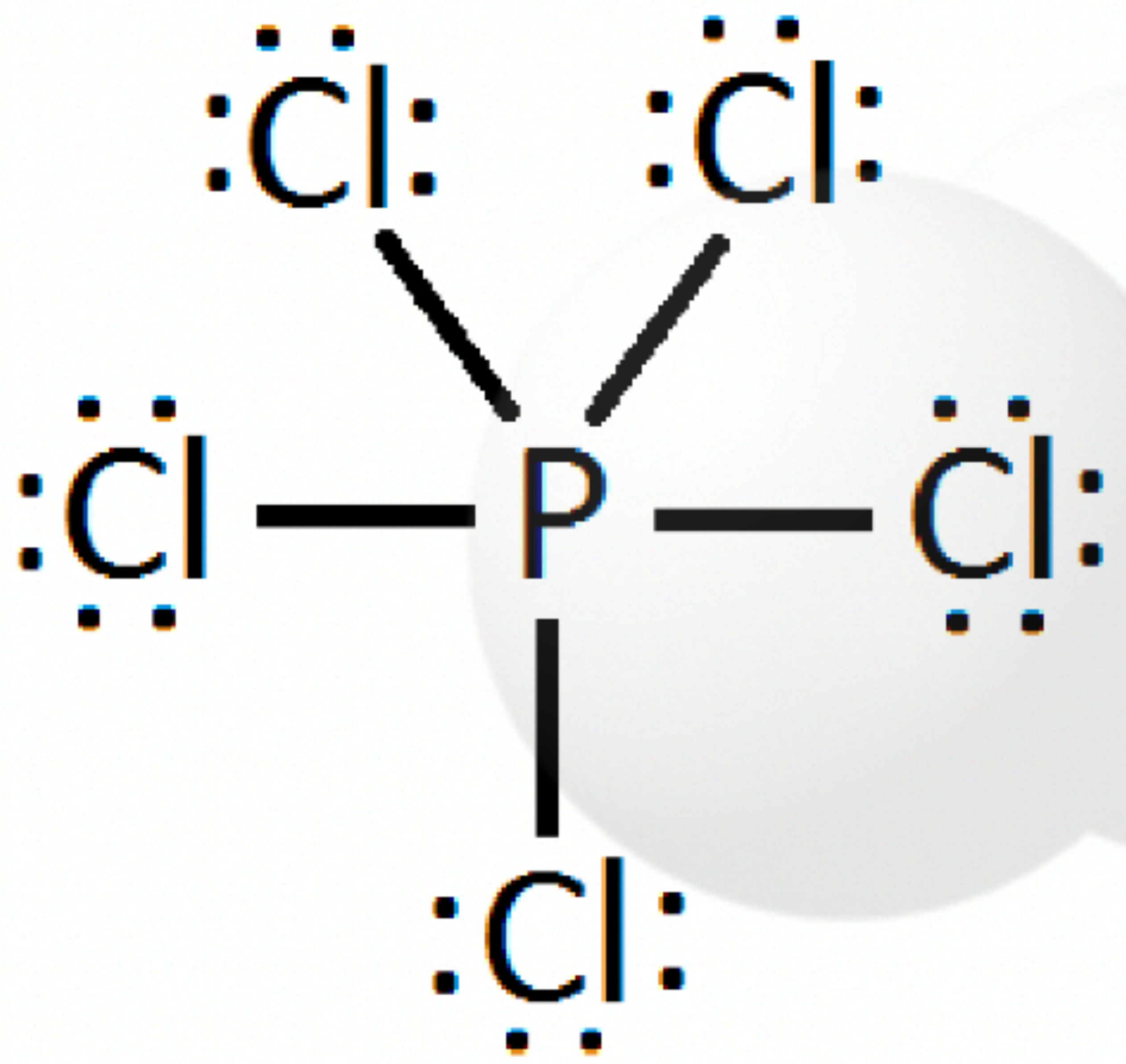
4 Charge Clouds (H_2O)

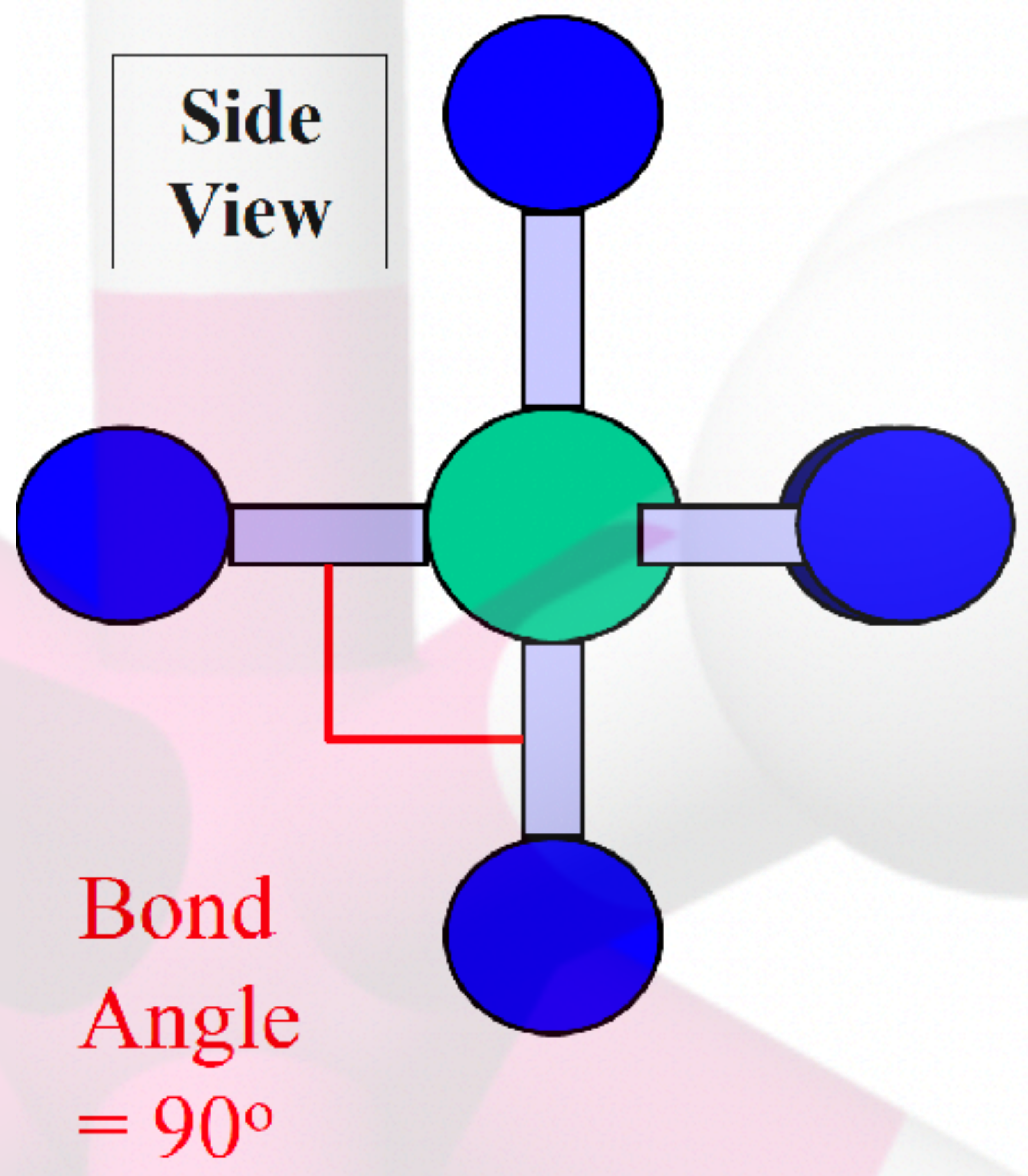


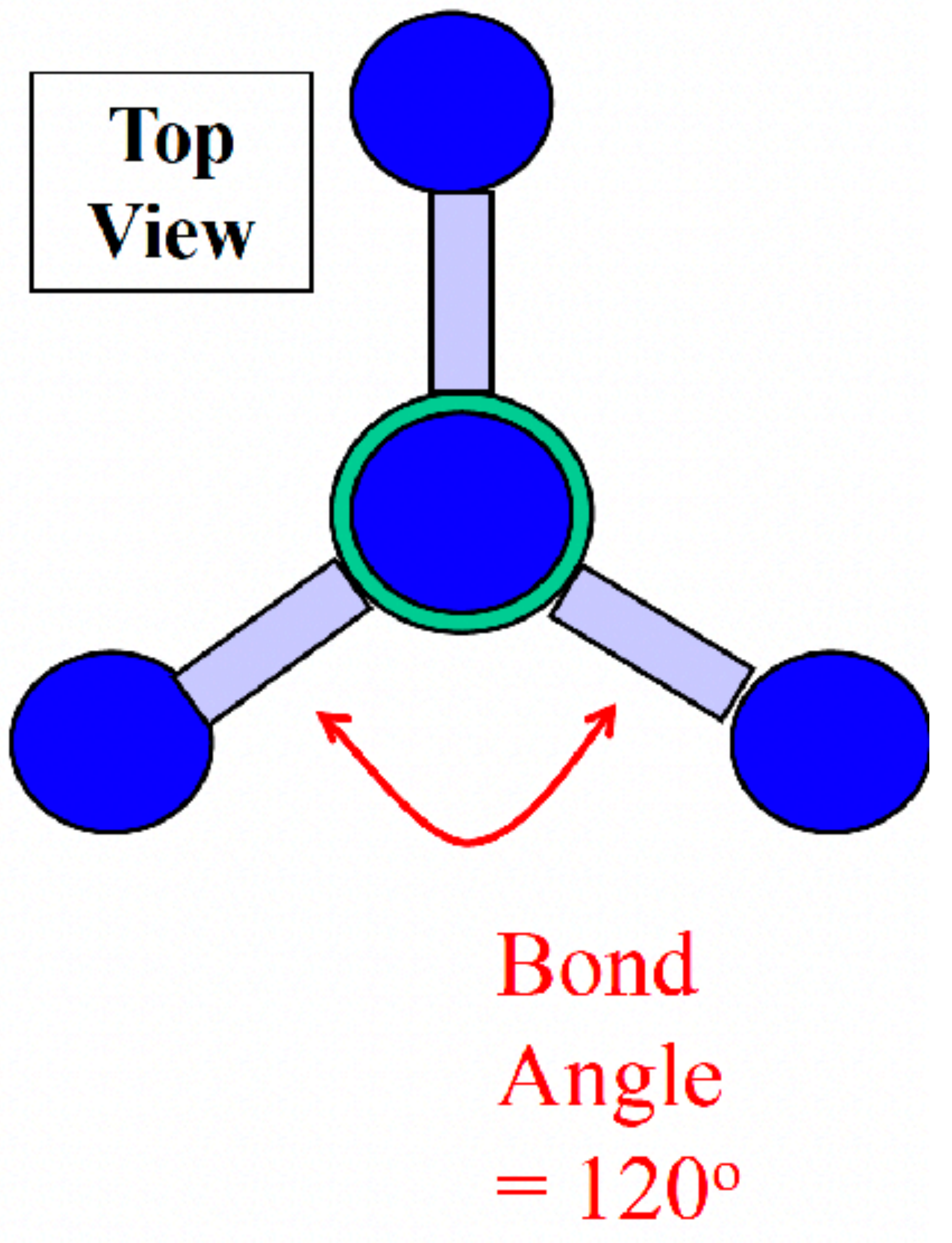


Charge Clouds	Bonds	Lone Pairs	Shape
4	2	2	Bent

5 Charge Clouds (PCl_5)

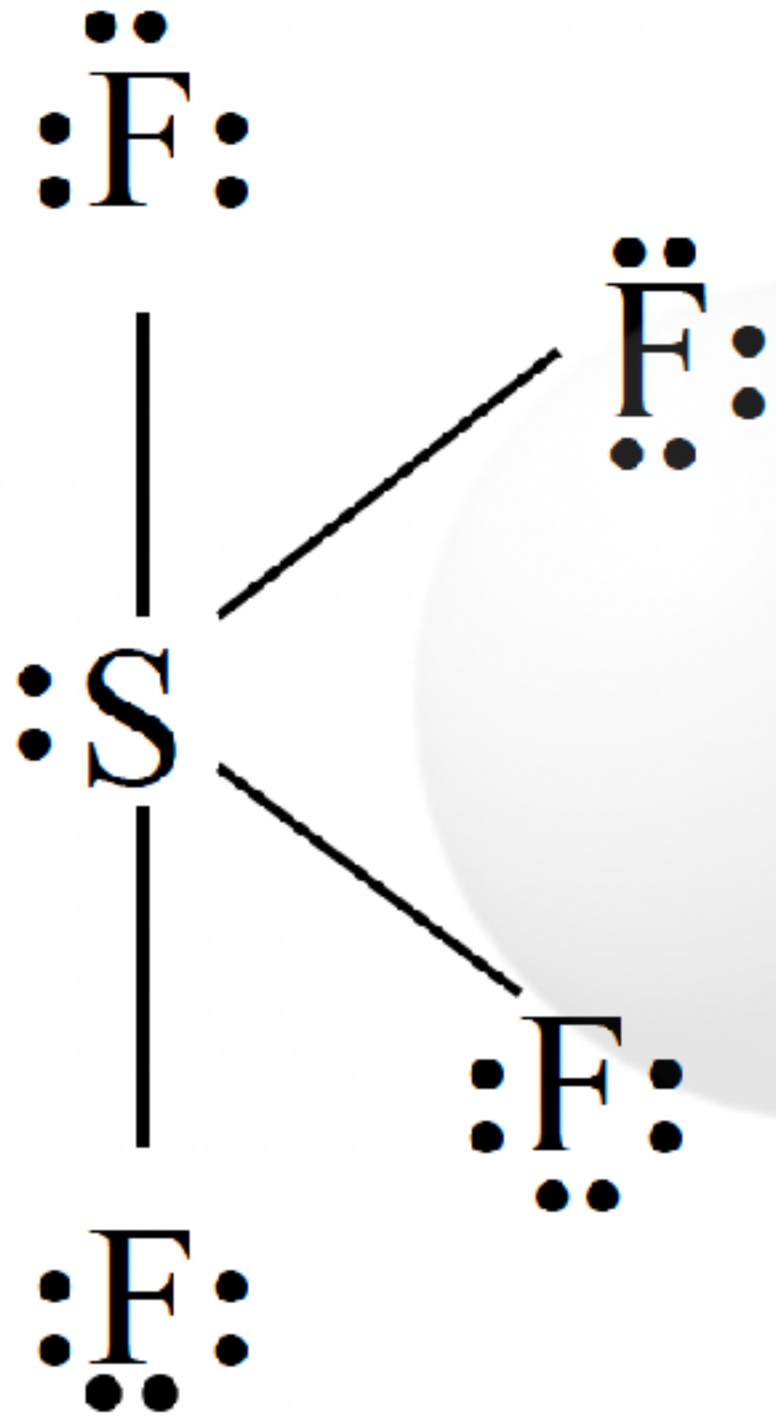


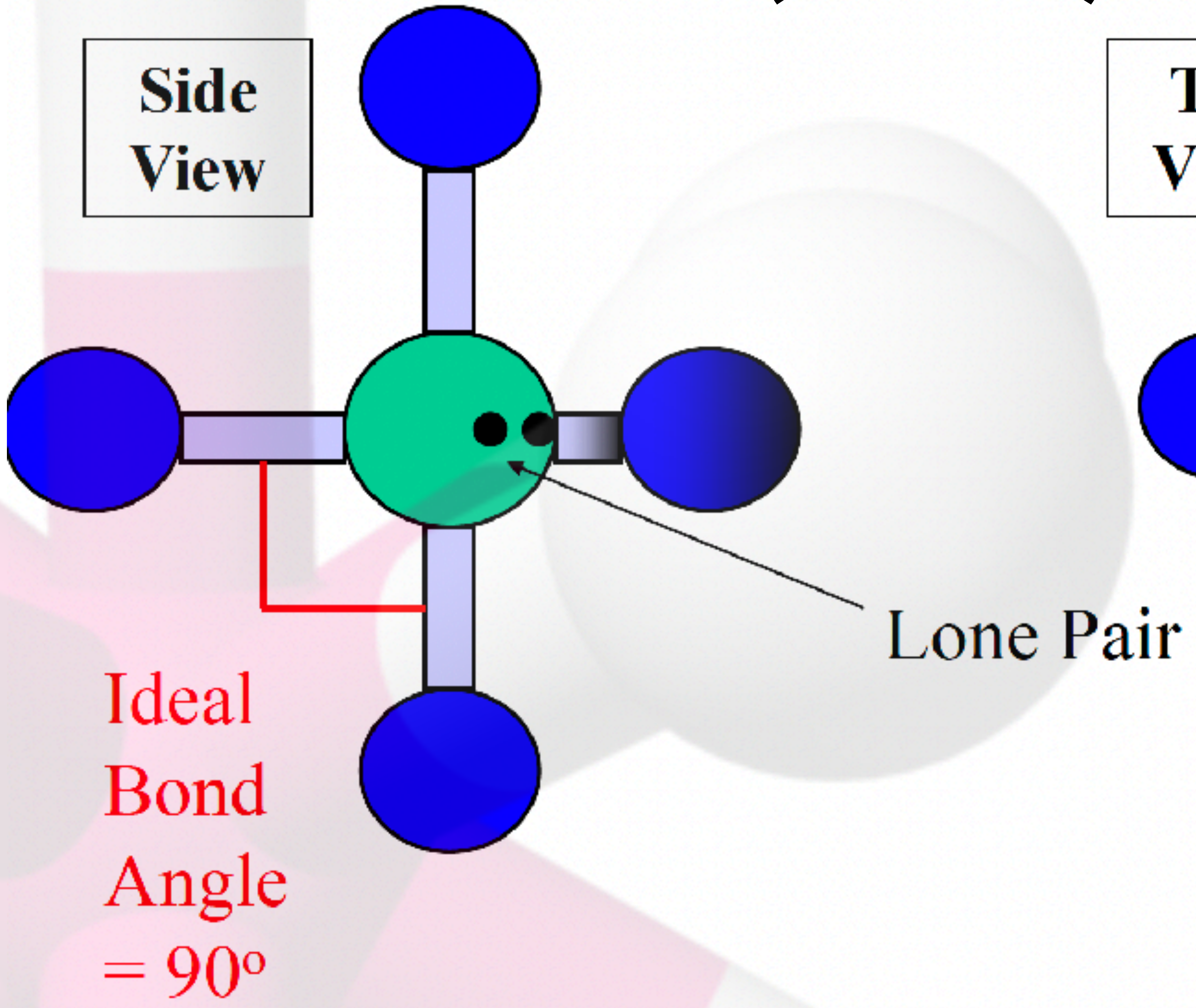


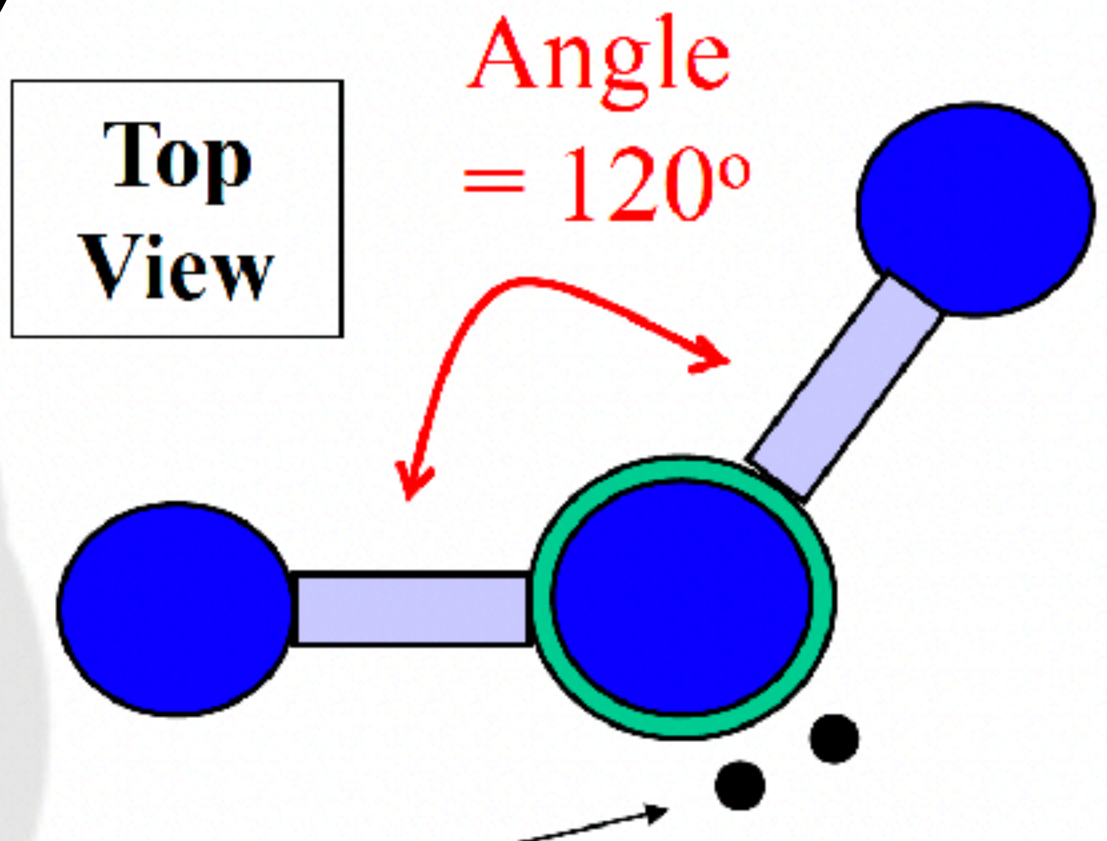


Charge Clouds	Bonds	Lone Pairs	Shape
5	5	0	Trigonal Bipyramidal

5 Charge Clouds (SF_4)

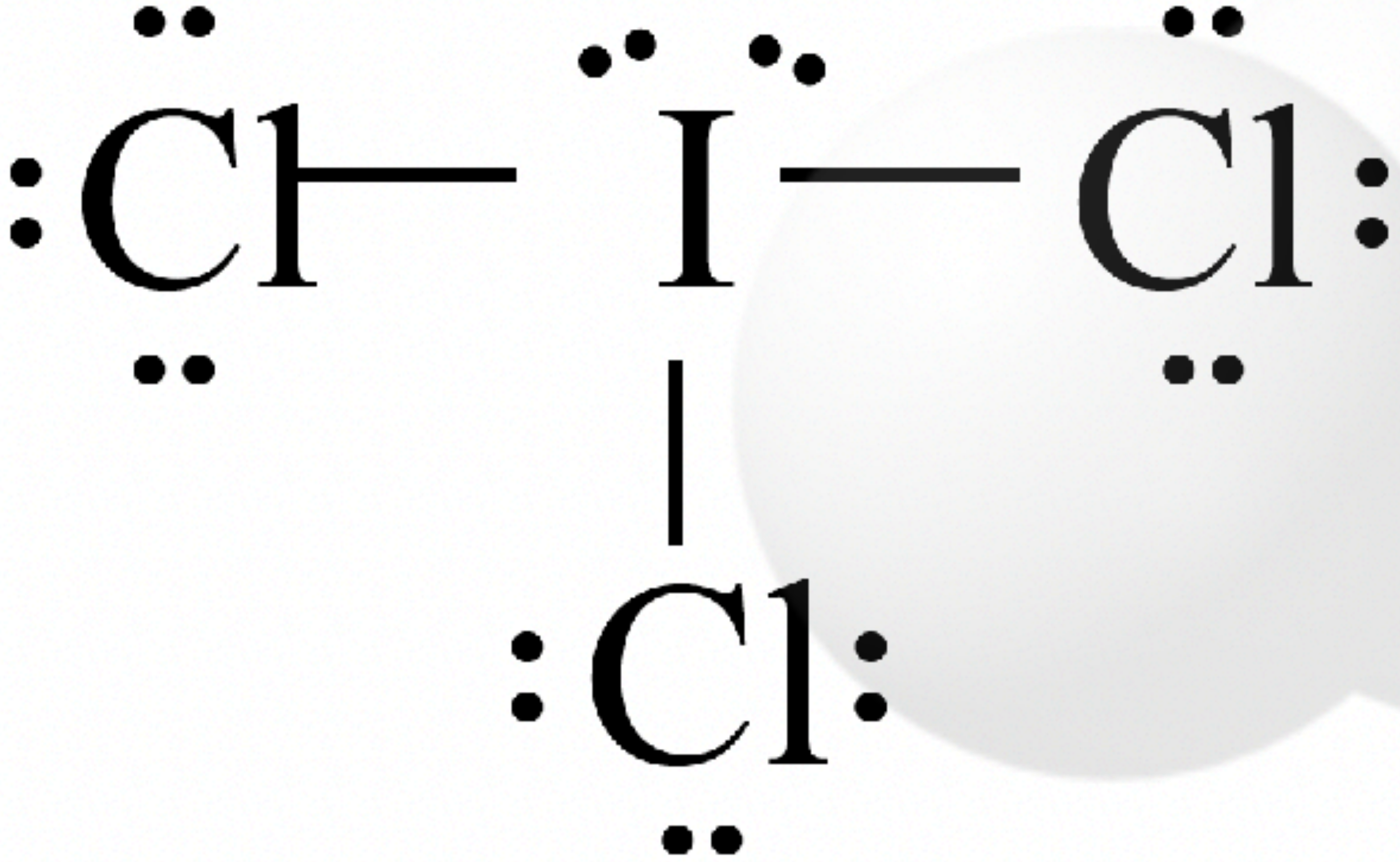


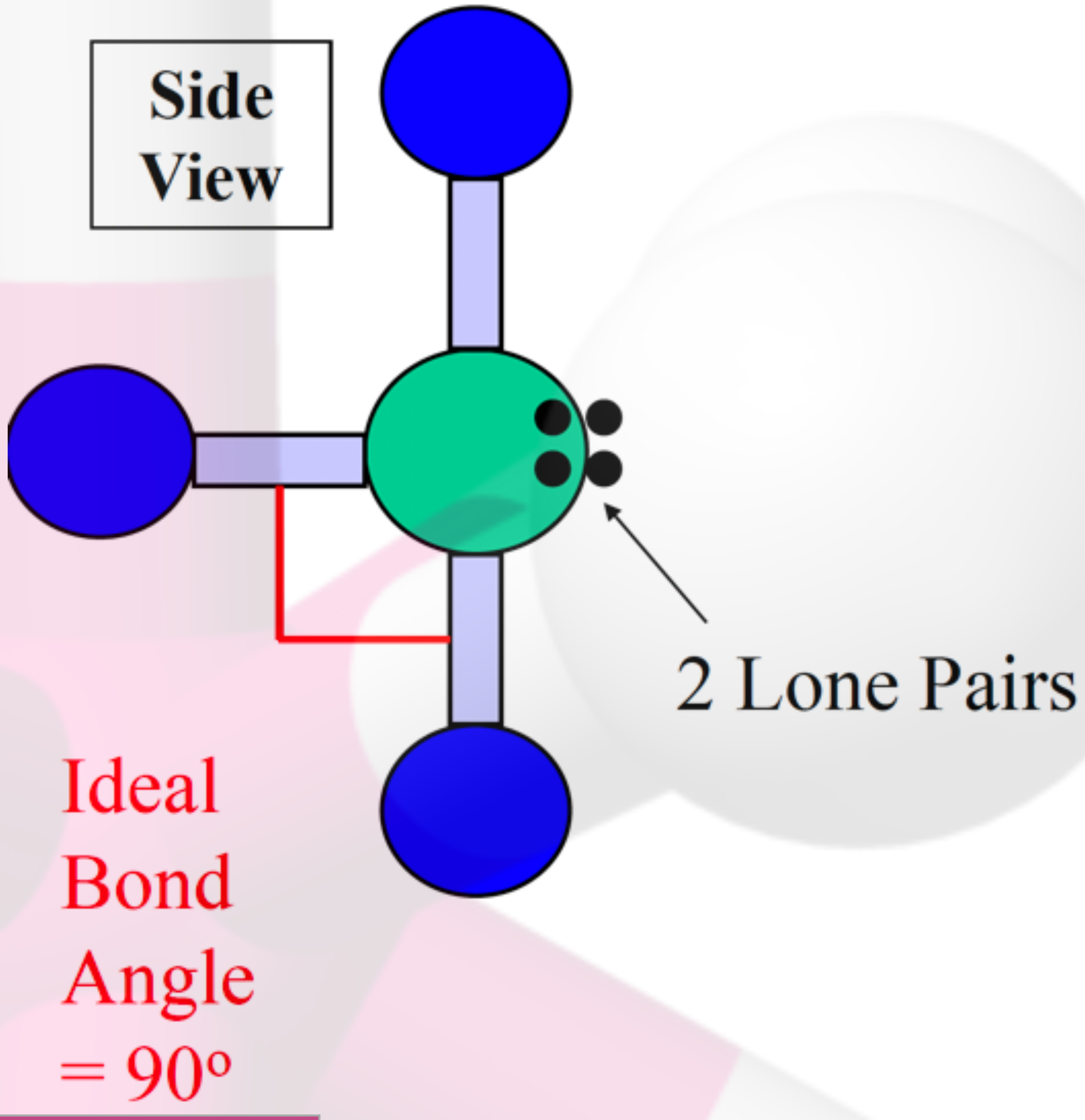


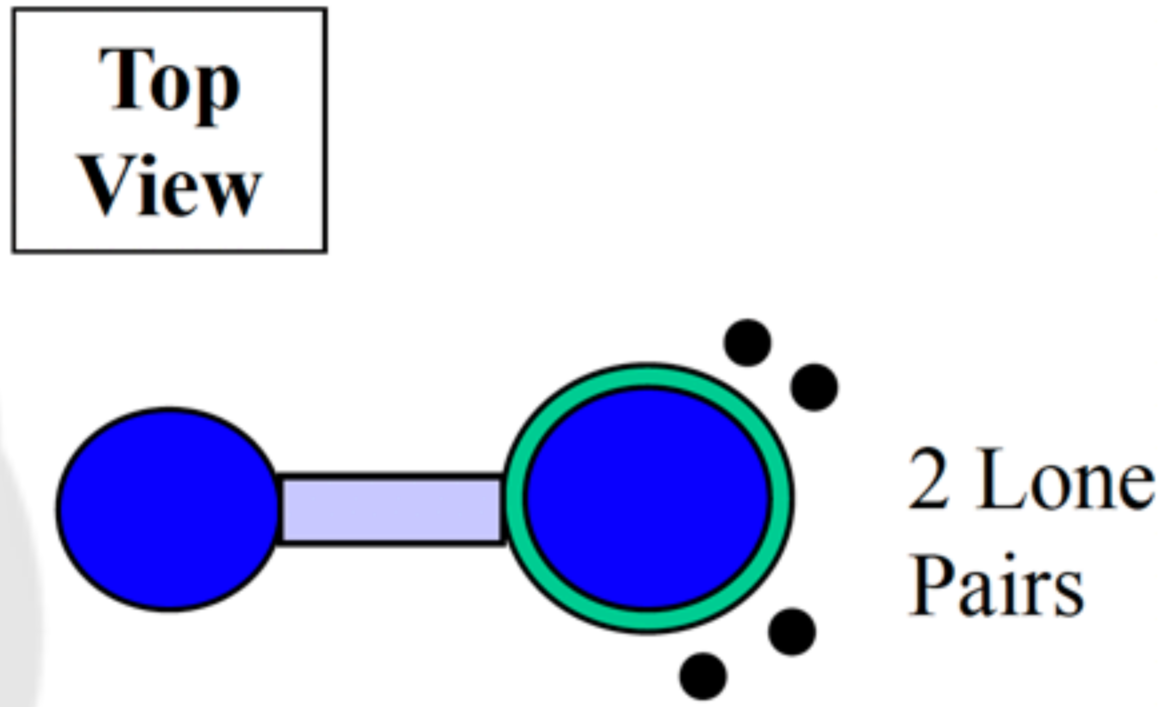


Charge Clouds	Bonds	Lone Pairs	Shape
5	4	1	Seesaw

5 Charge Clouds (ICl_3)

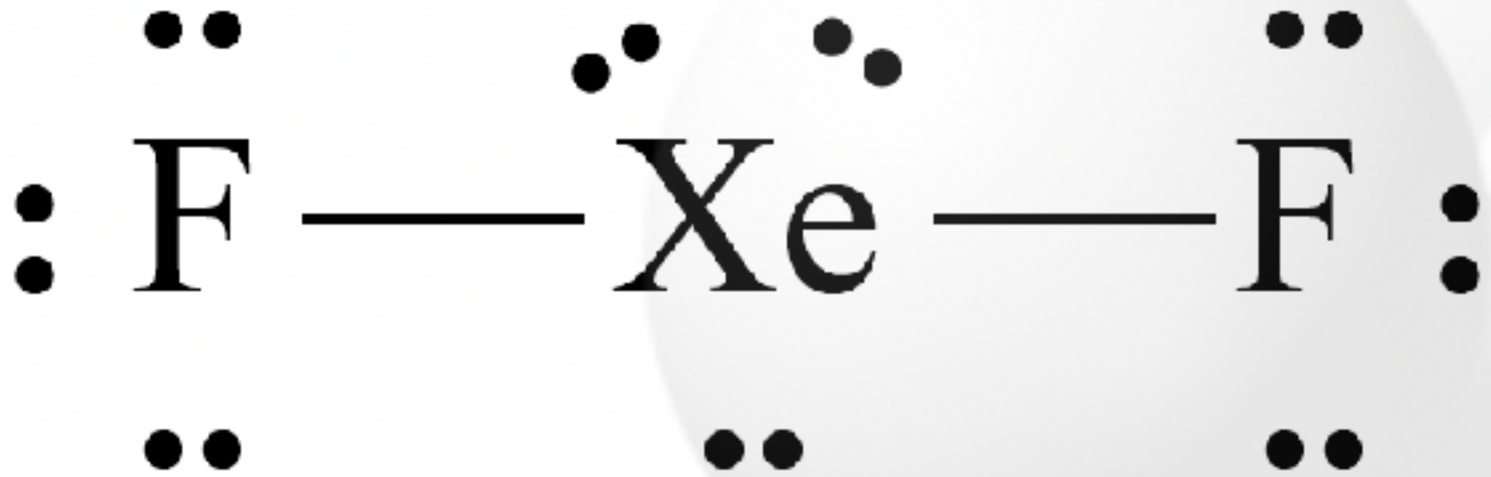


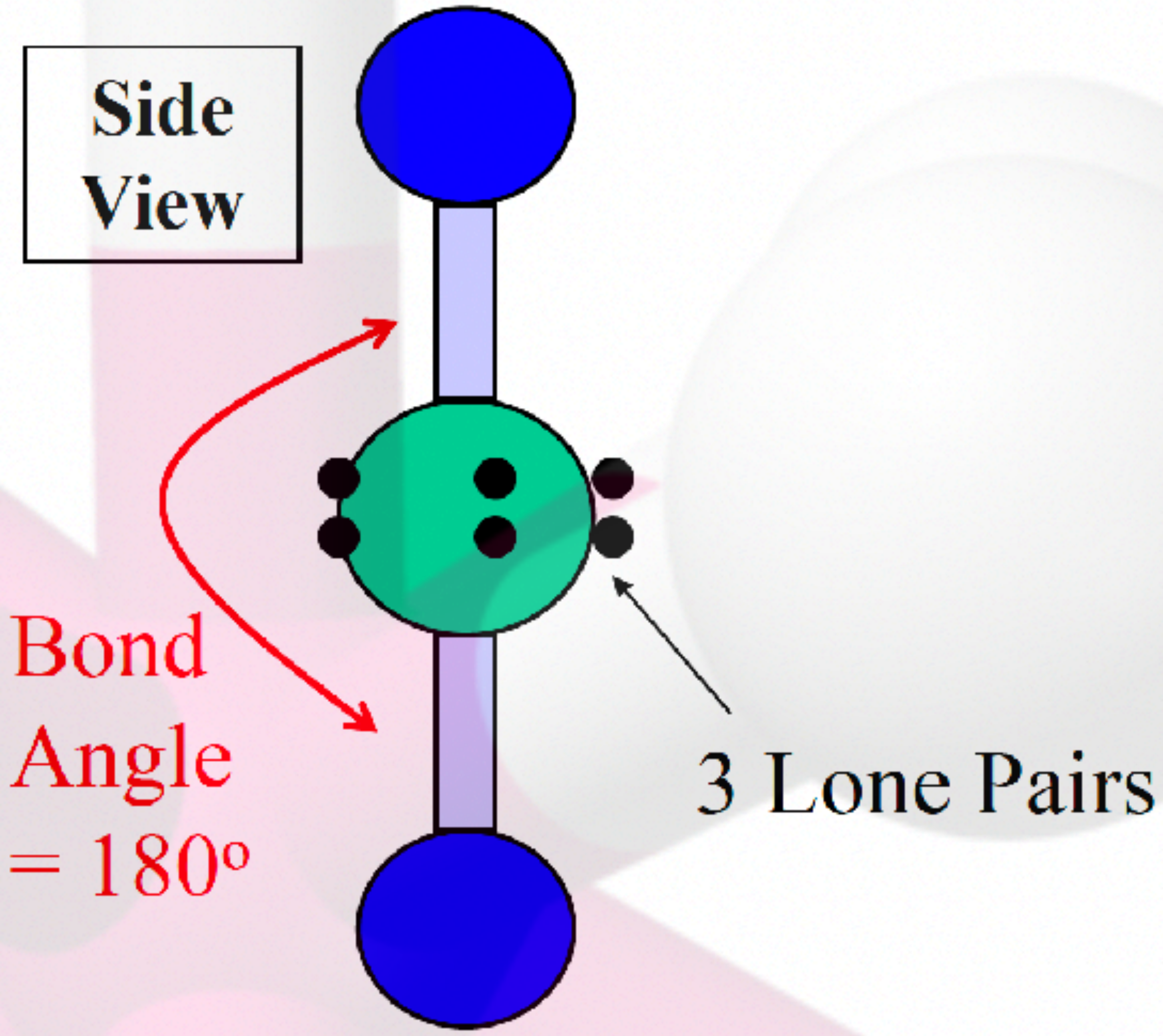


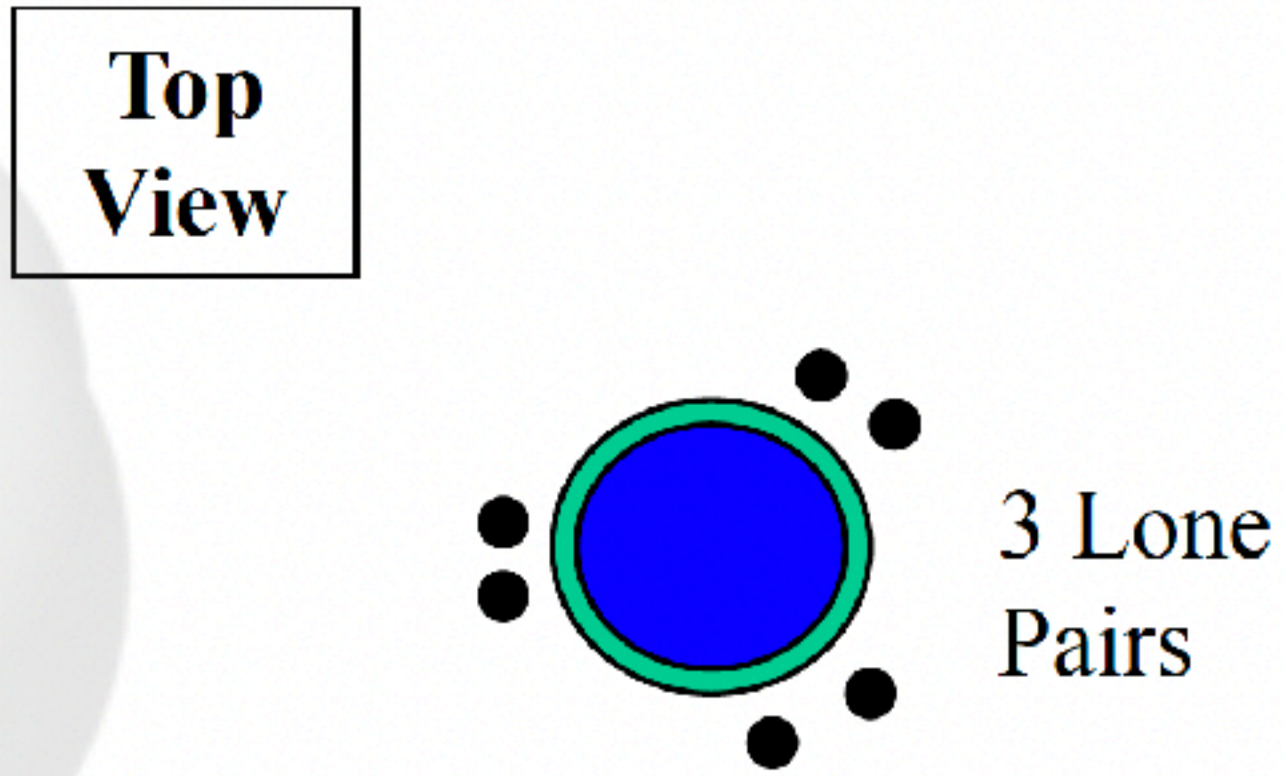


Charge Clouds	Bonds	Lone Pairs	Shape
5	3	2	T-shaped

5 Charge Clouds (XeF_2)

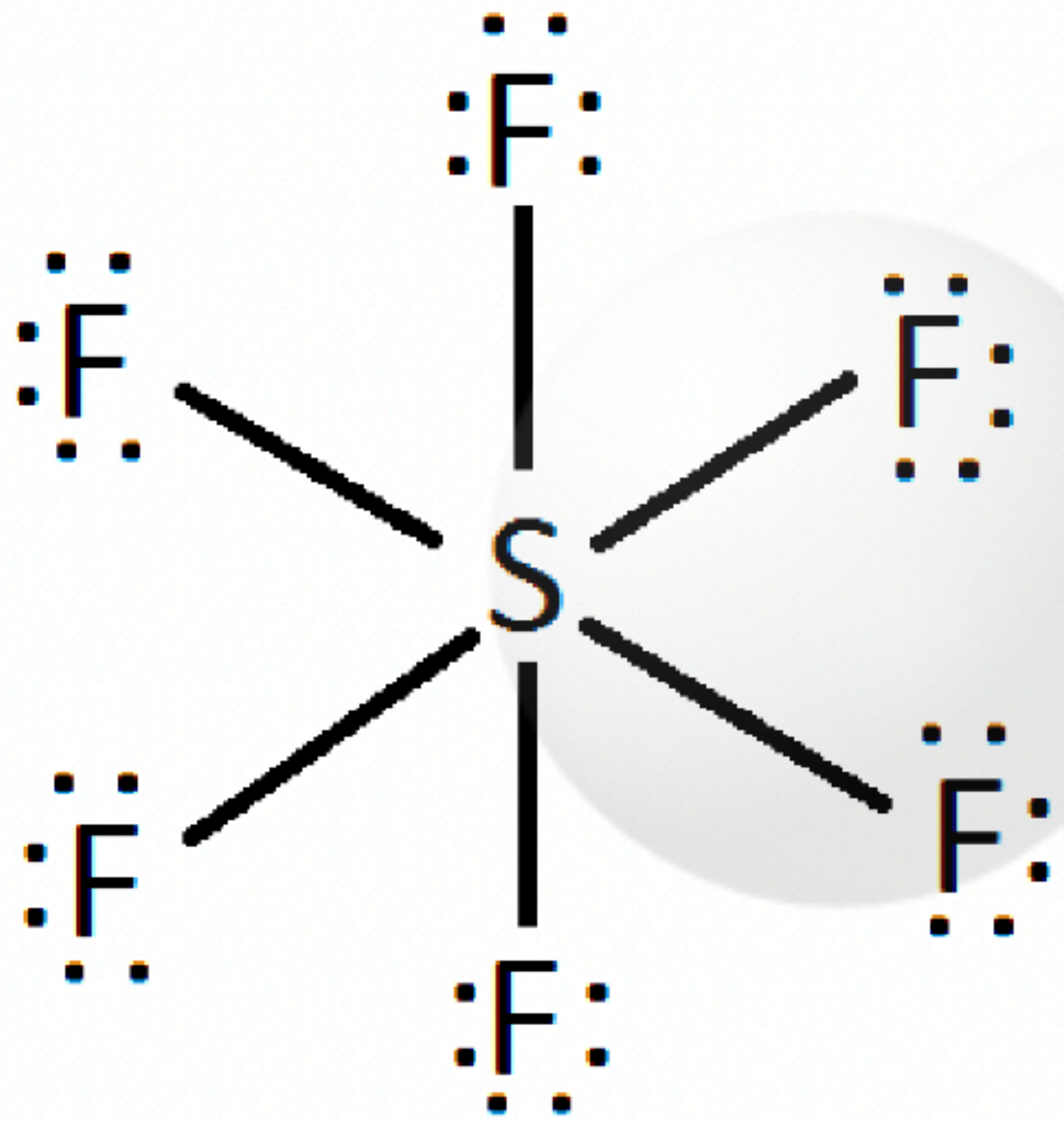


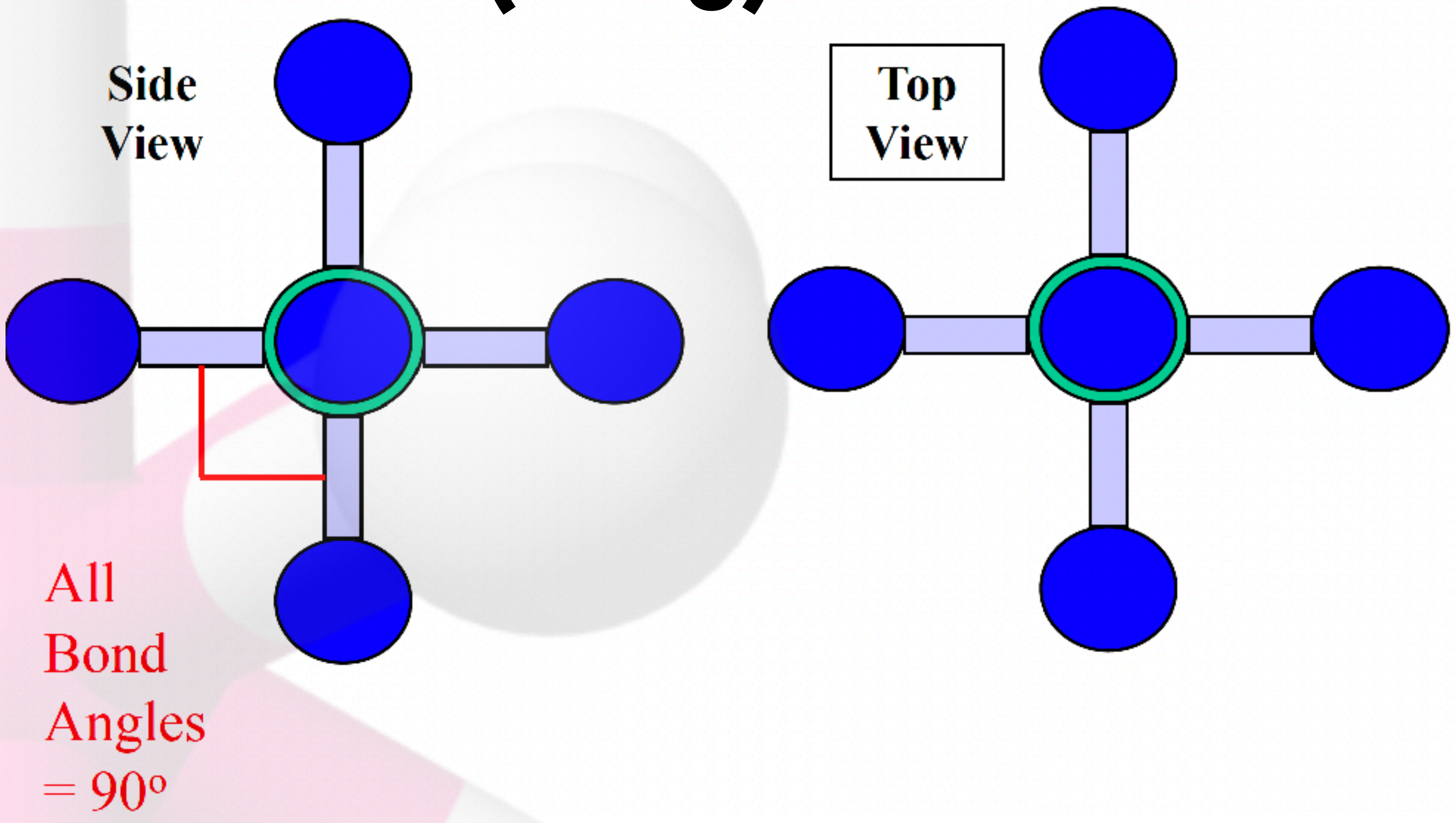




Charge Clouds	Bonds	Lone Pairs	Shape
5	2	3	Linear

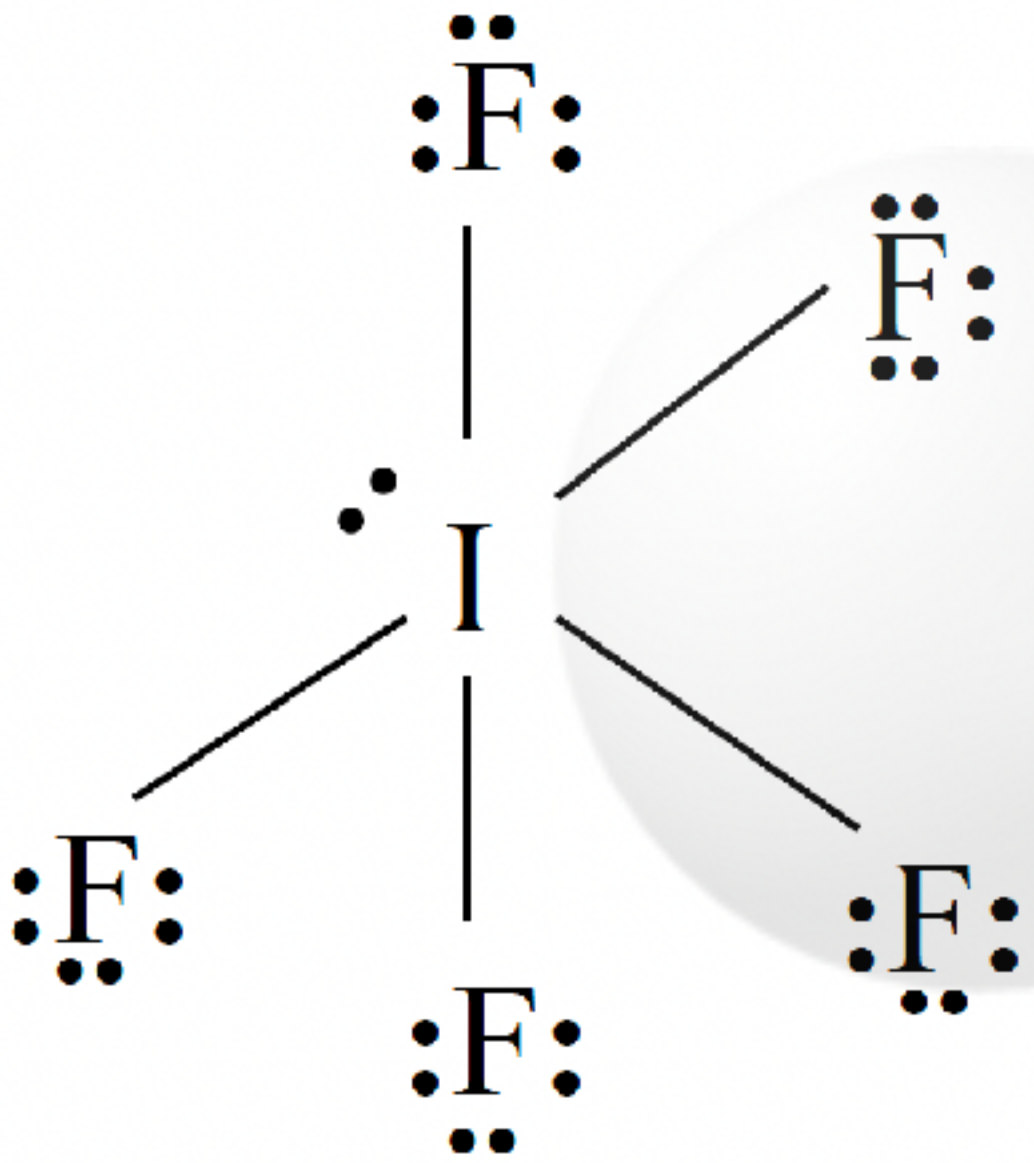
6 Charge Clouds (SF_6)

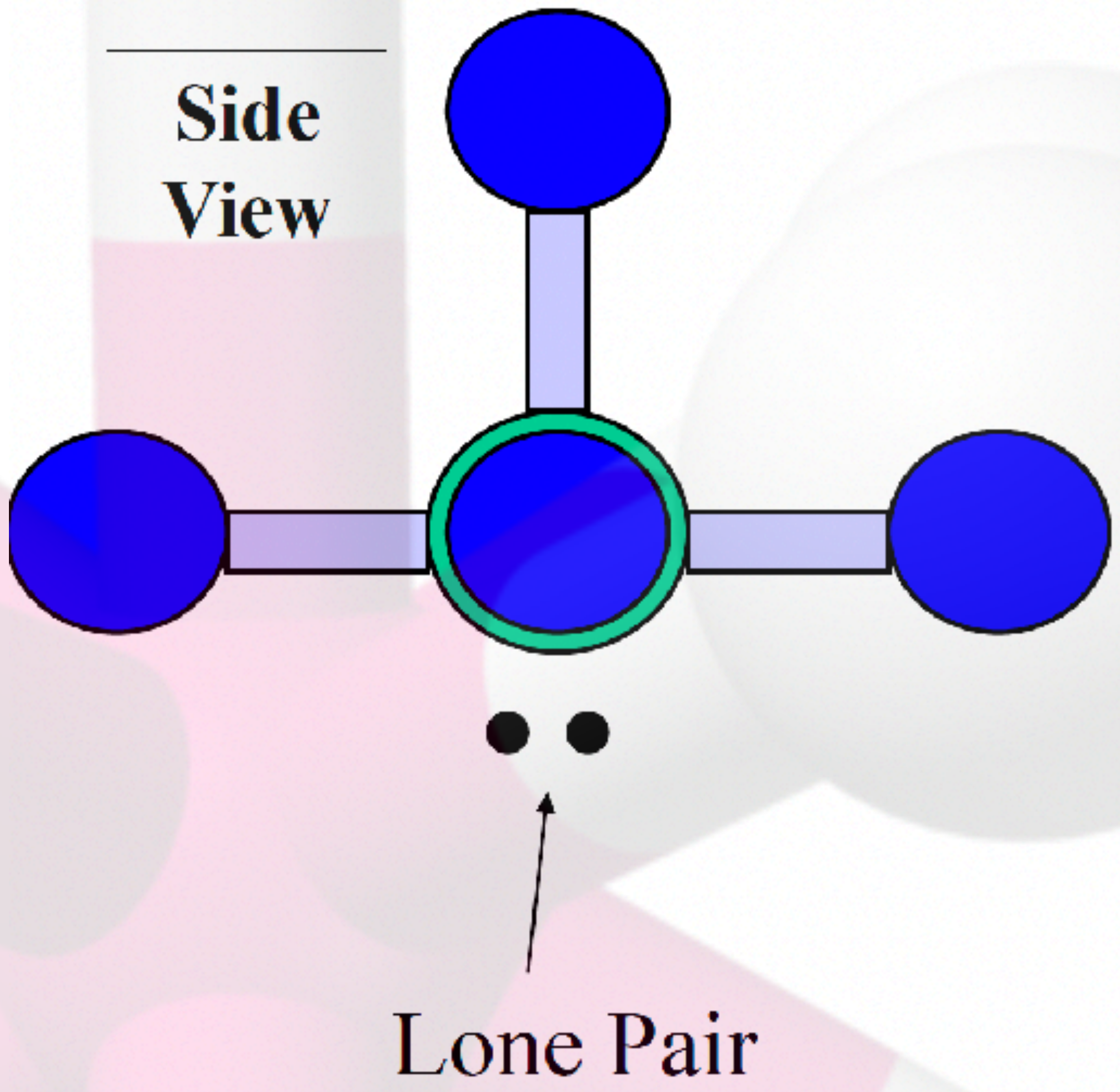


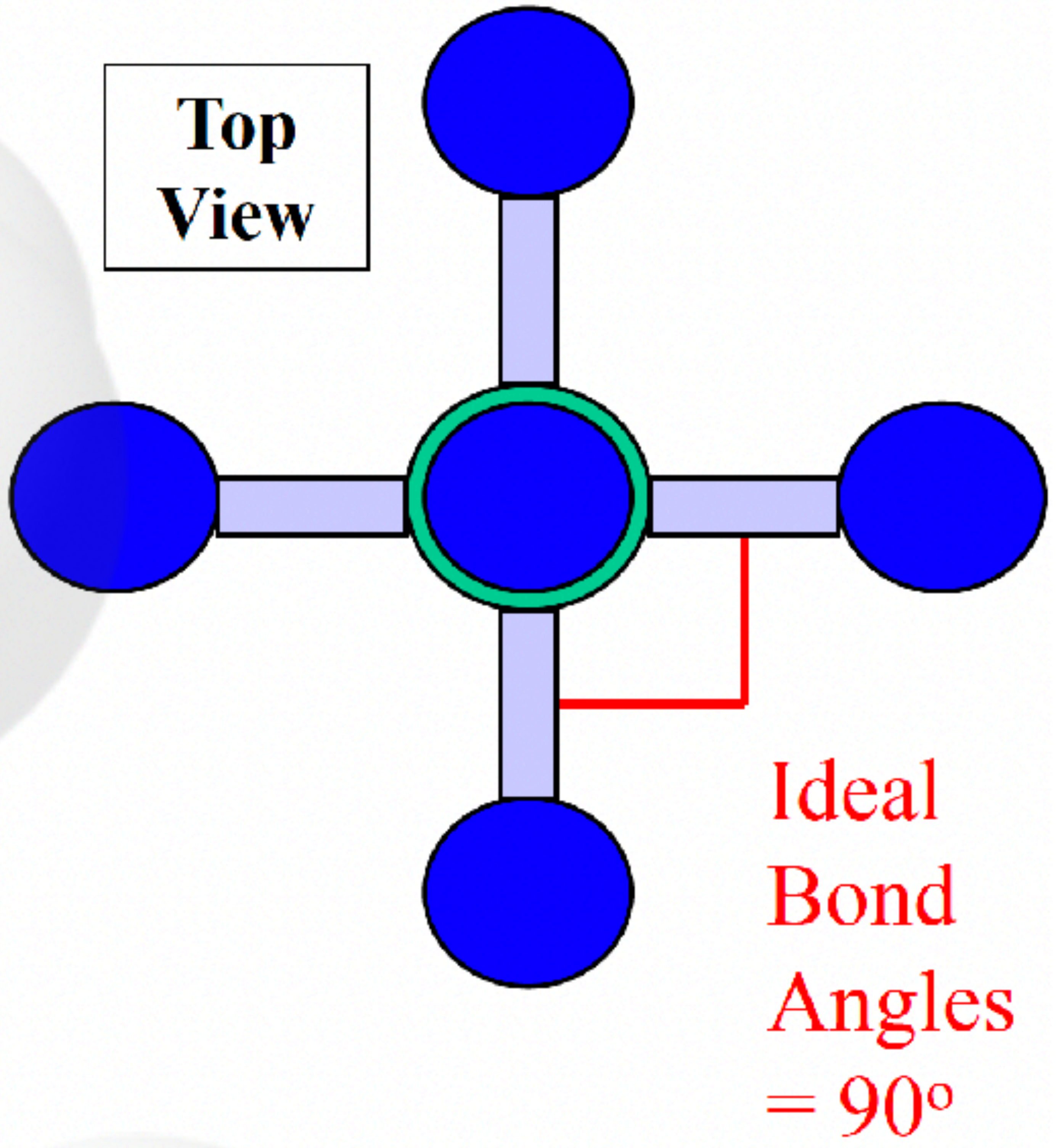


Charge Clouds	Bonds	Lone Pairs	Shape
6	6	0	Octahedral

6 Charge Clouds (IF_5)

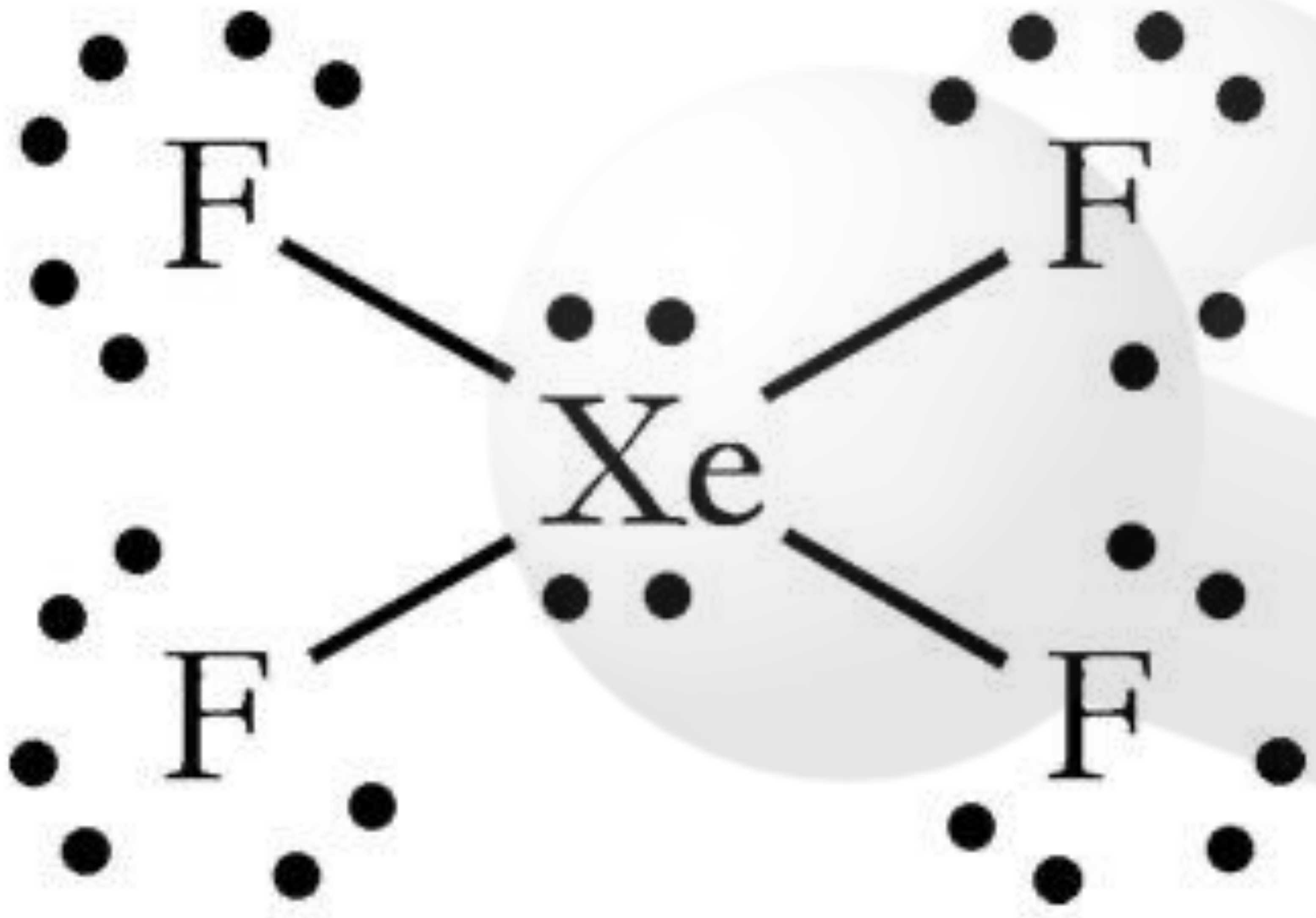


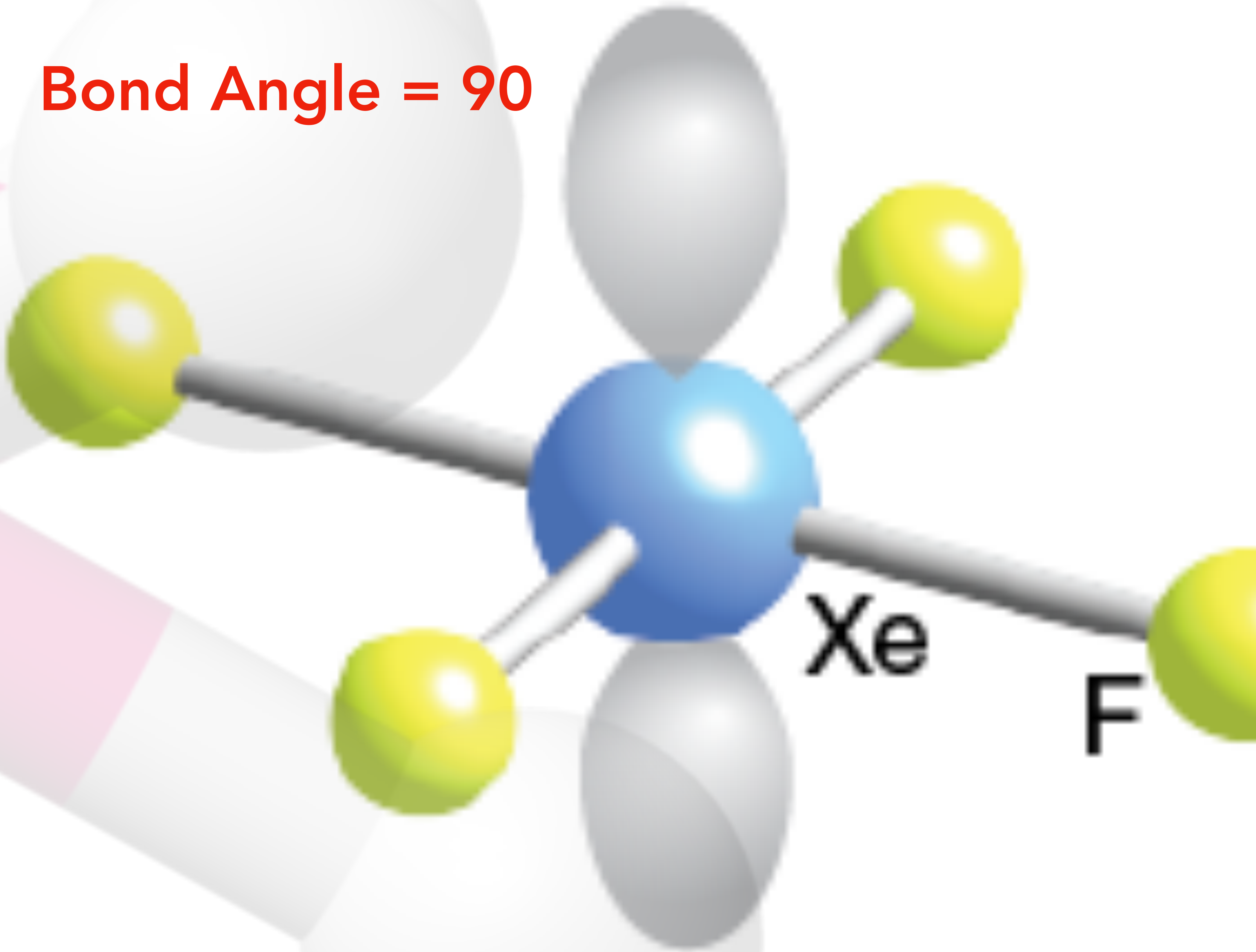




Charge Clouds	Bonds	Lone Pairs	Shape
6	5	1	Square Pyramidal

6 Charge Clouds (XeF_4)

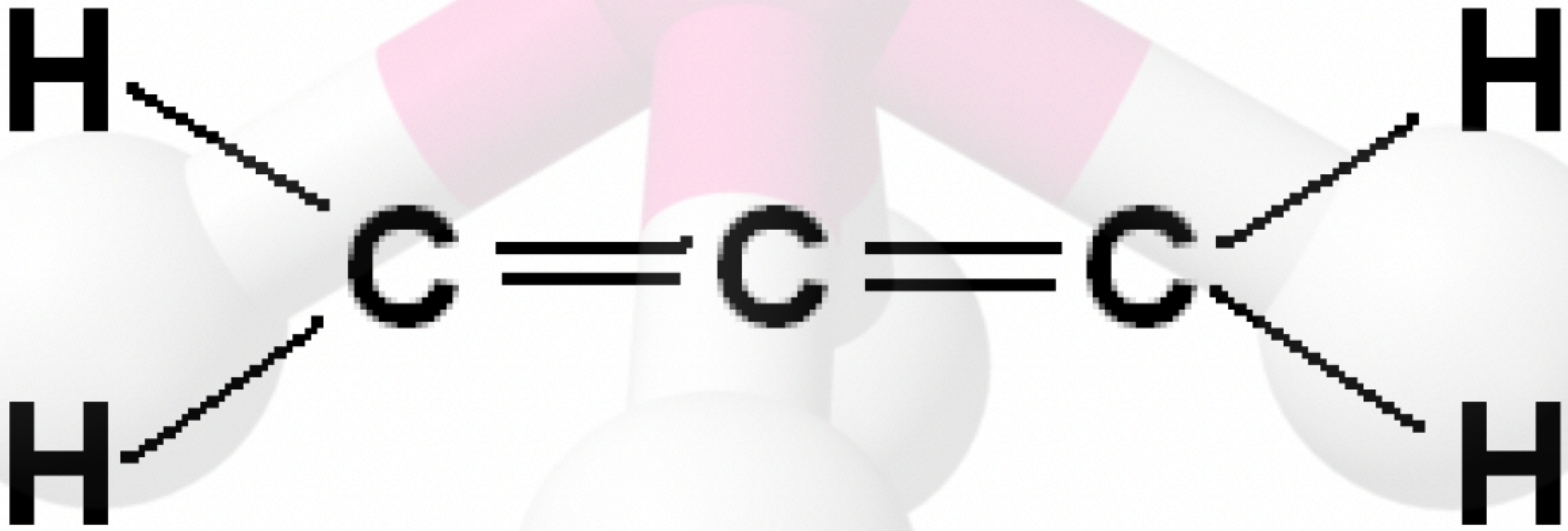




Charge Clouds	Bonds	Lone Pairs	Shape
6	4	2	Square Planar

Compounds with Multiple Central Atoms

1. Look at each central atom on its own.
   - everything it's bonded to is considered to be a terminal atom.
2. Count the charge clouds and bonds around it.
3. Predict the shape around it.
4. Isolate the next central atom and repeat steps 1 through 3.

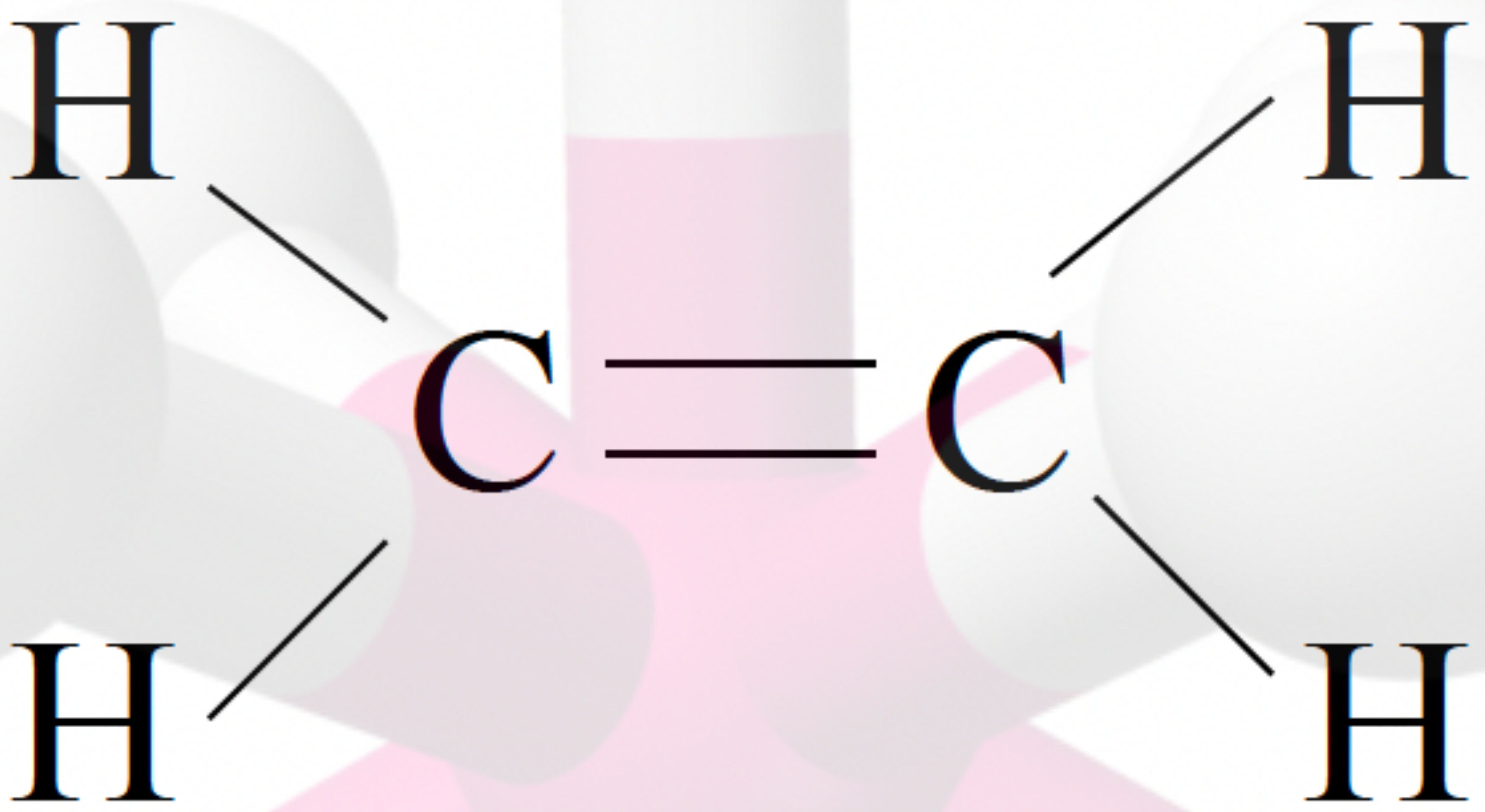


Hybrid Orbitals

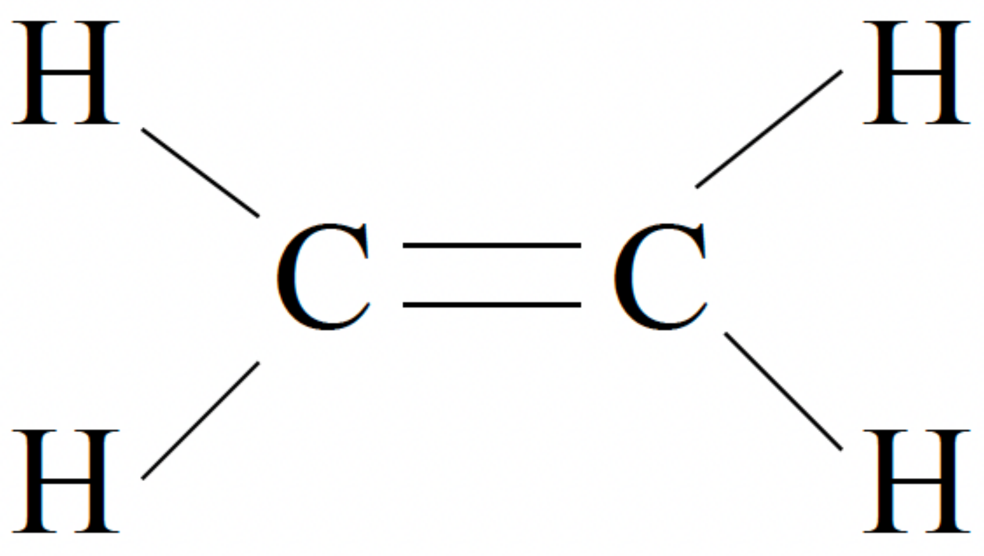
- The atomic orbitals around the central atom in a molecule must hybridize in order for bonding to occur.
- There are 3 types of hybrid orbitals (and bond angles) that you must know.

Charge Clouds	Determining Hybridization	Hybridization	Ideal Bond Angle
4	s + p + p + p	sp^3	109.5°
3	s + p + p	sp^2	120°
2	s + p	sp	180°

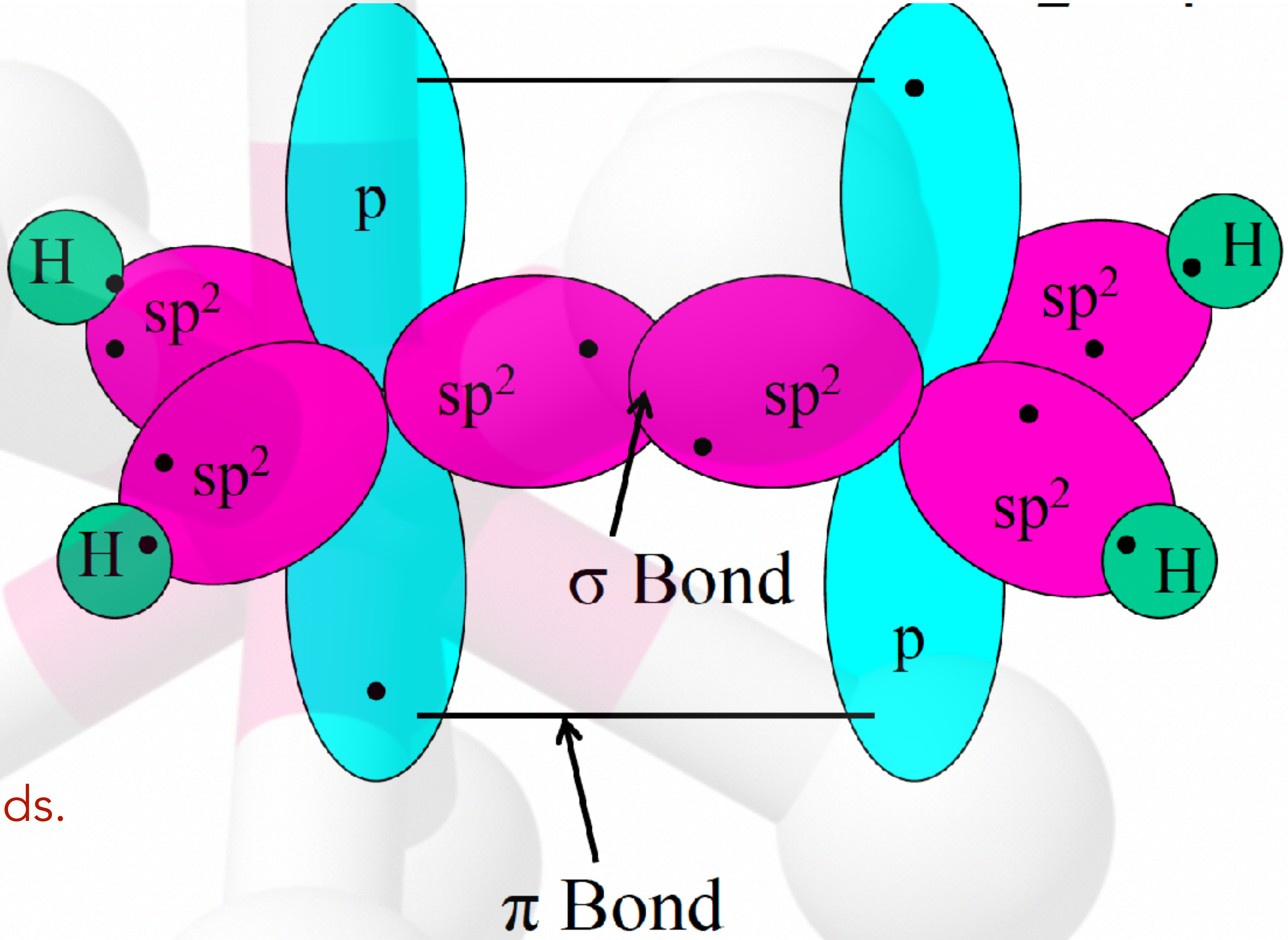
Double Bonds (C_2H_4)



- Each carbon has 3 charge clouds.
- sp^2 hybridization (120°)
- Double bonds consist of one sigma bond an one pi bond.



Double Bonds (C_2H_4)



- Each carbon has 3 charge clouds.
- sp^2 hybridization (120°)
- **Double bonds consist of one sigma bond an one pi bond.**

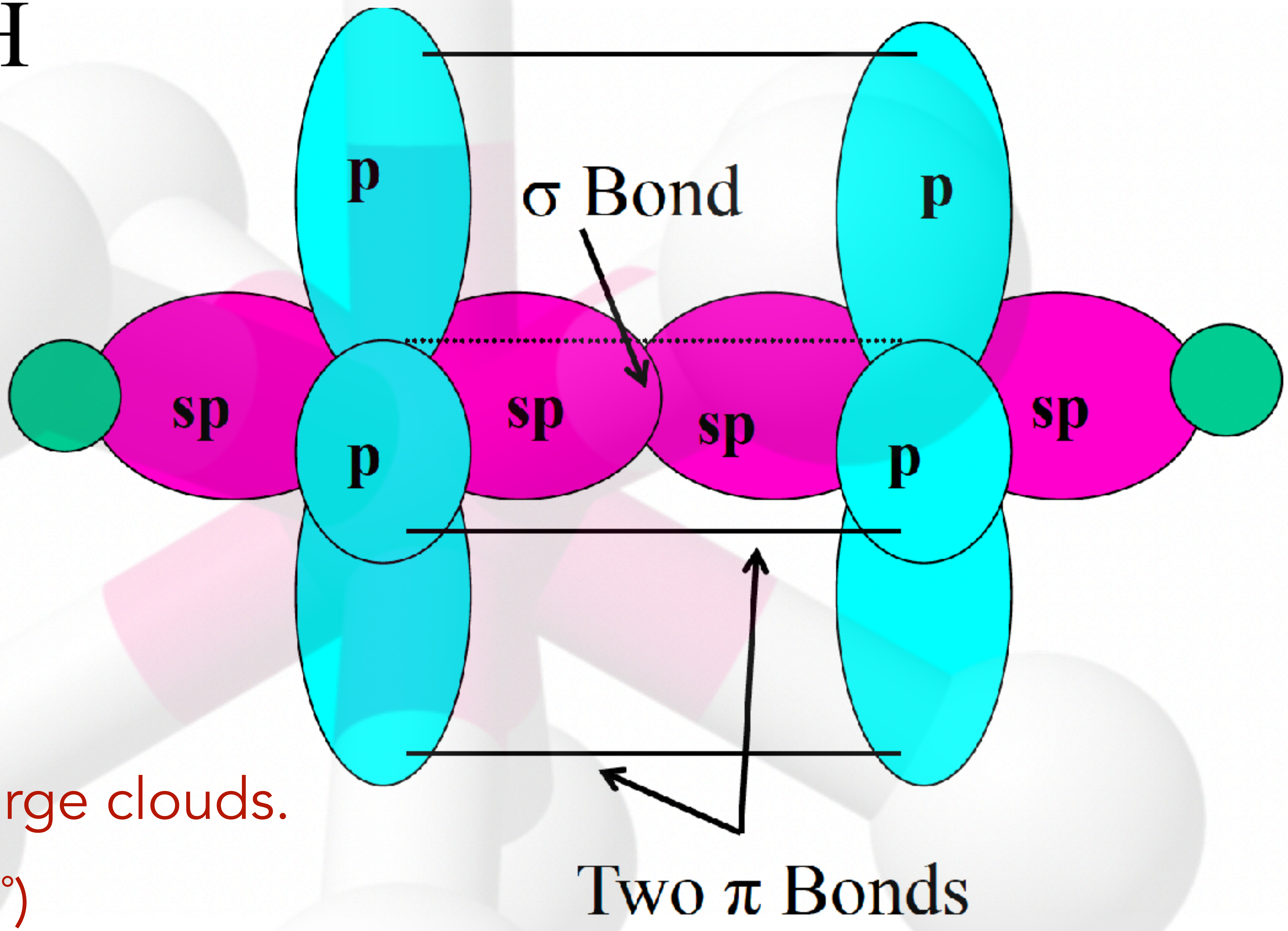
Triple Bonds (C_2H_2)

$$H-C\equiv C-H$$

- Each carbon has 2 charge clouds.
- sp hybrid orbitals (180°)
- Triple bonds consist of one sigma bond and 2 pi bonds.

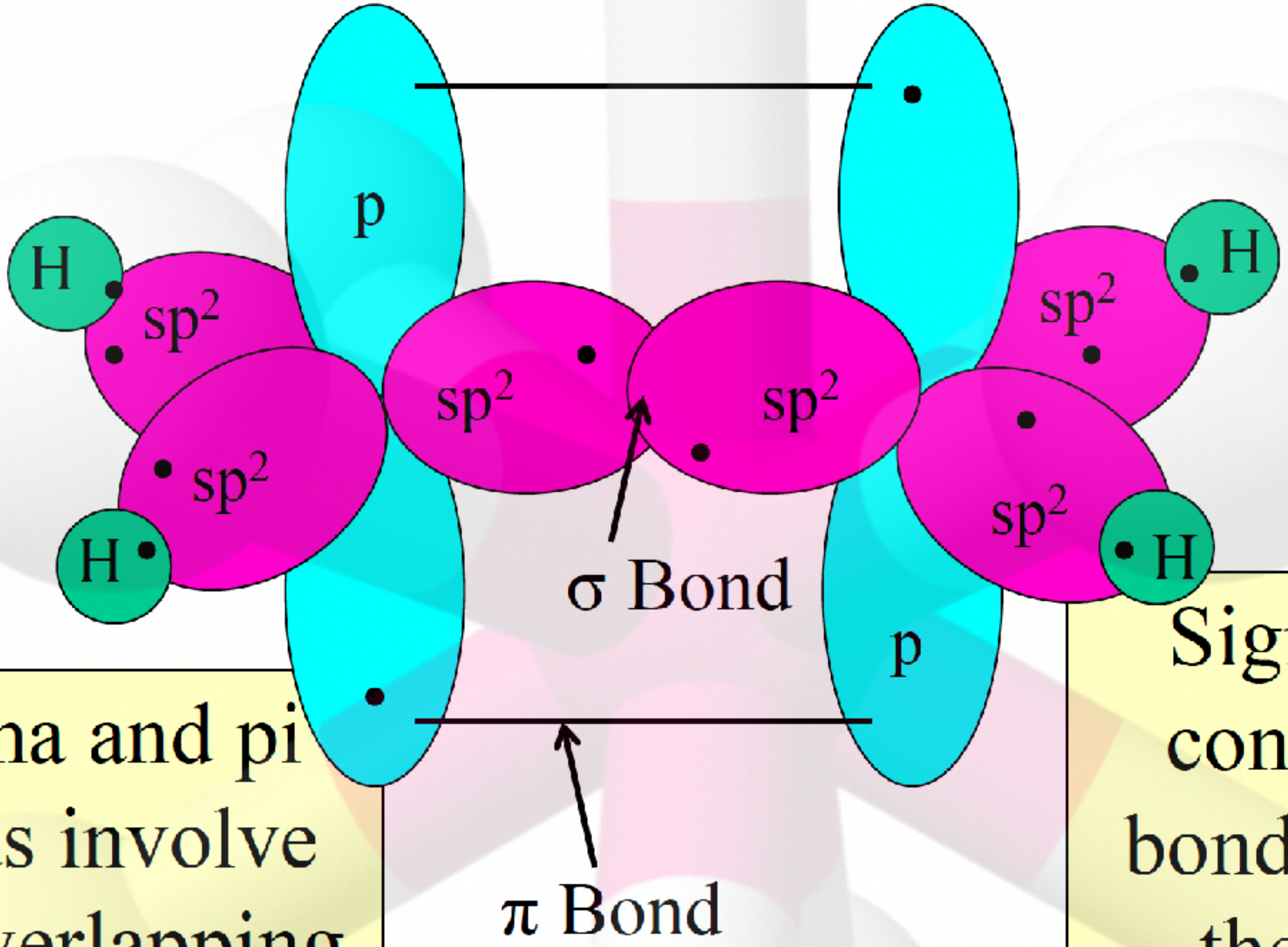
Triple Bonds (C_2H_2)

$H - C \equiv C - H$



- Each carbon has 2 charge clouds.
- sp hybrid orbitals (180°)
- **Triple bonds consist of one sigma bond and 2 pi bonds.**

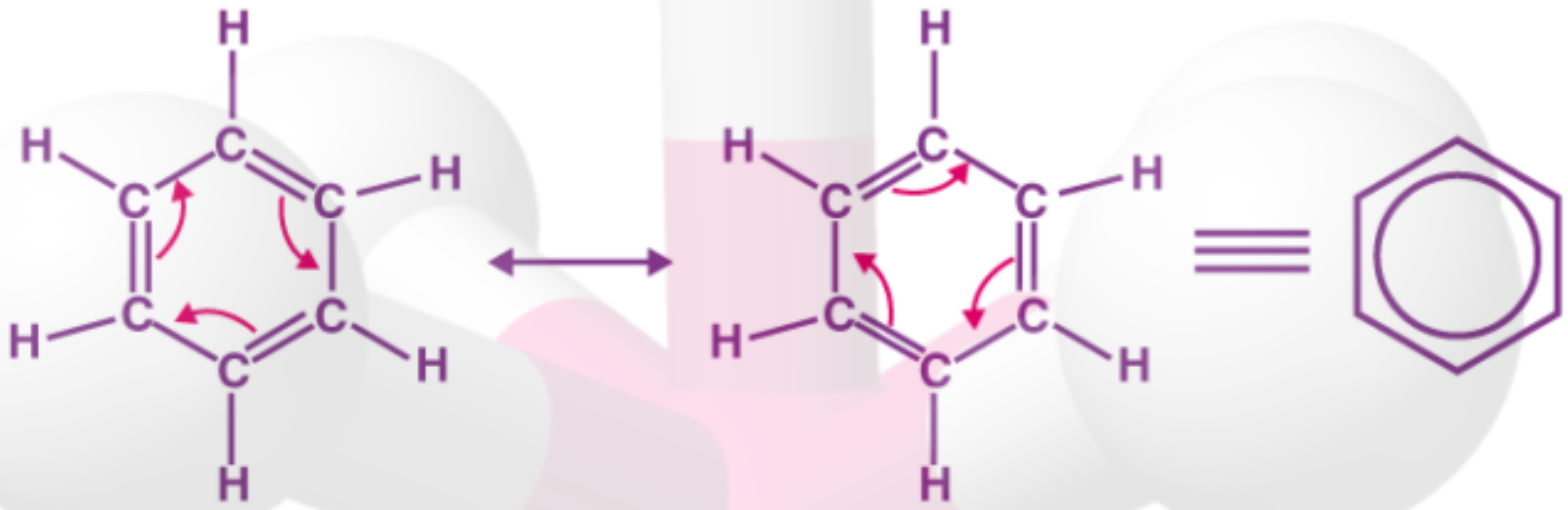
σ-Bond & π-Bond Energy



Sigma and pi bonds involve the overlapping of atomic orbitals.

Sigma bonds contain more bond energy, as the overlap between orbitals is stronger.

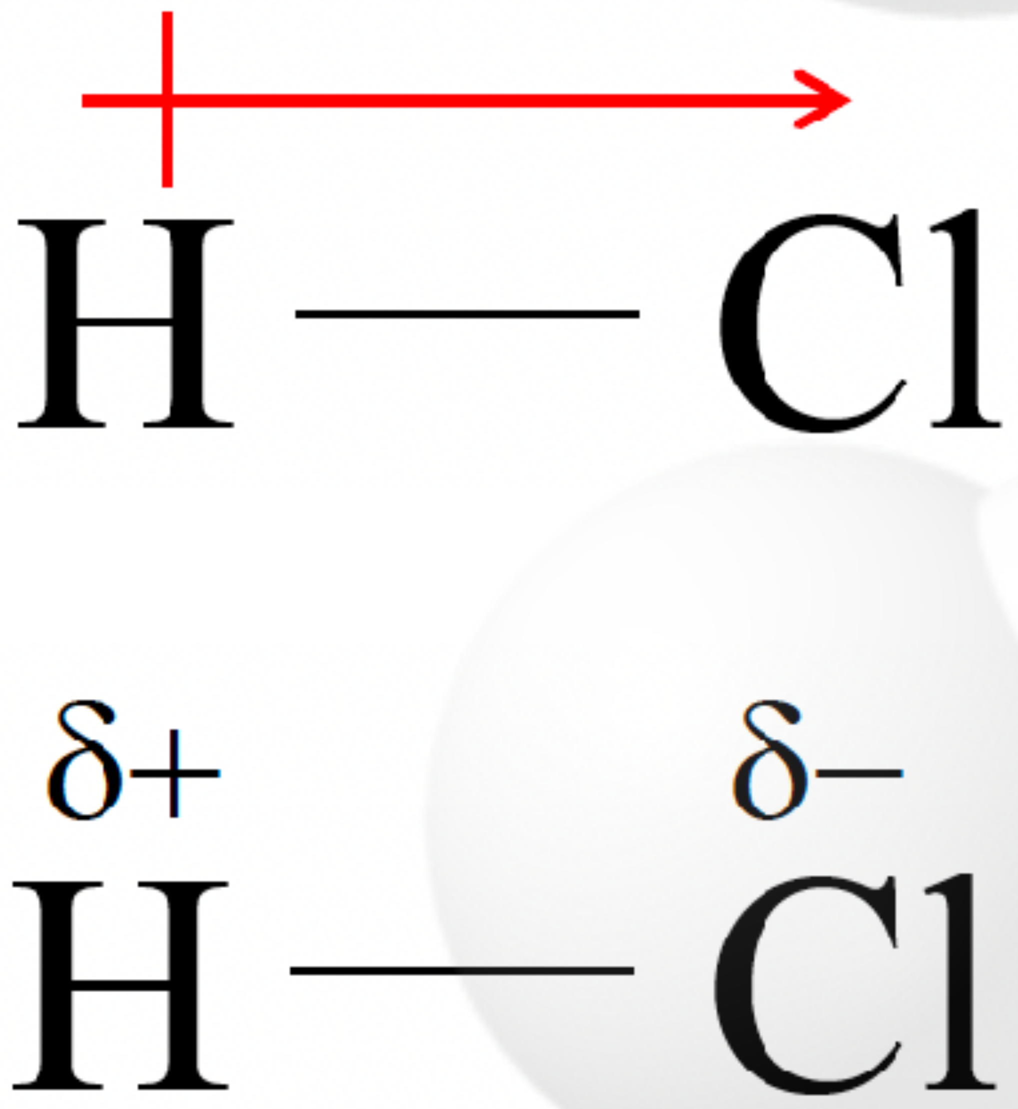
Extended π-Bonding (Benzene, C_6H_6)



- Alternating single and double bonds that move.
- Each p-orbital can overlap with 2 different p-orbitals.
- Results in **delocalization** of electrons — used to explain resonance in Lewis structures.

Bond Polarity

- Shared electrons spend more time around the most electronegative element in the chemical bond.
- Gives the more electronegative element a slightly negative charge and the less electronegative element a slightly positive charge.



Greater electronegativity values lead to greater partial charges and greater **bond dipoles**.

Polar and Non-Polar Molecules

- If a molecule is polar, it must have a dipole moment, *u*.

$$\mu = Q \times r$$

Q = absolute value of the net partial charge at each end of a molecule
r = distance between positive and negative poles of a molecule.

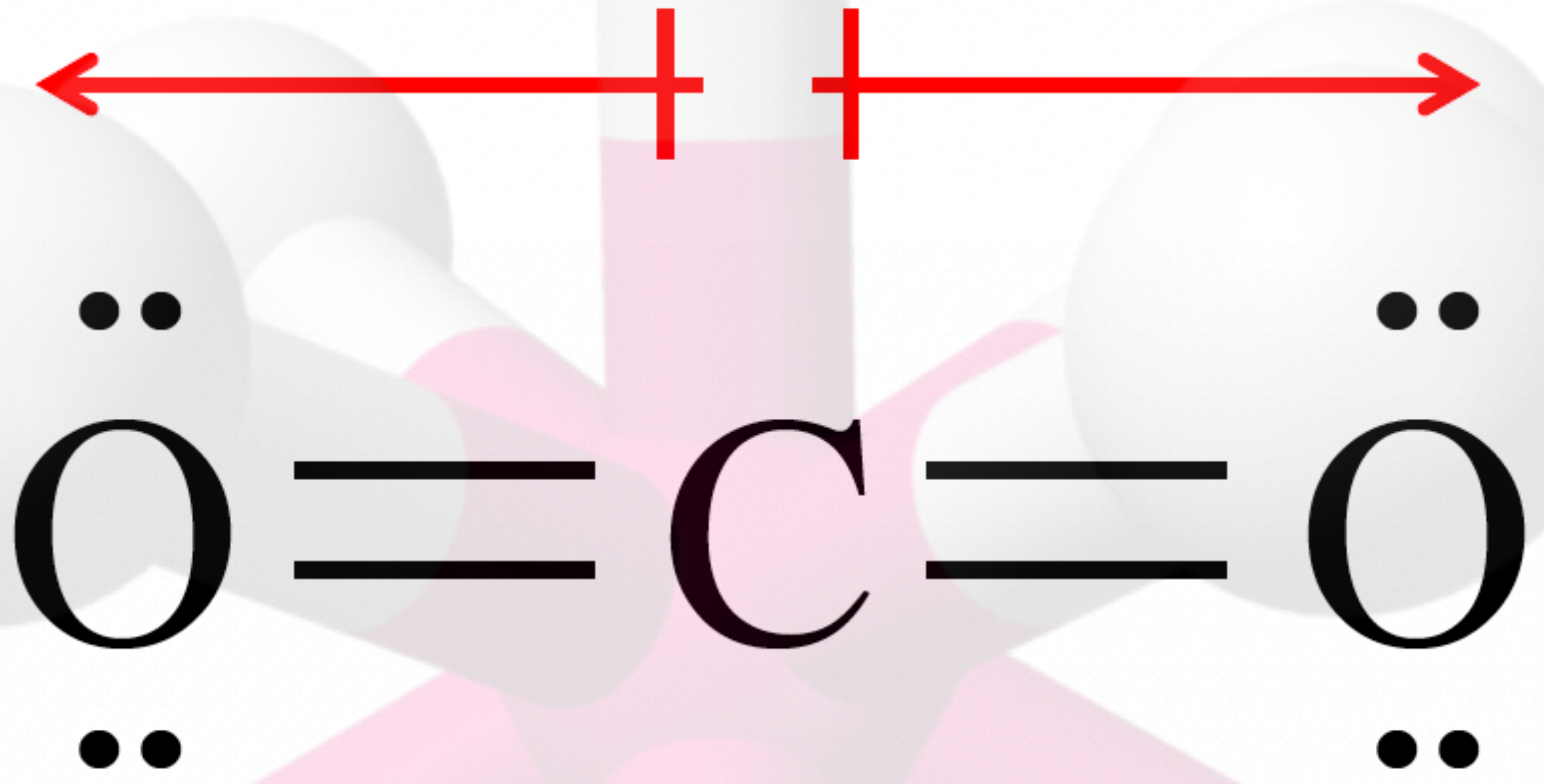
- To know if a molecule is polar:
  - you must know if the bonds are polar
  - you must know the overall shape of the molecule

Polar and Non-Polar Molecules

- **Polar** - bond dipoles do not cancel, so the molecule has a dipole moment

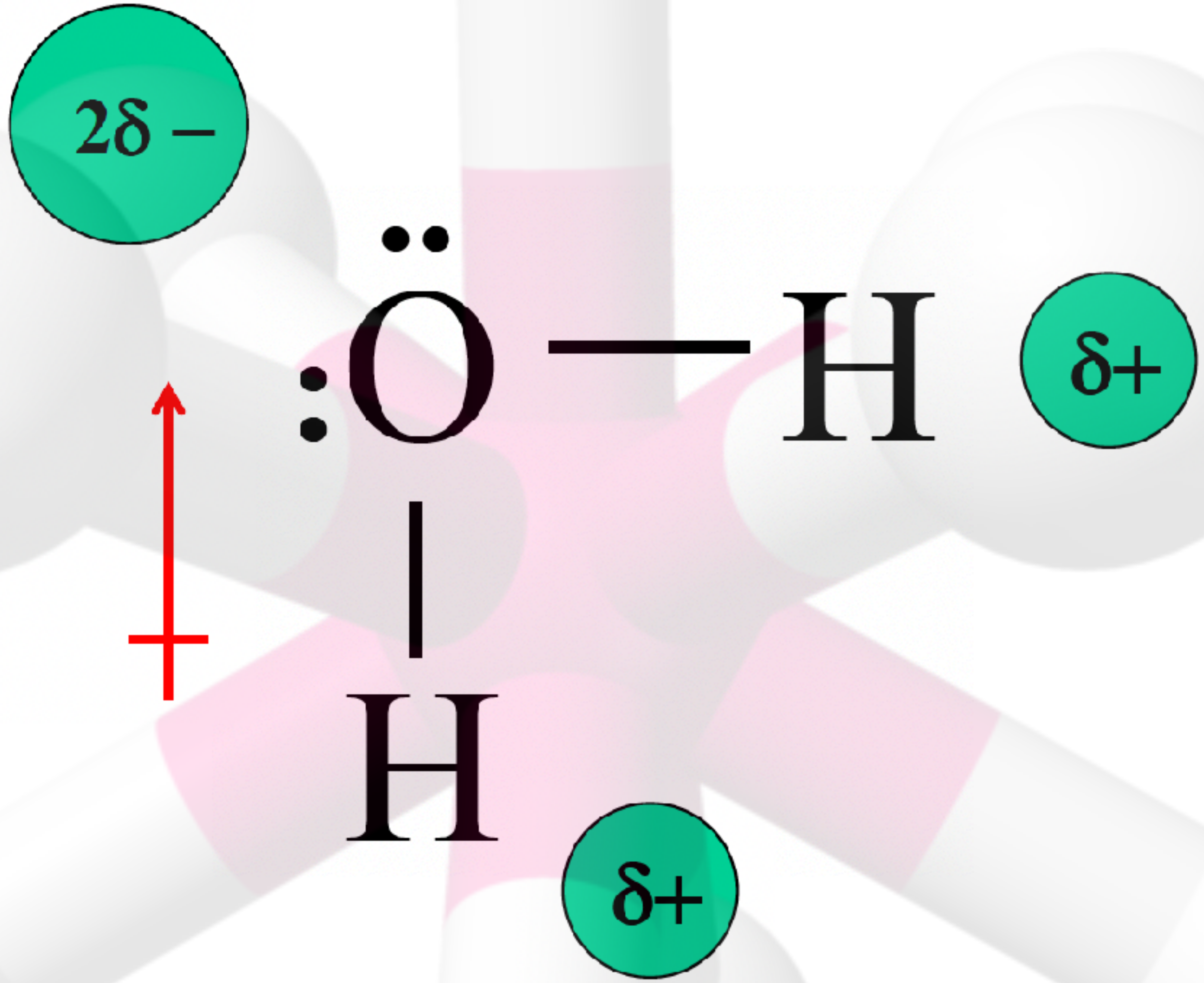
For polar molecules consisting ot two atoms, the partial negative charge on the more electronegative atom is always equal in magnitude to the partial positive charge on the less electronegative atom.

Polar and Non-Polar Molecules



- **Non-Polar** - Two polar C=O bonds are symmetrical so bond dipoles cancel. No dipole moment

Polar and Non-Polar Molecules



- **Polar** - Two polar bonds asymmetrically arranged around the central oxygen. Dipoles do not cancel.

Diatomic Molecules

- **Two diatomic molecules that contain atoms from the same group in the same proportions:**
  - will have the same shape will both be either polar or non-polar.
- **This can help chemists design new materials.**
  - Replacing an element from one group with another from the same group could lead to a new substance with similar properties.
  - SiO_2 can be used to make ceramics. SnO_2 might work just as well — or better.