Let's consider $_{16}S$

$$2H + S = H_2S$$
$$2O + S = SO_2$$
$$3O + S = SO_3$$

2 unpaired electrons
(valence II)

4 unpaired electrons
(valence IV)

Remember: one square – one orbital, on one orbital we can have up to two electrons.

3s 3p

Cl (ground state) [↑↓] [↑↓][↑↓][↑]

3d

Cl (excited state) [↑↓] [↑↓][↑][↑] [↑]□□□□

[↑↓] [↑↓][↑↓][↑]   [↑↓] [↑↓][↑↓][↑]   [↑↓] [↑↓][↑↓][↑]

F   F   F

Could you tell me if fluorine (F)can have valency
of III, V or VII? And why?

$:\ddot{F}:$

$:\overset{..}{\underset{..}{Cl}}—\overset{..}{\underset{..}{F}}:$

$:\ddot{F}:$

Valency of Cl I, III, V, VII

Cl_2 (I) $Cl-Cl$

HCl (I) $H-Cl$

HCl (V) $HClO_3$ $O=\overset{..}{Cl}=O$
                              |
                              OH

HCl(III)O_2 $O=Cl=O-H$

HCl (VII)O_4 $O=Cl=O$
                        ‖
                        O
                        |
 OH

Molecular geometry

How can we predict the molecule shape? We can use the principle that electron pairs must avoid each other. The want to be far away from each other as possible.

Molecular geometry

Valence shell electron pair repulsion (VSEPR) theory

- Molecular geometry is the 3D arrangement of atoms within a molecule

- Chemical bonds and unbonded electron pairs or single electrons in a molecule repel, so they try to stay as far as possible from each other.

- The repulsion between unbound electrons (u.e.) is stronger than repulsion between bound electrons (b.e.). The repulsion decreases in the row:
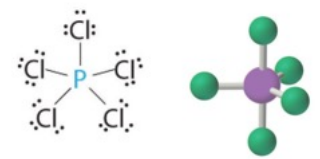
(u.e. / u.e. > u.e. / b.e. > b.e. /b.e.)
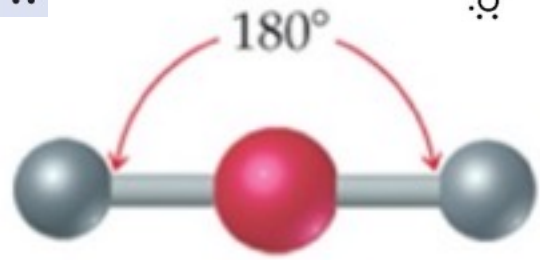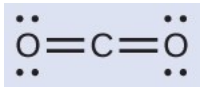
Linear
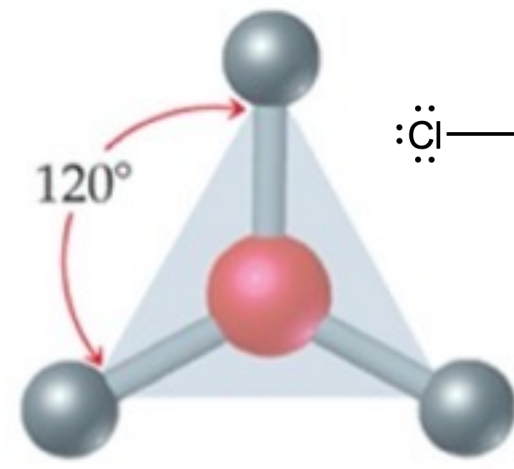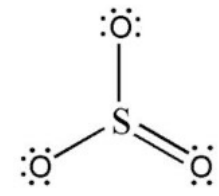
Trigonal planar
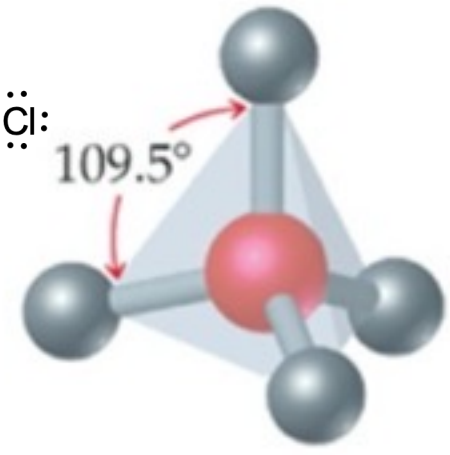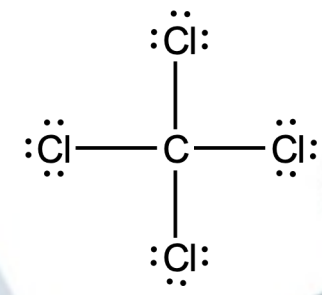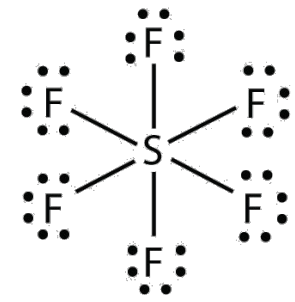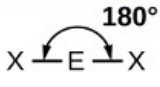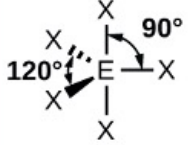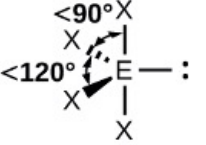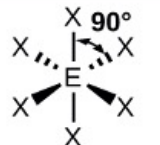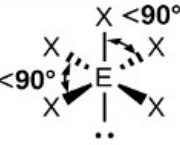
Tetrahedral
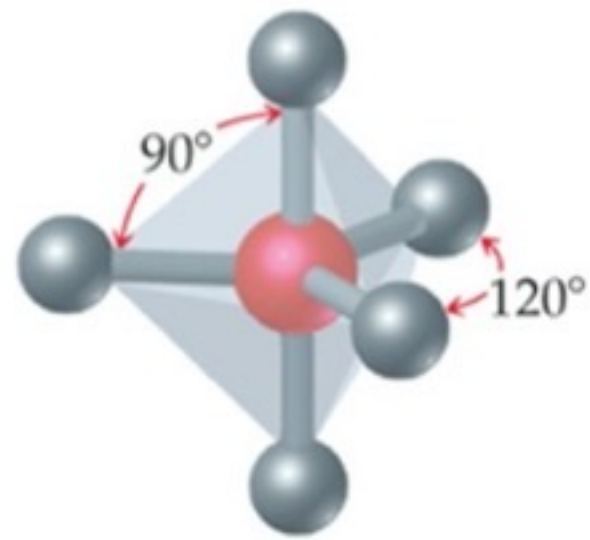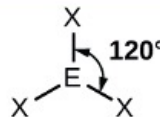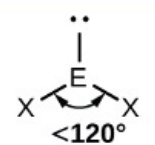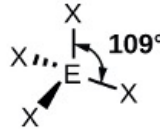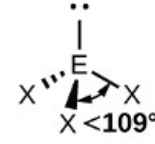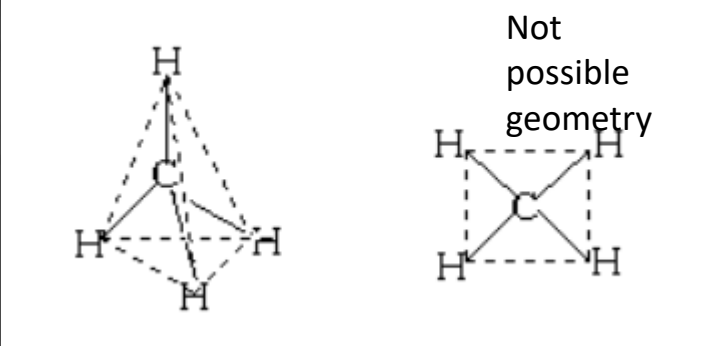
Trigonal bipyramidal
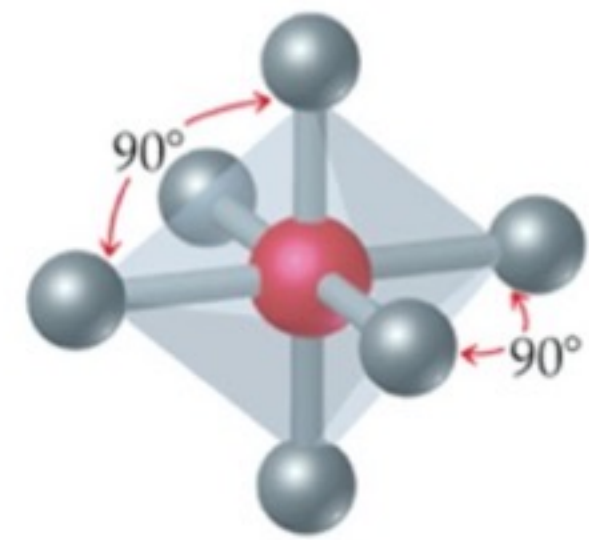
Octahedral

Electron domain
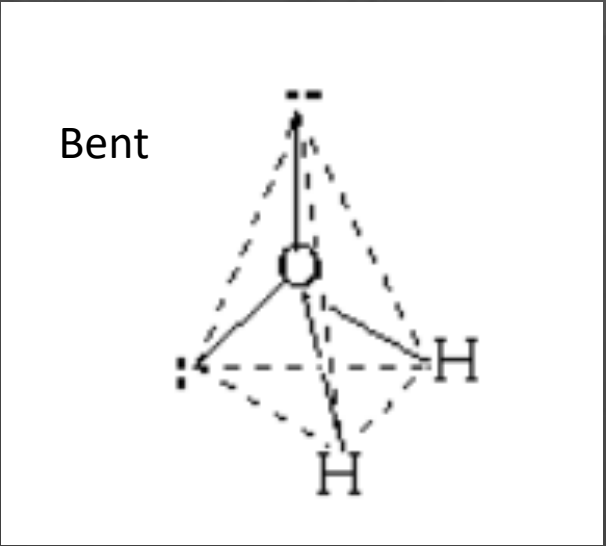
Number of electron pairs	Shape 0 lone pair	1 lone pair
2	180° X—E—X Linear	
3	X 120° E X X Trigonal planar	E X X <120° Bent or angular
4	X 109° E X X Tetrahedral	E X X X <109° Trigonal pyramid
5	X X 90° 120° E—X X X Trigonal bipyramid	<90° X X <120° E—: X X Sawhorse or seesaw
6	X 90° X X E X X X Octahedral	X <90° X X <90° E X X Square pyramid

How to predict the shapes of the molecules?
1. Draw the Lewis structure
2. Count up the numbers of electron pairs (bonding pairs and lone pairs) in the valence shell of the central atom. Double or triple bonds here will be counted as a single electron pair. This gives total number of electron domains (2, 3, 4, etc.)
3. Look at the number of electron domain and correspond it to the shape.
4. A lone pair will contribute to the overall shape of the molecule. This is due to greater repulsion from lone pairs than from bonding pairs. The molecule will be bent.

Cl—Be—Cl

F
|
B
/ \
F   F

Not possible geometry

~109º

Bent

~105º

"The main idea behind molecular orbitals is that the electrons in a molecule can be described as being distributed in a set of mathematical functions, called molecular orbitals. These orbitals are based on the individual atomic orbitals of the atoms in the molecule, and they are used to describe the distribution of the electrons in the molecule. This allows chemists to predict the shape and behavior of a molecule, and to understand how it will react with other molecules. Molecular orbitals are an important concept in chemistry, and they are often used in conjunction with other theories, such as valence bond theory, to provide a more complete description of the behavior of molecules. "
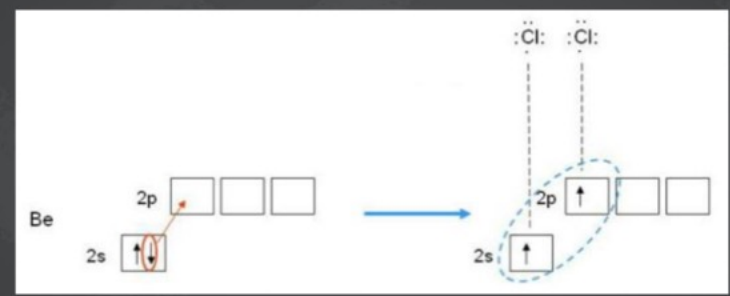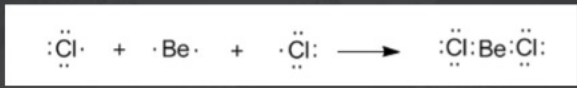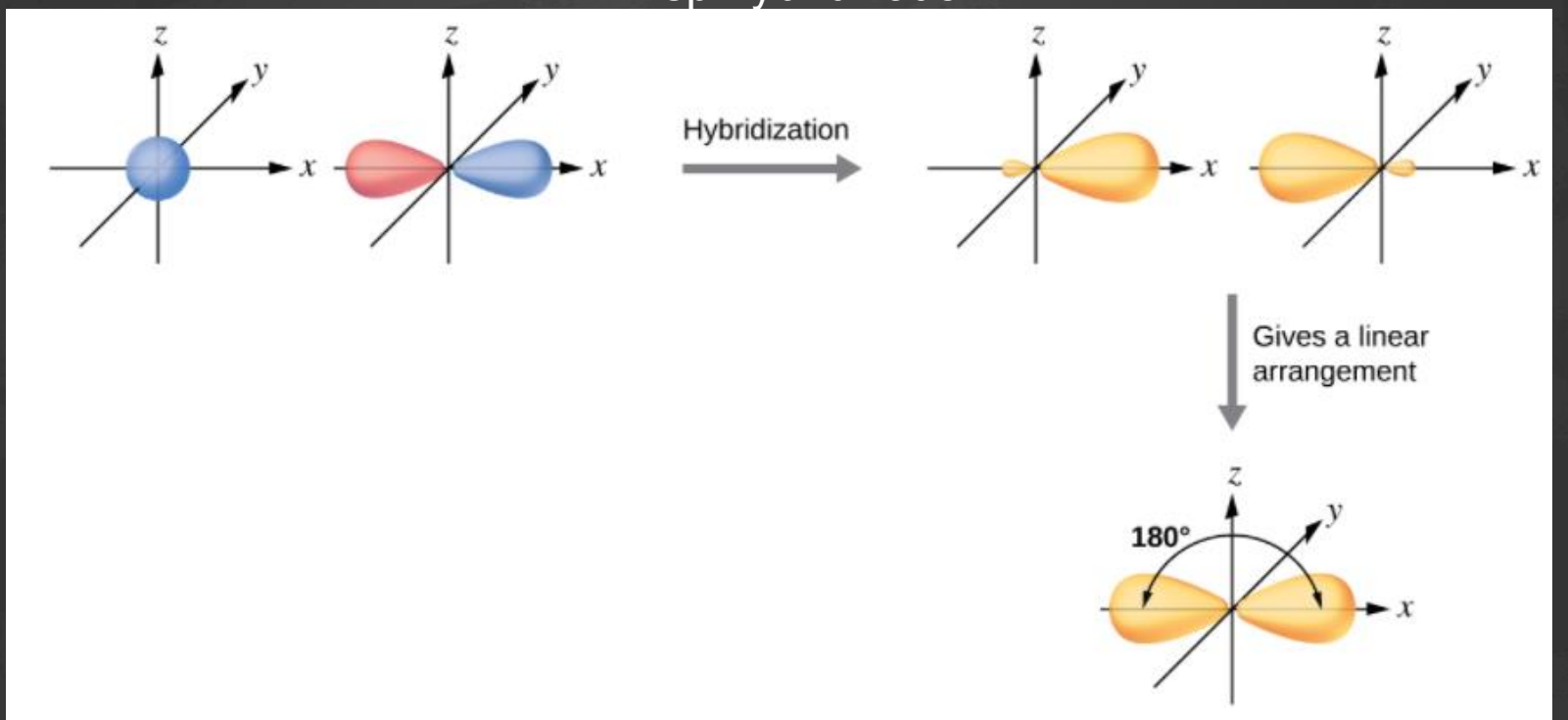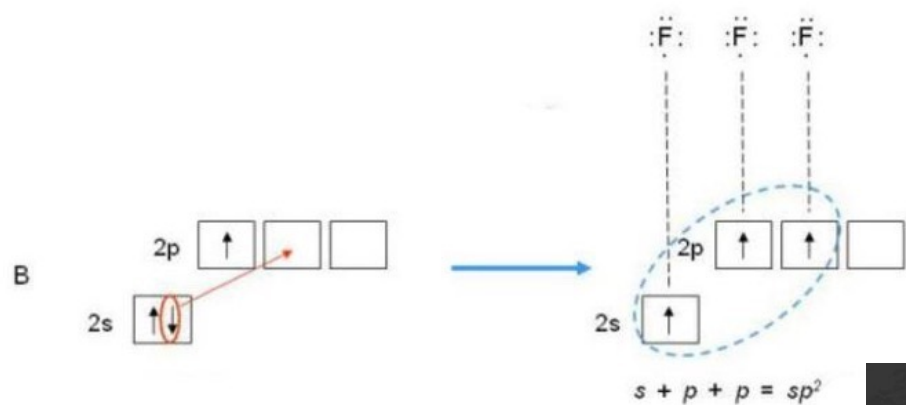
To form a covalent bond, two orbitals each containing one electron are required.
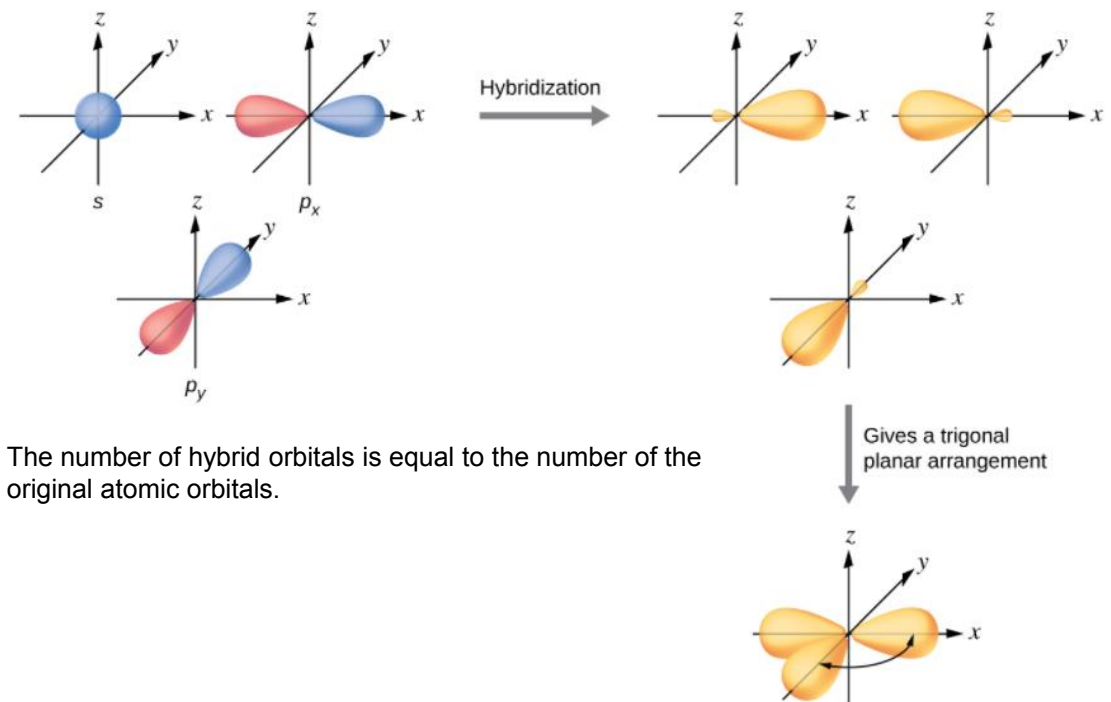
Hybridisation is the mixing of atomic orbitals in an atom to produce a new set of orbitals (the same number as originally) that are better arranged in space for covalent bonding. We will call new orbitals – hybrid orbitals.
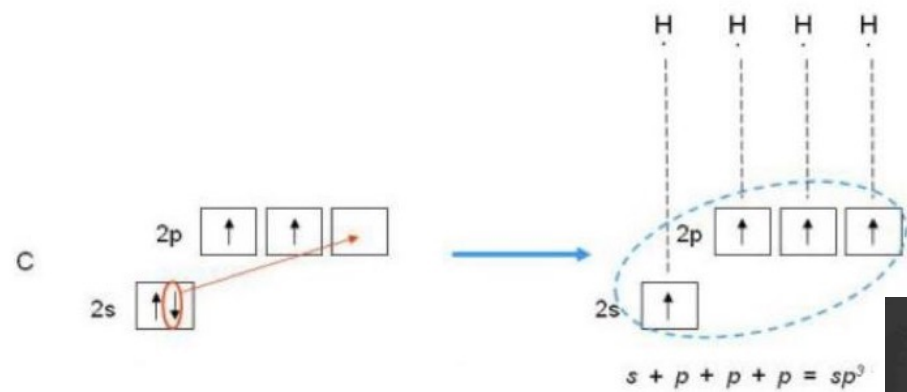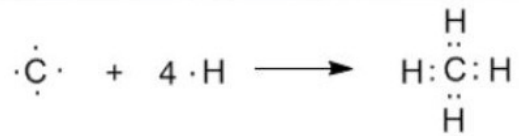
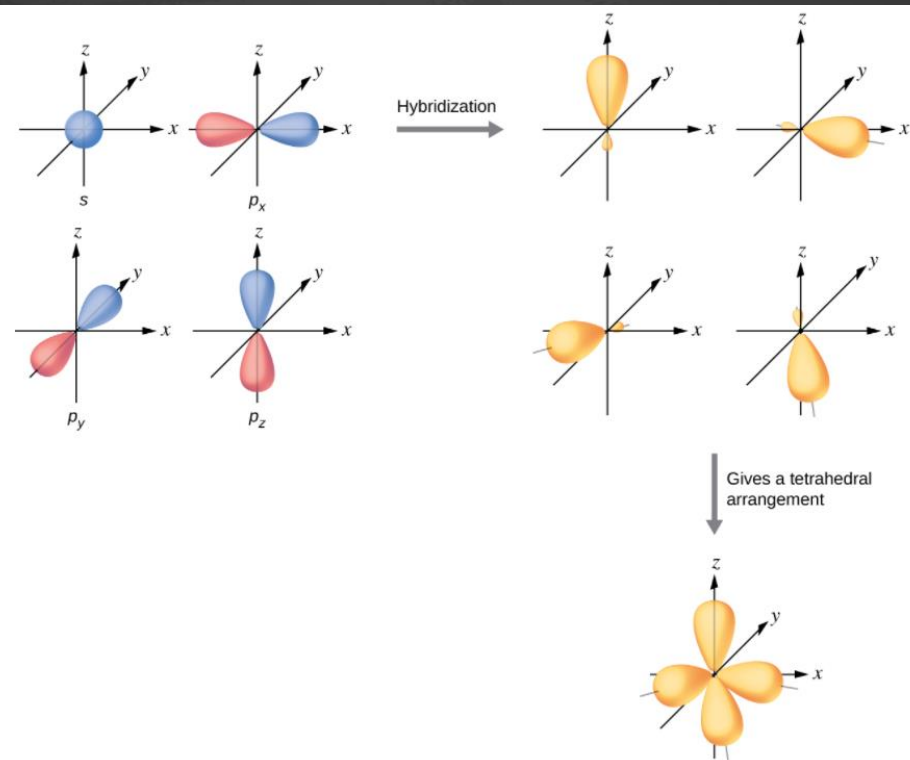Linear combination of atomic orbitals (LCAO) – hybridization
1. sp hybridization

$$\cdot B \cdot \quad + \quad 3 \cdot \ddot{F} : \quad \longrightarrow \quad : \ddot{F} : B : \ddot{F} : \\ \qquad\qquad\qquad\qquad\qquad :\ddot{F}:$$

B

2p

2s

2p

2s

$s + p + p = sp^2$

2. sp² hybridization
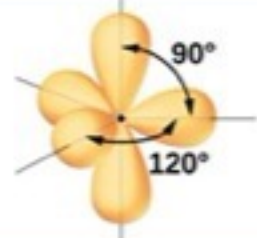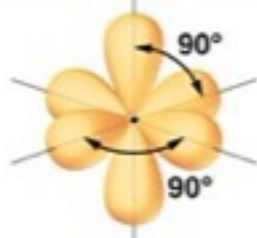

Hybridization

The number of hybrid orbitals is equal to the number of the original atomic orbitals.
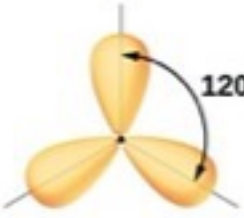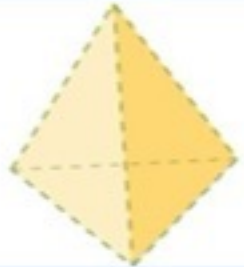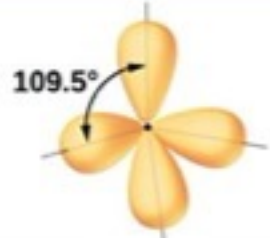
Gives a trigonal planar arrangement

2. sp³ hybridization

Regions of Electron Density	Arrangement		Hybridization
2		linear	sp 180°
3		trigonal planar	sp^2 120°
4		tetrahedral	sp^3 109.5°
5		trigonal bipyramidal	sp^3d 90° 120°
6		octahedral	sp^3d^2 90° 90°

Consider the following molecules:

PCl₃ PCl_3

CF₄ CF_4

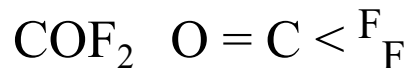HCN $H:C:::N:$

COF₂ $O = C <^F_F$

CS₂ $S = C = S$

FNO $F - \dot{N} = O$

O₃
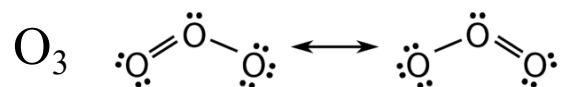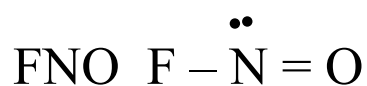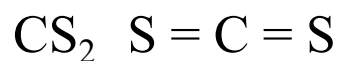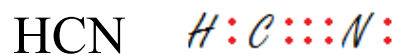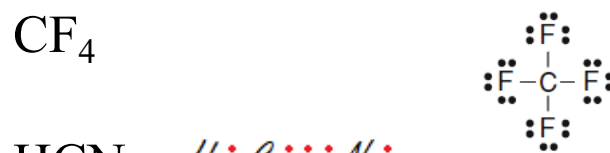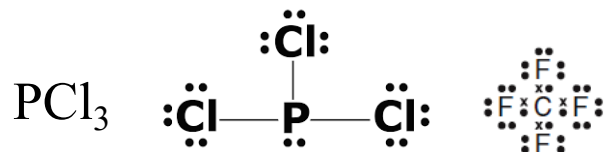
Can you tell their shape?

Number of electron pairs	Shape	
	0 lone pair	1 lone pair
2	180° X—E—X Linear	
3	120° X—E, X Trigonal planar	<120° X—E—X Bent or angular
4	109° X—E(X)(X)(X) Tetrahedral	X<109° X—E—X Trigonal pyramid
5	90° 120° Trigonal bipyramid	<90°X <120° Sawhorse or seesaw
6	X 90° Octahedral	X <90° Square pyramid

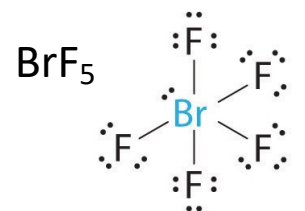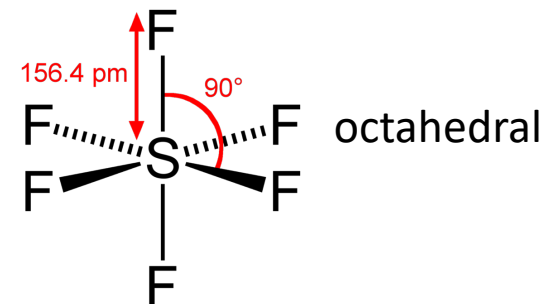This Photo by Unknown Author is licensed under CC BY

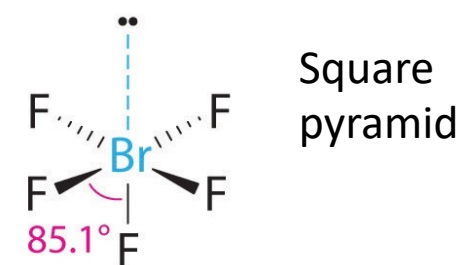How to predict the shapes of the molecules?
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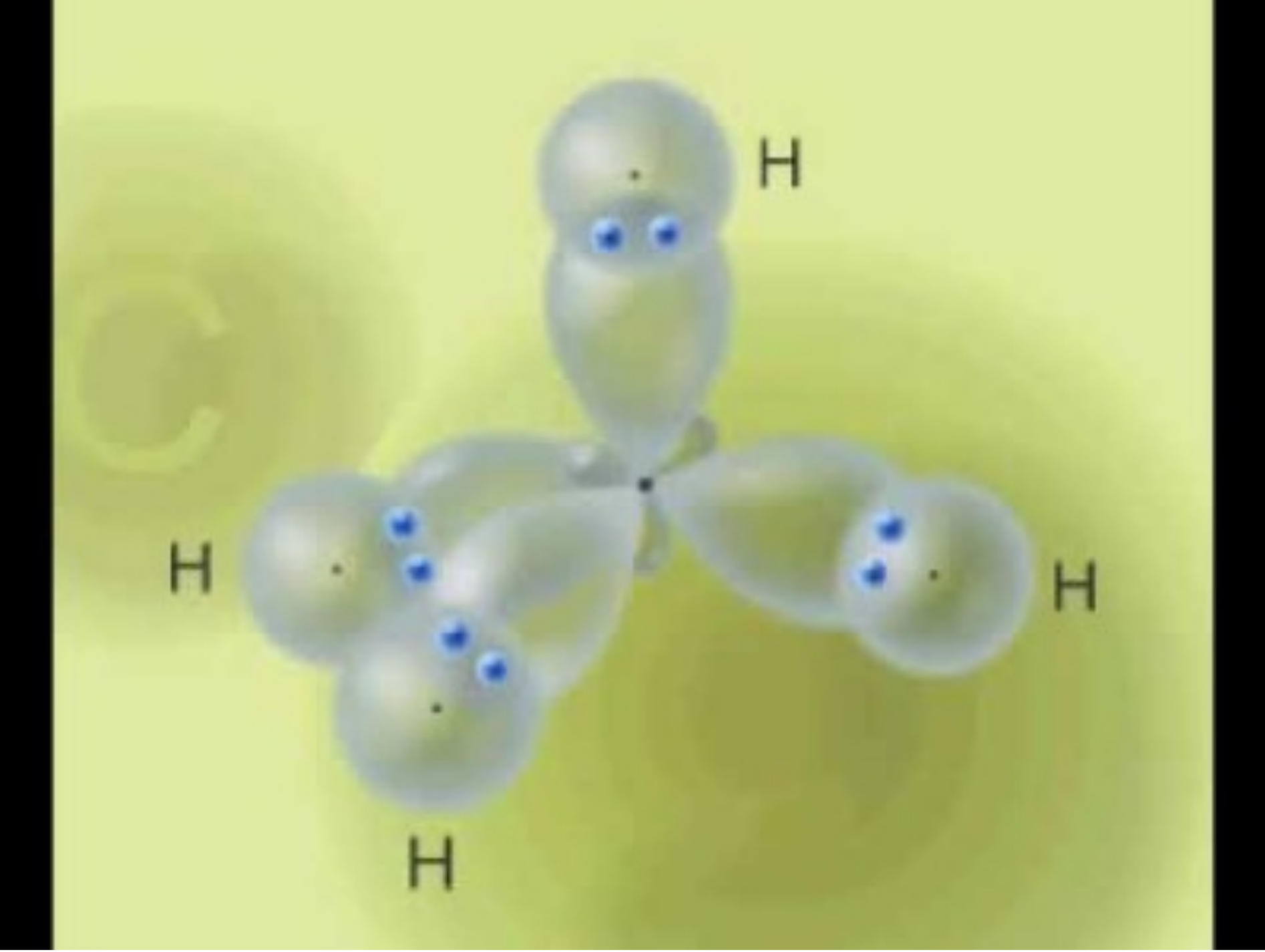
SF₆ SF_6

Lewis structure

156.4 pm   90°

octahedral

BrF₅ BrF_5

Lewis structure

Square pyramid

85.1°

https://youtu.be/1Mg97CoaWwg