Unit 1, Lesson 10: VSEPR Theory and Molecular Shape

http://www.chem.ufl.edu/~chm2040/Notes/Chapter_11/shapes.html

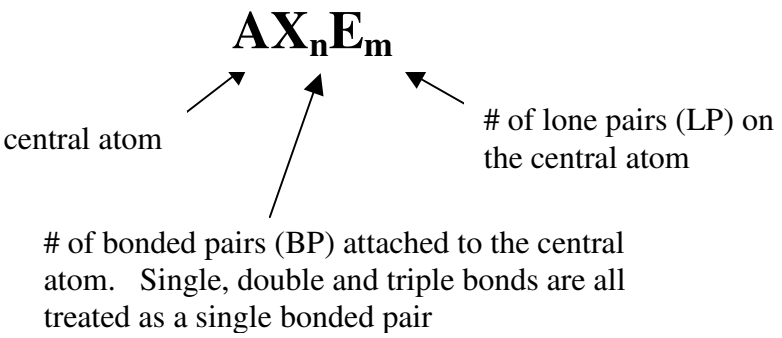
Lewis structures are two-dimensional representations of molecules; however, most molecules are three-dimensional. A molecule's shape depends on the number of bonded pairs (BP) and lone pairs (LP) around the central atom.

Dr. Gillespie at McMaster University in Hamilton developed the VSEPR Theory to explain the shapes of molecules. He was one of Mrs. Chiasson's chemistry professors.

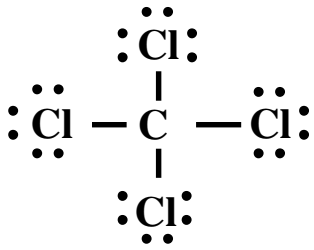
VSEPR (pronounced "vesper") stands for **V**alence **S**hell **E**lectron **P**air **R**epulsion Theory:

- states that the shape of a molecule depends on the repulsion between the electron pairs in the valence shell around the molecule's central atom
- electron pairs can be either bonded pairs (BP, single, double and triple bonds are all treated as one "bonded pair") or lone pairs (LP) around the central atom
- the electron pairs will repel each other so they are as far apart as possible
- lone pairs spread out and take up more room than bonded pairs so they will push the bonded atoms closer together

The number of bonded pairs and lone pairs around a central atom is determined from the Lewis diagram for the molecule and can be written using the general VSEPR notation:



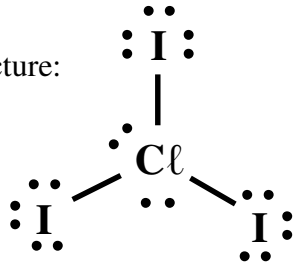
eg. $CC\ell_4$ has the Lewis structure:



- the central atom has 4 BP and 0 LP
- in VSEPR notation we would write:

AX_4E_0

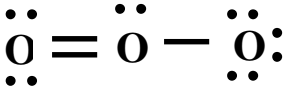
eg. $IC\ell_3$ has the Lewis structure:



- the central atom has 3 BP and 2 LP
- in VSEPR notation we would write:

AX_3E_2

eg. O_3 has the Lewis structure:



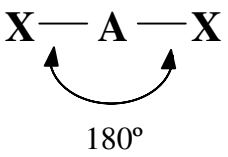
- the central atom has 2 BP and 1 LP
- in VSEPR notation we would write:

AX_2E_1

The Lewis structure determines the number of bonded pairs and lone pairs on the central atom.
The number of bonded pairs and lone pairs on the central atom determines the shape of the molecule.

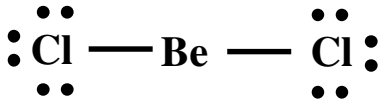
The shapes of molecules are grouped by the # of BP + # of LP around the central atom:

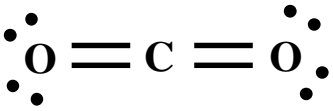
1. # of BP + # of LP on the central atom = 2



- VSEPR notation: $\mathbf{AX_2E_0}$
- the two BP spread out as far as possible
- the X – A – X bond angle is 180º
- the basic shape is linear

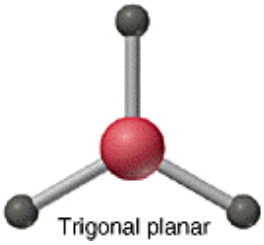
eg. $BeCl_2$ HCN CS_2 and CO_2
(remember, a multiple bond is treated as a one electron group)

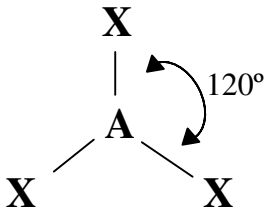




2. # of BP + # of LP on the central atom = 3

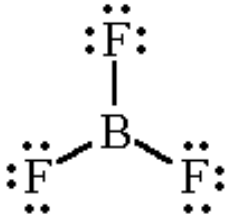
a) 3 BP and no LP, VSEPR notation: $\mathbf{AX_3E_0}$

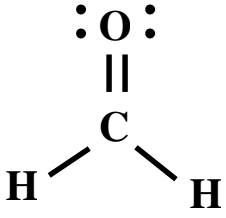


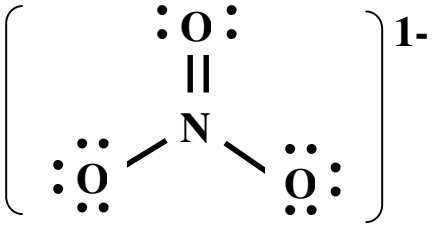


- the three BP spread out as far as possible
- the X – A – X bond angle is 120º
- the basic shape is trigonal planar

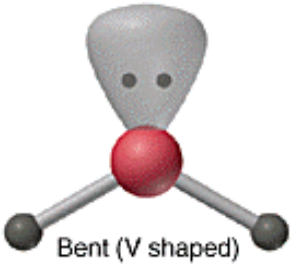
eg. BF_3 CH_2O and NO_3^{1-}

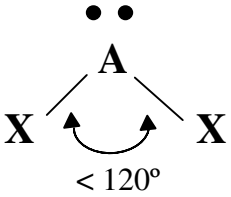






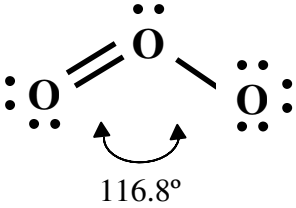
b) 2 BP and one LP, VSEPR notation: $\mathbf{AX_2E_1}$

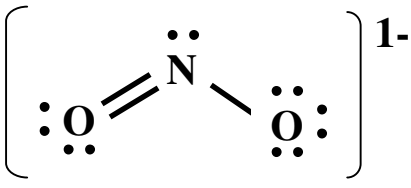




- the two BP are pushed closer together by the lone pair
- the X – A – X bond angle is <120º
- the basic shape is bent or V-shaped

eg. O_3 and NO_2^{1-}



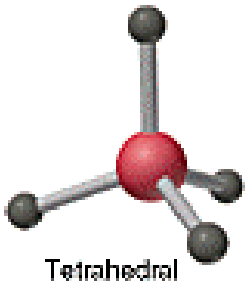


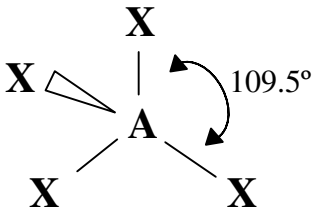
3. # of BP + # of LP on the central atom = 4

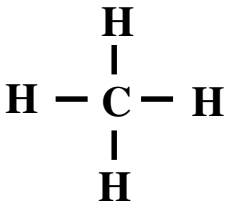
a) 4 BP and no LP, VSEPR notation: $\mathbf{AX_4E_0}$

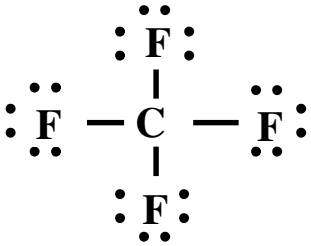
- the four BP spread out as far as possible
- the X – A – X bond angle is 109.5º
- the basic shape is tetrahedral

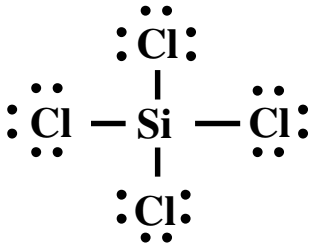
eg. CH_4 CF_4 $SiCl_4$ and $SnCl_4$







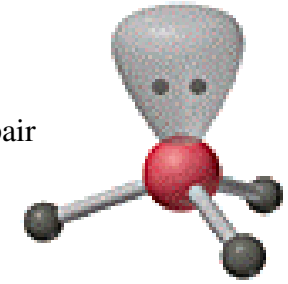


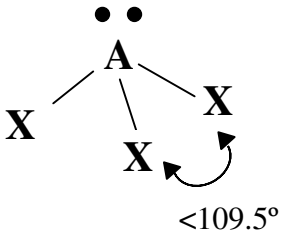


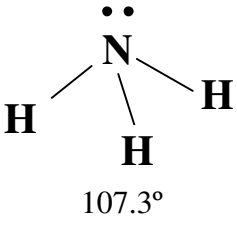
b) 3 BP and one LP, VSEPR notation: $\mathbf{AX_3E_1}$

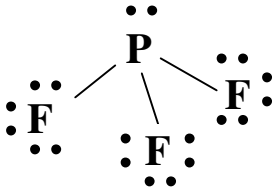
- the three BP spread out as far as possible
- the three BP are pushed closer together by the lone pair
- the X – A – X bond angle is <109.5º
- the basic shape is trigonal pyramidal

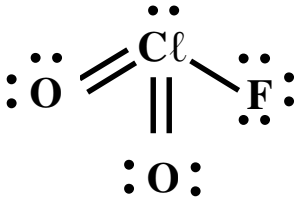
eg. NH_3 PF_3 $C\ell O_2F$ and $AsC\ell_3$







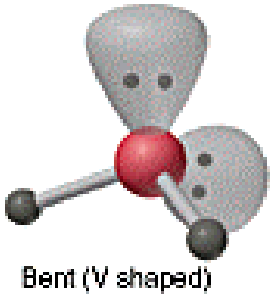


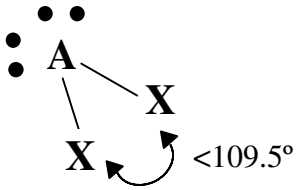


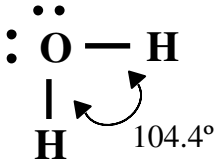
c) 2 BP and two LP, VSEPR notation: $\mathbf{AX_2E_2}$

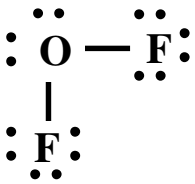
- the two BP spread out as far as possible
- the two BP are pushed closer together by two lone pairs
- the X – A – X bond angle is <109.5º
- the basic shape is bent or V-shaped

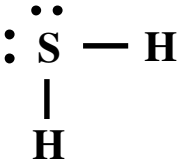
eg. H_2O OF_2 H_2S and SF_2









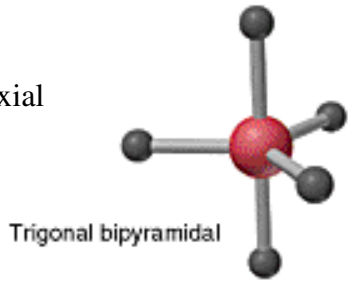


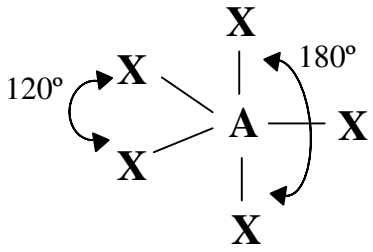
4. # of BP + # of LP on the central atom = 5 (expanded valence)

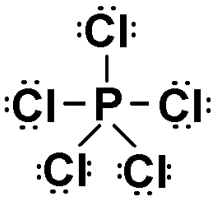
a) 5 BP and no LP, VSEPR notation: **AX_5E_0**

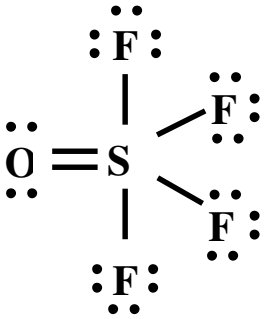
- the five BP spread out as far as possible
- the X – A – X bond angle between the two axial atoms is 180º
- the X – A – X bond angle between the three equatorial atoms is 120º
- the basic shape is trigonal bipyramidal

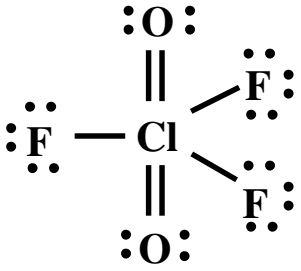
eg. $PC\ell_5$ SOF_4 $C\ell F_3O_2$







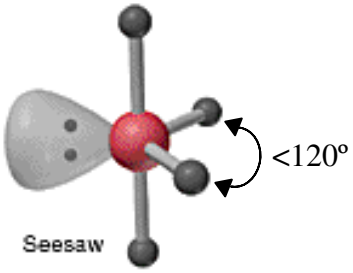


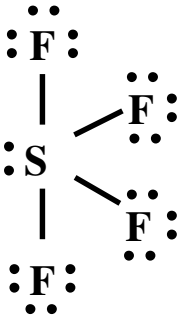


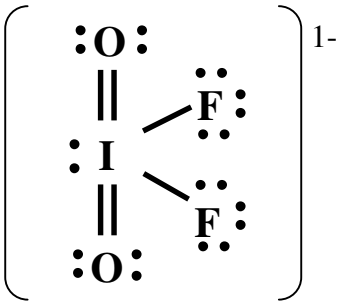
b) 4 BP and one LP, VSEPR notation: **AX_4E_1**

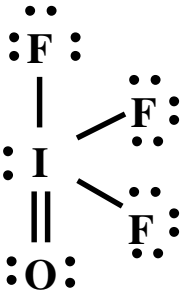
- the four BP spread out as far as possible
- it is lower energy if the lone pair is found in an equatorial position
- the lone pair will push the remaining equatorial atoms closer together, so the equatorial X – A – X bond angle is <120º
- the basic shape is "seesaw"

eg. SF_4 $IF_2O_2^{1-}$ IOF_3 BrF_4^{1+}





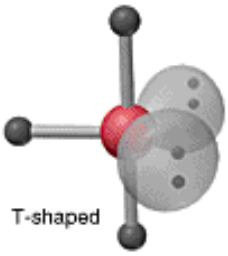


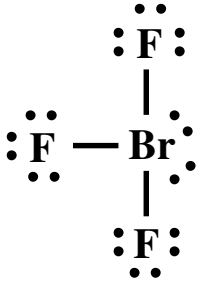


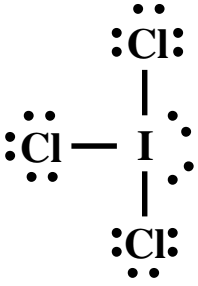
c) 3 BP and two LP, VSEPR notation: **AX_3E_2**

- the three BP spread out as far as possible
- it is lower energy if the two lone pairs are found in equatorial positions
- the basic shape is "T-shaped"

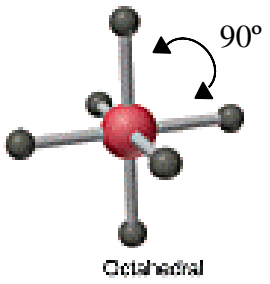
eg. BrF_3 $IC\ell_3$ $C\ell F_3$







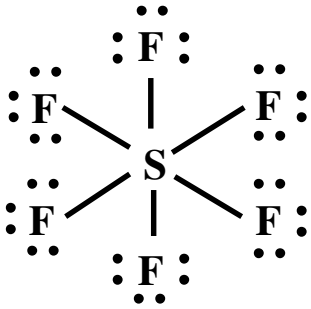
5. # of BP + # of LP on the central atom = 6 (expanded valence)

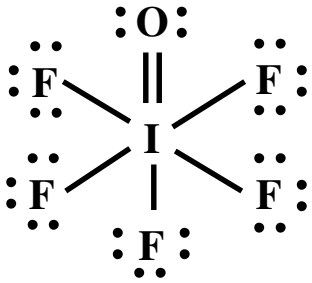


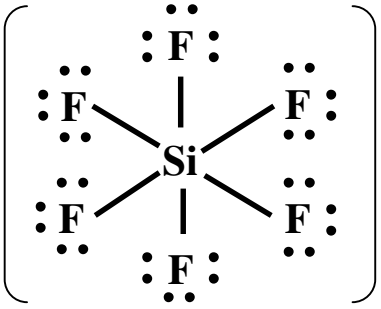
a) 6 BP and no LP, VSEPR notation: **AX_6E_0**

- the six BP spread out as far as possible
- the X – A – X bond angle between all atoms is 90º
- the basic shape is "octahedral"

eg. SF_6 IOF_5 $C\ell F_6^{1+}$ SiF_6^{2-}



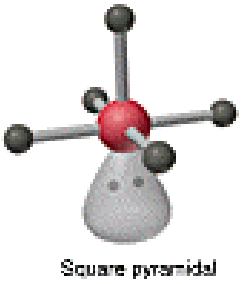


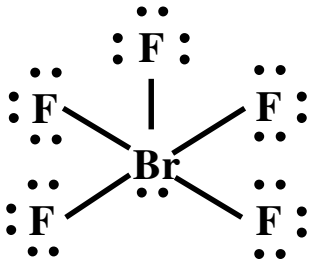


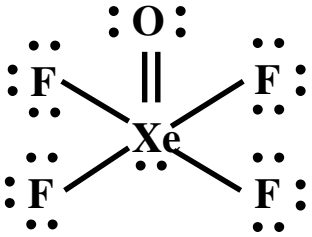
b) 5 BP and one LP, VSEPR notation: **AX_5E_1**

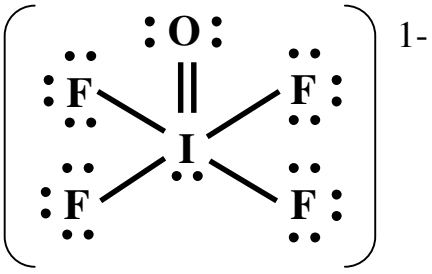
- the five BP spread out as far as possible
- the lone pair is found in one corner of the octahedral
- the X – A – X bond angles are very close to 90º
- the basic shape is "square-based pyramid"

eg. BrF_5 $XeOF_4$ IOF_4^{1-} $IC\ell_5$





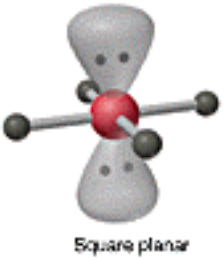


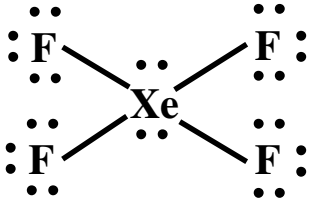


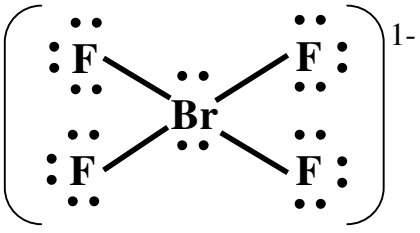
c) 4 BP and two LP, VSEPR notation: **AX_4E_2**

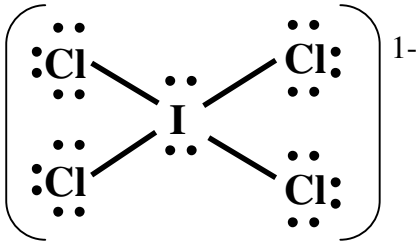
- the four BP spread out as far as possible
- the lone pairs are found above and below the plane of the bonded atoms
- the basic shape is square planar

eg. XeF_4 BrF_4^{1-} $IC\ell_4^{1-}$









VSEPR Summary

To predict the shape of a molecule:
1. Draw the Lewis structure for the molecule.
2. Count the number of bond pairs (BP) and lone pairs (LP) around the central atom.
3. Decide on the total number of electron groups (treat multiple bonds as single electron groups).
4. Consider the locations of lone pairs and any distortions from "regular" shapes.
5. Name the shape based on the arrangement of the bonding **atoms** as outlined below:

a) If the total number of electron groups (bond pairs + lone pairs) is **TWO**:
- two bond pairs and no lone pairs ( ): the molecule is linear

b) If the total number of electron groups (bond pairs + lone pairs) is **THREE**:
- three bond pairs and no lone pairs ( ): the molecule is trigonal planar
- two bond pairs and one lone pair ( ): the molecule is bent or V-shaped

} Trigonal Planar or Variation

c) If the total number of electron groups (bond pairs + lone pairs) is **FOUR**:
- four bond pairs and no lone pairs ( ): the molecule is tetrahedral
- three bond pairs and one lone pair ( ): the molecule is trigonal pyrimidal
- two bond pairs and two one pairs ( ): the molecule is bent or V-shaped

} Tetrahedral or Modified Tetrahedral

d) If the total number of electron groups (bond pairs + lone pairs) is **FIVE**:
- five bond pairs and no lone pairs ( ): the molecule is trigonal bipyramidal
- four bond pairs and one lone pair ( ): the molecule is a "see-saw" shape
- three bond pairs and two lone pairs ( ): the molecule is "T-shaped"
- two bond pairs and three lone pairs ( ): the molecule will be linear

} Trigonal Bipyramidal or Modified Trigonal Bipyramidal

e) If the total number of electron groups (bond pairs + lone pairs) is **SIX**:
- six bond pairs and no lone pairs ( ): the molecule is octahedral
- five bond pairs and one lone pair ( ): the molecule is a square-based pyramid
- four bond pairs and two lone pairs ( ): the molecule is square planar

} Octahedral or Modified Octahedral

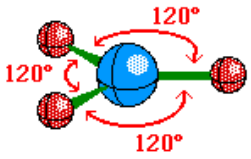
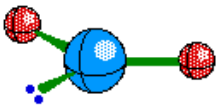
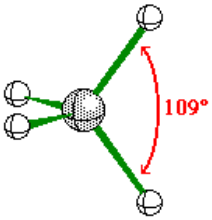
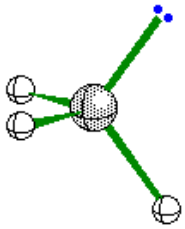
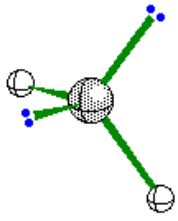
Homework:
1. Read pages178 to 185

2. Identify the molecular shape associated with the following VSEPR notations

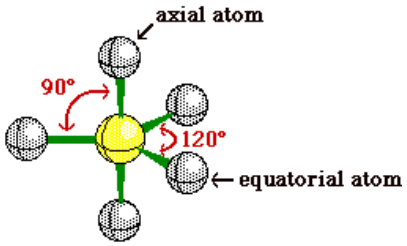
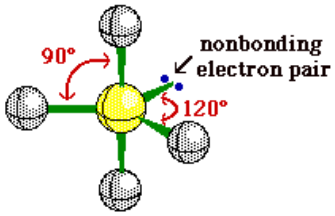
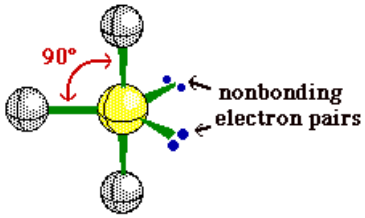
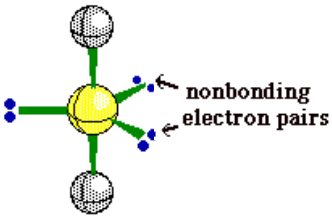
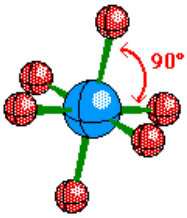
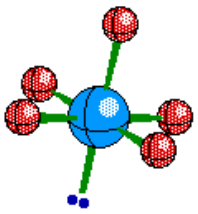
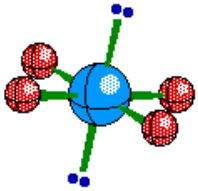
a) AX_5E_1	e) AX_6E_0
b) AX_3E_0	f) AX_3E_2
c) AX_4E_2	g) AX_3E_1
d) AX_2E_1	h) AX_5E_0
e) AX_4E_1	i) AX_4E_0
f) AX_2E_2	j) AX_2E_3

3. On pages 185 – 186, do questions18 to 21 (refer to the examples on pages184 to 185)

VSEPR Theory and Molecular Shape

Total # of e- groups (BP + LP) in valence level of central atom (basic shape)	# of bonded e- pairs (BP) around central atom (X)	# of unbonded e- pairs (lone pairs, LP) around central atom (E)	General Formula (VSEPR notation) AX_nE_m	Lewis Structure (use A as the central atom and X as the bonded atoms)	Diagram and Name of Molecular Shape	Example
2						$BeC\ell_2$ CO_2 HCN
3						$BC\ell_3$ CH_2O BF_3
3						O_3 NO_2^{1-}
4						$CC\ell_4$ NH_4^+ $C\ell O_4^{1-}$
4						NH_3 PF_3 $C\ell O_2F$
4						H_2O OF_2 I_3^{1+}

* when determining molecular shape, a double or triple bond is a single electron group. Treat multiple bonds as a single bonded pair (BP)

Total # of e- groups (BP + LP) in valence level of central atom (basic shape)	# of bonded e- pairs (BP) around central atom (X)	# of unbonded e- pairs (lone pairs, LP) around central atom (E)	General Formula	Lewis Structure	Diagram and Name of Molecular Shape	Example
5						$PC\ell_5$ $C\ell F_3O_2$ SOF_4
5						SF_4 $IF_2O_2^{1-}$ BrF_4^{1+}
5						BrF_3 $IC\ell_3$
5						XeF_2 I_3^{1-} $IC\ell_2^{1-}$
6						SF_6 IOF_5 $C\ell F_6^{1+}$
6						BrF_5 $XeOF_4$ IOF_4^{1-}
6						XeF_4 BrF_4^{1-} $I\,C\ell_4^{1-}$