A.AravinthanB.sc.(Hons)Spl.Chem,PGDE

VSEPRtheory

Valence shell electron pair repulsion (VSEPR) theory (1957) is a model in chemistry, which is used for predictingthe shapes of individual molecules, based upon their extent of electron-pair electrostatic repulsion, determined usingsteric numbers[1] .

The theory is also called the **Gillespie-Nyholm theory** after the two main developers. The premise of VSEPR is that a constructed Lewis structure is expanded to show all lone pairs of electrons alongsideprotruding and projecting bonds, for predicting the geometric shape and lone-pair behavior of a compound throughconsideration of the total coordination number.

VSEPR theory is based on the idea that the geometry of a molecule or polyatomic ion is determined primarily byrepulsion among the pairs of electrons associated with a central atom.

The pairs of electrons may be bonding ornonbonding (also called lone pairs). Only valence electrons of the central atom influence the molecular shape in ameaningful way.

Basic assumptions

1. Pairs of electrons in the valence shell of a central atom repel each other.
2. These pairs of electrons tend to occupy positions in space that minimize repulsions and maximize the distance ofseparation between them.
3. The valence shell is taken as a sphere with electron pairs localizing on the spherical surface at maximum distancefrom one another.
4. A multiple bond is treated as if it is a single electron pair and the two or three electron pairs of a multiple bondare treated as a single super pair.
5. Where two or more resonance structures can depict a molecule the VSEPR model is applicable to any such

structure. Three types of repulsion take place between the electrons of a molecule:

1. The lone pair-lone pair repulsion
2.The lone pair-bonding pair repulsion
3.The bonding pair-bonding pair repulsion.

A molecule must avoid these repulsions to remain stable. When repulsion cannot be avoided, the *weaker repulsion* (i.e. the one that causes the smallest deviation from the ideal shape) is preferred. The lone pair-lone pair (lp-lp) repulsion is considered to be stronger than the lone pair-bonding pair (lp-bp)

repulsion, which in turn is stronger than the bonding pair-bonding pair (bp-bp) repulsion. Hence, the weaker bp-bprepulsion is preferred over the lp-lp or lp-bp repulsion.

VSEPR theory is usually compared (but not part of) and contrasted with valence bond theory, which addresses

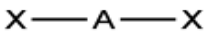
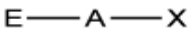
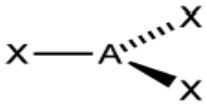
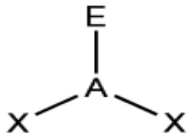
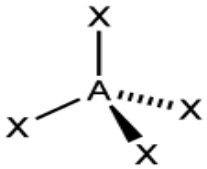
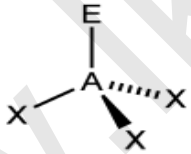
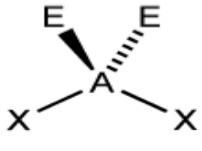
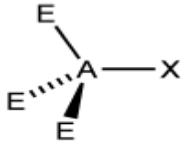
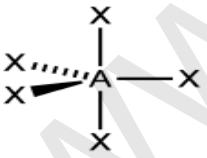
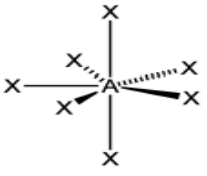
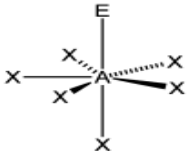
molecular shape through orbitals that are energetically accessible for bonding. Valence bond theory concerns itself with the formation of sigma and pi bonds. Molecular orbital theory is another model for understanding how atoms and electrons are assembled into molecules and polyatomic ions.

www.lkcou.lk

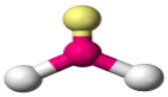
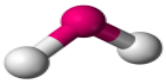
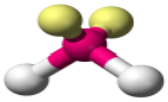
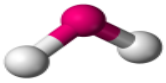
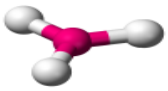
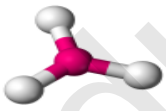
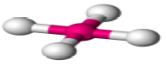
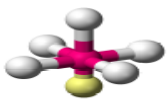
VSEPR theory has long been criticized for not being quantitative, and therefore limited to the generation of "crude",even though structurally accurate, molecular geometries of covalent molecules. However, molecular mechanics force fields based on VSEPR have also been developed.[2]

AXE Method

The "AXE method" of electron counting is commonly used when applying the VSEPR theory. The *A* represents thecentral atom and always has an implied subscript one. The *X* represents how many sigma bonds are formed betweenthe central atoms and outside atoms. Multiple covalent bonds (double, triple, etc) count as one X. The *E* representsthe number of lone electron *pairs* present outside of the central atom. The sum of *X* and *E*, sometimes known as thesteric number, is also associated with the total number of hybridised orbitals used by valence bond theory.

Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs
1	 linear			
2	 linear	 Linear		
3	 trigonal planar	 bent	 Trigonal Planar	
4	 tetrahedral	 trigonal pyramid	 bent	 linear
5	 trigonal bipyramid	 seesaw (chemistry)	 T-shaped (chemistry)	 linear
6	 octahedral	 square pyramid	 square planar	
7	 Pentagonal bipyramid	 pentagonal pyramid		

www.ikedu.lk

Type	Shape	Geometry†	Geometry‡	Examples
AX_1E_*	Diatomic			HF, O_2
AX_2E_0	Linear			$BeCl_2$, $HgCl_2$, CO_2
AX_2E_1	Bent			NO_2^-, SO_2, O_3
AX_2E_2	Bent			H_2O, OF_2
AX_2E_3	Linear			XeF_2, I_3^-
AX_3E_0	Trigonal planar			BF_3, CO_3^{2-}, NO_3^-, SO_3
AX_3E_1	Trigonal pyramidal			NH_3, PCl_3
AX_3E_2	T-shaped			ClF_3, BrF_3
AX_4E_0	Tetrahedral			CH_4, PO_4^{3-}, SO_4^{2-}, ClO_4^-
AX_4E_1	Seesaw			SF_4
AX_4E_2	Square Planar			XeF_4
AX_5E_0	Trigonal Bipyramidal			PCl_5
AX_5E_1	Square Pyramidal			ClF_5, BrF_5
AX_6E_0	Octahedral			SF_6
AX_6E_1	Pentagonal pyramidal			XeF_6
AX_7E_0	Pentagonal bipyramidal			IF_7

www.ikeou.lk

When the substituent (X) atoms are not all the same, the geometry is still approxmiately valid, but the bond anglesmay be slightly different than the ones where all the outside atoms are the same. For example, the double-bondcarbons in alkenes like C2H4 are AX3E0, but the bond angles are not all exactly 120 Å. Similarly, SOCl2 is AX3E1,but because the X substituents are not identical, the XAX angles are not all equal.

The methane molecule (CH4) is tetrahedral because there are four pairs of electrons. The four hydrogen atoms are

positioned at the vertices of a tetrahedron, and the bond angle is cos-1(-1/3) Å 109Å28'. This is referred to as an AX4type of molecule. As mentioned above, A represents the central atom and X represents all of the outer atoms.

The ammonia molecule (NH3) has three pairs of electrons involved in bonding, but there is a lone pairof electrons on the nitrogen atom. It is not bonded with another atom; however, it influences the overall shape through repulsions. As in methane above, there are four regions of electron density. Therefore, the overall orientation of the regions of electron density is tetrahedral. On the other hand, there are only three outer atoms. This is referred to as an AX3E

type molecule because the lone pair is represented by an E. The overall shape of the molecule is a trigonal pyramid because the lone pair is not "visible." The shape of a molecule is found from the relationship of the atoms even though it can be influenced by lone pairs of electrons.

A steric number of seven is possible, but it occurs in uncommon compounds such as iodine heptafluoride. The base geometry for this is pentagonal bipyramidal.

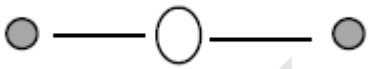
www.AAravinthan.lk

Shapes of molecules – Valence Shell Electron Pair Repulsion (VSEPR) Model.

A. Approach.

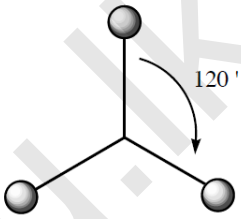
1. Draw Lewis diagram.
2. Count the number of **lone pairs (L) + atoms bonded(B)** around each central atom.
At this point, it does not matter whether the atoms are bonded by single, double, or triple bonds.
3. These groups will repel one another and arrange themselves about the central atom so as to get as far away from one another as possible. The order of repulsion is:
lone pairs >> triple bonds > double bonds > single bonds.
4. If the sum of L+B about a central atom is equal to

a. 2, the arrangement is linear.

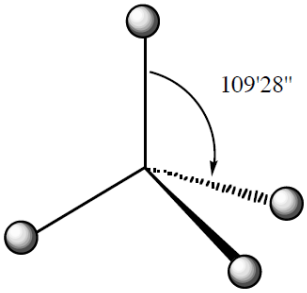


b. 3, the arrangement is trigonal planar.

All three sites are equivalent

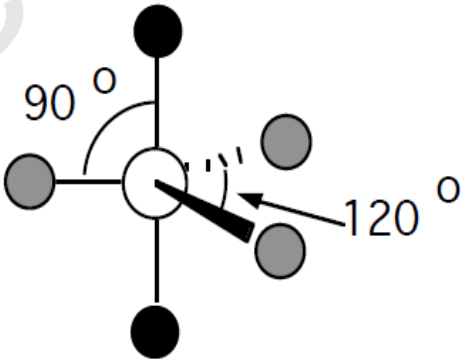


c. 4, All four positions are equivalent.



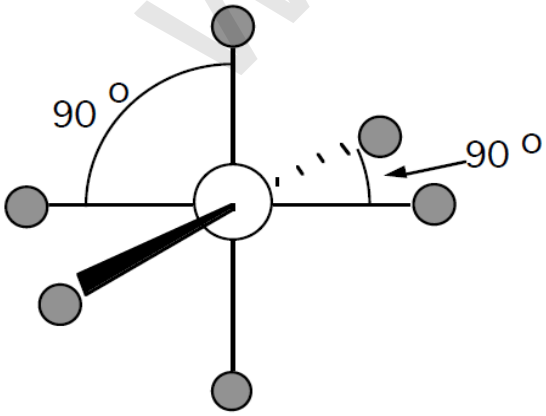
d. 5, the arrangement is trigonal bipyramidal.

1) All five positions are not equivalent.
2) The three positions in the trigonal plane are the **equatorial** positions.
3) The two above and below the equatorial plane are the **axial** positions.



e. 6, the arrangement is octahedral.

All six positions are equivalent



www.Aravinthar.uk

B. Examples.

1. B+L=2; Linear



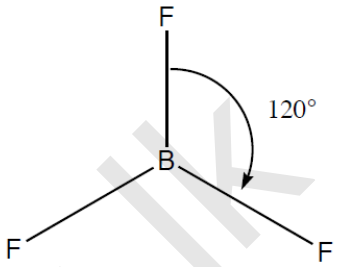
$\overline{O} = C = \overline{O}$ H - C ≡ C - H

2. L+B = 3 F

a. B = 3, L = 0

TRIGONAL PLANAR or

PLANAR TRIANGULAR

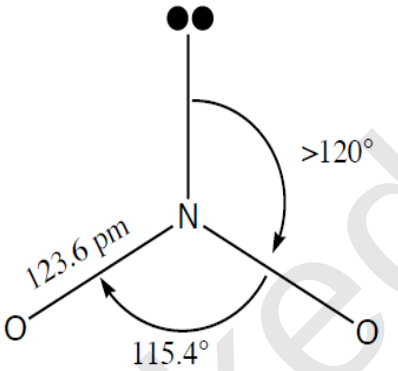


3. b. B = 2, L = 1

Example NO_2^-

(18 e- system)

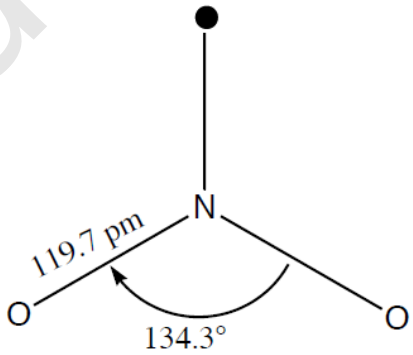
V SHAPED or BENT

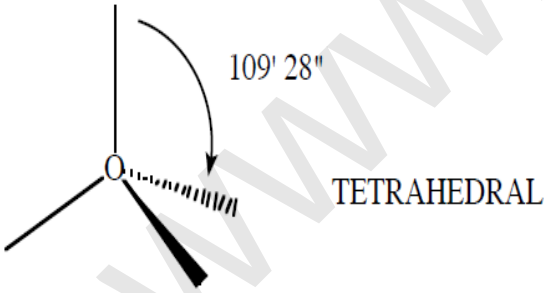


NO2

(17 e- system)

Note that one electron takes up less room than either a bonded pair or a lone pair.

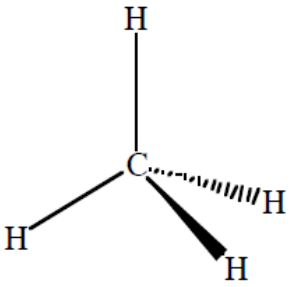


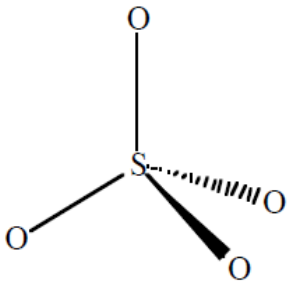


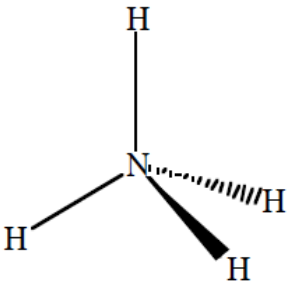
3. L + B = 4; Tetrahedral.

a. B = 4, L = 0

CH4, SO42-, NH4+

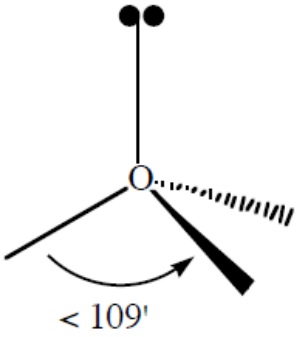


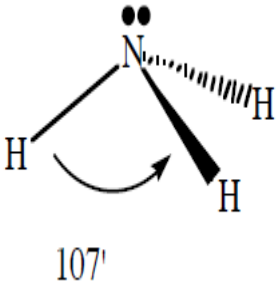


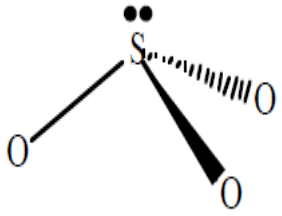


www.lkedu.lk

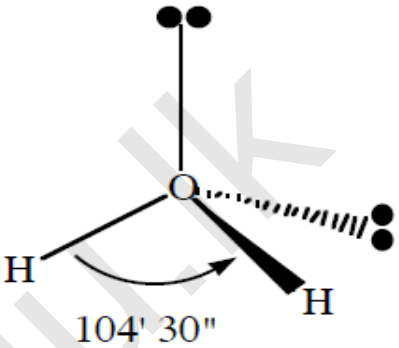
b. B = 3, L = 1
NH3 SO_3^{2-}
TRIGONAL
PYRAMID



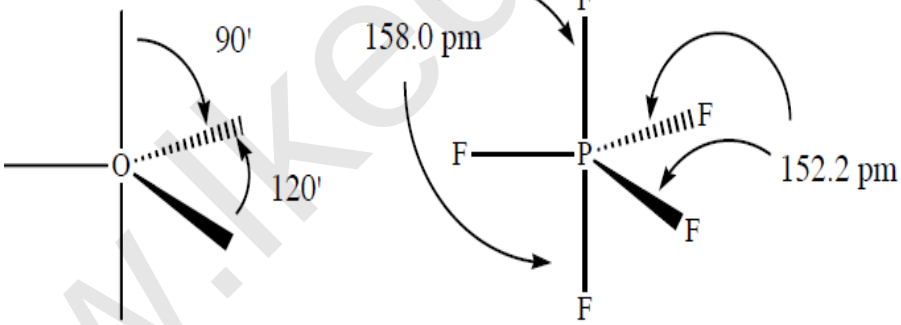




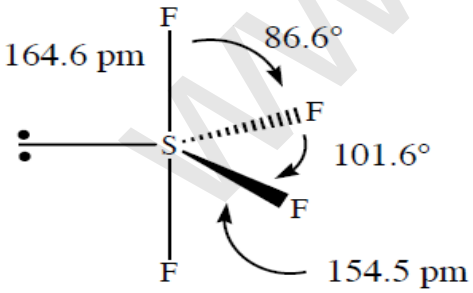
c. B = 2, L = 2 H2O
V SHAPED or
BENT



4. L + B = 5; Trigonal
Bipyramid.
a. B = 5, L = 0 PF5
The F's are not equivalent.
The two axial bonds are158
pm and the three equatorial
bonds are152 pm

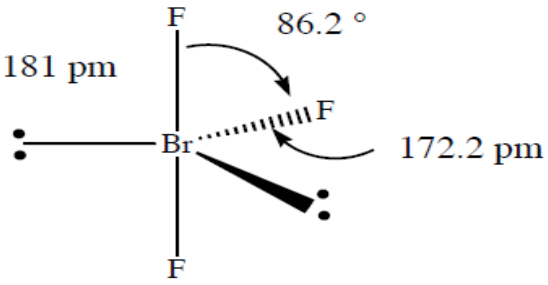


b. B = 4, L = 1 SF4



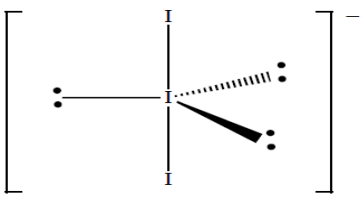
SHAPED

c. B
= 3,
L =2
BrF3
"T"



d. B = 2, L = 3 I_3^-

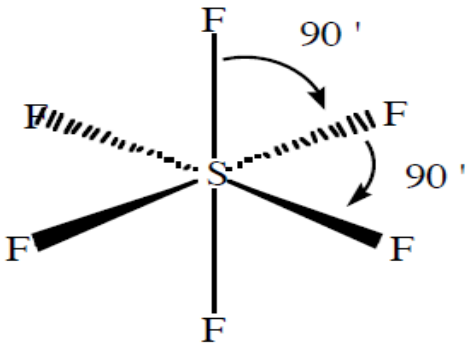
LINEAR



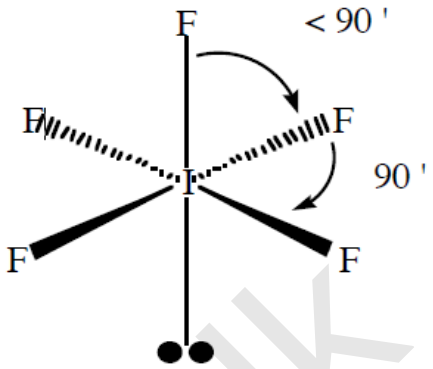
www.tkeduk

5. L + B = 6; Octahedral

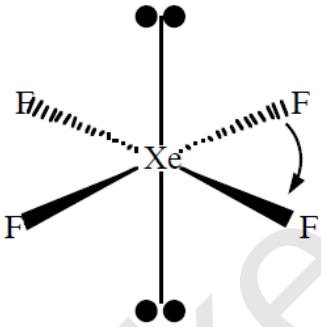
a. B = 6, L = 0 SF_4
OCTAHEDRAL



b. B = 5, = 1 IF_5 SQUAREPYRAMID



c. B = 4, L = 2 XeF4
SQUARE PLANAR



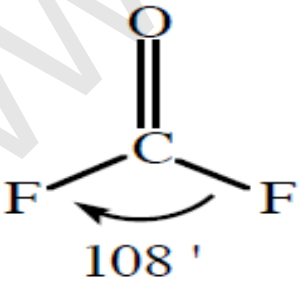
C. Other Considerations.

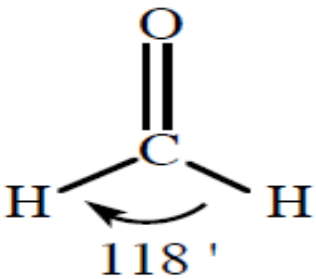
1. Electronegativity differences.

a. Electron-electron repulsion increases the closer the electrons are to the central atom. The electron density in a bond formed between the central atom and a very electronegative atom will be polarized away from the central atom and will be less effective in repelling electrons than if the central atom was bonded to an element with lower electronegative.

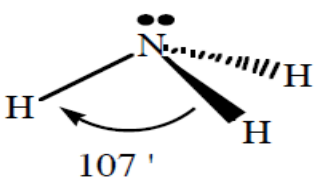
b. Therefore, bond angles involving very electronegative will tend to be smaller than those involving less

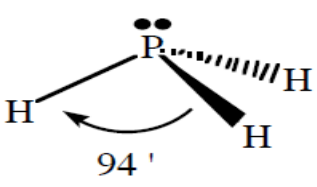
c. Example

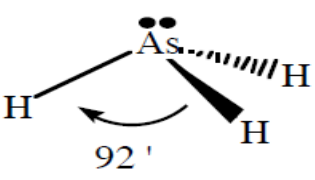




2. When lone pairs are present, the bond angles decrease as the size of the central atom increases.







www.Arkedu.lk

1. The shape of the cationic species PCl_4^+

1. Planer 2. Tirgonal pyramid 3. Trigonal bipyramidal 4. Tetrahedral 5.None of the above

2. . The shape of the cationic species PF_4^+

1. Planer 2. Tirgonal pyramid 3. Trigonal bipyramidal 4. Tetrahedral 5.None of the above

3. The shape of the POClBrF is?

1.is planer 2. Takes the form of the squre pyramid 3. Octahetral 4. tetrahedral 5. Trigonal bipyramidal.

4. Which one of the following statements concerning the shape of the ClO_3^- anions is most appropriate.

1. tetrahedral 2. Planer 3.T-shape 4. Trigonal bipyramidal. 5.ithas the shape of the SO_3

5. Which one of the following species has a shape that shows close simillaries to the shape of the ammonia molecules ?

1. SO_3 2. $SOCl_2$ 3.$COCl_2$ 4. CO_2 5. BF_3

6. Which one of the following statements/statement is/are true about the notronium ion (NO_2^+)

a.It is a linear shape b. There are only σ bonds c. It is a angular shape d. valence shell of N has less than 8 electrons.

7. The ion/molecule which has a shape significantly different from the SO_4^{2-}

1. NH_4^+ 2. BCl_4^- 3. SF_4 4. S_2O_32- 5. CH_4

8. Which one of the following statements concerning the shape of the ICl_2^- anions is most appropriate.

.1. SO_2 2. O_3 3.$BeCl_2$ 4. H_2S 5. HOCl

9.Noble gas Xenon forms a covalent compound XeF_4. The likely geometry of XeF_4 is?

1. tetrahedral 2. Square Planer 3.octrahetral 4. Trigonal bipyramidal. 5. see- saw

10. The ion/molecule which has a shape significantly different from the PO_4^{2-}

1. ICl_4^- 2. $SiCl_4$ 3. $POCl_3$ 4. SO_42- 5. CH_4

11. The shape of the BrF_5 is?

1. tetrahedral 2. Square Planer 3.octrahetral 4. Trigonal bipyramidal. 5. None of the above

12.Which of the following pairs contains species with different shapes?

1. CO_2,$BeCl_2$ 2. PO_4^{3-},$S_2O_3^{2-}$ 3. NO_3-,SO_32- 4. HOBr,H_2S 5. NCl_3,BCl_3

13.In which of the following do the two molecules have an unpaired electron each.

1.SO_2&NO 2. NO&CO 3. NO_2&N_2O 4. SO_2&NO_2 5. NO_2&NO

14.Of the molecules / ions given below , which one has a shape different from the shape of the others

1. SO_4^{2-} 2. $S_2O_3^{2-}$ 3. PCl_4^+ 4.NH_4^+ 5. SF_4

15. Among the following the molecules /ions having the same shape are?

A. NH_3 B. H_3O^+ c. ClF_3 D. BCl_3 E. PCl_3

1. A&C 2. C&D 3. A,B&E 4. C,D,&E 5. A,B&E

www.Aravinthan.lk

16. Identify the molecule or ion from those given below whose shape is distinctly different from that of SO_3^{2-} ion

1. ClO_3- 2. PCl_3 3. $SOCl_2$ 4. H_3O^+ 5. NO_3^-

17. The electron pair geometry & the molecular shape of $XeOF_4$ are respectively.

1. trigonal bipyramidal & octahedral 2. Square pyramidal & Trigonal bipyramidal

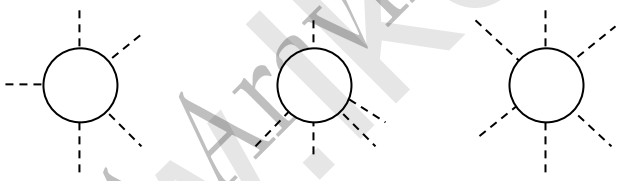
3. trigonal bipyramidal &square pyramidal 4. square pyramidal& octahedral

5. octahedral &square pyramidal

18.The shape & electron pair geometry of F_4ClO^- ion are respectively.

1. trigonal bipyramidal & square pyramidal 2. square pyramidal& octahedral
3. . trigonal bipyramidal & octahedral 4. Square pyramidal & Trigonal bipyramidal
5. octahedral &square pyramidal

(1) மூலக்கூறுகளிலுள்ள தள்ளும் அலகுகளின் (பிணைப்புகளினதும் தனிச்சோடிகளினதும்) சாத்தியமான ஒழுங்கமைப்புகளைக் காட்டக்கூடிய மூன்று வடிவங்கள் கீழே தரப்பட்டுள்ளன. இவற்றுள் பொருத்தமான வடிவத்தைத் தேர்ந்தெடுத்து SiF_4,XeF_4,SF_4 ஆகிய மூலக்கூறுகளிலுள்ள நடு அணுவைச் சுற்றியுள்ள தள்ளும் அலகுகளின் ஒழுங்கமைப்புகளைக் குறிப்பிடுக. இதற்காக நடு அணுவை ஒவ்வொரு வட்டத்துள்ளும் பிணைப்புகளைத் திண்மக் கோடுகளாலும் (-) தனிச்சோடிகளை ஆலும் குறிப்பிடுக.

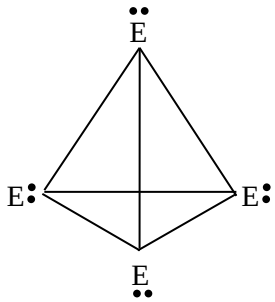


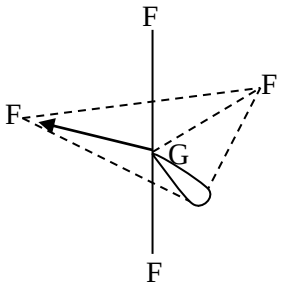
(2) N_2O_4,O_3 ஆகிய மூலக்கூறுகளின் எல்லா அணுக்களினதும் வலுவளவு இலத்திரன்களைக் காட்டும் புள்ளி – புள்ளடி வரிப்படங்களை கீழே உள்ள பொருத்தமான பெட்டிகளில் வரைக.

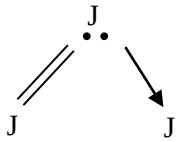
(i) N_2O_4	(i) O_3

www.Aravinthan.lk

(3) கீழே தரப்பட்ட E_4,GF_4,J_3 ஆகிய மூலக்கூறுகளின் கட்டமைப்புகளிலுள்ள E,G,J ஆகிய மூலகங்களை இனங்காண்க.







E = …… G = ……..…… J = ……

3ம் பக்கத்தில் தரப்பட்டுள்ள ஆவர்த்தன அட்டவணைக் கூட்டின் பொருத்தமான பெட்டிகளில் E,G,J ஆகியவற்றிற்குரிய இரசாயனக் குறியீடுகளை எழுதுக.

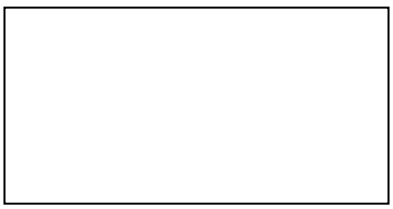
1																	2
3	4											5	6	7	8	9	10
11	12											13	14	15	16	17	18
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36

(4) A எனும் மூலகம் AF_2^-, AF_4^- ஆகிய அன்னயன்களை உண்டாக்குகின்றது வடிவத்தில் AF_2^- நேர்கோடாகவும் AF^-_4 தளசதுரமாகவும் உள

i. தனிச்சோடி இலத்திரன்கள் ஏதாவது நடு அணுவில் இருப்பின் அவற்றின் ஒழுங்கமைப்புகளைச் சுட்டிக் காட்டி AF^-_2 இனதும் வடிவங்களை வரைக.



AF^-_2



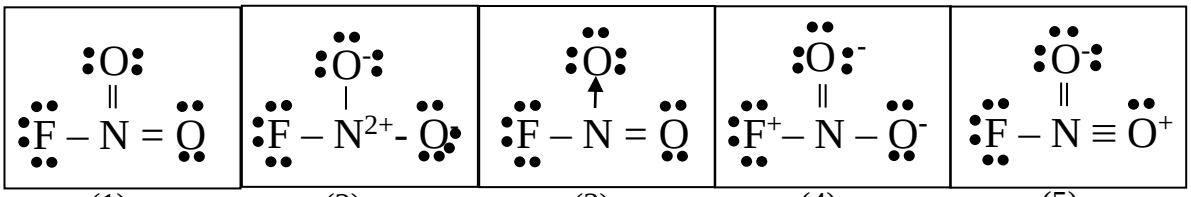
AF^-_4

ii. ஆவர்த்தன அட்டவணையில் A இற்குரிய கூட்டத்தைத் தருக.

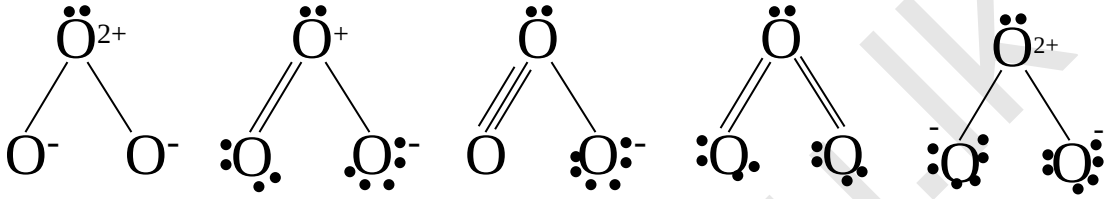
……

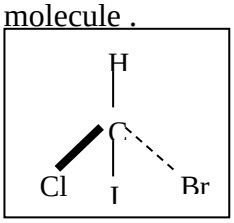
www.Aravinthan.lk

19. **The most acceptable Lewis strcture for** NO_2F



27. The most acceptable Lewis strcture for O_3



	1st statement	**2nd statement**
21	ICl_2- **&** NO_2 are both linear in shape	**Molecules/ions that have the same number of atoms generally have the sameshape bond**
22.	**The** PF_3 molecule is planer	**In** PF_3 phosphorus is trivalent
23.	**H**$_3O^+$ is planer	**There are three O−H** bonds in H_3O+
24.	PCl_5 exist but NCl_5 does not	**The Phosphorous atom is larger than the nitrogen atom**
25.	**I**Cl_4- ion is tetrahetral	**There** are four repulsion units around the iodine atom in ICl_4-
26.	Each bond angle in the molecule . Is equal to109.5˚ 	**The** carbon atom in this molecules is SP3 hybridised.

www.AravinthanTN.lk