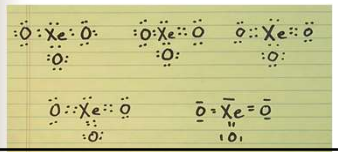
VSEPR Theory

Problem

- Give possible Lewis structures for XeO_3, an explosive compound of xenon. Which Lewis structure or structures are most appropriate **according to the formal charges**?

- The top three all have formal charges although the are closer to obeying the octet rule.
- The bottom is the most correct **by formal charge**, as 0 is assigned to everything.



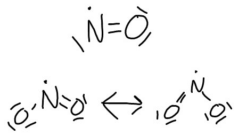
Current AP Grading

- If the problem does explicitly say "by formal charge", any of the resonance structures on the previous slide for XeO_3 would have been acceptable.
- Older research said formal charges rarely exist, new research is contradicting that.

Odd electron problems

- Although rare, it is possible to have compounds that have an odd number of electrons.
- Obviously it is not possible to satisfy the octet rule with an odd number of electrons, ONE CANNOT BE A PAIR!
- Two compounds are NO and NO_2
- They will have a free electron.

Lewis dot



Nitrous Oxide Systems, Inc.

- The formal charge is appropriate for each atom and the molecule
- Compounds with a free electron, unpaired electron, are called free radicals.
- They are highly reactive.
- These two compounds are used in nitrous oxide systems in cars

VSEPR theory

- Valence shell electron pair repulsion theory
- Simply stated it says- all atoms and electrons pairs will stay as far apart from one another as possible in 3-D space.
- This is because electrons and the electron shells of each atom are negative and therefore repel each other.
- We will only deal with the simple shapes around <u>one</u> *center* atom

Steric number

- Steric number- how many spots an atom has for pairs of electrons or bonds
- steric number = bonds + unshared electron pairs
- Steric number can go from 2-6
- Double/Triple bonds count as 1 bond.
- *only get the steric number for the **<u>ONE</u>** center atom

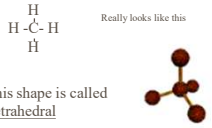
Other designation

- AB_mN_n designation, where *m* and *n* are integers, A is the central atom, B is a surrounding atom, and N is a nonbonding valence-electron group, is also used
- Bond angle, the angle formed by two surrounding atoms with the central atom at the vertex, is also measured in the VSEPR model.

Steric number 4 AB_4

So something like methane - CH_4

The bond angle is 109.5°



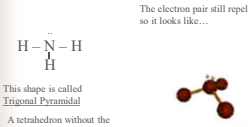
Really looks like this

This shape is called Tetrahedral

Unbonded pair of electrons… Steric number 4 AB_3N

Something like ammonia NH_3

The electron pair still repels the atoms so it looks like…



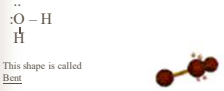
This shape is called Trigonal Pyramidal

A tetrahedron without the top piece, or a triangle that is bent downwards

Steric number 4 AB_2N_2

Something like water H_2O

You get a shape that looks like



This shape is called Bent

A "V" shape

Steric number 4 ABN_3

Something like Chlorine gas, Cl_2

It looks exactly like we draw it

This shape is called Linear

A straight line

Steric number of 3 AB_3

Like BF_3 or CH_2O

Will look like this

The bond angle is 120°

This is called Trigonal Planar

A flat triangle

Steric number of 2 AB_2

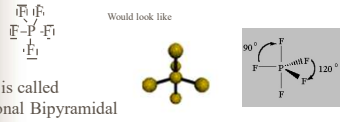
Like CO_2 carbon dioxide

Is again a linear shape it looks exactly as it is drawn

The bond angle is 180°

Steric number of 5 AB_5

Like PF_5 Phosphorus pentafluoride



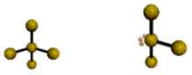
Would look like

This is called Trigonal Bipyramidal

The bond angle is either 90° or 120°

Steric # 5 with unbonded pairs of electrons

- With one pair of unbonded electrons it is a See-saw shape (SF_4, IOF_4) AB_4N_1
- With two pairs of unbonded electrons it is T-Shaped (ClF_3, BrF_3) AB_3N_2
- With 3 unbonded pairs of electrons it is linear (XeF_2)



Steric number of 6 AB_6

Like SF_6 sulfur hexafluoride

Would look like

This shape is Octahedral

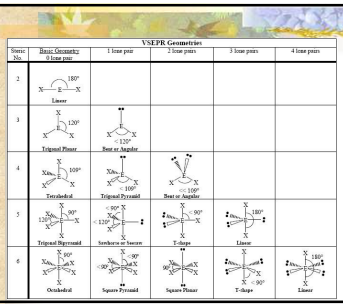
The bond angle is 90^0

Steric # of 6 with unbonded pairs of electrons

- With one unbonded pair of electrons it is square pyramidal. ($XeOF_4$) AB_5N_1
- With two unbonded pairs of electrons it is square planar. (XeF_4) AB_4N_2

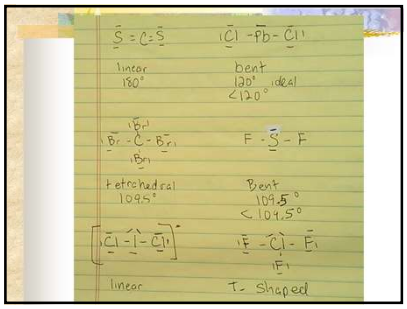
Table of all shapes

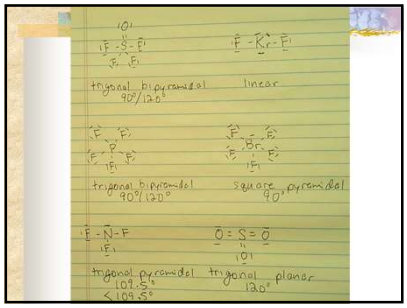
e⁻ pairs	Steric # 2	Steric # 3	Steric # 4	Steric # 5	Steric # 6
Bond angle	180°	120°	109.5°	90° and 120°	90°
0	Linear	Trigonal planar	tetrahedral	Trigonal Bipyramidal	octahedral
1	(Linear)	(bent)	trigonal pyramidal	Seesaw	Square pyramidal
2	n/a	(linear)	bent	T-Shaped	Square Planar
3	n/a	n/a	Linear	Linear	n/a



Problems

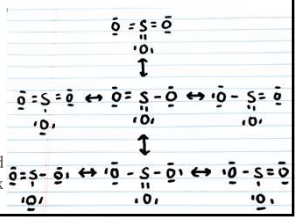
- Draw the Lewis dot structure and name the shape and predict the ideal bond angles, and any deviations from them, for the following molecules CS_2, $PbCl_2$, CBr_4, SF_2, ICl_2^-, ClF_3, SOF_4, KrF_2, PF_5, BrF_5, NF_3, and SO_3.





SO_3 possible resonance structures

- No FC, expanded valence
- FC on 1 O and S
- No expanded valence, max FC

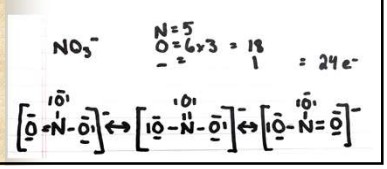


Resonance

- When a molecule exhibits resonance, any one of the resonance structures can be used to predict the molecular structure using the VSEPR model.
- Draw the structures and predict the shape of nitrate ion

Nitrate

- The shape is trigonal planar. The angles are 120°



Molecules with no single central atom

- Like C_2H_4 or CH_3COOH
- These molecule are just different shapes joined together