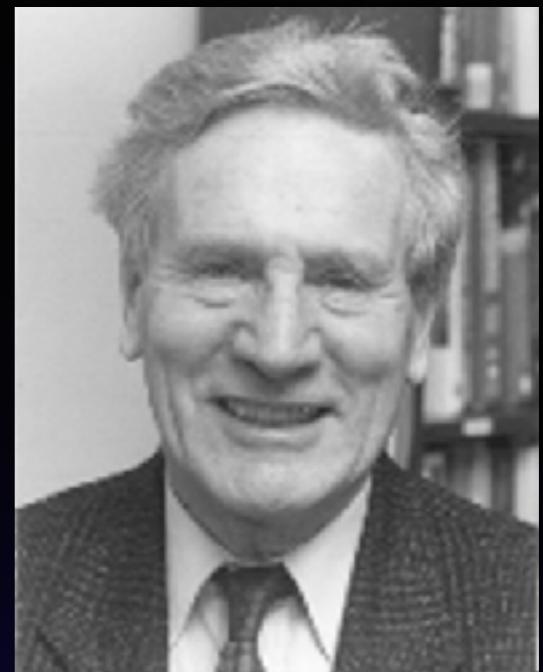


Previously in Molecularity...

Valence-shell electron-pair repulsion theory (VSEPR)

- Assign a geometric shape around an atom based on a **steric number, SN**
- **SN** = # bonded atoms + # lone pairs
- SN 2–8 correspond to specific geometric shapes.
- Lone pairs occupy positions just like bonded atoms.



Ronald Gillespie
archive.cnx.org
graphics1.jpg



Ronald Nyholm
images.npg.org.uk
mw86253.jpg

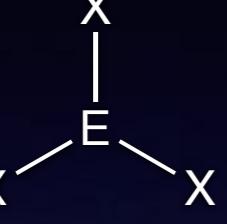
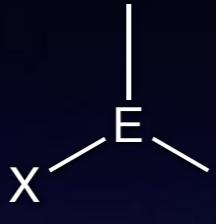
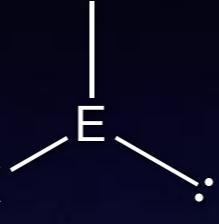
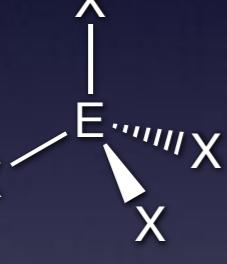
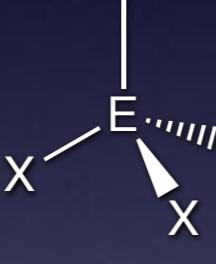
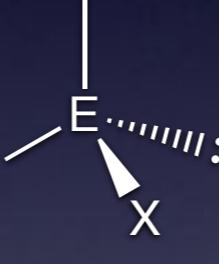
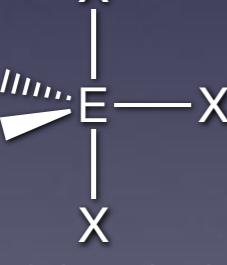
SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	$\begin{array}{c} \text{X} \\ \\ \text{X}-\text{E}-\text{X} \end{array}$ Trigonal planar	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\text{X} \end{array}$ 120° Bent	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\cdot\cdot \\ \\ \text{X} \end{array}$			
4	$\begin{array}{c} \text{X} \\ \\ \text{X}-\text{E}-\cdot\cdot\cdot\cdot\text{X} \\ \\ \text{X} \end{array}$ Tetrahedral	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\cdot\cdot\cdot\cdot\text{X} \\ \\ \text{X} \end{array}$ Trig. pyramidal	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\cdot\cdot\cdot\cdot\text{X} \\ \\ \text{X} \end{array}$ 109.5° Bent	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\cdot\cdot\cdot\cdot\text{X} \\ \\ \cdot\cdot \end{array}$		
5						
6						

A photograph of a silver fork standing upright in a field of dry, yellowish-brown grass. In the background, there's a paved road curving to the left, some green trees, and a bright sky.

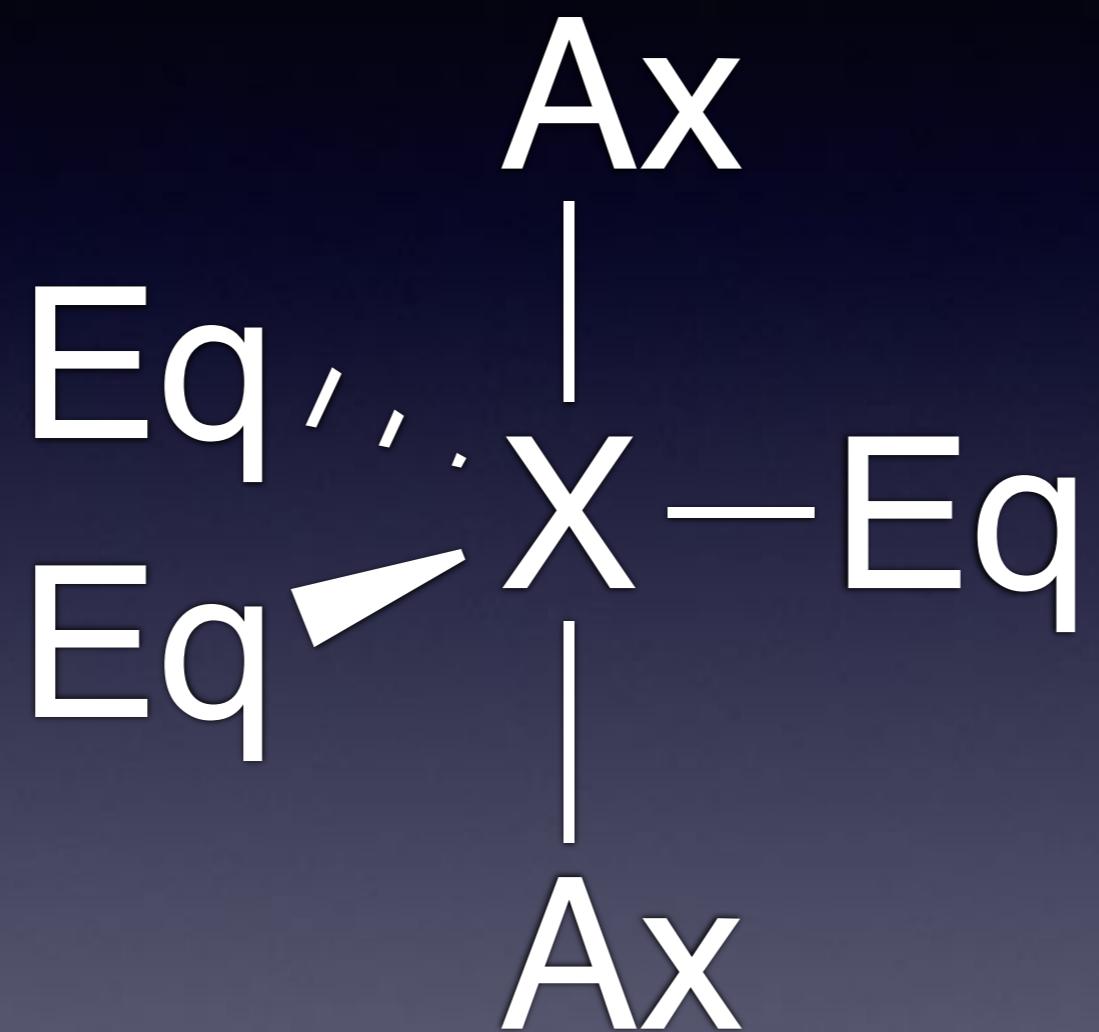
Where are we going today?

Ch1010-A17-A03 Lecture 16

- §5.7 VSEPR: Fundamental Structures
- §5.8 VSEPR: Effect of Lone Pairs
- §5.9 VSEPR: Predicting Geometries

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyramidal					
6						

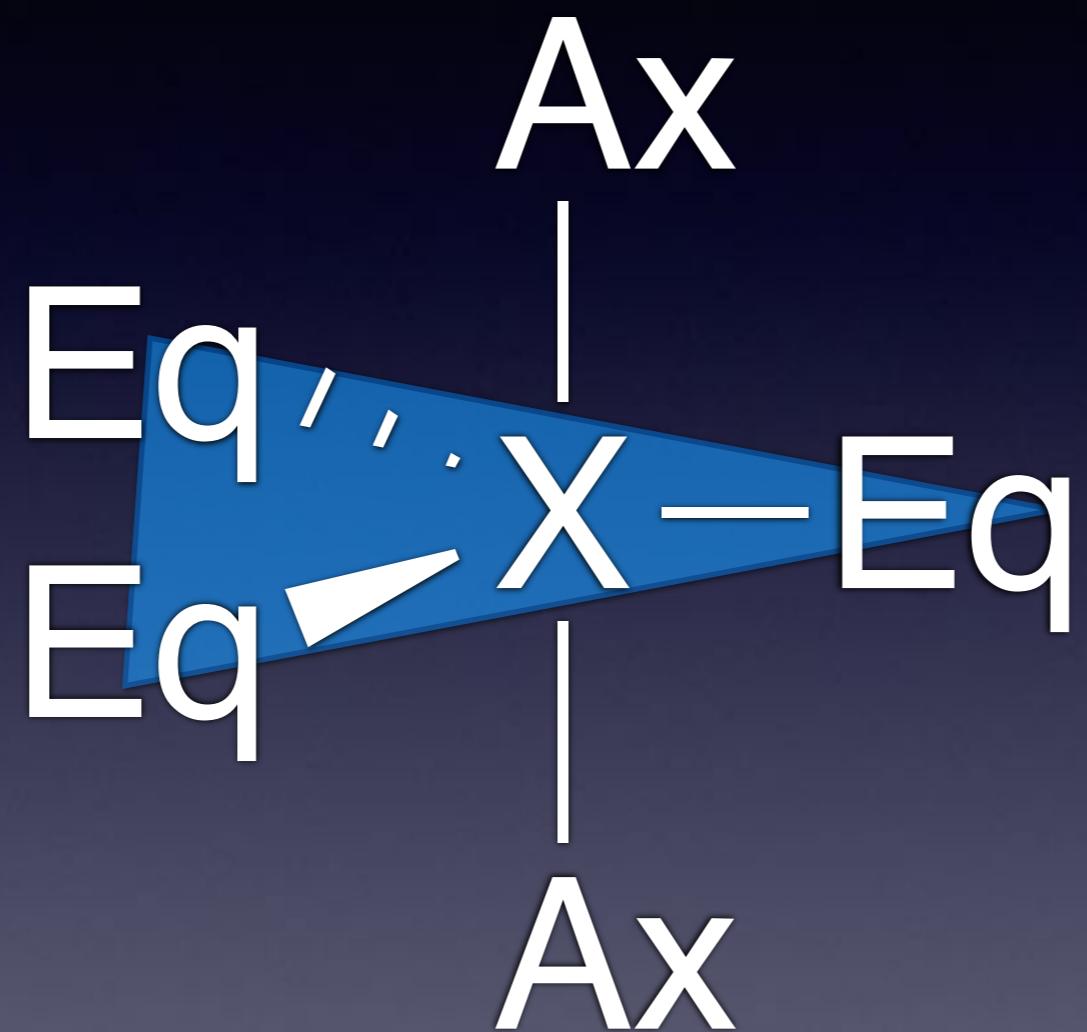
SN 5: Trigonal bipyramidal



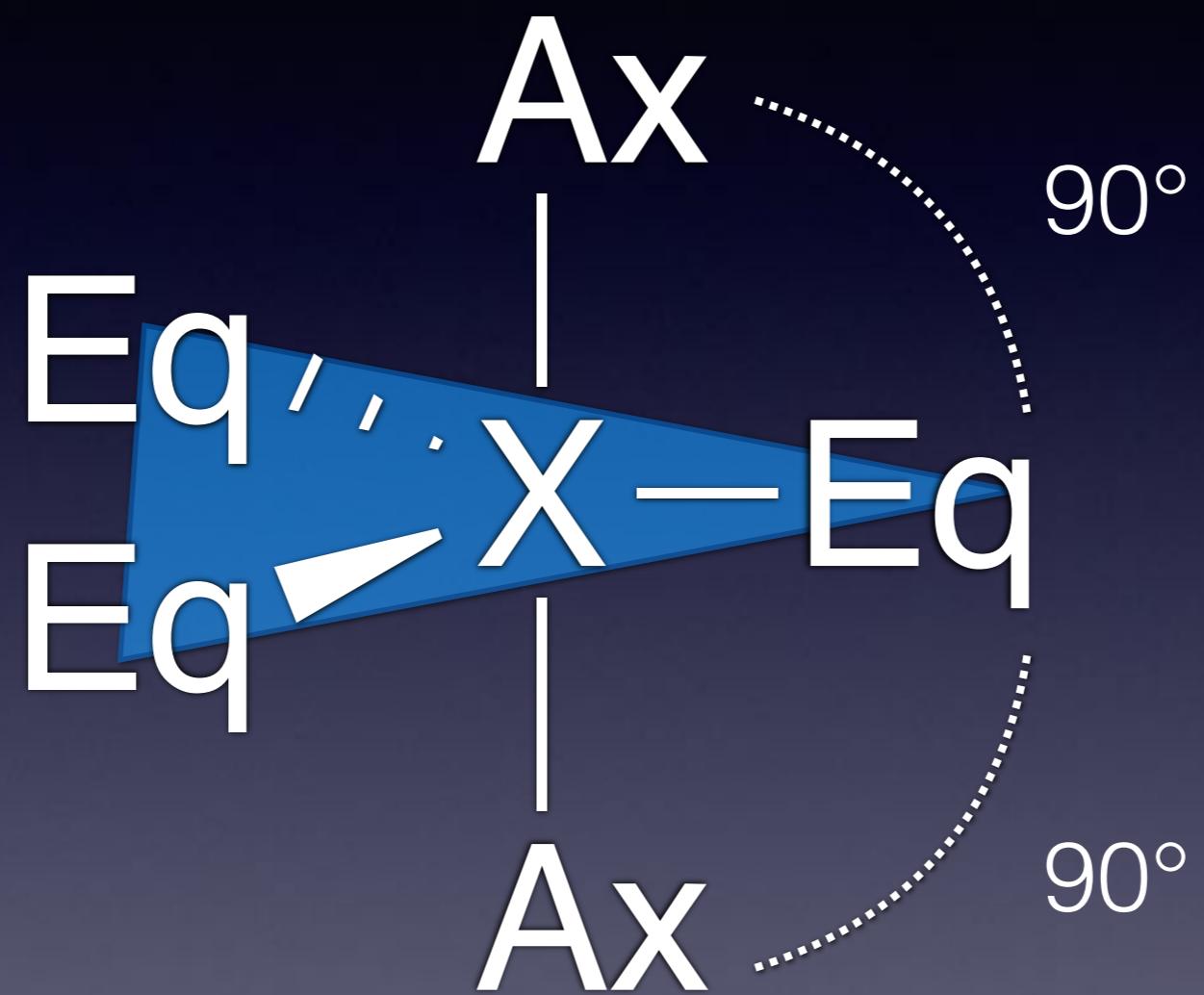
Ax: Axial position

Eq: equatorial position

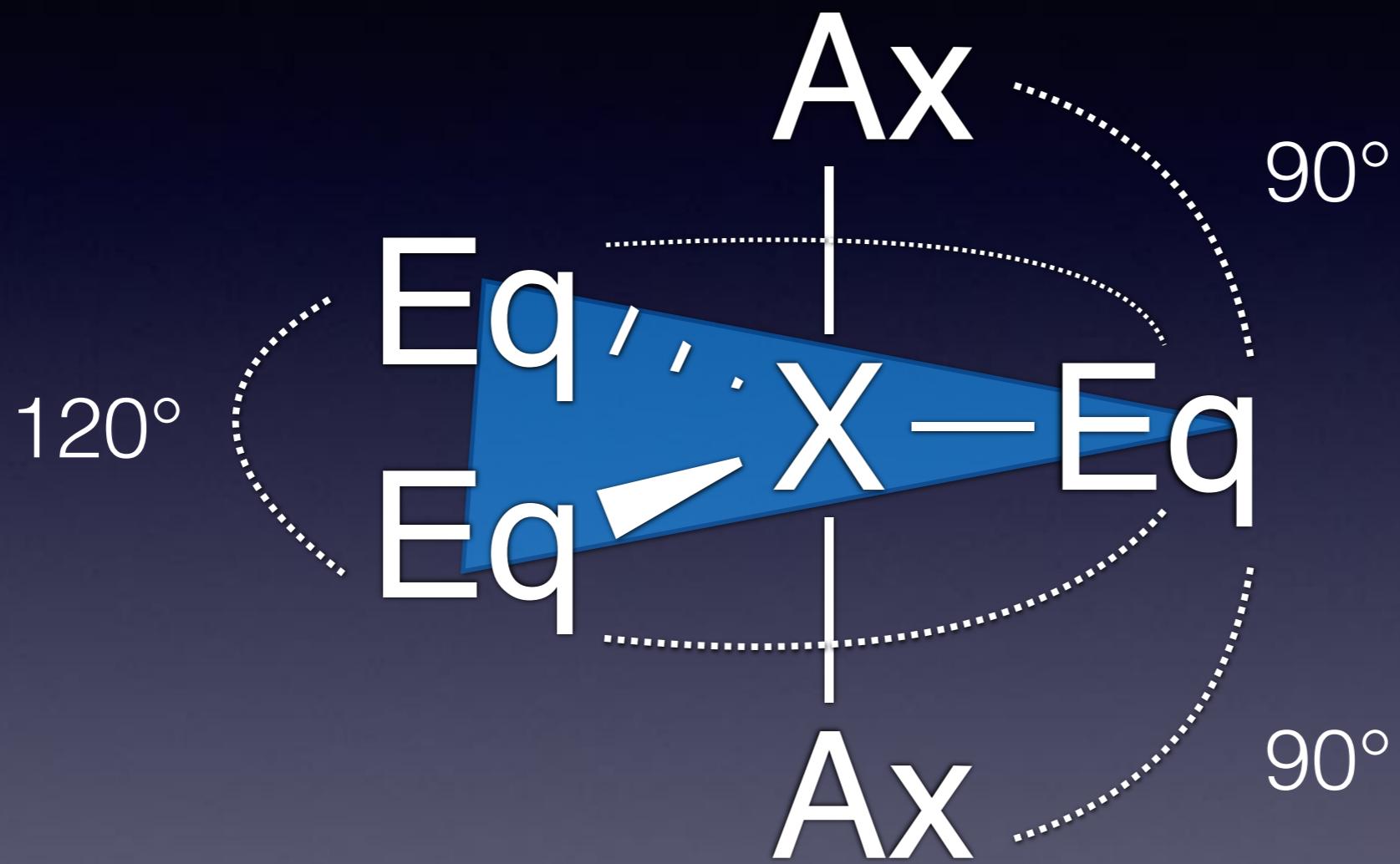
SN 5: Trigonal bipyramidal



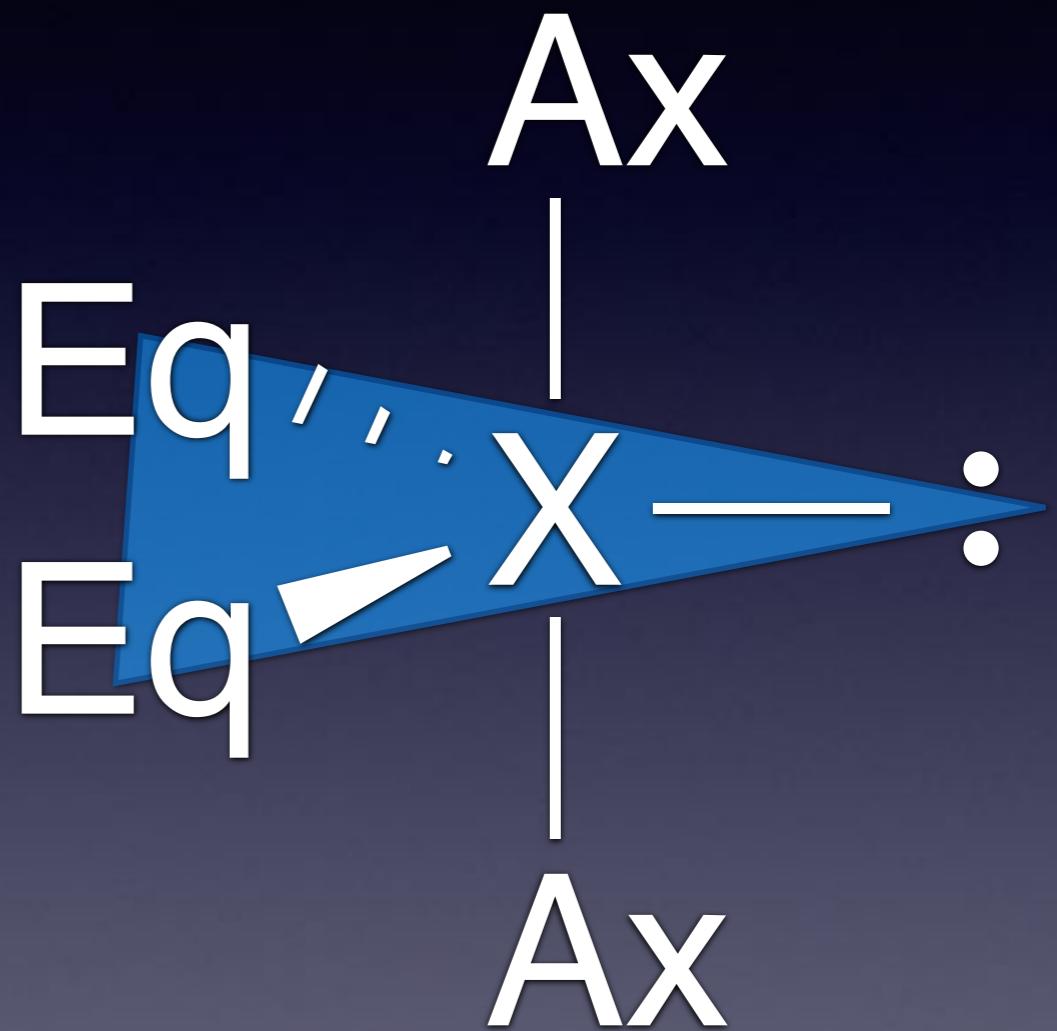
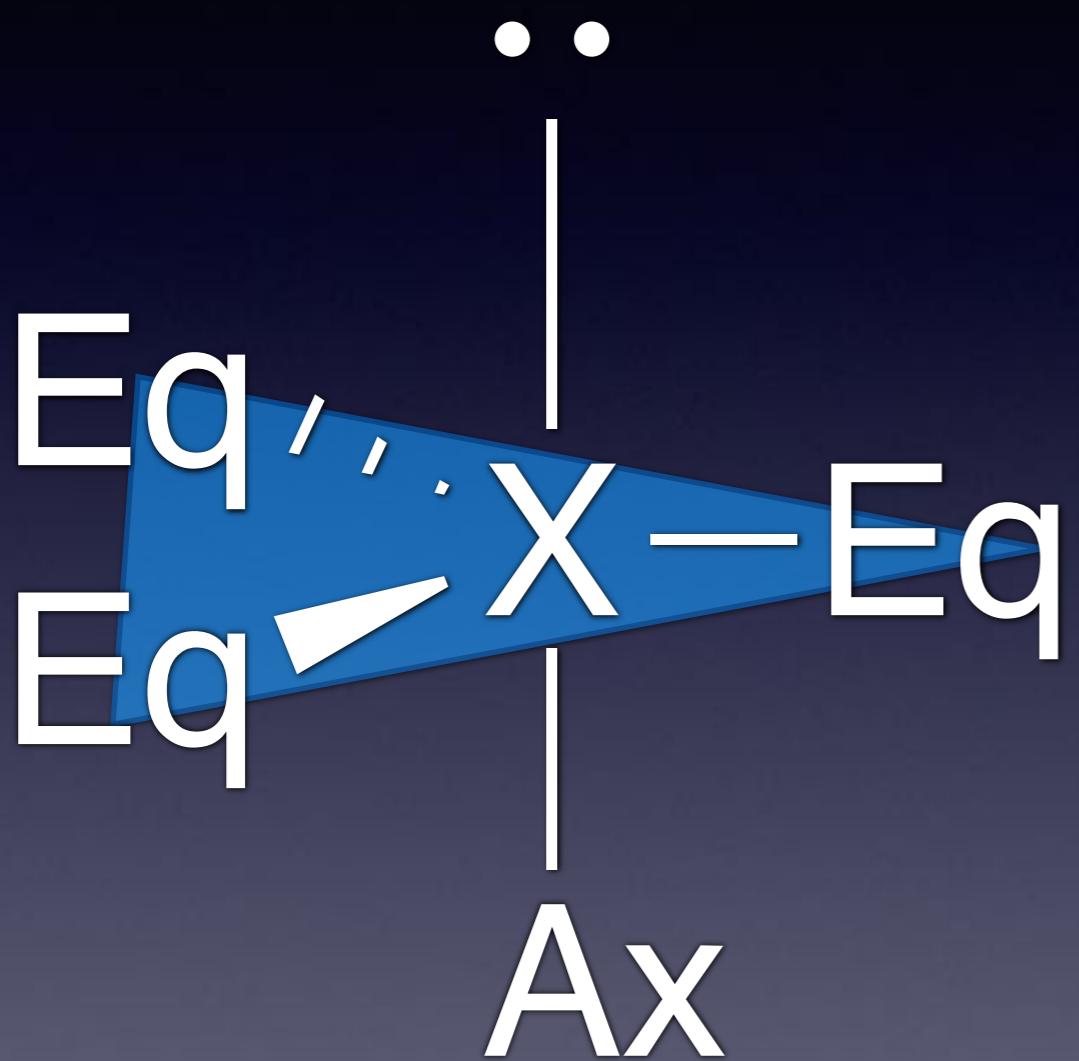
SN 5: Trigonal bipyramidal



SN 5: Trigonal bipyramidal

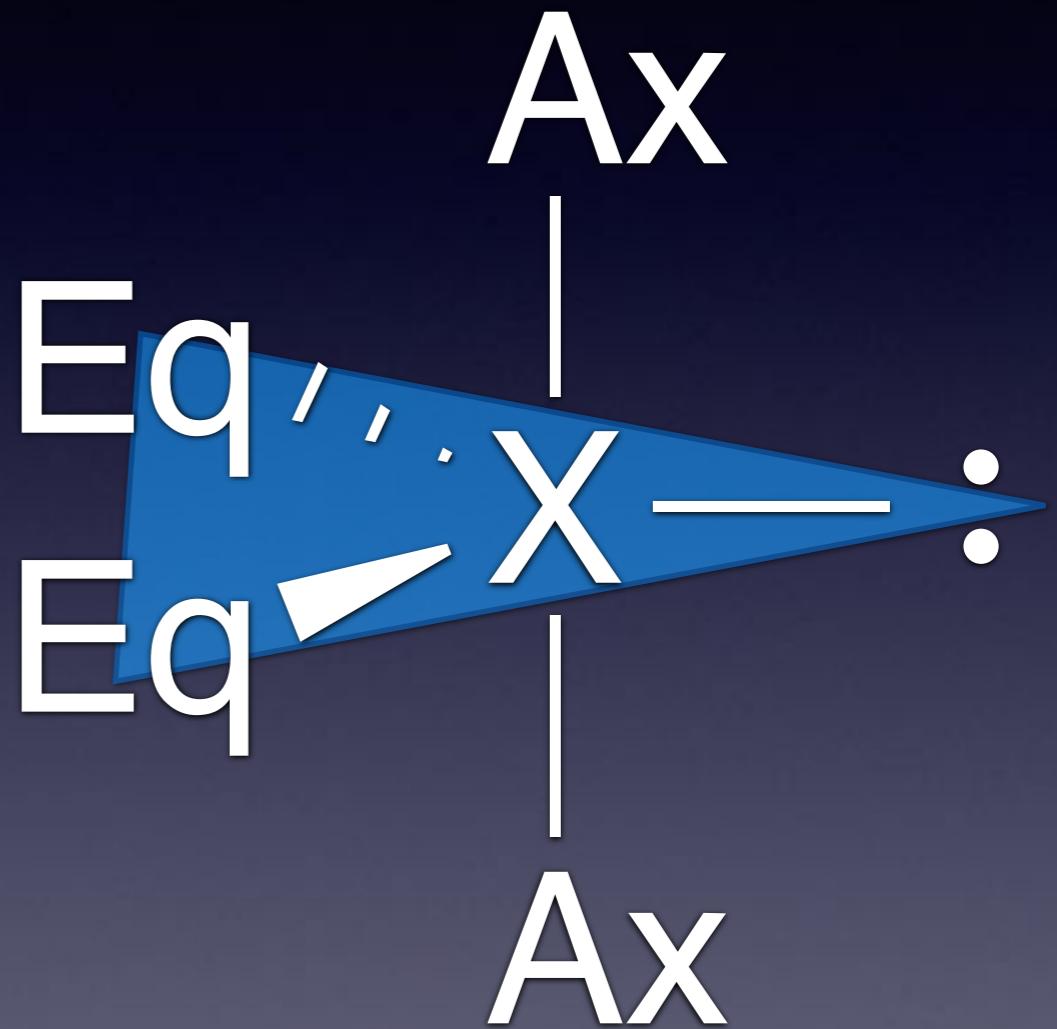


SN 5: where would a lone pair go?



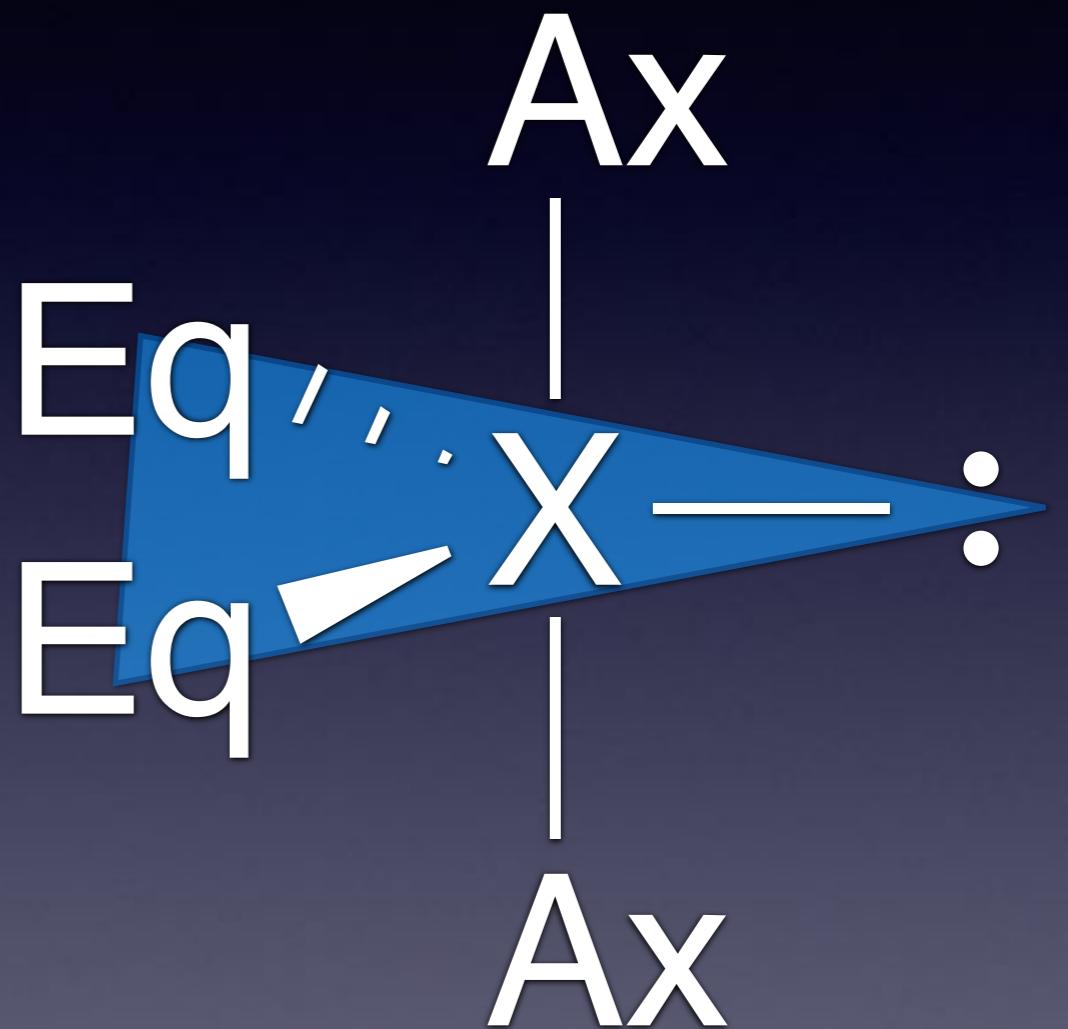
SN 5: where would a lone pair go?

- Lesson: Lone pairs occupy more space than atoms. In other words, lone pairs are fat!

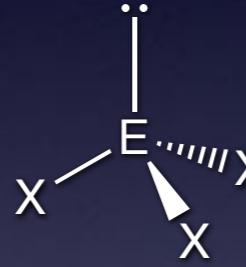
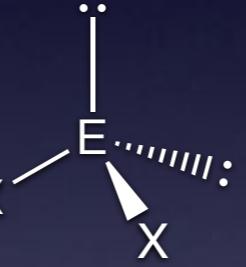
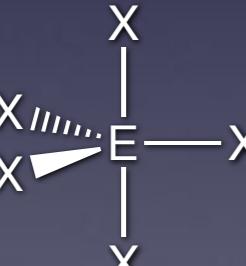


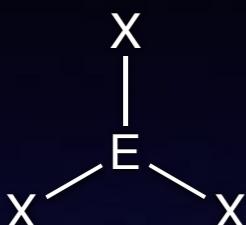
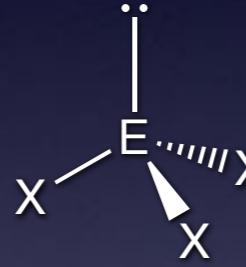
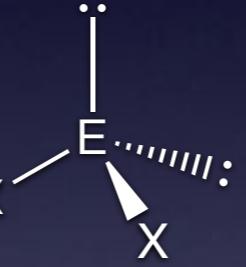
Lone pairs are fat #1

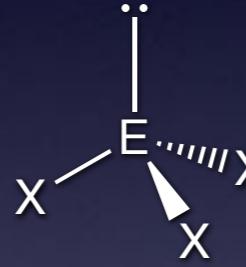
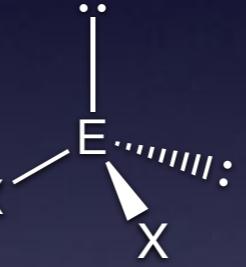
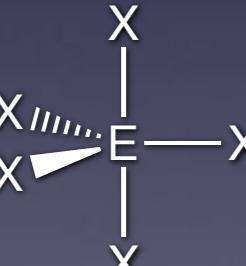
- Lone pairs occupy more space than atoms.
- Lone pairs will occupy the least sterically crowded location around the central atom.

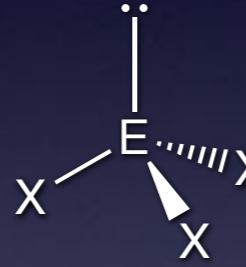
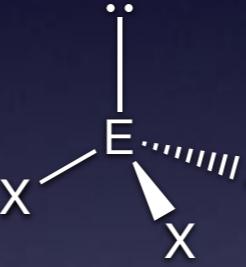
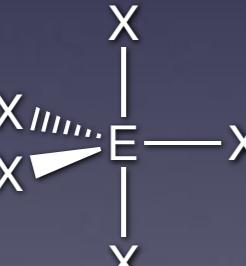
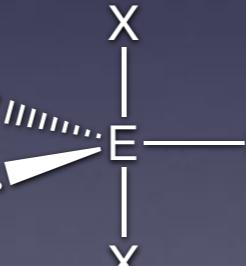
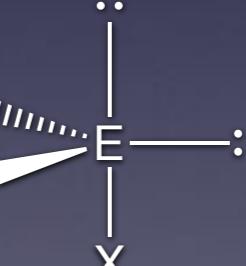


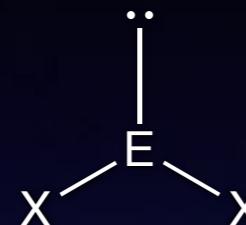
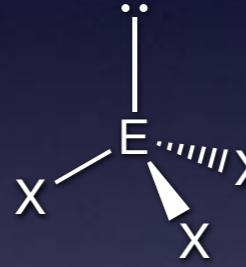
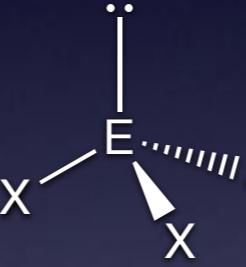
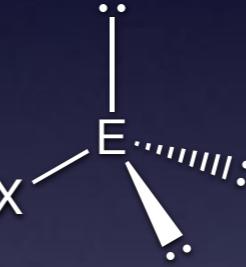
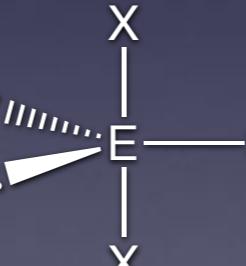
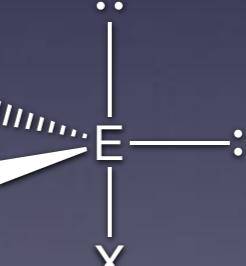
SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	$\begin{array}{c} \text{X} \\ \\ \text{X}-\text{E}-\text{X} \end{array}$ Trigonal planar	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\text{X} \end{array}$ 120° Bent	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\cdot\cdot \\ \\ \text{X} \end{array}$			
4	$\begin{array}{c} \text{X} \\ \\ \text{X}-\text{E}-\cdot\cdot\cdot\cdot\text{X} \\ \\ \text{X} \end{array}$ Tetrahedral	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\cdot\cdot\cdot\cdot\text{X} \\ \\ \text{X} \end{array}$ Trig. pyramidal	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\cdot\cdot\cdot\cdot\text{X} \\ \\ \text{X} \end{array}$ 109.5° Bent	$\begin{array}{c} \cdot\cdot \\ \\ \text{X}-\text{E}-\cdot\cdot\cdot\cdot\cdot\cdot\cdot\text{X} \\ \\ \text{X} \end{array}$		
5	$\begin{array}{c} \text{X} \\ \\ \text{X}-\text{E}-\text{X} \\ \\ \text{X} \end{array}$ Trig. bipyramidal					
6						

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyramidal	 See-saw				
6						

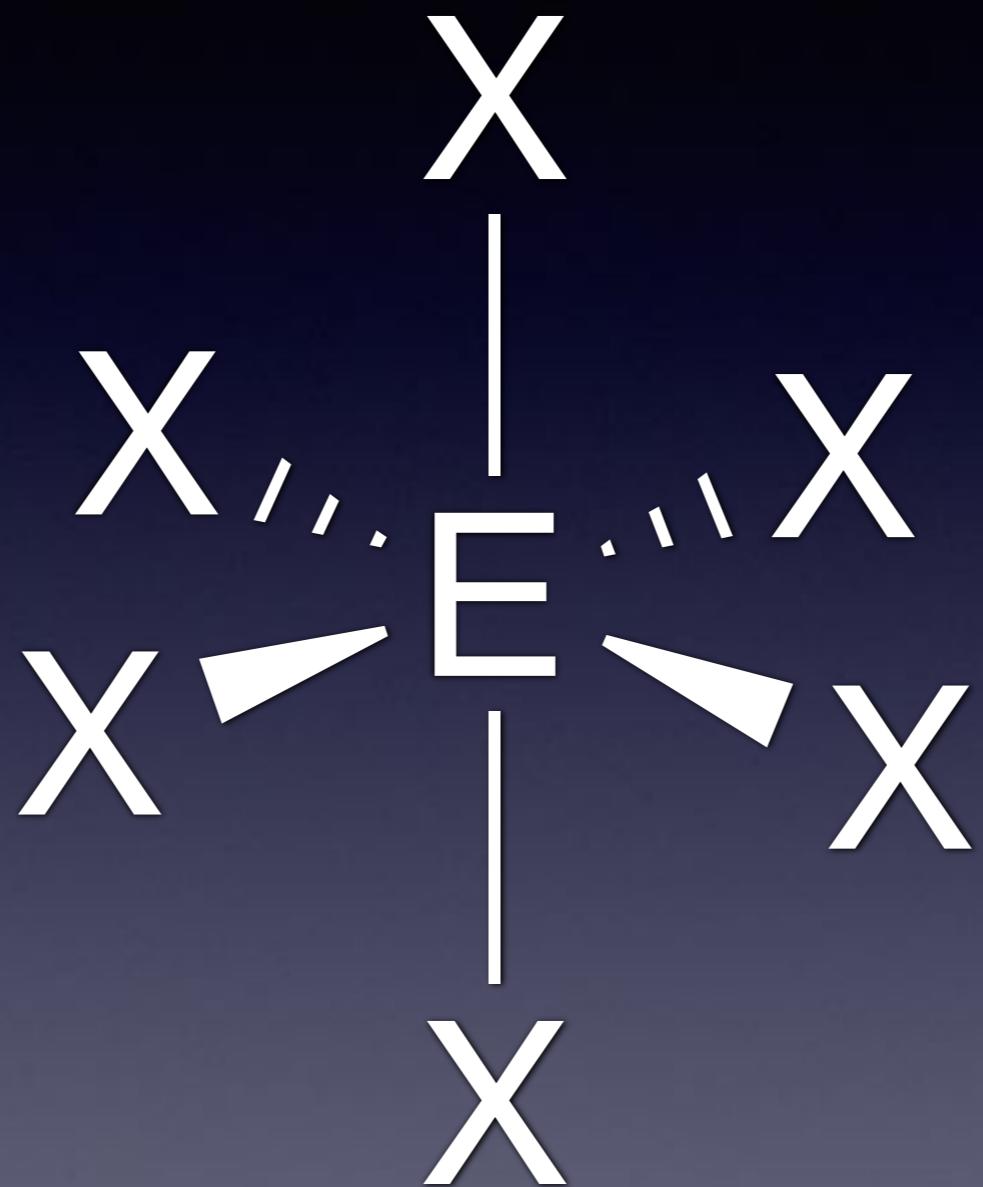
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2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyrimidal	 See-saw	 T-shaped			
6						

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyrimidal	 See-saw	 T-shaped	 Linear		
6						

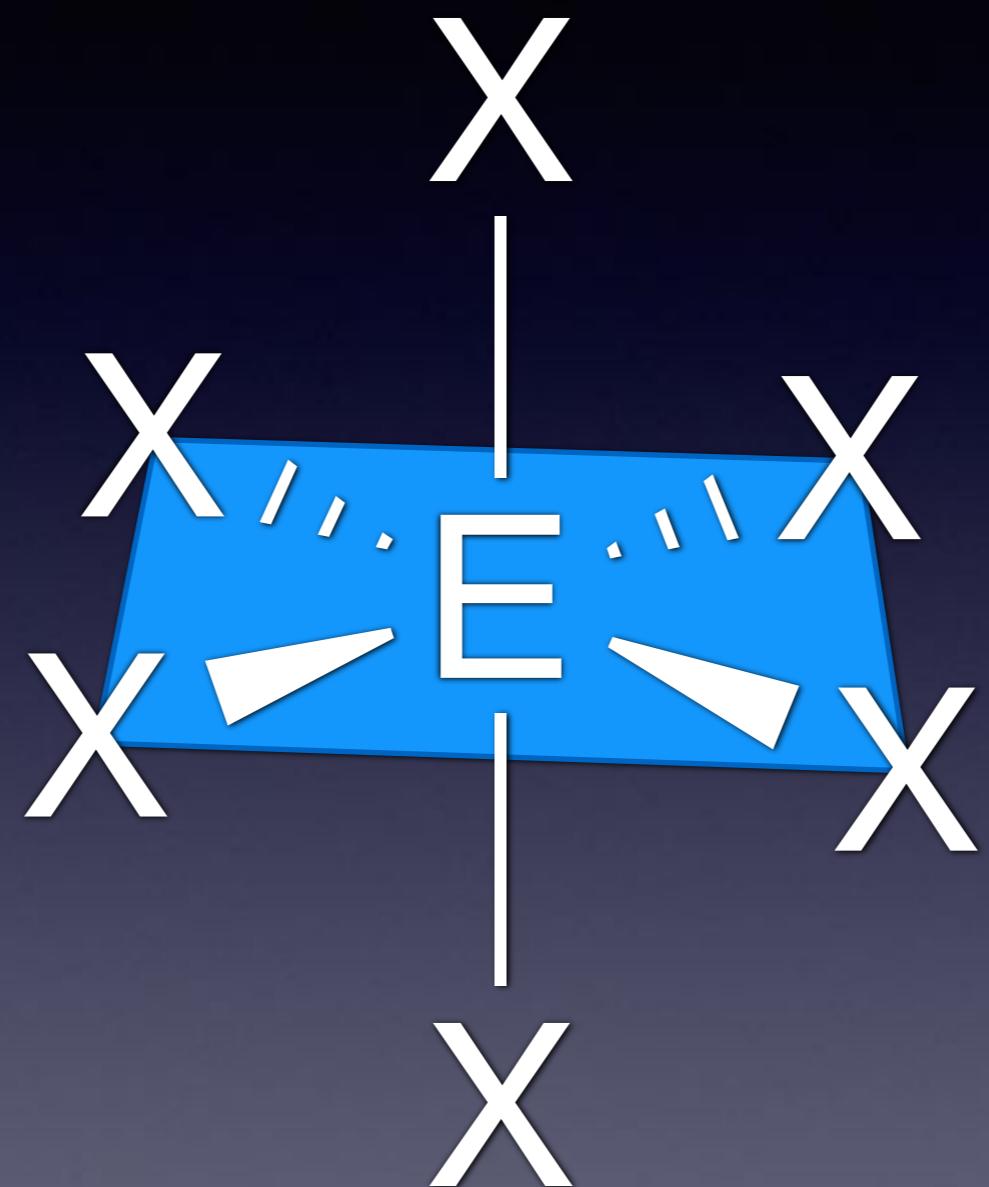
SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyramidal	 See-saw	 T-shaped	 Linear		
6						

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyramidal	 See-saw	 T-shaped	 Linear		
6	 Octahedral					

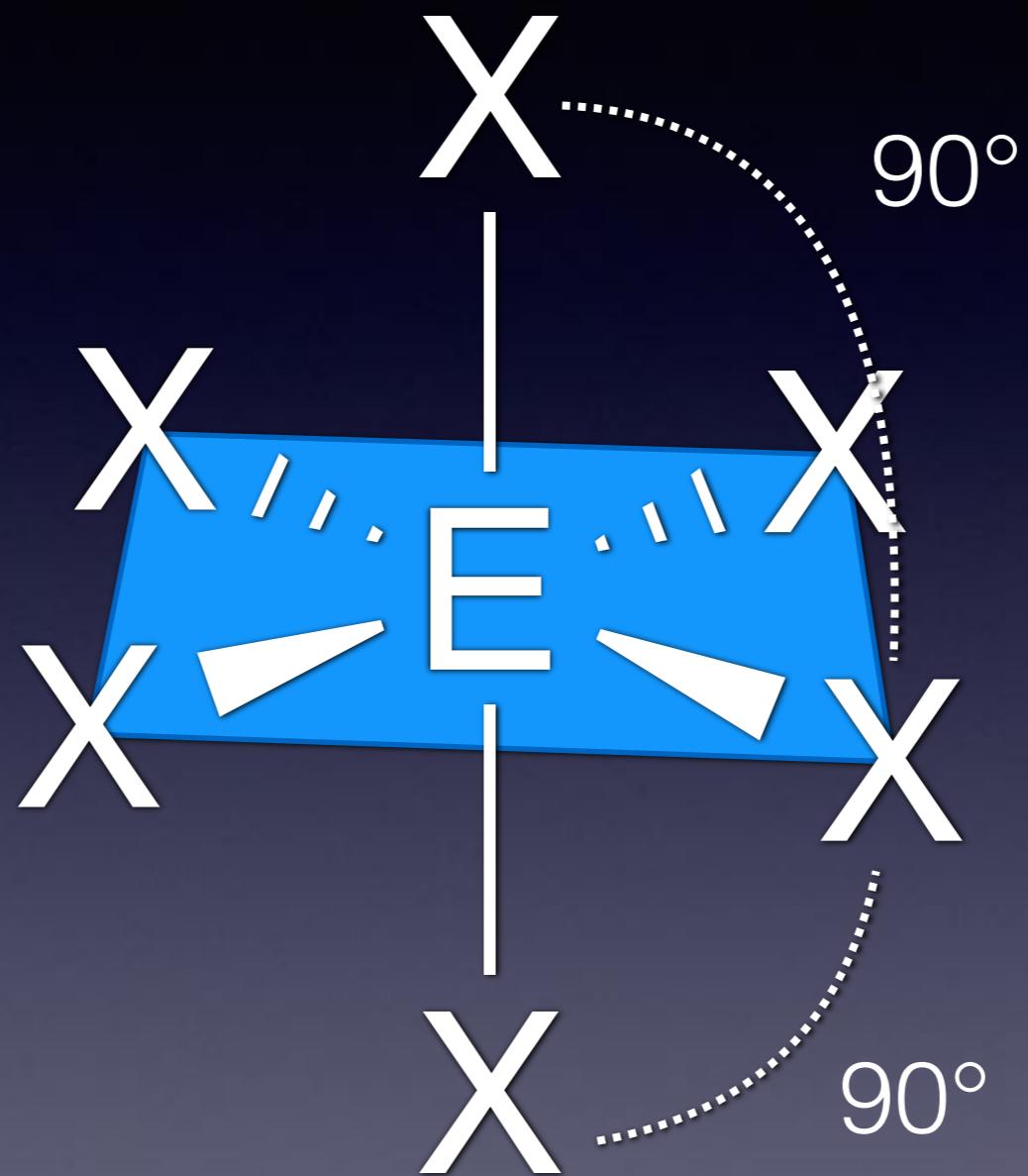
SN 6: Octahedral



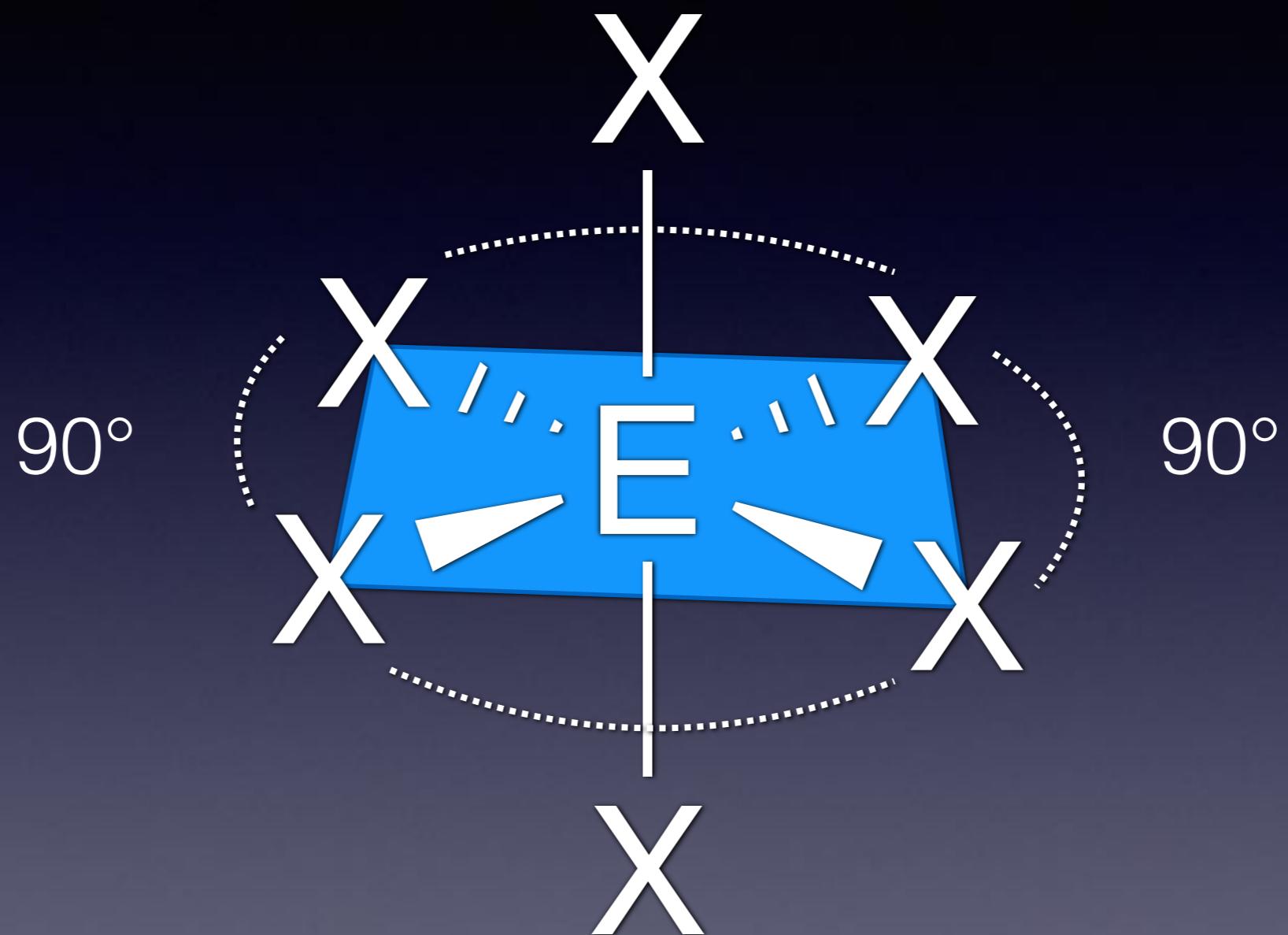
SN 6: Octahedral



SN 6: Octahedral

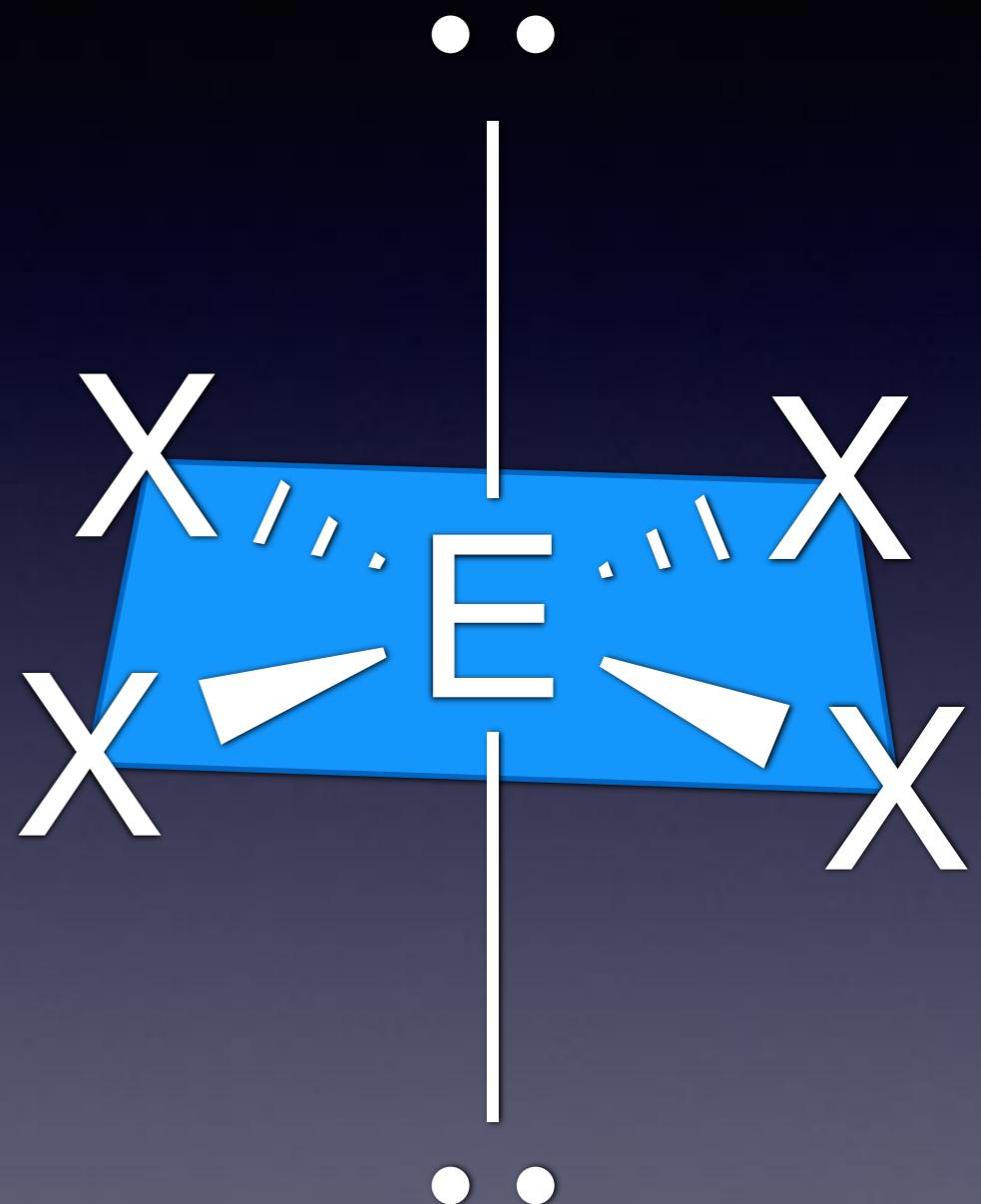


SN 6: Octahedral

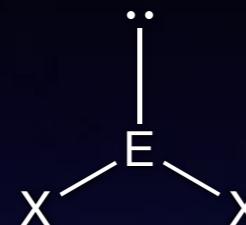
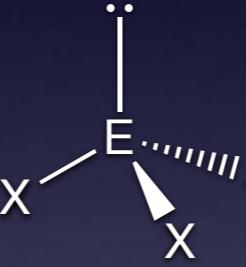
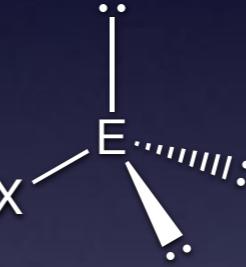
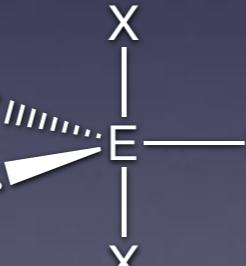
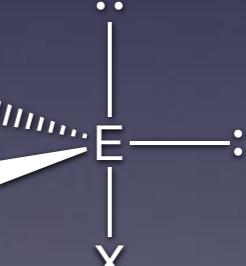
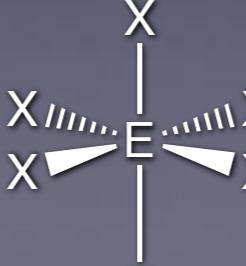
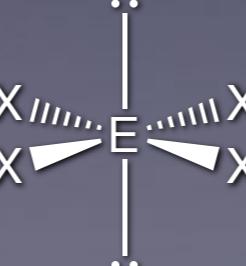


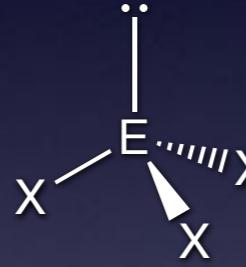
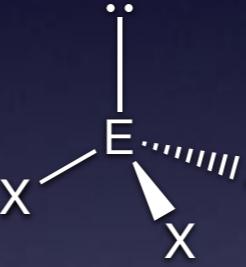
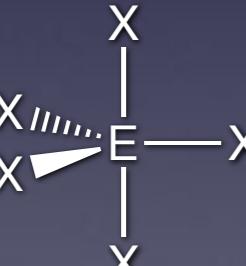
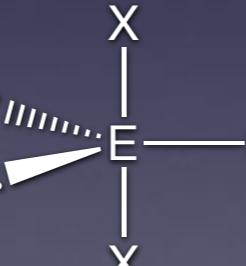
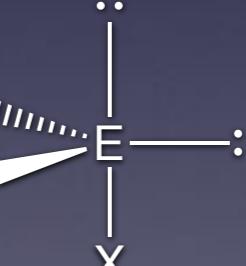
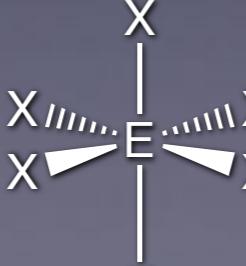
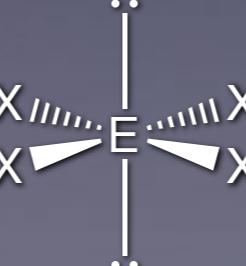
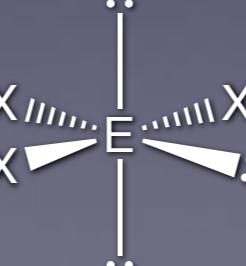
Lone pairs are fat #2

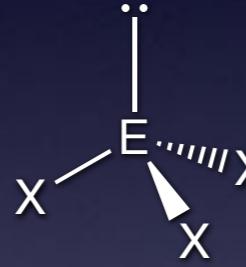
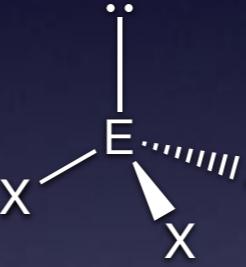
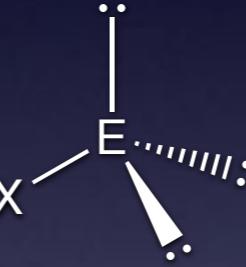
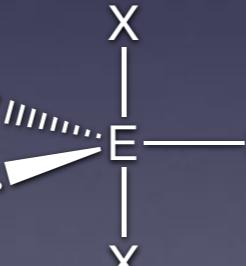
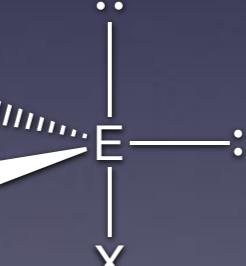
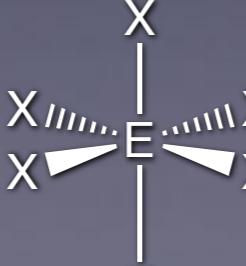
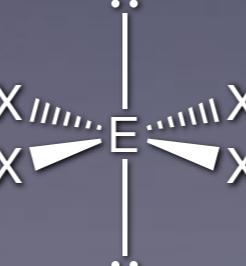
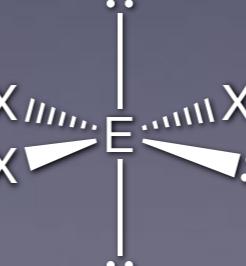
- In an octahedral arrangement with two lone pairs...
- ... lone pairs will occupy the opposite positions around that central atom

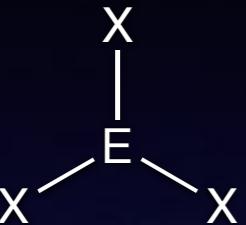
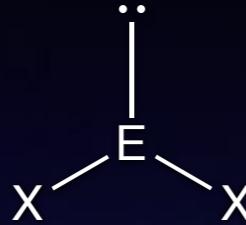
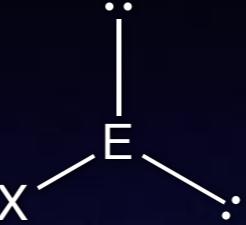
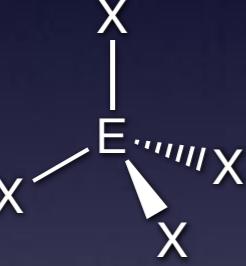
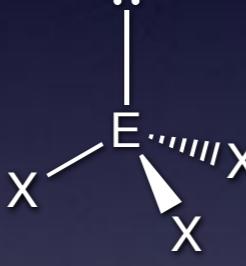
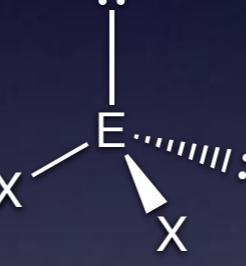
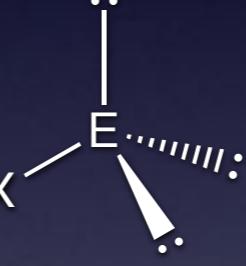
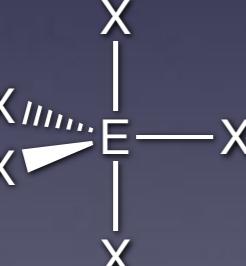
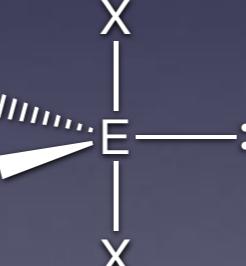
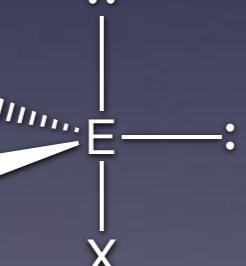
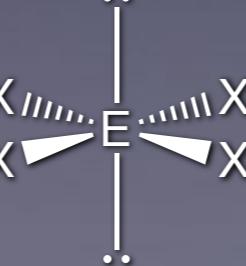
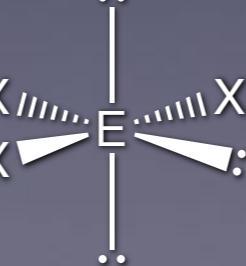
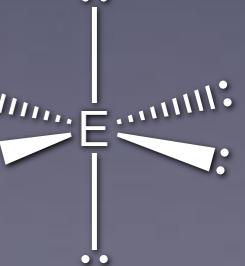


SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent	 109.5° Bent			
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyrimidal	 See-saw	 T-shaped	 Linear		
6	 Octahedral	 Sq. pyramidal				

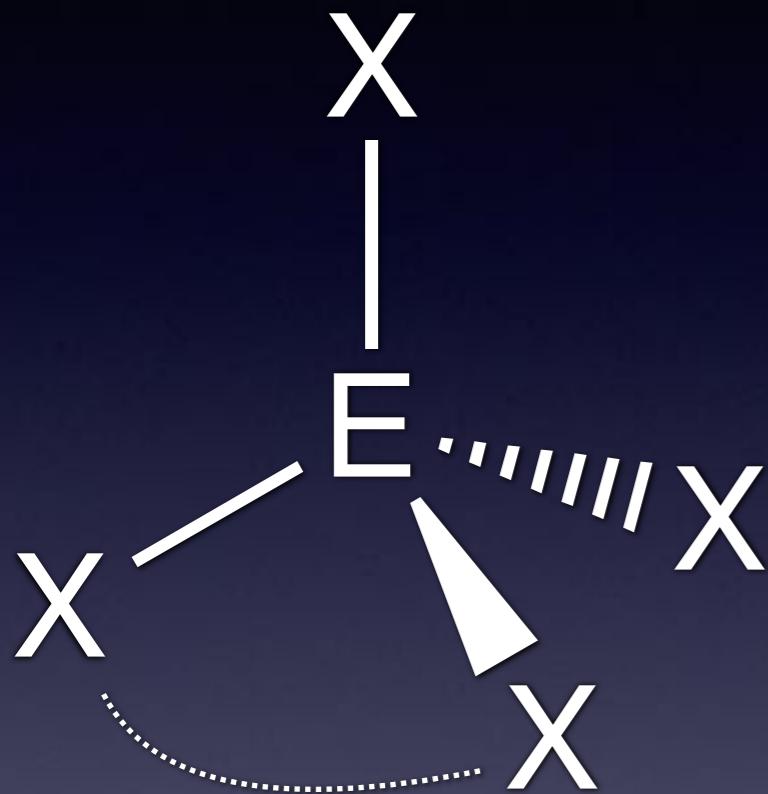
SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyramidal	 See-saw	 T-shaped	 Linear		
6	 Octahedral	 Sq. pyramidal	 Sq. planar			

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyrimidal	 See-saw	 T-shaped	 Linear		
6	 Octahedral	 Sq. pyramidal	 Sq. planar	 T-shaped		

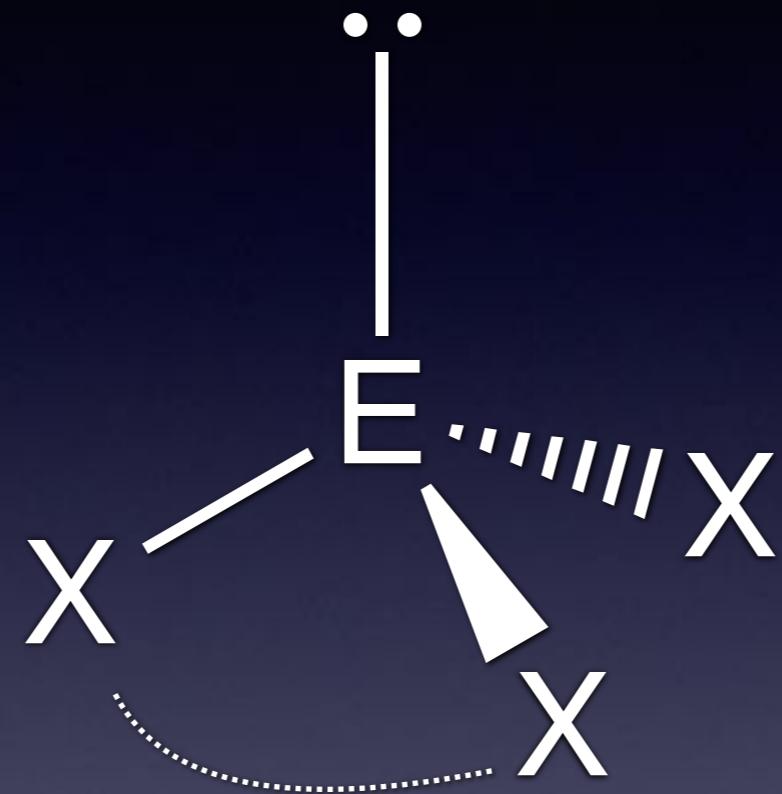
SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyrimidal	 See-saw	 T-shaped	 Linear		
6	 Octahedral	 Sq. pyramidal	 Sq. planar	 T-shaped		Linear

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	$\text{X}-\text{E}-\text{X}$ Linear	$\text{X}-\text{E}-:$				
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
5	 Trig. bipyrimidal	 See-saw	 T-shaped	 Linear		
6	 Octahedral	 Sq. pyramidal	 Sq. planar	 T-shaped		 Linear

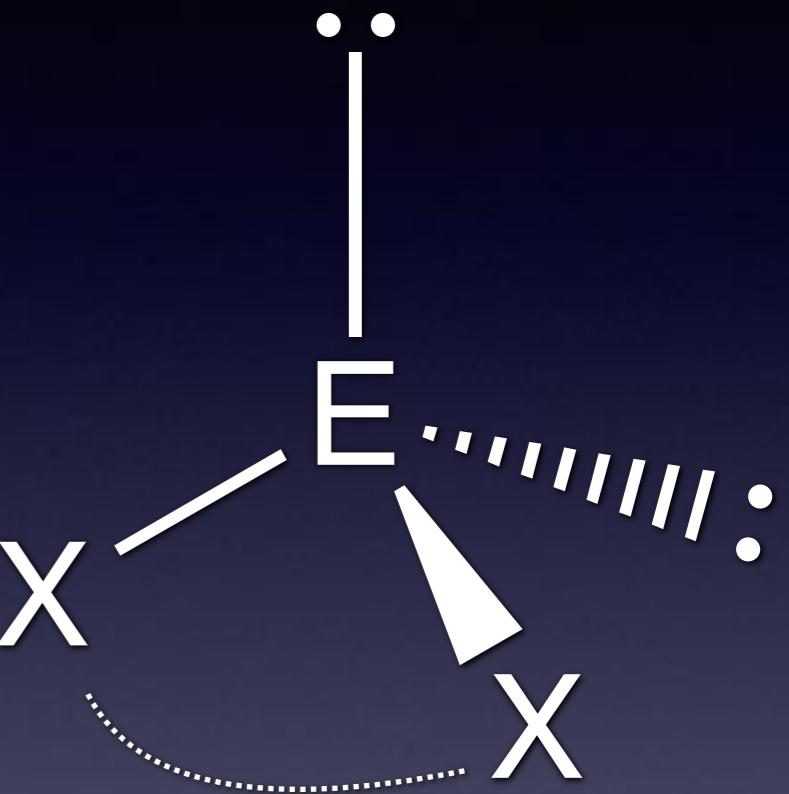
Lone pairs are fat #3



109.5° in CH₄



107° in NH₃



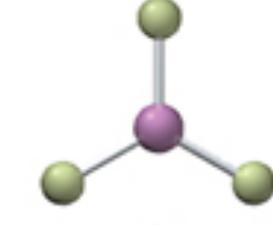
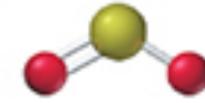
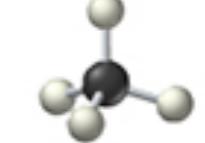
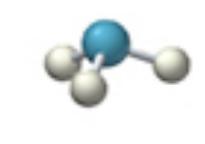
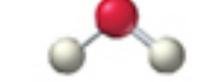
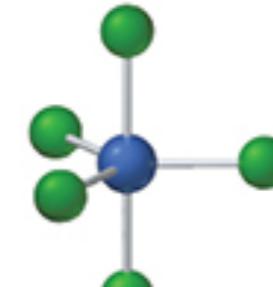
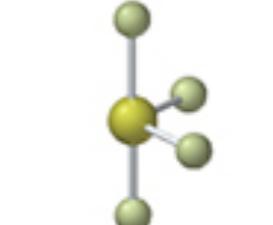
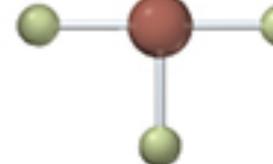
104.5° in H₂O

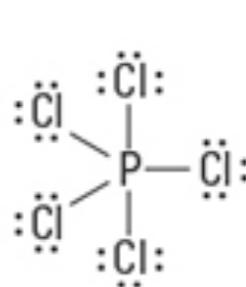
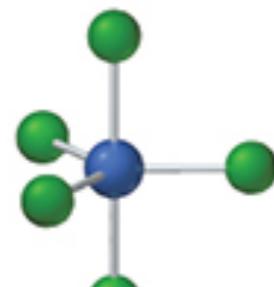
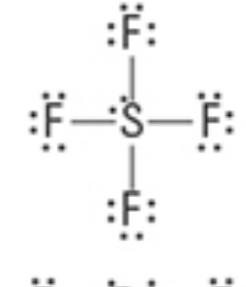
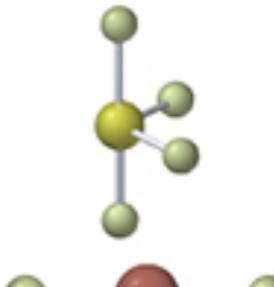
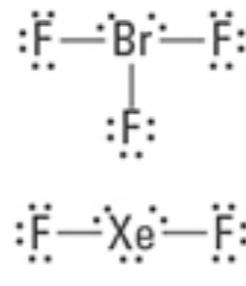
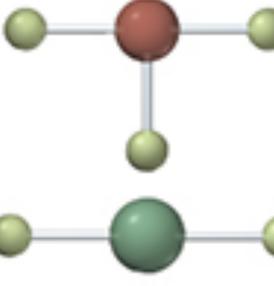
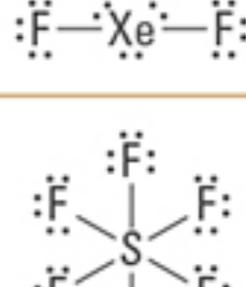
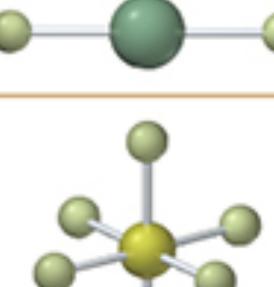
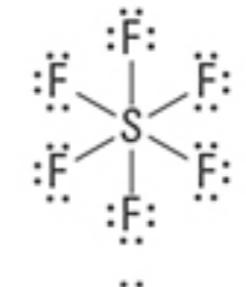
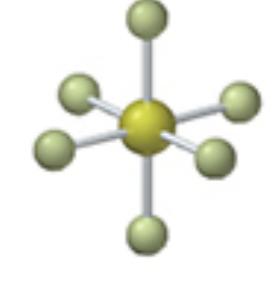
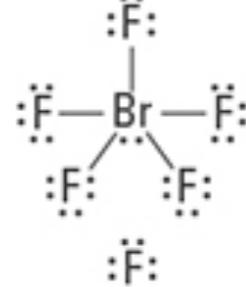
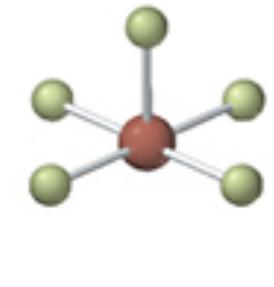
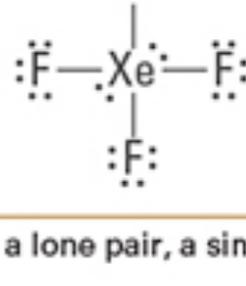
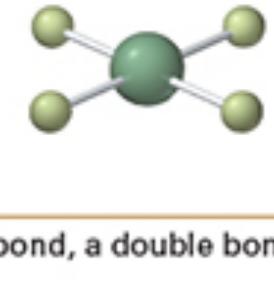
Can you predict changes to bond angles from lone pairs?

VSEPR Expectations

- Given a chemical formula (or name), can you...
- ...draw the correct Lewis dot structure that identifies the correct number of atoms and lone pairs around a central atom?
- ...identify the steric number of the central atom
- ...properly place bonded atoms and lone pairs around the central atom?
- ...draw the correct structure with particular attention to in-plane and out-of-plane bonds?
- ...name the geometric structure of bonded atoms around the central atom? (*i.e.* tetrahedral, 109.5° bent, trigonal planar, trigonal bipyramidal, etc.)
- ... estimate how lone pairs affect bond angles (*i.e.* why is H–O–H 104.5° in water?)

TABLE 5.5 Electron and Molecular Geometries

Electron Groups*	Bonding Groups	Lone Pairs	Electron Geometry	Molecular Geometry	Approximate Bond Angles	Example
2	2	0	Linear	Linear	180°	: $\ddot{\text{O}}$ =C= $\ddot{\text{O}}$: 
3	3	0	Trigonal planar	Trigonal planar	120°	: $\ddot{\text{F}}$: : $\ddot{\text{F}}$ -B- $\ddot{\text{F}}$: 
3	2	1	Trigonal planar	Bent	<120°	: $\ddot{\text{O}}$ =S= $\ddot{\text{O}}$: 
4	4	0	Tetrahedral	Tetrahedral	109.5°	H—C—H 
4	3	1	Tetrahedral	Trigonal pyramidal	<109.5°	H—N—H 
4	2	2	Tetrahedral	Bent	<109.5°	H— $\ddot{\text{O}}$ —H 
5	5	0	Trigonal bipyramidal	Trigonal bipyramidal	120° (equatorial) 90° (axial)	: $\ddot{\text{Cl}}$: : $\ddot{\text{Cl}}$ -P- $\ddot{\text{Cl}}$: : $\ddot{\text{Cl}}$: 
5	4	1	Trigonal bipyramidal	Seesaw	<120° (equatorial) <90° (axial)	: $\ddot{\text{F}}$: : $\ddot{\text{F}}$ -S- $\ddot{\text{F}}$: : $\ddot{\text{F}}$: 
5	3	2	Trigonal bipyramidal	T-shaped	<90°	: $\ddot{\text{F}}$ -Br- $\ddot{\text{F}}$: : $\ddot{\text{F}}$: 

5	5	0	Trigonal bipyramidal	Trigonal bipyramidal	120° (equatorial) 90° (axial)		
5	4	1	Trigonal bipyramidal	Seesaw	<120° (equatorial) <90° (axial)		
5	3	2	Trigonal bipyramidal	T-shaped	<90°		
5	2	3	Trigonal bipyramidal	Linear	180°		
6	6	0	Octahedral	Octahedral	90°		
6	5	1	Octahedral	Square pyramidal	<90°		
6	4	2	Octahedral	Square planar	90°		

*Count only electron groups around the central atom. Each of the following is considered one electron group: a lone pair, a single bond, a double bond, a triple bond, or a single electron.

VSEPR Practice

- Find the most stable or preferred structure for:
 PCl_5 , PCl_4I , PCl_3I_2 , PCl_2I_3 , PClI_4 , PI_5
- Try Problems 5.57–68...
Problems like 5.63–68 might end up on the exam (hint, hint)



Where did we go today?

Ch1010-A17-A03 Lecture 16

- §5.7 VSEPR: Fundamental Structures
- §5.8 VSEPR: Effect of Lone Pairs
- §5.9 VSEPR: Predicting Geometries

Next time...

- § 5.10 Bond polarity & dipole moment