Previously in Molecularity…

Odd-electron example: Methylborane CH_3BH_2

- Sum valence e^- including overall charge.
  (This determines total # of bonds and lone pairs)
- Arrange around a central atom…
  1. Greatest bonding capacity
  2. Lowest electronegativity
- Draw single bonds to central atom
- Complete octets around periphery
- Fix central atom octet by converting peripheral lone pairs to bonds as needed
- Determine resonance / formal charge

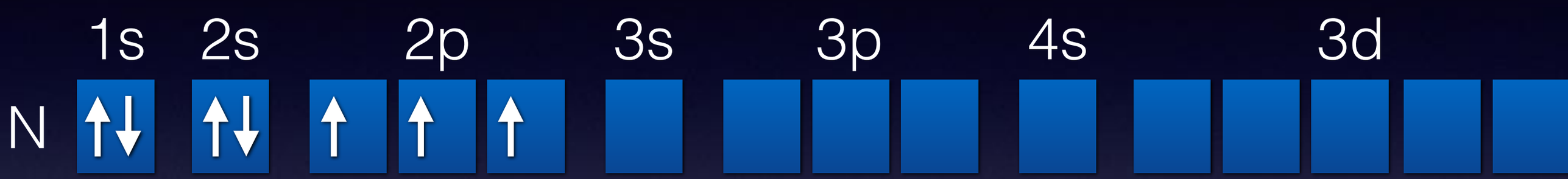
Where are we going today?

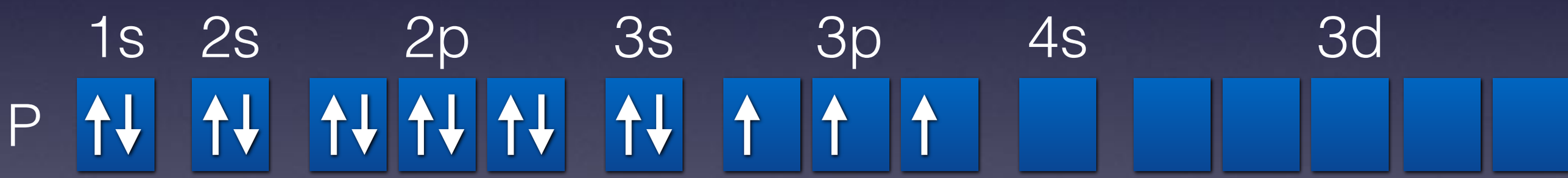
Ch1010-A17-A03 Lecture 15

- Lewis wrap-up
- Valence Shell Electron Pair Repulsion Theory!

http://stevedeace.com/wp-content/uploads/2012/11/

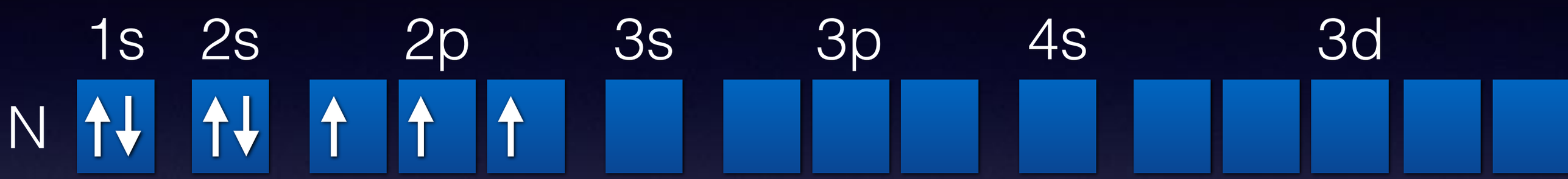
Hypervalency or Expanded Octets

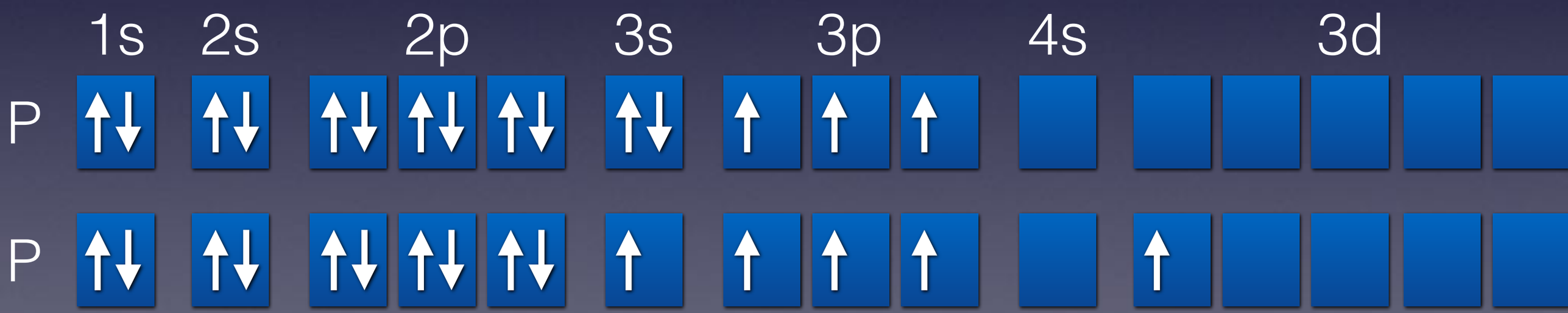




Both should only be able to bond to three other atoms…

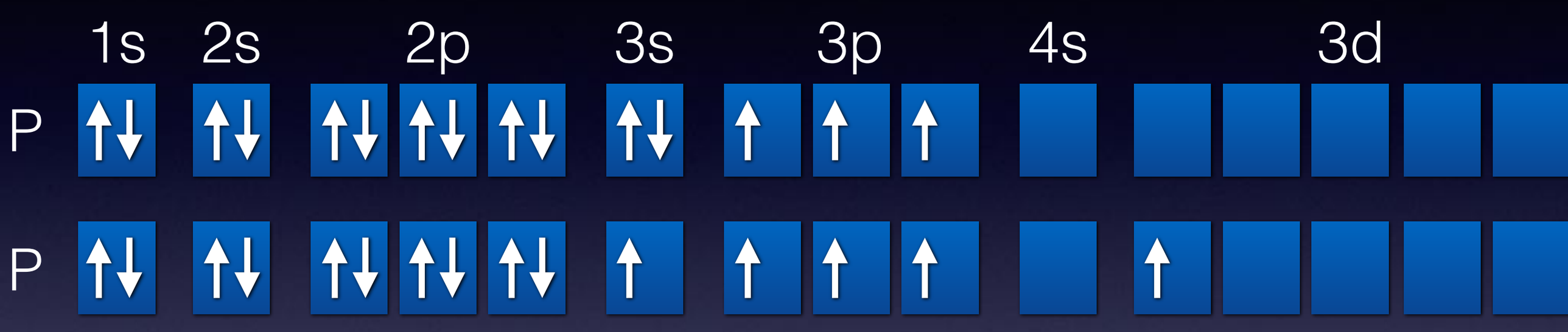
Hypervalency or Expanded Octets





…but phosphorous can form **five** bonds!

Conditions for expanded octets



- Requires d orbitals, therefore, it only occurs for $n \geq 3$!
- Only occurs for group 15–18 elements (pnictogens, chalcogenides, halogens, noble gases)
- This is **not** hybridization, but rather this **enables** d-orbitals to participate in hybridization (more detail in chapter 5).

Example: Phosphate anion, PO_4^{3-}

- Sum valence e^- including overall charge.
  (This determines total # of bonds and lone pairs)
- Arrange around a central atom…
  1. Greatest bonding capacity
  2. Lowest electronegativity
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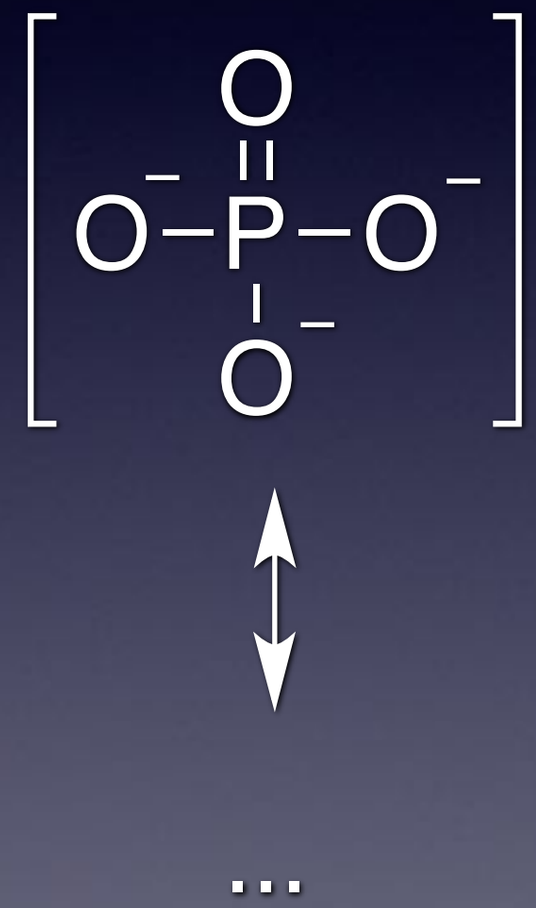
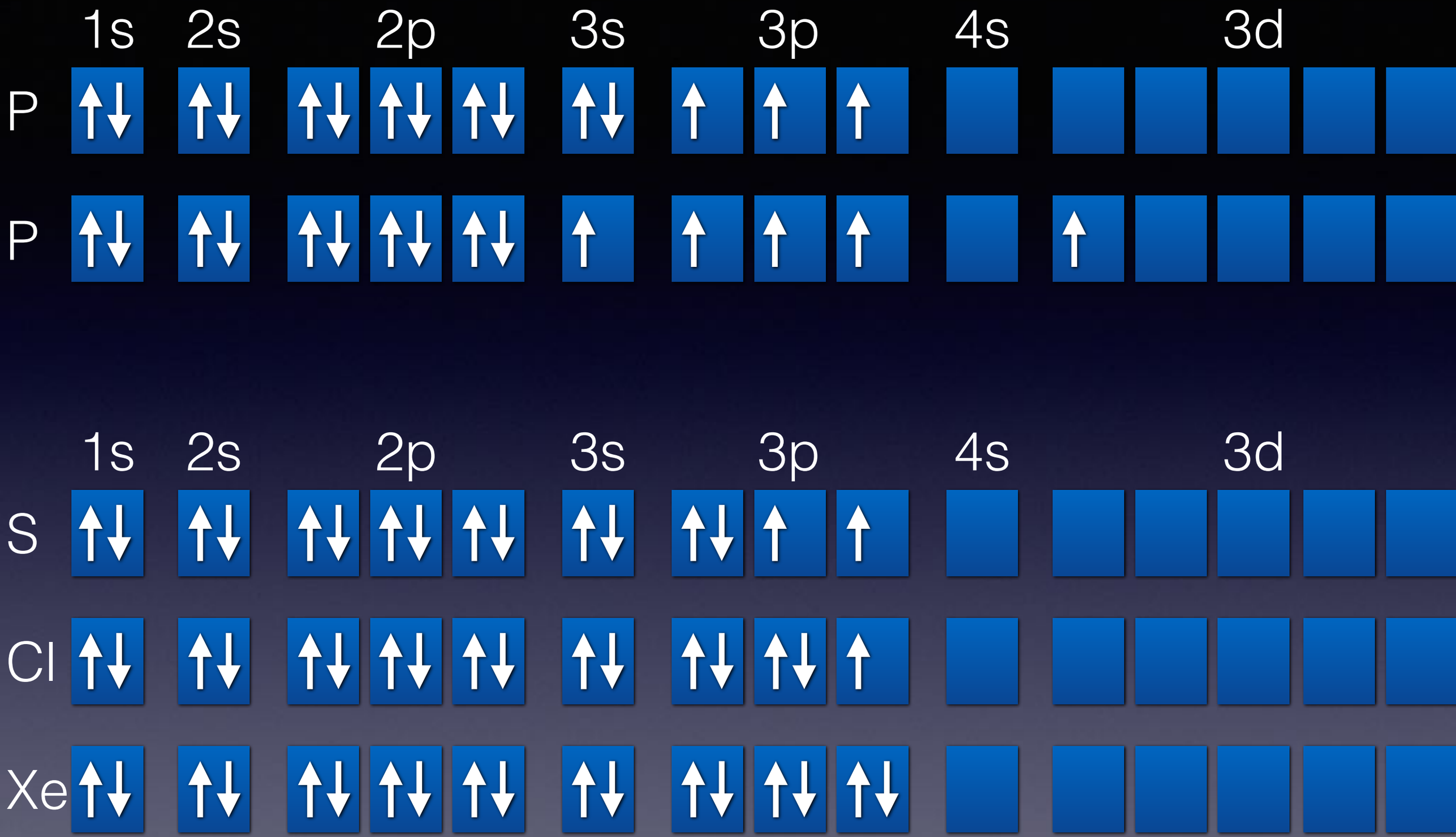




How many bonds could chalcogenides and halides form?

Great example molecules

- Determining “best” Lewis dot structure
  Formyl azide CHN_3O (connected OCNNN, H bonded to C)

- Incomplete octets:
  Aluminum chloride, magnesium hydride

- Odd-electron molecules:
  Chlorine monoxide, chlorine dioxide
  (unstable species in the atmosphere)

- Hypervalent / expanded octets
  Sulfuryl chloride SO_2Cl_2, Chlorate anion, Perchlorate anion

What you're responsible for in Lewis Dot structures

- Bond lengths vs bond order (single, double, triple)
- Bond energies vs bond order
- How bond lengths and energies support resonance structures in the Lewis model
- How resonance structures give us an "average" picture that is different than the component frames

Lewis dot expectations

- Given a compound (either by name or by formula)

  Can you…

  - Identify number of valence electrons and net charge?
  - Recognize and account for exceptions to normal rules?
  - Draw Lewis structures(s)?
  - Identify best structure from formal charge / electronegativity?
  - Recognize need for multiple resonances and draw them…
    …and visualize an “average” from component structures?

Lewis dot structure examples…

- Perchlorate, ClO_4^-
- Chlorate, ClO_3^-
- Chlorite, ClO_2^-
- Hypochlorite, ClO^-

Chapter 4 expectations: Bond lengths and strengths

- Carbon bonding to other things…

C–H	C–N	C–O
0.110 nm	0.147 nm	0.143 nm
413 kJ mol^{-1}	293 kJ mol^{-1}	358 kJ mol^{-1}

- Single vs double vs triple bonds…

$H_3C–CH_3$	$H_2C=CH_2$	$HC\equiv CH$
0.154 nm	0.134 nm	0.120 nm
348 kJ mol^{-1}	614 kJ mol^{-1}	839 kJ mol^{-1}

Chapter 4 expectations: Bond lengths and strengths

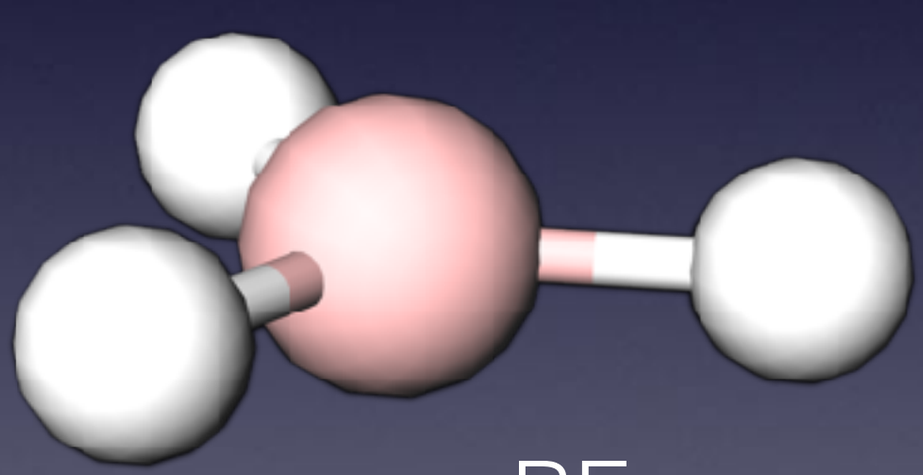
- Estimate bond length and strength in HI given…

H–F	H–Cl	H–Br
0.092 nm	0.127 nm	0.141 nm
567 kJ mol^{-1}	431 kJ mol^{-1}	366 kJ mol^{-1}

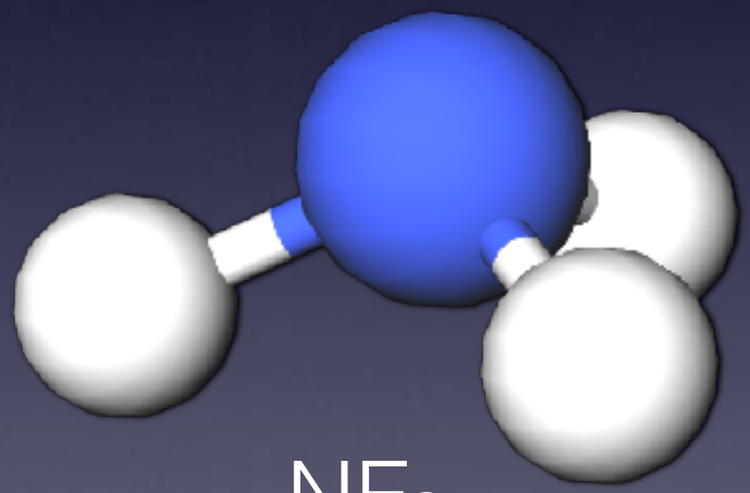
- Great problems in GKF: 4.145,147,150–152

Molecular structure

- Boron trifluoride vs nitrogen trifluoride:



BF_3

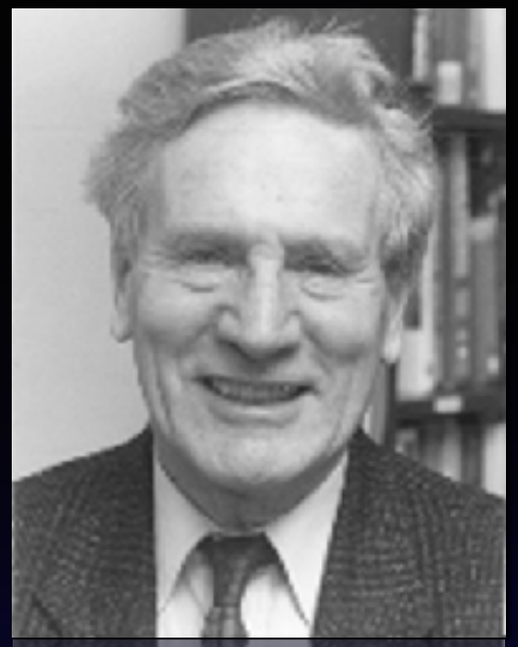


NF_3

- Why is one co-planar and one is not?
- Can we predict these geometries?

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

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Ronald Nyholm

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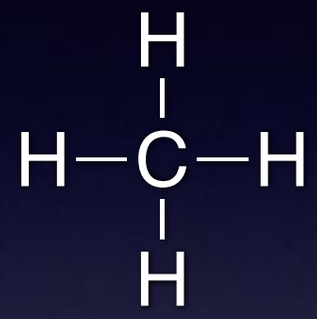
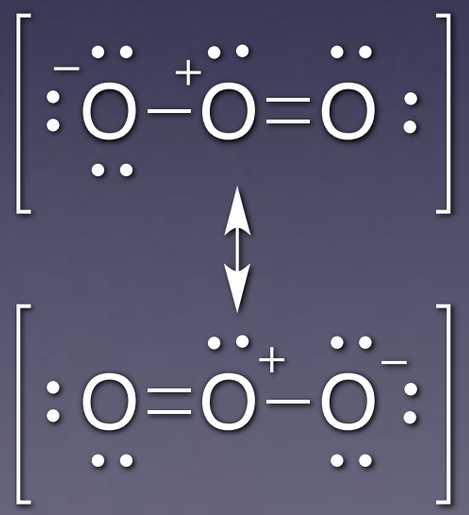
Steric number practice

- Methane
  Steric number: ?



- Magnesium hydride
  Steric number: ?

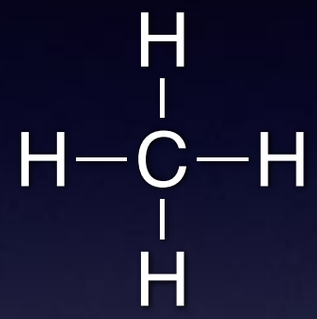
- Ozone
  Steric number: ?



- Water
  Steric number: ?

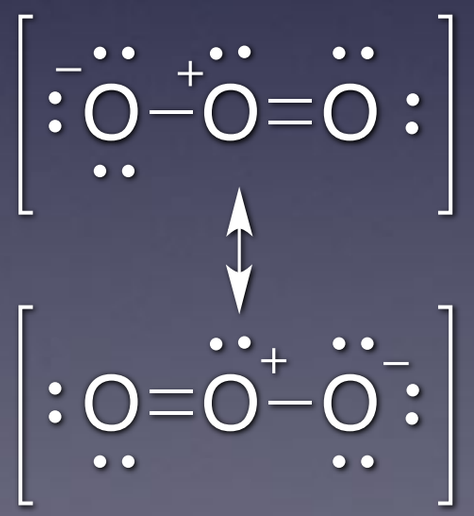
Steric number practice

- Methane
  Steric number: 4



- Magnesium hydride
  Steric number: 2

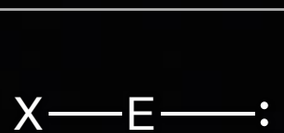
- Ozone
  Steric number: 3

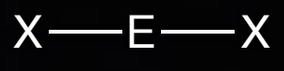
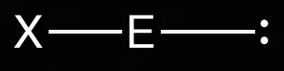
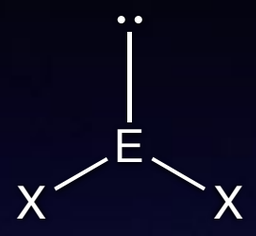


- Water
  Steric number: 4

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	X—E—X Linear					
3						
4						
5						
6						

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	X—E—X Linear	X—E—:				
3						
4						
5						
6						

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	 Linear					
3	 Trigonal planar					
4						
5						
6						

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	 Linear					
3	 Trigonal planar	 120° Bent				
4						
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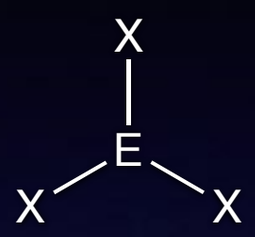
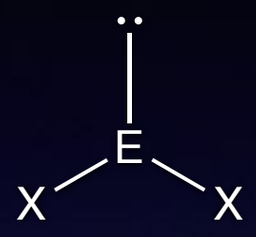
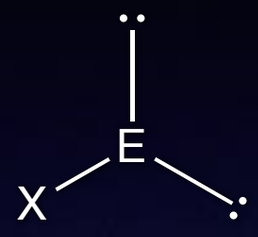
6						

SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	 Linear					
3	 Trigonal planar	 120° Bent				
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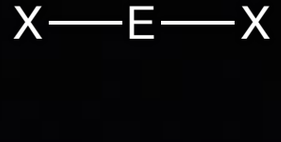
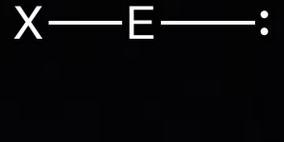
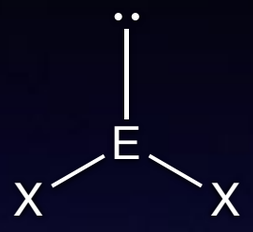
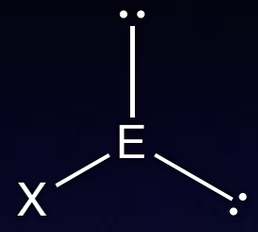
SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	 Linear					
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral					
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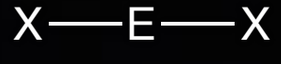
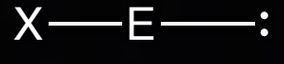
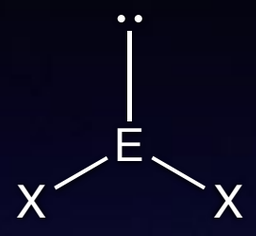
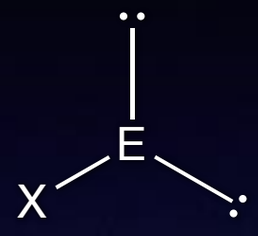
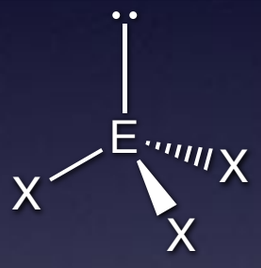
SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	 Linear					
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal				
5						
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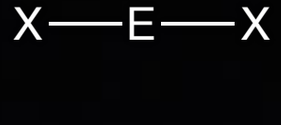
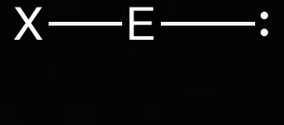
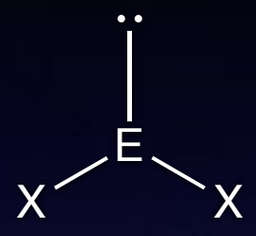
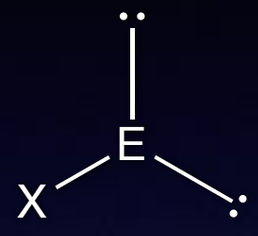
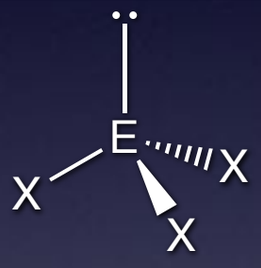
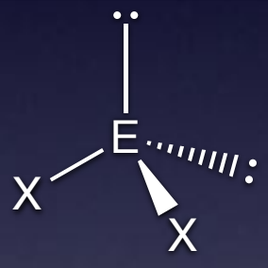
SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	 Linear					
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
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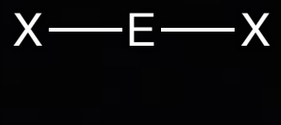
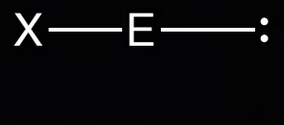
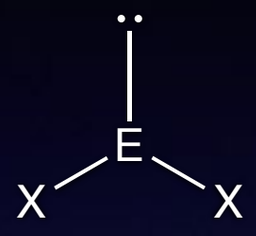
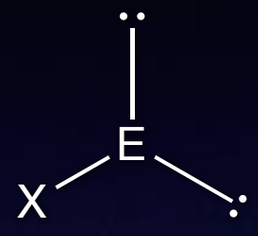
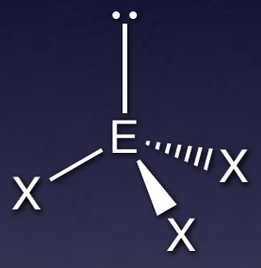
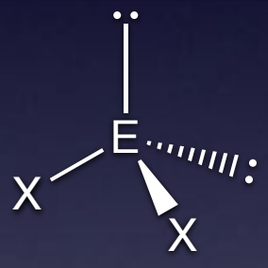
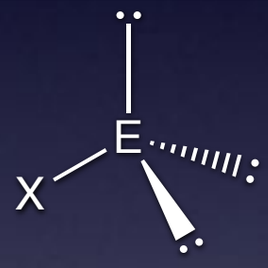
SN	0 LP	1 LP	2 LP	3 LP	4 LP	5 LP
2	 Linear					
3	 Trigonal planar	 120° Bent				
4	 Tetrahedral	 Trig. pyramidal	 109.5° Bent			
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Where did we go today?

Ch1010-A17-A03 Lecture 15

- §5.7 The Fundamental Structures

Next time…

- § 5.8 The Effect of Lone Pairs

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