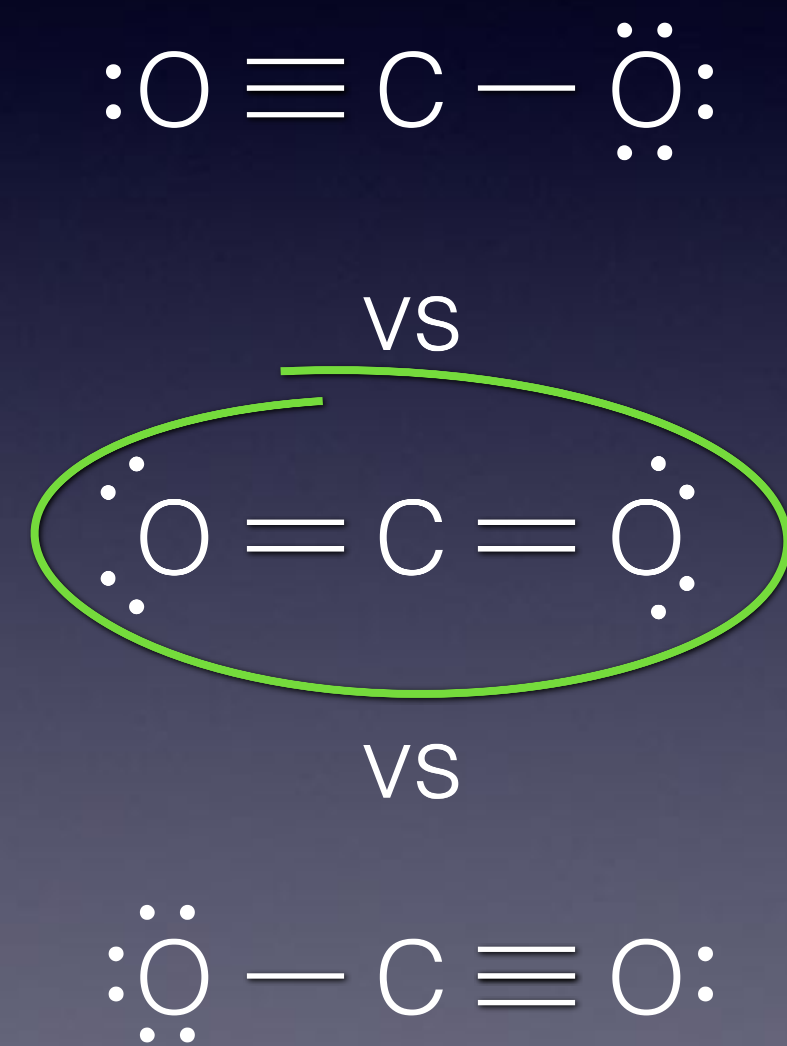
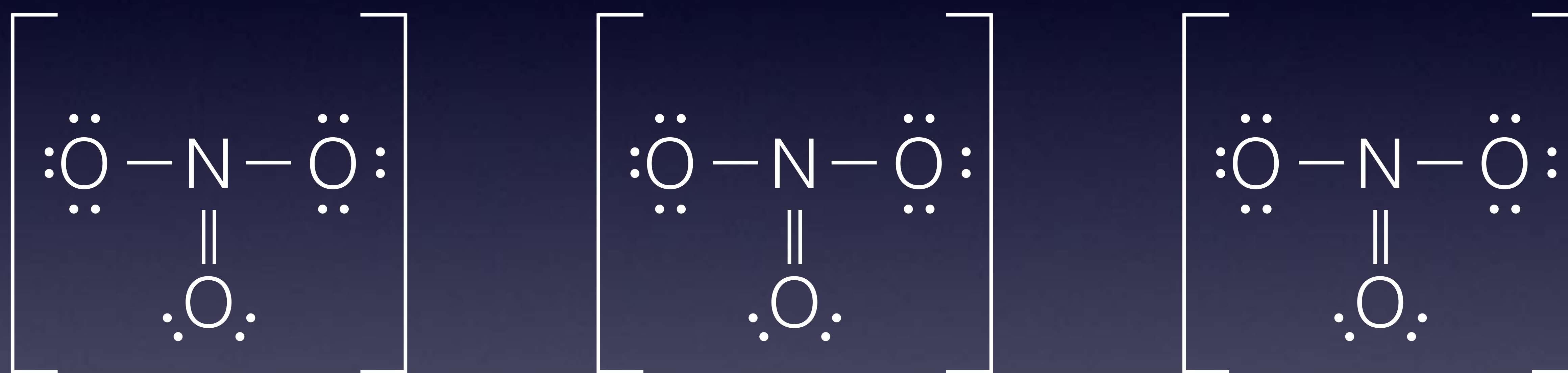
Previously in Molecularity…

Formal charge: which is “right”?

- Compare number of electrons around an atom relative to the valence electrons
  - Add up number of lone pair electrons
  - Only count one e– from a bond
- Electron deficient: positive formal charge
  Electron rich: negative formal charge
- Choose dot structure with formal charges closest to zero!



Nitrate anion, $[NO_3]^-$



What are the charges on each atom in each structure?

What might the “average” charge look like in reality?

Notable s- and p-block exceptions

- Hydrogen $1s^1$ and helium $1s^2$ follow a *duet* rule
(n = 1 can only hold two electrons)

- Alkaline earths and the boron family sometimes do their own thing
Example: magnesium hydride (MgH_2)
Example: boron trifluoride (BF_3)

- Molecules with an odd total of valence electrons
(one atom will end up with an odd count, duh!)
Example: nitrogen monoxide

- *Hypervalent* molecules or *expanded octets*:
large atoms in the 3p, 4p, … block

Where are we going today?

Ch1010-A17-A03 Lecture 14

- §5.6 Exceptions, hyperconjugation, etc.

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Example: Nitrogen monoxide

- 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

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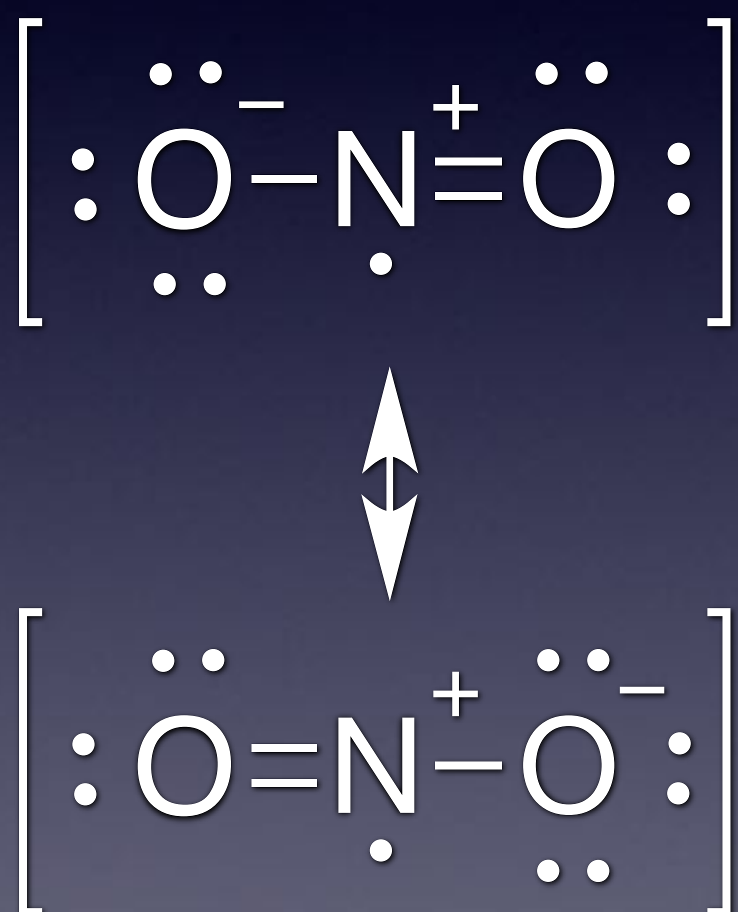

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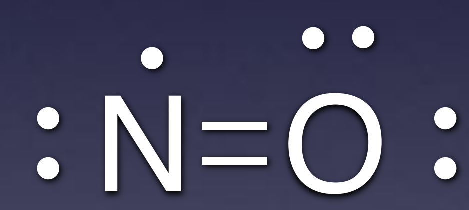

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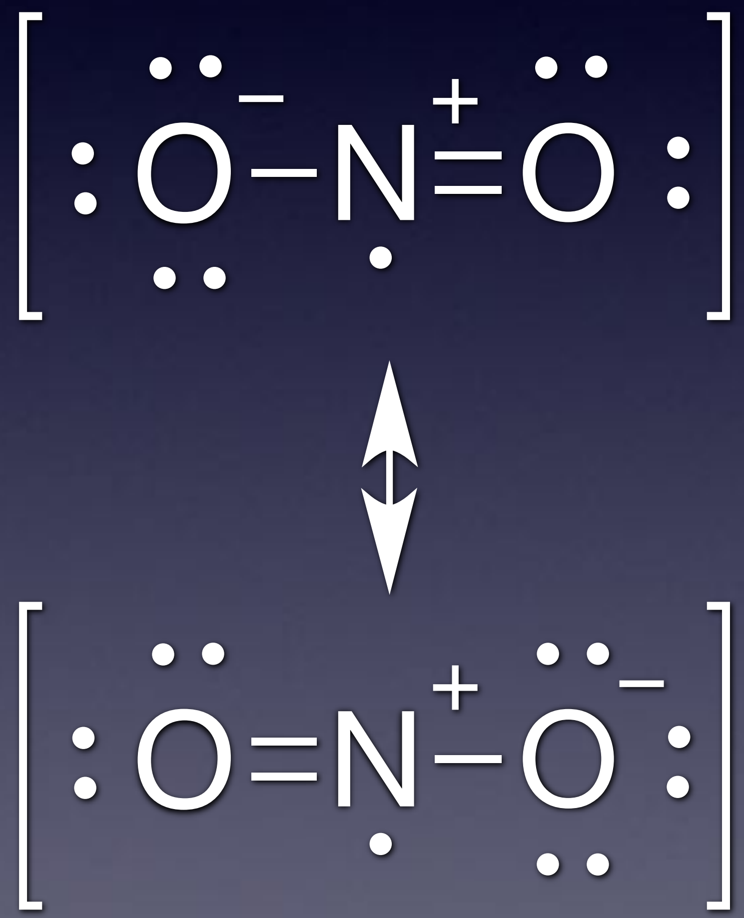
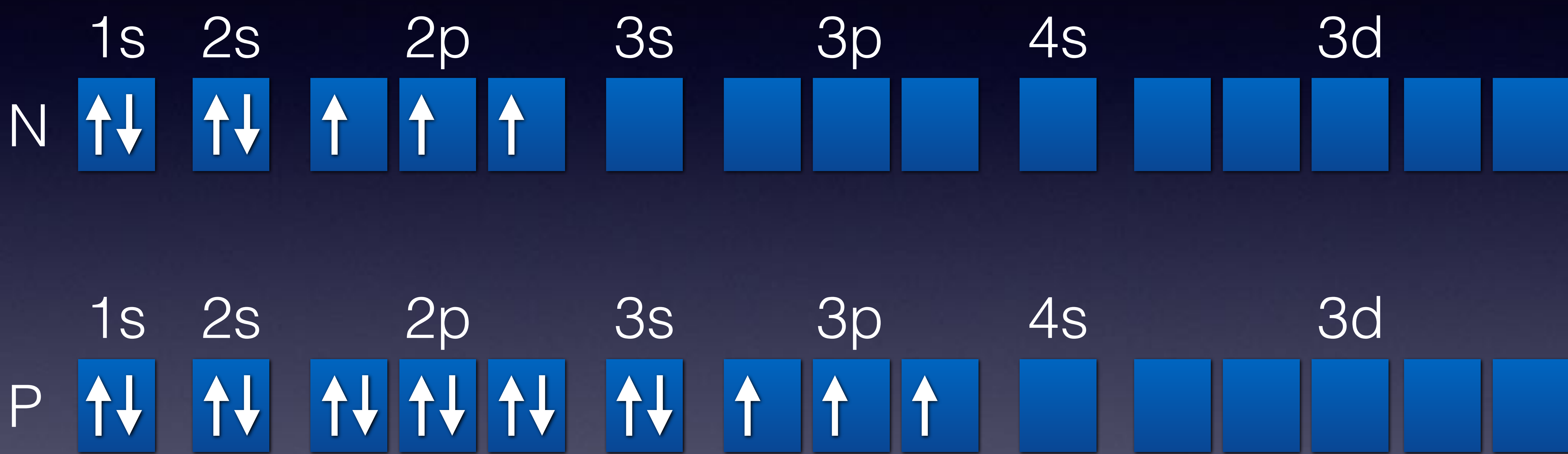
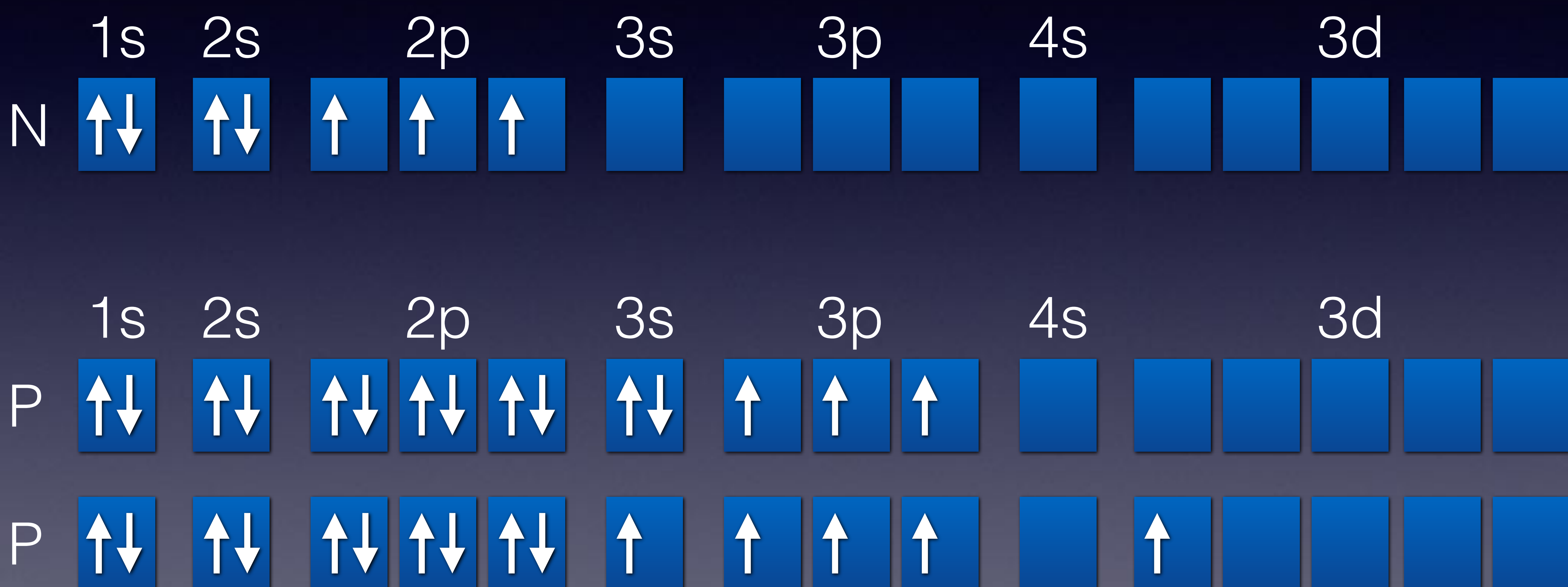


Hypervalency or Expanded Octets

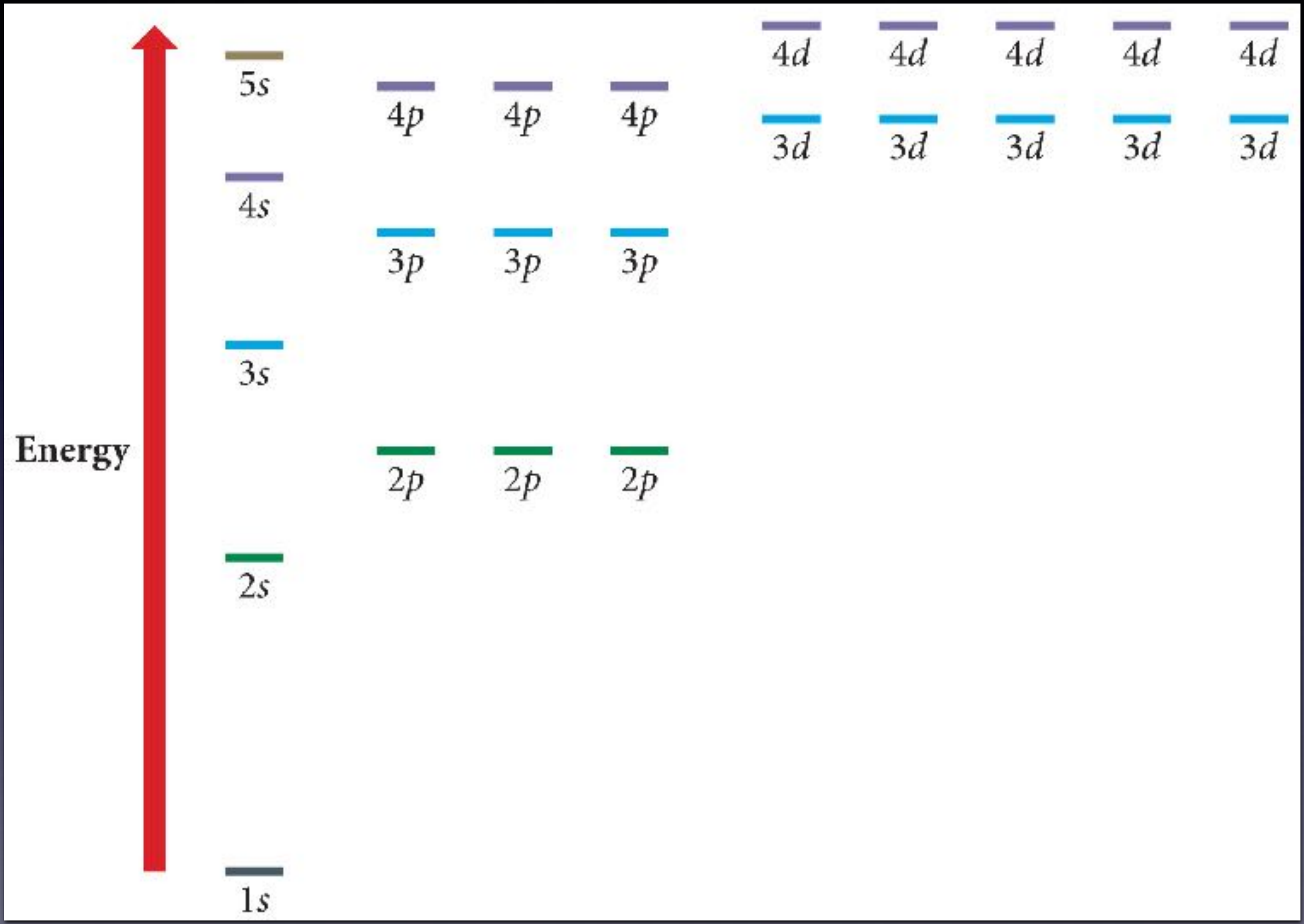


Both should only be able to bond to three other atoms…

Hypervalency or Expanded Octets

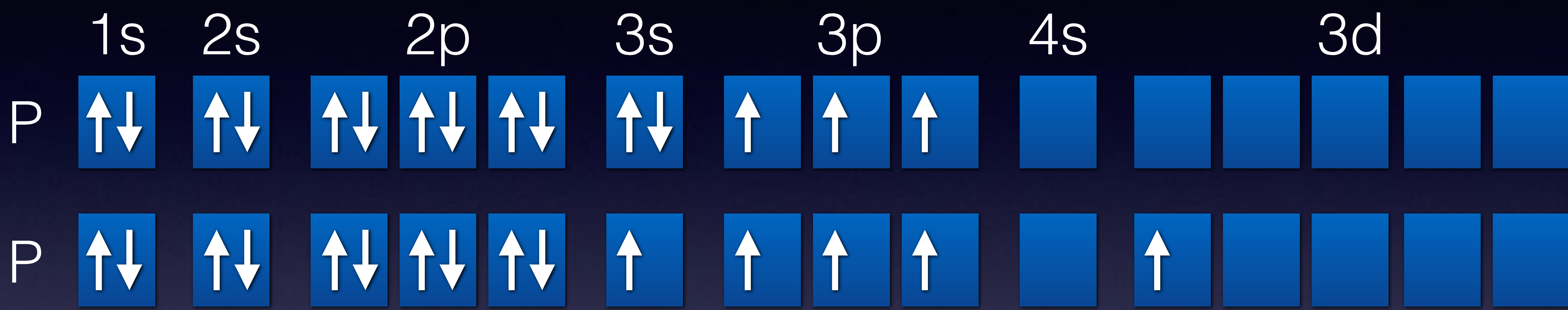


…but phosphorous can form **five** bonds!


Energy
5s
4s
3s
2s
1s
4p 4p 4p
3p 3p 3p
2p 2p 2p
4d 4d 4d 4d 4d
3d 3d 3d 3d 3d

Tro
Fig. 8.5

Conditions for expanded octets



- Requires d orbitals, therefore, it only occurs for $n \geq 3$!
- Only occurs for group 15–18 elements (pnictides, 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-}

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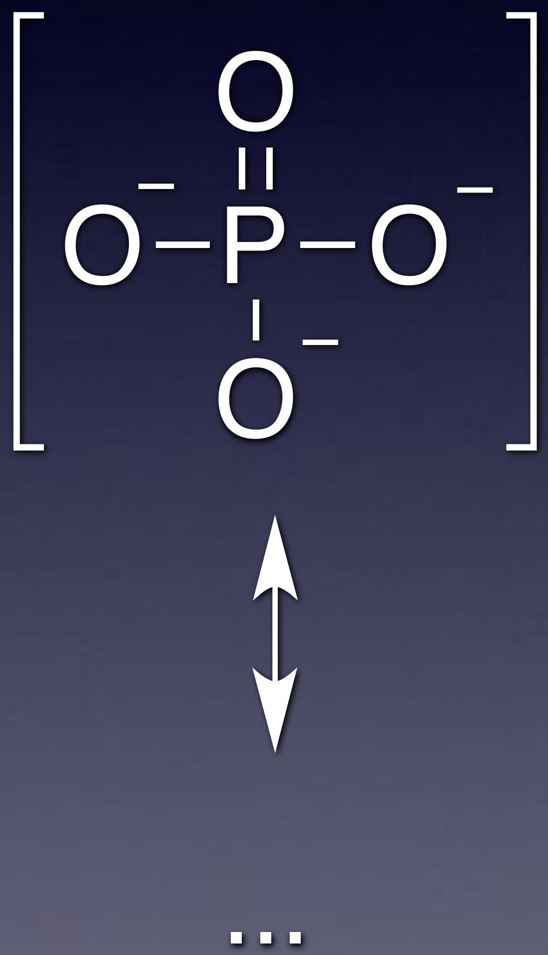

	1s	2s		2p		3s		3p		4s			3d		
P	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑						
P	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑	↑		↑				

	1s	2s		2p		3s		3p		4s			3d		
S	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑						
Cl	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑						
Xe	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓						

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:
  Boron trichloride, magnesium hydride
  $AlCl_3$ and AlF_3 do something different…

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

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

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Where did we go today?

Ch1010-A17-A03 Lecture 14

- §5.6 Exceptions, hyperconjugation, etc.

Next time…

- §5.7 VSEPR theory: the five basic shapes
- §5.8 VESPR theory: lone pairs are fat
- §5.9 VSEPR theory: predicting molecular geometries