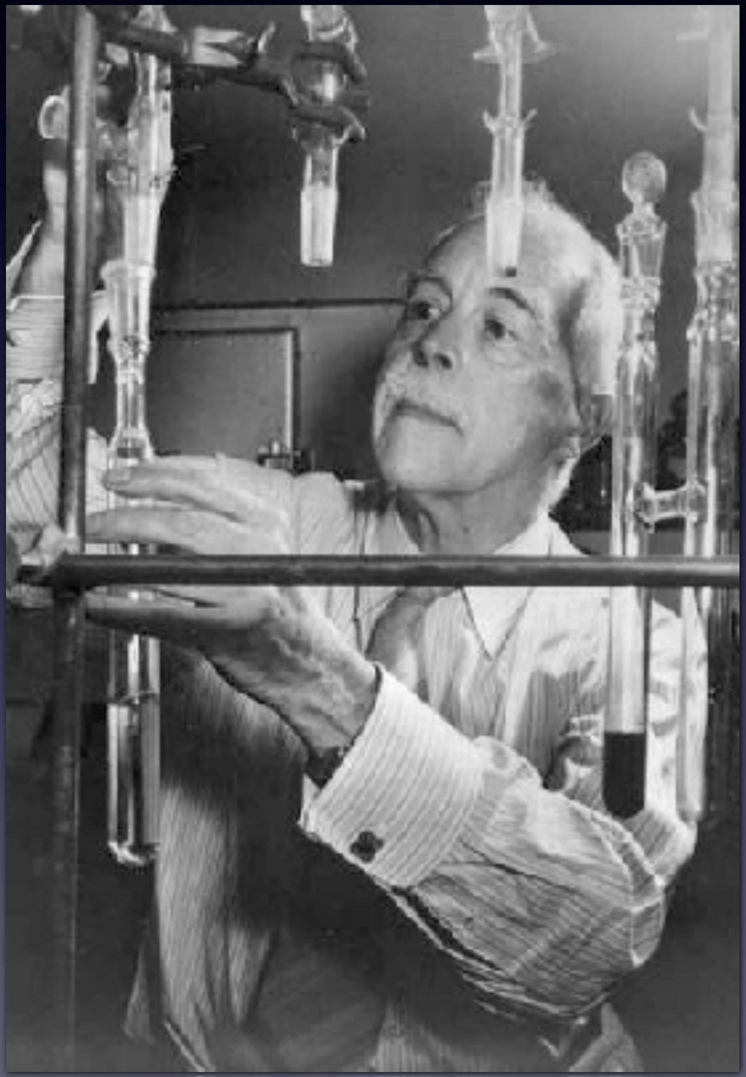
Previously in Molecularity…

The Octet "Rule"

- Atoms form chemical bonds by sharing electrons
- Atoms tend to gain, loose, or share electrons to have 8 valence electrons
- Theory predates quantum mechanics
- <u>Generally</u> accurate for s- and p-block.
- Totally fails for d-block (see 18 e^- rule) and totally fails for f-block (crazytown)



G. N. Lewis

www.atomicheritage.org
Gilbert%20Lewis.jpg

Exam[illegible]ass

need more examples

- Some easy ones:
  - Difluorodichloromethane (which is a CFC by the way) CCl_2F_2
  - Phosphine (PH_3)

- Organic molecules including ethene, C_2H_4, formaldehyde CH_2O, formic acid HCOOH (both oxygens connect to carbon), and ethanol C_2H_5OH ($H_3C–CH_2OH$)

- More challenging ones involving ions… we'll only get partway…
  - Perchlorate anion $[ClO_4]^-$
  - Chlorate anion $[ClO_3]^-$
  - Ammonium cation $[NH_4]^+$

Notable s- and p-block exceptions

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

- Alkali 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 13

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- §5.4 Resonance & formal charge

Example: carbon dioxide, CO_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

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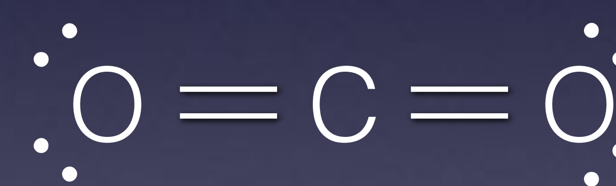
vs



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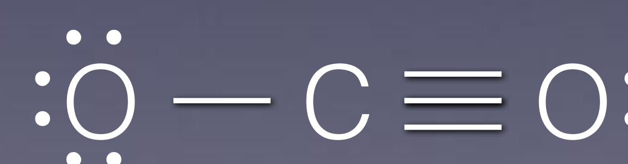
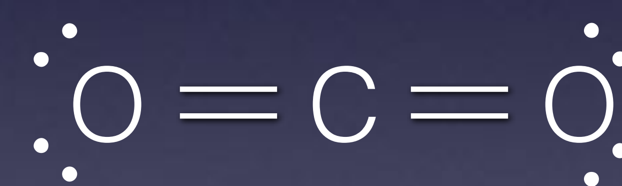


Formal charge: which is “right”?

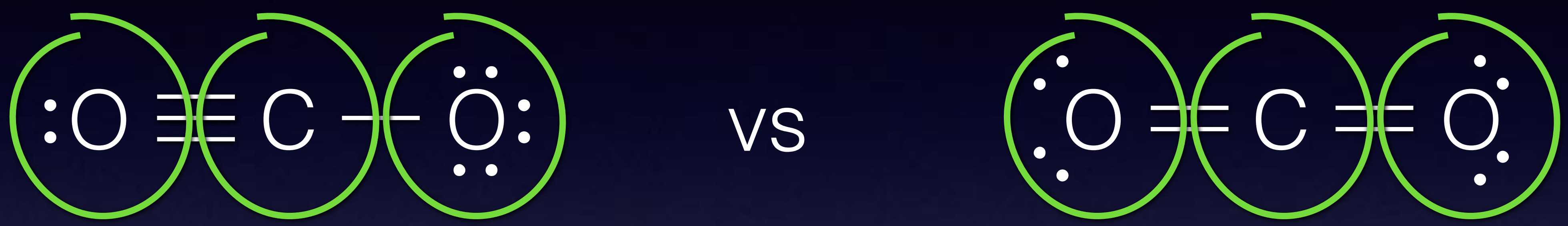
- Compare number of electrons around an atom relative to the valence electrons
    - Add up number of lone pair electrons
    - Only count one e– from a bond
- Electron deficient: positive formal charge
  Electron rich: negative formal charge
- Choose dot structure with formal charges closest to zero!

vs



vs

FC: Can only count one e⁻ from a bond



$$FC = \begin{pmatrix}\text{number of} \\ \text{valence e}^-\end{pmatrix} - \left[\begin{matrix}\text{number of} \\ \text{unshared e}^-\end{matrix} + \frac{1}{2}\begin{matrix}\text{number of e}^- \\ \text{in bonding pairs}\end{matrix}\right]$$

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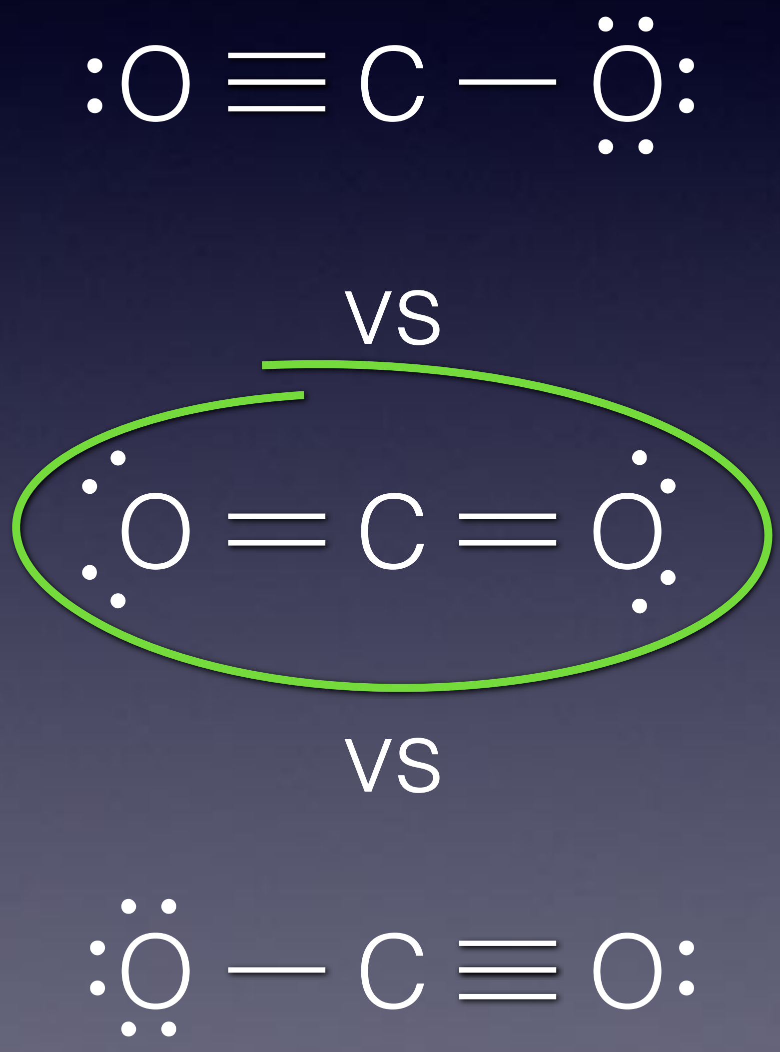

Formal charge examples

- Cyanide ion, $(CN)^{-}$
- Hydrogen cyanide, HCN
- Hydrogen isocyanide, HNC

HCN and HNC both exist, but one is much more common. Why?

Nitrate anion, $[NO_3]^-$

- Sum valence e^- incl. charge (of ions), determine # of bonds and lone pairs
- Arrange around a central atom…
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  2. Lowest electronegativity
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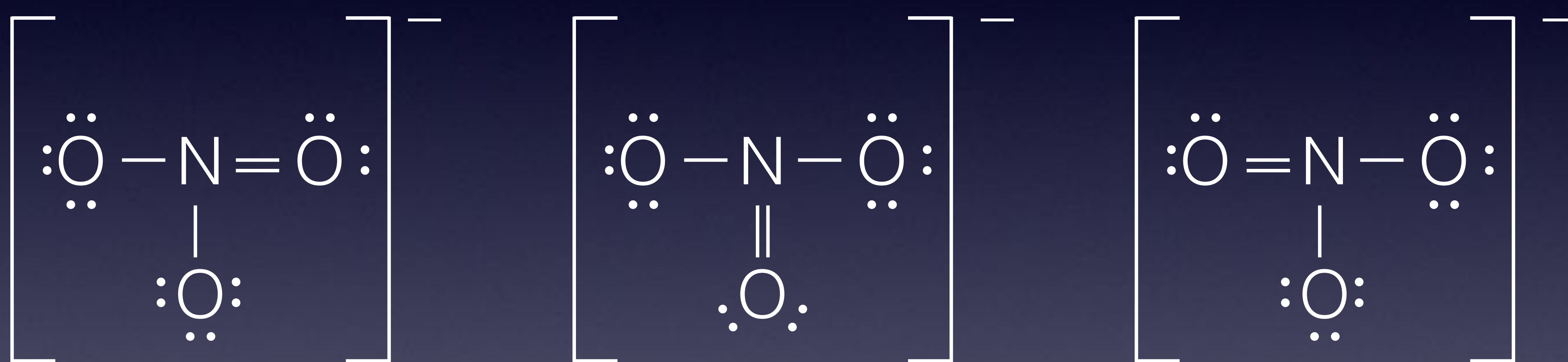
Nitrate anion, $[NO_3]^-$



What are the charges on each atom in each structure?

What might the "average" charge look like in reality?

Bisulfate anion, $[HSO_4]^-$

- Sum valence e^- incl. charge (of ions), determine # of bonds and lone pairs
- Arrange around a central atom…
  1. Greatest bonding capacity
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Where did we go today?

Ch1010-A17-A03 Lecture 13

- §5.4 Resonance & formal charge

Next time…

- §5.5 Exceptions to the octet rule
- The 18 e^- rule for transition metals

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