Essential Question

How do we choose the best Lewis structure?

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Resonance Structures

- Sometimes more than one valid Lewis structure can be drawn for the same molecule or ion.
- These are called **resonance structures**. The atoms stay in the same places; only the electrons are arranged differently.

Ozone, O_3, has 18 valence electrons (3 × 6).

Drawing Resonance Structures

- Move only lone pairs and double bonds.
- Atoms never move. Moving an atom gives a different molecule, not a resonance structure.
- Every resonance structure has the same total number of electrons.

The nitrate ion, NO_3^-, has 5 + 3(6) + 1 = 24 valence electrons.

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The Resonance Hybrid

- The real molecule is a blend of all its resonance structures, called the **resonance hybrid**.
- It does not flip back and forth between the structures.

Think of a mule, a cross between a horse and a donkey: a mule isn't a horse one second and a donkey the next.

Bond Order in a Hybrid

- Average bond order = total bonds ÷ number of bond locations
- Ozone: one double bond (2) + one single bond (1) = 3 bonds, shared over 2 locations, so 3 ÷ 2 = 1.5
- Higher bond order → shorter, stronger bond. A bond order of 1.5 falls between a single and a double bond, and so does the bond length.

Bond order is the number of bonds between two atoms: 1 for a single bond, 2 for a double bond, and 3 for a triple bond.

Formal Charge

- ***V*** = valence electrons of the neutral atom (from the group number)
- ***N*** = nonbonding electrons on that atom (count every dot)
- ***B*** = bonding electrons on that atom (2 for every line)

$$FC = V - N - \tfrac{1}{2}B$$

Adding Up Formal Charges

- Find the formal charge on every atom.
- The sum of the formal charges equals the overall charge of the molecule or ion.

The sum is 0, which matches neutral O_3.

Choosing the Best Structure

1. **Octets:** give atoms octets. C, N, O, and F never go over an octet.
2. **Formal charges as close to zero as possible:** fewer and smaller formal charges make a more stable structure.
3. **The tiebreaker:** any negative formal charge should be on the most electronegative atom, the one that pulls electrons the hardest.

Exam tip: when you justify which structure is best, name these rules as your evidence.

Equivalent vs. Nonequivalent

- **Equivalent structures** have the same pattern with the bonds in different spots (examples: O_3, NO_3^-). Every structure is equally good, so use resonance and blend them.

Equivalent vs. Nonequivalent

- **Nonequivalent structures** have different formal charge patterns (examples: CO_2, OCN^-). They are not equally good, so use formal charge to pick the best one. The best structure is the best model for predicting the molecule's shape and properties.

Limitations of the Lewis Model

- Every model has limits.
- An odd number of valence electrons means one electron is left unpaired.
- At least one atom can’t have an octet.

Nitrogen monoxide, NO, has 5 + 6 = 11 valence electrons.

Example: Drawing Resonance Structures

Try it first!

Draw all resonance structures for the nitrite ion, NO_2^-.

Example: Calculating Formal Charge

Try it first!

Calculate the formal charge on each atom in this Lewis structure of the thiocyanate ion, SCN^-.

Diagram: Lewis structure of the thiocyanate ion in brackets with a minus charge: S=C=N, with two lone pairs on sulfur, none on carbon, and two lone pairs on nitrogen.

Example: Choosing the Best Structure

Try it first!

Two Lewis structures for N_2O are shown. Which is the better model? Justify your answer using formal charge.

Diagram: Two Lewis structures for N2O. Structure A: N=N=O with two lone pairs on the end nitrogen and two on oxygen. Structure B: N≡N-O with one lone pair on the end nitrogen and three on oxygen.

Example: Average Bond Order

Try it first!

One resonance structure of the carbonate ion, CO_3^{2-}, is shown. Find the average C-O bond order. How do the three C-O bond lengths compare?

Diagram: One resonance structure of the carbonate ion in brackets with a 2− charge: carbon in the center double-bonded to the top oxygen and single-bonded to two lower oxygens, with lone pairs on each oxygen.

Example: Odd Electrons

Try it first!

Nitrogen dioxide, NO_2, has 17 valence electrons. Explain why no Lewis structure for NO_2 can give every atom an octet.

Big Ideas

- Resonance: more than one valid Lewis structure can be drawn.
- The real molecule is the resonance hybrid.
- FC = $V - N - \frac{1}{2}B$ (valence − dots − lines).
- Best structure: formal charges near 0, with any negative formal charge on the most electronegative atom.