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# Topic 2.6: Resonance and Formal Charge

Revision Notes · AP Chemistry

UNIT 2 · COMPOUND STRUCTURE AND PROPERTIES

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## When One Lewis Diagram Is Not Enough

Some species cannot be represented honestly by a single Lewis diagram. Draw carbonate, $CO_3^{2-}$, by the Topic 2.5 sequence and one C−O bond comes out double, the other two single, yet nothing picks out one oxygen for the double bond: any of the three could carry it. The three resulting diagrams are resonance structures, or contributors, of one and the same ion. Measured bond lengths prove it: all three C−O bonds are identical, each shorter than a single bond but longer than a double bond, which no single contributor matches.

## What May and May Not Change Between Contributors

Resonance structures share everything except the placement of electrons: atoms, connectivity, total valence electrons and overall charge are all identical. Only multiple bonds and lone pairs trade places: a lone pair beside a multiple bond can join it, and a multiple bond can collapse into a lone pair on one of its atoms.

Contributors may be equivalent or nonequivalent. Carbonate's three are equivalent: same arrangement, same charges, same energy, contributing equally. $NCO^-$'s are nonequivalent, with different charge patterns, and contribute unequally; judging between them is the work of formal charge, below.

## The Resonance Hybrid and Average Bond Order

The real species is a resonance hybrid: one static structure blending the contributors, its bonding spread over every position the contributors use. It does not switch or oscillate between them. The contributors are bookkeeping drawings; the hybrid is the molecule.

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Because the bonding is shared, a bond that is double in one contributor and single in another has an intermediate, fractional bond order in the hybrid: total bond order across the equivalent positions, divided by the number of positions. Formate, $HCOO^-$: (2 + 1) / 2 = 1.5 over its two C−O positions. Carbonate and nitrate: (2 + 1 + 1) / 3 = 4/3, about 1.33, over three positions. Benzene's two contributors give every C−C bond an order of 1.5.

Bond order still predicts length and strength, as in Topic 2.2. Nitrate's N−O bonds (order 1.33) are longer than nitrite's (order 1.5, from (2 + 1) / 2), because the same bonding is spread over more positions. Delocalization also lowers the energy: the hybrid is more stable than any single contributor, its electrons spread over more atoms.

## Formal Charge: The Bookkeeping Formula

Formal charge audits a finished diagram: the charge each atom would carry if every bonding pair were split exactly equally between the two atoms it joins:

Formal charge = valence electrons − (nonbonding electrons + ½ × bonding electrons)

The working shortcut counts lines instead of electrons: formal charge = valence electrons − dots − bonds, where dots are nonbonding electrons and bonds are the bond lines touching the atom. A double bond counts as two bonds, since the atom is assigned half of four bonding electrons.

Two checks make the arithmetic self-verifying. First, a diagram's formal charges must sum to the species' overall charge: zero for a neutral molecule, −1 for $NO_3^-$. Any other sum exposes a counting error. Second, formal charge is a bookkeeping device, not a measured charge: it splits shared electrons equally, ignoring electronegativity, so never confuse it with oxidation state, which hands both bonding electrons to the more electronegative atom.

## Worked Example: Nitrate, Atom by Atom

$NO_3^-$ owns 5 + (3 × 6) + 1 = 24 valence electrons. In each contributor nitrogen is double bonded to one oxygen, single bonded to two, and carries no lone pair; the double bonded oxygen carries two lone pairs, each single bonded oxygen three.

Nitrogen: 5 − (0 + 4) = +1. Double bonded oxygen: 6 − (4 + 2) = 0. Each single bonded oxygen: 6 − (6 + 1) = −1. The sum, +1 + 0 − 1 − 1 = −1, matches the ion's charge, and the placed electrons audit too: 8 bonding + 16 in lone pairs = 24. The same audit on ozone gives +1, 0 and −1 across its three oxygens, summing to zero as a neutral molecule must.

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## Judging Structures: The Stability Hierarchy

Formal charge exists to rank diagrams. Apply the tests in this order.

**Complete the octets first.** A contributor with complete octets, especially on period 2 atoms, beats one without, even at the price of formal charges. Carbon monoxide proves it: 10 electrons cannot give both atoms an octet through a double bond (that takes 12 placed electrons), so the accepted diagram is the triple bond, completing both octets at the price of −1 on carbon and +1 on oxygen.

**Then minimize formal charges.** Fewer and smaller formal charges mean a better contributor. Sulfate, $SO_4^{2-}$, drawn with four single bonds puts +2 on sulfur and −1 on every oxygen. Converting two lone pairs into double bonds (legal for period 3 sulfur) puts 12 electrons around sulfur, with sulfur and the double bonded oxygens at 0 and only the single bonded oxygens at −1. Both diagrams place exactly 32 electrons; the second wins purely on smaller formal charges.

**Then place unavoidable charges well.** Negative formal charge belongs on the more electronegative atom, positive charge on the less electronegative one. In $NCO^-$, the contributor $[:N{\equiv}C{-}O]^-$ (charges 0, 0, −1, with the −1 on oxygen) dominates $[N{=}C{=}O]^-$ (−1 on nitrogen), although both have complete octets and one charge each.

**But formal charge never licenses a bad octet trade.** $BF_3$ is the counterweight to sulfate. Its standard diagram leaves boron with 6 electrons and every formal charge zero. A B=F double bond completes boron's octet only by putting +1 on fluorine, the most electronegative element there is, and −1 on boron. The incomplete octet with zero formal charges is the accepted structure. Octets first governs period 2 atoms and reasonable charges; it is not an instruction to complete an octet at any cost.

One limit case: NO, with 11 valence electrons, always leaves one electron unpaired, so no diagram completes every octet.

## Traps That Cost Marks in Topic 2.6

**Describing resonance as movement.** The hybrid never flips between contributors. Saying the double bond "moves around" or the molecule "alternates" misdescribes a static blend; the credited language is delocalized electrons and equal bond lengths.

**Offering a different skeleton as a resonance structure.** Moved atoms, changed connectivity, or a broken and remade single bond all mean a different species. Resonance rearranges electrons only.

**Formal charges that do not sum to the charge.** The sum is a free error check, so run it before trusting any individual value: +1 with two −1s suits a −1 ion, not a neutral molecule.

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**Counting a double bond as one bond in the shortcut.** Formal charge = valence − dots − bonds counts bond lines; a double bond is two lines, assigning the atom 2 of the 4 bonding electrons. Halving wrongly here is the commonest arithmetic slip in the topic.

**Assuming the zero formal charge diagram always wins.** CO keeps a triple bond with charges of −1 and +1 because the octet matters more; $BF_3$ keeps an incomplete octet because the alternative charges fluorine positively. Quote one rung as the whole rule and exactly these species catch you.

### Key Relationships to Remember

- Resonance (SAP-4.B): needed when one Lewis diagram cannot represent the species; contributors share connectivity, electron total and charge, differing only in where multiple bonds and lone pairs sit
- Resonance hybrid: the single real structure, a static blend of the contributors; more stable than any contributor alone because its electrons are delocalized over more atoms
- Average bond order: total bond order over the equivalent positions divided by the number of positions ($HCOO^-$ 1.5, $CO_3^{2-}$ and $NO_3^-$ 4/3, $PO_4^{3-}$ 5/4, benzene C−C 1.5); higher order means shorter, stronger bonds
- Formal charge = valence electrons − (nonbonding electrons + ½ bonding electrons), or valence − dots − bonds; a diagram's formal charges always sum to the species' overall charge
- Stability order: complete octets first (period 2 above all), then smallest formal charges, then least charge separation, then negative charge on the most electronegative atom ($SO_4^{2-}$ two double bonds; $NCO^-$ −1 on oxygen; CO and $BF_3$ mark the limits)

### Continue Revising

Topic 2.6 Quiz: Resonance and Formal Charge

Topic 2.6 Worksheet

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