Atomic Structure, Lewis Structures, and Formal Charge — Study Guide

Organic chemistry is the chemistry of carbon compounds, and every reaction you will learn is ultimately a story about where electrons are and where they move. This guide builds the electron bookkeeping skills that every later topic depends on: electron configuration, valence electrons, the octet rule, drawing correct Lewis structures, assigning formal charge, reading bond-line drawings, and using a molecular formula to count rings and π bonds.

Companion guides: Hybridization, Molecular Geometry, and Polarity; Resonance; Intermolecular Forces and Functional Groups. Drawing on Klein, Clayden, Wade, McMurry, Chemistry LibreTexts, and G. N. Lewis's original 1916 paper.

Section	Topic
1	Atomic Structure and Electron Configuration
2	Valence Electrons, the Octet Rule, and Bonding Patterns
3	Ionic and Covalent Bonds
4	Drawing Lewis Structures Step by Step
5	Formal Charge
6	Reading and Drawing Organic Structures
7	Molecular Formulas and Degrees of Unsaturation

1. Atomic Structure and Electron Configuration

An atom has a dense nucleus of protons (positive) and neutrons (neutral) surrounded by electrons (negative). The number of protons is the atomic number, Z, and it defines the element: every carbon atom has Z = 6. Chemistry happens almost entirely in the electrons, so that is where we focus.

Orbitals: Where Electrons Live

Electrons occupy orbitals, regions of space where an electron is likely to be found. Each orbital holds at most two electrons. For organic chemistry you need only the first two shells and two orbital shapes.

Orbital	Shape	Number per shell	Key point for organic chemistry
s	Sphere centred on the nucleus	1	Lower in energy and held closer to the nucleus than p in the same shell
p	Dumbbell (two lobes) with a node at the nucleus	3 (px, py, pz), mutually perpendicular	Sideways overlap of p orbitals makes π bonds

Three Rules for Filling Orbitals

- **Aufbau principle:** fill the lowest-energy orbital first (1s, then 2s, then 2p, then 3s, 3p…).
- **Pauli exclusion principle:** an orbital holds at most two electrons, and they must have opposite spins.
- **Hund's rule:** when orbitals have equal energy (the three 2p orbitals), put one electron in each before pairing any.

Electron Configurations of Common Organic Atoms

Element	Z	Configuration	Valence electrons
H	1	$1s^1$	1
B	5	$1s^2\ 2s^2\ 2p^1$	3
C	6	$1s^2\ 2s^2\ 2p^2$	4
N	7	$1s^2\ 2s^2\ 2p^3$	5
O	8	$1s^2\ 2s^2\ 2p^4$	6
F	9	$1s^2\ 2s^2\ 2p^5$	7
P	15	[Ne] $3s^2\ 3p^3$	5
S	16	[Ne] $3s^2\ 3p^4$	6
Cl	17	[Ne] $3s^2\ 3p^5$	7

Shortcut: for main-group elements, the number of valence electrons equals the group number in the A-group system (C is in group 4A, so 4 valence electrons; O in 6A, so 6). You will use this number constantly when drawing Lewis structures and computing formal charge.

2. Valence Electrons, the Octet Rule, and Bonding Patterns

Only valence electrons (those in the outermost shell) take part in bonding. Second-row atoms (C, N, O, F) are most stable with eight valence electrons around them, the configuration of the noble gas neon. This is the octet rule, first stated in recognisable form by G. N. Lewis in 1916.

Octet rule: second-row atoms gain, lose, or share electrons until each is surrounded by eight valence electrons. Hydrogen is satisfied with two (a duet).

The Four Neutral Bonding Patterns

Each shared pair (bond) counts toward the octet of both atoms. A neutral atom therefore forms a characteristic number of bonds: its valence electrons minus the electrons it keeps as lone pairs. Memorising these four patterns lets you spot errors in a structure instantly.

Atom	Valence e^-	Bonds (neutral)	Lone pairs (neutral)	Example
H	1	1	0	H–C in CH_4
C	4	4	0	CH_4, $H_2C{=}CH_2$
N	5	3	1	NH_3, CH_3NH_2
O	6	2	2	H_2O, CH_3OH
F, Cl, Br, I	7	1	3	CH_3Cl

Exceptions You Must Know

- **Hydrogen** never exceeds two electrons and always forms exactly one bond.
- **Boron and aluminum** are often electron-deficient: BF_3 and BH_3 have only six electrons around boron, which is why they act as Lewis acids (you saw this with hydroboration).
- **Carbocations and radicals** are electron-deficient carbon: a carbocation has six electrons, a radical has seven. Their instability is the reason they are reactive intermediates.
- **Third-row elements (P, S, Cl)** can exceed eight electrons because they have accessible d orbitals in older models (or more accurately, because they are larger). You will see this in H_2SO_4, $SOCl_2$, and PCl_5. Second-row atoms (C, N, O, F) can never exceed eight.

Exam trap: a second-row atom with more than eight electrons, such as a carbon with five bonds or a nitrogen with four bonds and a lone pair, is always wrong. Check every C, N, and O in your answer before moving on.

3. Ionic and Covalent Bonds

Atoms reach a stable electron configuration in two ways. In an ionic bond, one atom transfers electrons to another, and the resulting oppositely charged ions attract. In a covalent bond, two atoms share a pair of electrons. Most organic bonds are covalent, though many are polarised.

Feature	Ionic bond	Covalent bond
How the octet is reached	Electron transfer	Electron sharing
Typical partners	Metal + nonmetal (Na^+ Cl^-)	Nonmetal + nonmetal (C–H, C–O)
Electronegativity difference	Large (above about 1.7 Pauling units)	Small to moderate (below about 1.7)
Organic examples	Sodium acetate (CH_3COO^- Na^+), NaOH, alkoxides	Nearly every bond in an organic molecule

The boundary between the two is not sharp: bond polarity is a continuum set by the electronegativity difference between the bonded atoms. That continuum, and how it creates partial charges (δ+ and δ−), is covered in detail in the companion guide on Hybridization, Molecular Geometry, and Polarity.

Ionic reagents in organic chemistry (NaOH, $NaOCH_3$, $NaNH_2$, NaH) are written with the metal counter-ion, but the reactive species is the anion. In mechanisms you usually draw only the anion: HO^-, CH_3O^-, H_2N^-, H^-.

4. Drawing Lewis Structures Step by Step

A Lewis structure shows every valence electron: bonds as lines (each line is two shared electrons) and lone pairs as pairs of dots. Drawing them correctly is a mechanical procedure; the steps below work for any neutral molecule or ion.

The Five-Step Method

- **Count total valence electrons.** Add the valence electrons of every atom. Add one for each negative charge; subtract one for each positive charge.
- **Build the skeleton.** Connect atoms with single bonds. Hydrogen and halogens are always terminal (one bond). Carbon forms the backbone; the least electronegative non-hydrogen atom usually goes in the centre.
- **Subtract the bonding electrons** (2 per bond) from the total.
- **Distribute the remaining electrons as lone pairs,** completing octets on the outer atoms first, then the central atoms.
- **Fix any incomplete octets** by converting a lone pair on a neighbouring atom into a shared pair (forming a double or triple bond). Then assign formal charges (Section 5).

Worked Example A — Methanol, CH_3OH

- Valence electrons: C (4) + 4 H (4 × 1) + O (6) = 14.
- Skeleton: C bonded to three H and to O; O bonded to one H. That is 5 single bonds.
- Bonding electrons used: 5 × 2 = 10. Remaining: 14 − 10 = 4.
- Place the 4 remaining electrons as 2 lone pairs on O. Oxygen now has 2 bonds + 2 lone pairs = octet. Carbon has 4 bonds = octet. Done; every formal charge is zero.

```
     H
     |
  H — C — O — H      (O carries two lone pairs)
     |
```

```
    H
```

Worked Example B — Formaldehyde, CH_2O

- Valence electrons: C (4) + 2 H (2) + O (6) = 12.
- Skeleton: C in the centre bonded to 2 H and O (3 single bonds, 6 electrons). Remaining: 6.
- Put the 6 electrons on O as 3 lone pairs. Oxygen has an octet, but carbon has only 3 bonds = 6 electrons.
- Fix: move one lone pair from O into a C=O double bond. Now C has 4 bonds (octet) and O has 2 bonds + 2 lone pairs (octet). This is the carbonyl group.

```
H
  \
   C = O       (O carries two lone pairs)
  /
H
```

Worked Example C — Hydrogen Cyanide, HCN

- Valence electrons: H (1) + C (4) + N (5) = 10.
- Skeleton H–C–N (2 bonds, 4 electrons). Remaining: 6, placed on N as 3 lone pairs.
- Carbon has only 4 electrons. Convert two lone pairs on N into bonds: H–C≡N with one lone pair left on N. Now C has 4 bonds and N has 3 bonds + 1 lone pair.

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H – C ≡ N:
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Worked Example D — The Hydroxide Ion, HO^-

- Valence electrons: O (6) + H (1) + 1 for the negative charge = 8.
- One O–H bond (2 electrons). Remaining 6 go on O as 3 lone pairs.
- Oxygen: 1 bond + 3 lone pairs. Its formal charge is −1 (Section 5), which locates the ion's charge on oxygen.

Never forget to count lone pairs. Lone pairs are not decoration: they are the electrons that act as nucleophiles and bases in nearly every mechanism you will draw. A structure missing its lone pairs is incomplete on an exam.

5. Formal Charge

Formal charge is a bookkeeping tool that tells you which atom in a structure carries a charge. It compares how many valence electrons an atom "owns" in the structure with how many it has as a free, neutral atom. The sum of all formal charges always equals the overall charge of the molecule or ion.

Formal charge = (valence electrons of the free atom) − (nonbonding electrons) − (number of

bonds)

Equivalently: formal charge = V − (lone-pair electrons) − ½(bonding electrons). Each bond contributes one electron to each atom, and each lone pair contributes two electrons to the atom that holds it.

Worked Calculations

Species	Atom	V	Lone-pair e⁻	Bonds	Formal charge
Hydronium, H_3O^+	O	6	2	3	6 − 2 − 3 = +1
Hydroxide, HO^-	O	6	6	1	6 − 6 − 1 = −1
Ammonium, NH_4^+	N	5	0	4	5 − 0 − 4 = +1
Amide ion, H_2N^-	N	5	4	2	5 − 4 − 2 = −1
Methyl cation, CH_3^+	C	4	0	3	4 − 0 − 3 = +1
Methyl anion, CH_3^-	C	4	2	3	4 − 2 − 3 = −1
Methyl radical, $CH_3\bullet$	C	4	1	3	4 − 1 − 3 = 0

The Pattern Shortcut

After a few weeks you should stop calculating and simply recognise the pattern. Compare each atom with its neutral pattern from Section 2: one extra bond (and one fewer lone pair) means +1; one fewer bond (and one more lone pair) means −1.

Atom	Formal charge +1	Formal charge 0	Formal charge −1
Carbon	3 bonds, 0 lone pairs (carbocation)	4 bonds, 0 lone pairs	3 bonds, 1 lone pair (carbanion)
Nitrogen	4 bonds, 0 lone pairs	3 bonds, 1 lone pair	2 bonds, 2 lone pairs
Oxygen	3 bonds, 1 lone pair	2 bonds, 2 lone pairs	1 bond, 3 lone pairs
Halogen	2 bonds, 2 lone pairs (halonium)	1 bond, 3 lone pairs	0 bonds, 4 lone pairs (halide)

The bromonium ion you met in alkene halogenation is the halogen +1 pattern: bromine with two bonds and two lone pairs. The oxonium ion in acid-catalysed hydration is the oxygen +1 pattern: three bonds and one lone pair.

Worked Example — Nitromethane, CH_3NO_2

- Valence electrons: C (4) + 3 H (3) + N (5) + 2 O (12) = 24.

- Skeleton: CH_3 bonded to N; N bonded to both O atoms (6 single bonds, 12 electrons). Remaining: 12.
- Complete the oxygen octets: 3 lone pairs on each O (12 electrons). Nitrogen now has only 3 bonds and no lone pair = 6 electrons.
- Fix: move one lone pair from one O to make N=O. Nitrogen: 4 bonds, no lone pairs, formal charge +1. The double-bonded O: 2 bonds, 2 lone pairs, formal charge 0. The single-bonded O: 1 bond, 3 lone pairs, formal charge −1.
- Check: (+1) + 0 + (−1) = 0, matching the neutral molecule. The two N–O bonds are actually equivalent; this is resonance, the subject of its own companion guide.

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           O         (double-bonded O: 2 lone pairs, FC 0)
          //
H₃C — N⁺
          \
           O⁻     (single-bonded O: 3 lone pairs, FC −1)
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Formal Charge Is Not Real Charge

Formal charge assumes every bond is shared perfectly equally, which is never quite true. In hydronium, the formal +1 sits on oxygen, but because oxygen is very electronegative, the actual positive charge density is spread mostly onto the three hydrogens. Formal charge tells you where to draw the charge symbol and how to track electrons; electronegativity tells you where the electron density really is.

6. Reading and Drawing Organic Structures

Full Lewis structures become unreadable for molecules with more than a few carbons. Organic chemists use three shorthand styles, and you must be able to move between them fluently.

Style	What is shown	Example: butan-1-ol
Lewis (Kekulé)	Every atom, every bond, every lone pair	All 15 atoms drawn individually
Condensed	Atoms grouped along the chain; bonds to H implied	$CH_3CH_2CH_2CH_2OH$
Bond-line (skeletal)	Zigzag lines; each vertex and line end is a carbon; H on carbon implied	A four-carbon zigzag ending in OH

Rules for Bond-Line Drawings

- Each vertex (corner) and each line end is a carbon atom, unless another atom is written there.
- Hydrogens on carbon are not drawn. Each carbon has enough implied hydrogens to make 4 bonds total.
- Heteroatoms (O, N, S, halogens) are always written, together with any hydrogens attached to them (OH, NH_2).

- Chains are drawn as zigzags because sp^3 carbons have ~109.5° bond angles. Double bonds keep the zigzag; triple bonds are drawn straight (180°).
- Formal charges and, in mechanisms, the lone pairs that react must be shown explicitly.

Counting Implied Hydrogens

The number of hydrogens on any carbon in a bond-line drawing is 4 minus the number of bonds drawn to that carbon (counting a double bond as 2 and a triple bond as 3).

Carbon in the drawing	Bonds drawn	Implied H	Type
Line end (one line)	1	3	CH_3
Simple vertex (two lines)	2	2	CH_2
Branch point (three lines)	3	1	CH
Four lines meet	4	0	Quaternary C
Vertex with one single + one double bond	3	1	=CH–
End of a triple bond	3	1	≡CH

Worked Example — From Condensed to Molecular Formula

Condensed formula: $(CH_3)_2CHCH_2C(O)CH_3$ (4-methylpentan-2-one).

- Expand the groups: two CH_3 groups on a CH, then CH_2, then a carbonyl carbon C(O), then CH_3.
- Count carbons: 2 + 1 + 1 + 1 + 1 = 6. Hydrogens: 6 + 1 + 2 + 0 + 3 = 12. Oxygens: 1.
- Molecular formula: $C_6H_{12}O$. In the bond-line drawing the carbonyl carbon is a vertex with a double bond to a written O and no hydrogens.

Showing Three Dimensions: Wedges and Dashes

A plain line is a bond in the plane of the page. A solid wedge points toward the viewer; a hashed (dashed) wedge points away. A tetrahedral carbon is conventionally drawn with two plain lines, one wedge, and one dash. These conventions are formalised in the IUPAC recommendations for graphical representation of stereochemistry (Brecher, 2006) and are essential for the stereochemistry guide.

Common errors in bond-line drawings: a carbon drawn with five lines; a heteroatom written without its hydrogens (writing O instead of OH at a chain end changes the molecule); and drawing a straight line through a triple bond but forgetting that the two attached carbons are also part of that straight line.

7. Molecular Formulas and Degrees of Unsaturation

A saturated acyclic hydrocarbon has the formula C_nH_{2n+2}. Every ring or π bond removes two hydrogens from that maximum. The degree of unsaturation (also called the index of hydrogen deficiency, IHD) counts how many rings plus π bonds a formula must contain. It is the first thing to calculate when you are given an unknown in a spectroscopy problem.

Degrees of unsaturation = (2C + 2 + N − H − X) ÷ 2, where C = carbons, N = nitrogens, H = hydrogens, X = halogens. Oxygen and sulfur are ignored.

Why the Formula Works

- Each **halogen** replaces one hydrogen (one bond), so it counts like H.
- Each **nitrogen** forms three bonds and so carries one extra hydrogen compared with carbon's chain; adding N corrects for it.
- **Oxygen and sulfur** insert into a chain with two bonds and change the hydrogen count by zero, so they are ignored.

What Each Degree Can Mean

Structural feature	Degrees of unsaturation
One ring	1
One C=C or C=O double bond	1
One C≡C or C≡N triple bond	2
One benzene ring (ring + 3 C=C)	4

Worked Examples

Formula	Calculation	Degrees	One possible structure
C_6H_{12}	(12 + 2 − 12) / 2	1	Cyclohexane or a hexene
C_4H_6	(8 + 2 − 6) / 2	2	But-1-yne, buta-1,3-diene, or cyclobutene
C_6H_6	(12 + 2 − 6) / 2	4	Benzene
C_3H_5Cl	(6 + 2 − 5 − 1) / 2	1	3-Chloroprop-1-ene (allyl chloride)
C_5H_5N	(10 + 2 + 1 − 5) / 2	4	Pyridine
C_7H_6O	(14 + 2 − 6) / 2	5	Benzaldehyde (ring 4 + C=O 1)

A degree of unsaturation of 4 or more in a formula with six or more carbons should make you think "benzene ring" first. This is one of the most useful pattern-recognition rules for structure determination.

Quick Recap

Concept	Key fact
Orbital filling	Aufbau (lowest first), Pauli (2 e^{-}, opposite spin), Hund (spread out before pairing)
Valence electrons	Equal to the A-group number: C 4, N 5, O 6, halogens 7
Octet rule	C, N, O, F reach 8 electrons and never exceed it; H reaches 2
Neutral patterns	C: 4 bonds/0 LP; N: 3/1; O: 2/2; X: 1/3
Formal charge	V − lone-pair electrons − bonds; sum equals the overall charge
Bond-line H count	4 minus bonds drawn to that carbon
Degrees of unsaturation	(2C + 2 + N − H − X) / 2; each ring or π bond = 1, triple bond = 2

- Count valence electrons first, including charges, before drawing any Lewis structure
- Check every C, N, and O for an octet, never more than eight
- Show lone pairs on heteroatoms; they are the reactive electrons
- Use the pattern table to assign formal charge at a glance
- Calculate degrees of unsaturation before guessing any structure from a formula
- Do not give carbon five bonds or nitrogen four bonds plus a lone pair
- Do not omit H on heteroatoms in bond-line drawings (O versus OH)
- Do not treat formal charge as the true charge distribution

References & Further Reading

- Lewis, G. N. The Atom and the Molecule. J. Am. Chem. Soc. 1916, 38 (4), 762–785. DOI: 10.1021/ja02261a002 (origin of the electron-pair bond and the octet picture)
- Klein, D. R. Organic Chemistry, 4th ed.; Wiley, 2021. Chapter 1 (Electrons, Bonds, and Molecular Properties).
- Clayden, J.; Greeves, N.; Warren, S. Organic Chemistry, 2nd ed.; Oxford University Press, 2012. Chapters 2 and 4.
- Wade, L. G.; Simek, J. W. Organic Chemistry, 9th ed.; Pearson, 2017. Chapters 1 and 2.
- McMurry, J. Organic Chemistry, 9th ed.; Cengage Learning, 2016. Chapter 1.
- Brecher, J. Graphical Representation of Stereochemical Configuration (IUPAC Recommendations 2006). Pure Appl. Chem. 2006, 78 (10), 1897–1970. DOI: 10.1351/pac200678101897 (wedge and dash conventions)
- Chemistry LibreTexts: Lewis Structures and Formal Charge. https://chem.libretexts.org
- Chemistry LibreTexts: Degree of Unsaturation. https://chem.libretexts.org