

Topic 1.5: Atomic Structure and Electron Configuration

Revision Notes · AP Chemistry

UNIT 1 · ATOMIC STRUCTURE AND PROPERTIES

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Shells, Subshells and Orbitals

The electrons in an atom occupy orbitals, and each orbital holds at most two electrons. Orbitals are grouped into subshells, and subshells into shells labelled by the principal quantum number $n = 1, 2, 3$ and so on.

Each shell contains subshells of the types s, p, d and f, appearing in that order as n increases. Shell 1 has only an s subshell. Shell 2 adds p, shell 3 adds d, and shell 4 adds f.

Capacities. An s subshell has 1 orbital and holds 2 electrons. A p subshell has 3 orbitals and holds 6. A d subshell has 5 orbitals and holds 10. An f subshell has 7 orbitals and holds 14.

An electron configuration is the written record of how the electrons are distributed: $1s^2 2s^2 2p^4$ means two electrons in the 1s orbital, two in 2s, and four spread across the 2p subshell. The superscripts always add up to the total number of electrons.

The Three Filling Rules

Aufbau principle. Electrons fill the lowest energy orbitals first. The filling order is 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p. The one surprise is 4s before 3d: the 4s subshell is lower in energy than 3d when empty, so it fills first.

Pauli exclusion principle. An orbital holds at most two electrons, and they must have opposite spins. In an orbital diagram they are drawn as one up arrow and one down arrow.

Hund's rule. Within a subshell, electrons occupy separate orbitals singly first, all with the same spin, and only pair up when every orbital already holds one. Electrons repel each other, so spreading out is lower in energy than pairing early.

Worked Example: Writing a Configuration

Sulfur has atomic number 16, so a neutral sulfur atom has 16 electrons.

Filling in order: $1s^2$ (2), $2s^2$ (4), $2p^6$ (10), $3s^2$ (12), $3p^4$ (16). The configuration is $1s^2 2s^2 2p^6 3s^2 3p^4$.

Noble gas shorthand. Everything up to the previous noble gas is replaced by its symbol in brackets. Neon is $1s^2 2s^2 2p^6$, so sulfur becomes $[\text{Ne}] 3s^2 3p^4$. The shorthand throws the spotlight on the outer electrons, which are the ones chemistry cares about.

Valence electrons. The valence electrons are those in the outermost shell, the highest n . Sulfur's are the $3s^2$ and $3p^4$ electrons: 6 valence electrons. The rest, the $[\text{Ne}]$ core, are the core electrons. Elements in the same group share the same valence count and the same outer pattern, which is why their chemistry rhymes.

Orbital Diagrams and Unpaired Electrons

An orbital diagram draws each orbital as a box, or a line, and each electron as an arrow. It shows what a written configuration hides: how electrons are spread within a subshell, and how many are unpaired.

Oxygen, $1s^2 2s^2 2p^4$, places its four 2p electrons as one pair and two singles, following Hund's rule. It has 2 unpaired electrons.

Paramagnetic and diamagnetic. A species with one or more unpaired electrons is paramagnetic and is attracted to a magnetic field. A species with all electrons paired is diamagnetic and is not attracted. Zinc, $[\text{Ar}] 4s^2 3d^{10}$, has every electron paired and is diamagnetic; the oxygen atom above is paramagnetic.

To count unpaired electrons, never guess from the configuration's superscripts alone. Spread the last subshell out orbital by orbital, singly first, and count what is left without a partner.

Ions: Adding and Removing Electrons

For anions, add electrons to the neutral atom's configuration, continuing the normal filling order. Cl^- has 18 electrons and the configuration $1s^2 2s^2 2p^6 3s^2 3p^6$, identical to argon.

For cations, remove electrons, but the removal order is not the filling order reversed at random. Electrons leave the subshell with the highest n first. For transition metals that means the ns electrons go before the $(n-1)d$ electrons, even though ns filled first.

Worked example. Iron, $Z = 26$, is $[\text{Ar}] 4s^2 3d^6$. Fe^{2+} loses both 4s electrons: $[\text{Ar}] 3d^6$, with 4 unpaired electrons. Fe^{3+} loses one more, from 3d: $[\text{Ar}] 3d^5$, with 5 unpaired electrons, one in each d orbital.

This is why transition metals commonly form $2+$ ions: the outer s electrons are the exposed ones, and they leave first.

The Chromium and Copper Exceptions

Two first row transition metals break the expected pattern, and the AP syllabus expects you to know both.

Chromium, $Z = 24$, is expected to be $[\text{Ar}] 4s^2 3d^4$ but is actually $[\text{Ar}] 4s^1 3d^5$. Copper, $Z = 29$, is expected to be $[\text{Ar}] 4s^2 3d^9$ but is actually $[\text{Ar}] 4s^1 3d^{10}$.

In each case one 4s electron is promoted into 3d, because a half filled ($3d^5$) or completely filled ($3d^{10}$) subshell is especially stable. Learn the two configurations directly; do not try to extend the pattern to their neighbours, which behave normally.

Traps That Cost Marks in Topic 1.5

Removing 3d electrons before 4s in cations. Filling order is not removal order. Fe^{2+} is $[\text{Ar}] 3d^6$, not $[\text{Ar}] 4s^2 3d^4$. Highest n leaves first, always.

Counting d electrons as valence for main group behaviour, or ignoring the shell. Valence electrons sit in the highest n shell. For selenium, $[\text{Ar}] 4s^2 3d^{10} 4p^4$, the valence count is 6 (the 4s and 4p electrons), not 16.

Pairing electrons too early in a subshell. A $2p^4$ subshell drawn as two pairs and an empty orbital violates Hund's rule. Singles first, in every orbital, then pair.

Superscripts that do not add up. Before anything else, sum the superscripts and compare with the electron count: atomic number for a neutral atom, adjusted for the charge on an ion. Most configuration errors are caught by this ten second check.

Writing configurations in strict n order. Configurations are conventionally written in filling order, so iron is written $[\text{Ar}] 4s^2 3d^6$, not $[\text{Ar}] 3d^6 4s^2$. Follow the filling order when you write, or a correct answer can be marked wrong.

Forgetting that anions gain into the same pattern. Cl^- is not written by removing anything; it has one more electron than chlorine, filled into 3p to complete the subshell.

Key Relationships to Remember

- Subshell capacities: s = 2, p = 6, d = 10, f = 14 electrons; orbitals hold at most 2 electrons with opposite spins
- Filling order: 1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d 6p (4s fills before 3d)
- Hund's rule: one electron in each orbital of a subshell, spins parallel, before any pairing
- Superscripts in a configuration sum to the total number of electrons
- Valence electrons = electrons in the highest n shell; same group means same valence count and pattern
- Cations: remove electrons from the highest n first (transition metals lose ns before (n-1)d); anions: add electrons in normal filling order
- Unpaired electrons mean paramagnetic; all paired means diamagnetic
- Exceptions: Cr is [Ar] 4s¹ 3d⁵ and Cu is [Ar] 4s¹ 3d¹⁰

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