Structure and Bonding; Acids and Bases

스마트헬스케어학부 의공학전공

임해균 교수

1. Structure and Bonding; Acids and Bases

Origins of Organic Chemistry

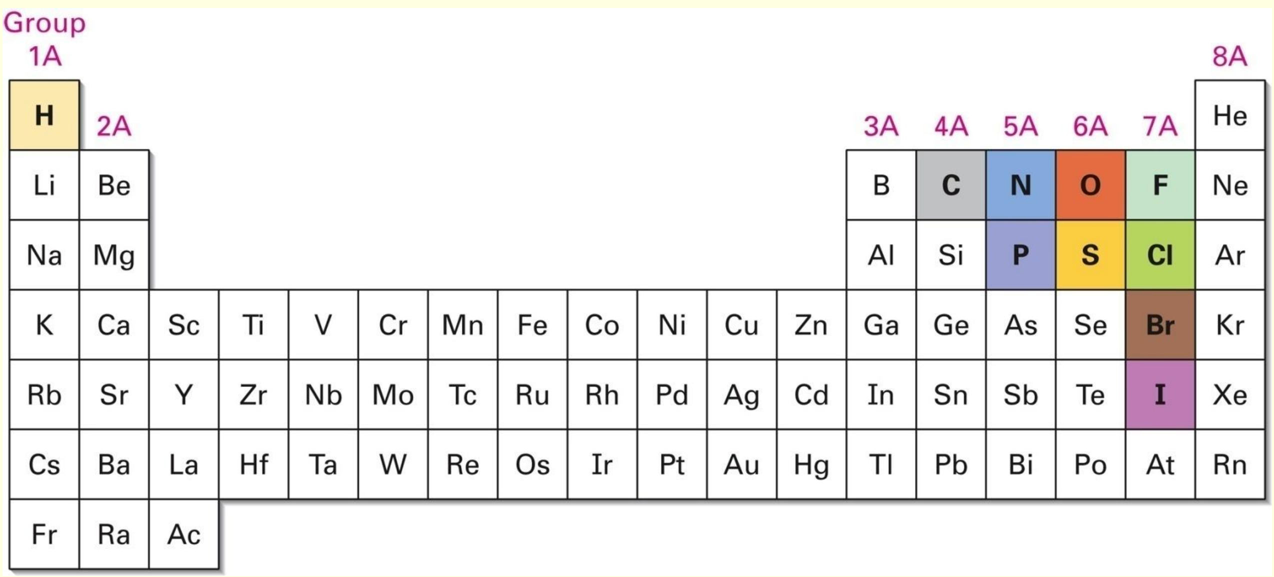
Foundations of organic chemistry from mid-1700’s.

The behavior of the “**organic**” substances isolated from **plants** and **animals** seemed different from that of the “**inorganic**” substances found in **minerals**.

Organic compounds were generally **low-melting** solids and were usually more difficult to isolate, purify, and work with than **high-melting inorganic compounds.**

The only distinguishing characteristic of **organic chemicals** is that all contain the element **carbon**

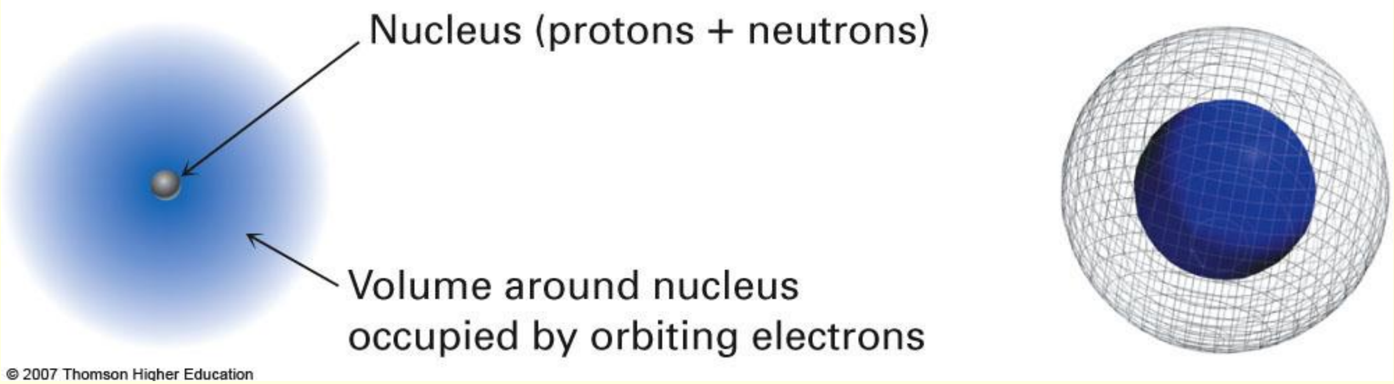
- Organic chemistry is study of carbon compounds.
- Why is it so special?
  - 90% of more than 30 million chemical compounds contain carbon.
  - Examination of carbon in periodic chart answers some of these questions.



Carbon is group 4A element, it can share 4 valence electrons and form 4 covalent bonds

1.1 Atomic Structure

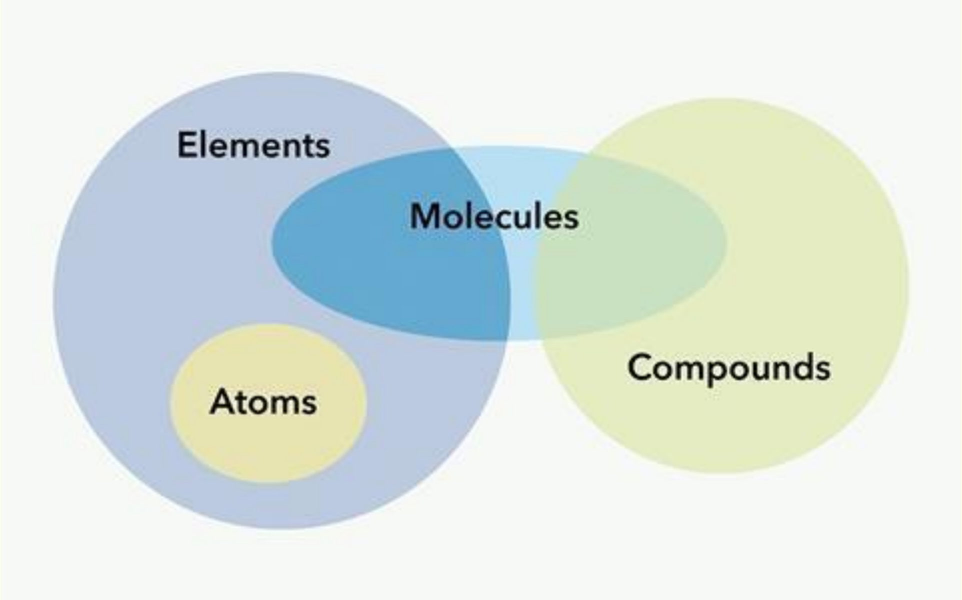
- Structure of an atom
  - **Positively charged *nucleus*** (very dense, protons and neutrons) and small (10^{-15} m)
  - **Negatively charged electrons** are in a cloud (10^{-10} m) around nucleus
- Diameter is about 2×10^{-10} m (200 *picometers* (pm)) [the unit *angstrom* (Å) is 10^{-10} m = 100 pm]

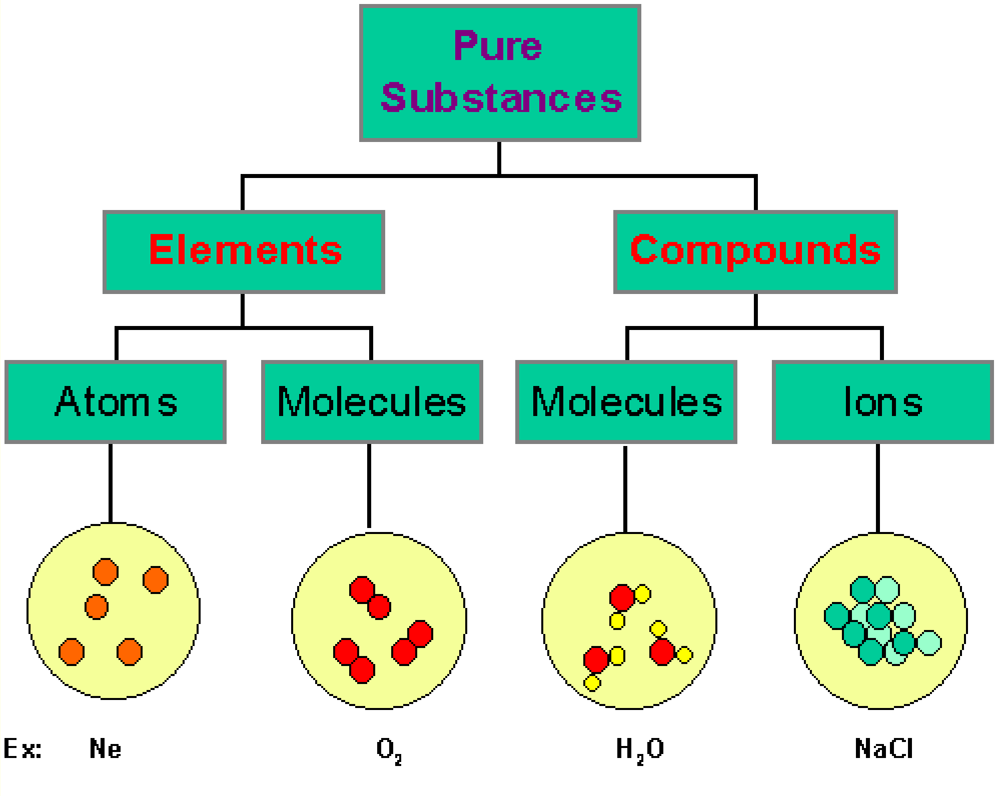


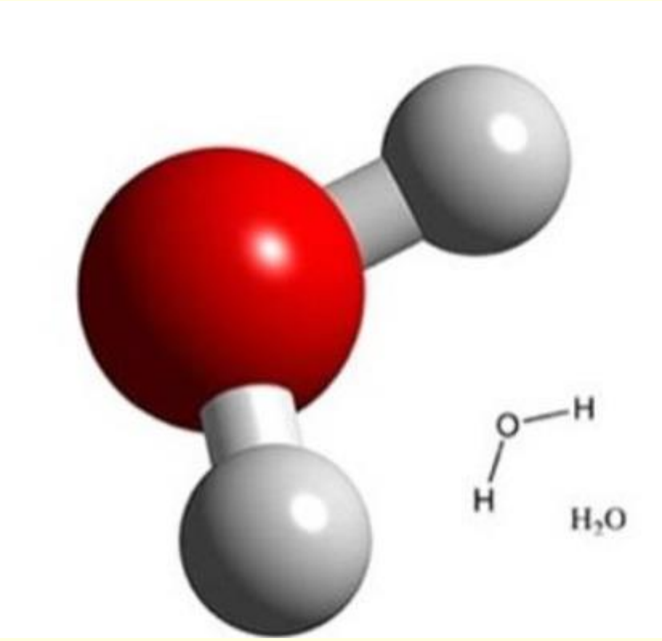
Atomic Number and Atomic Mass

- The *atomic number* (*Z*) is the number of protons in the atom's nucleus
- The *mass number* (*A*) is the number of protons plus neutrons
- All the **atoms** of a given **element** have the same atomic number
- **Isotopes** are **atoms of the same element** that **have different numbers of neutrons and therefore different mass numbers**
- The **atomic mass** (*atomic weight*) of an element is the weighted average mass in atomic mass units (amu) of an element’s naturally occurring **isotopes**

	1	2	3		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
①	Hydrogen 1 **H** 1.008																		Helium 2 **He** 4.0026
②	Lithium 3 **Li** 6.94	Beryllium 4 **Be** 9.0122												Boron 5 **B** 10.81	Carbon 6 **C** 12.011	Nitrogen 7 **N** 14.007	Oxygen 8 **O** 15.999	Fluorine 9 **F** 18.998	Neon 10 **Ne** 20.180
③	Sodium 11 **Na** 22.990	Magnesium 12 **Mg** 24.305												Aluminium 13 **Al** 26.982	Silicon 14 **Si** 28.085	Phosphorus 15 **P** 30.974	Sulfur 16 **S** 32.06	Chlorine 17 **Cl** 35.45	Argon 18 **Ar** 39.948
④	Potassium 19 **K** 39.098	Calcium 20 **Ca** 40.078	Scandium 21 **Sc** 44.956		Titanium 22 **Ti** 47.867	Vanadium 23 **V** 50.942	Chromium 24 **Cr** 51.996	Manganese 25 **Mn** 54.938	Iron 26 **Fe** 55.845	Cobalt 27 **Co** 58.933	Nickel 28 **Ni** 58.693	Copper 29 **Cu** 63.546	Zinc 30 **Zn** 65.38	Gallium 31 **Ga** 69.723	Germanium 32 **Ge** 72.630	Arsenic 33 **As** 74.922	Selenium 34 **Se** 78.971	Bromine 35 **Br** 79.904	Krypton 36 **Kr** 83.798
⑤	Rubidium 37 **Rb** 85.468	Strontium 38 **Sr** 87.62	Yttrium 39 **Y** 88.906		Zirconium 40 **Zr** 91.224	Niobium 41 **Nb** 92.906	Molybdenum 42 **Mo** 95.95	Technetium 43 **Tc** [98]	Ruthenium 44 **Ru** 101.07	Rhodium 45 **Rh** 102.91	Palladium 46 **Pd** 106.42	Silver 47 **Ag** 107.87	Cadmium 48 **Cd** 112.41	Indium 49 **In** 114.82	Tin 50 **Sn** 118.71	Antimony 51 **Sb** 121.76	Tellurium 52 **Te** 127.60	Iodine 53 **I** 126.90	Xenon 54 **Xe** 131.29
⑥	Caesium 55 **Cs** 132.91	Barium 56 **Ba** 137.33	Lanthanum 57 **La** 138.91	*	Hafnium 72 **Hf** 178.49	Tantalum 73 **Ta** 180.95	Tungsten 74 **W** 183.84	Rhenium 75 **Re** 186.21	Osmium 76 **Os** 190.23	Iridium 77 **Ir** 192.22	Platinum 78 **Pt** 195.08	Gold 79 **Au** 196.97	Mercury 80 **Hg** 200.59	Thallium 81 **Tl** 204.38	Lead 82 **Pb** 207.2	Bismuth 83 **Bi** 208.98	Polonium 84 **Po** [209]	Astatine 85 **At** [210]	Radon 86 **Rn** [222]
⑦	Francium 87 **Fr** [223]	Radium 88 **Ra** [226]	Actinium 89 **Ac** [227]	**	Rutherfordium 104 **Rf** [267]	Dubnium 105 **Db** [268]	Seaborgium 106 **Sg** [269]	Bohrium 107 **Bh** [270]	Hassium 108 **Hs** [270]	Meitnerium 109 **Mt** [278]	Darmstadtium 110 **Ds** [281]	Roentgenium 111 **Rg** [282]	Copernicium 112 **Cn** [285]	Nihonium 113 **Nh** [286]	Flerovium 114 **Fl** [289]	Moscovium 115 **Mc** [290]	Livermorium 116 **Lv** [293]	Tennessine 117 **Ts** [294]	Oganesson 118 **Og** [294]
				*	Cerium 58 **Ce** 140.12	Praseodymium 59 **Pr** 140.91	Neodymium 60 **Nd** 144.24	Promethium 61 **Pm** [145]	Samarium 62 **Sm** 150.36	Europium 63 **Eu** 151.96	Gadolinium 64 **Gd** 157.25	Terbium 65 **Tb** 158.93	Dysprosium 66 **Dy** 162.50	Holmium 67 **Ho** 164.93	Erbium 68 **Er** 167.26	Thulium 69 **Tm** 168.93	Ytterbium 70 **Yb** 173.05	Lutetium 71 **Lu** 174.97	
				**	Thorium 90 **Th** 232.04	Protactinium 91 **Pa** 231.04	Uranium 92 **U** 238.03	Neptunium 93 **Np** [237]	Plutonium 94 **Pu** [244]	Americium 95 **Am** [243]	Curium 96 **Cm** [247]	Berkelium 97 **Bk** [247]	Californium 98 **Cf** [251]	Einsteinium 99 **Es** [252]	Fermium 100 **Fm** [257]	Mendelevium 101 **Md** [258]	Nobelium 102 **No** [259]	Lawrencium 103 **Lr** [266]	







H atom : 2
O atom: 1

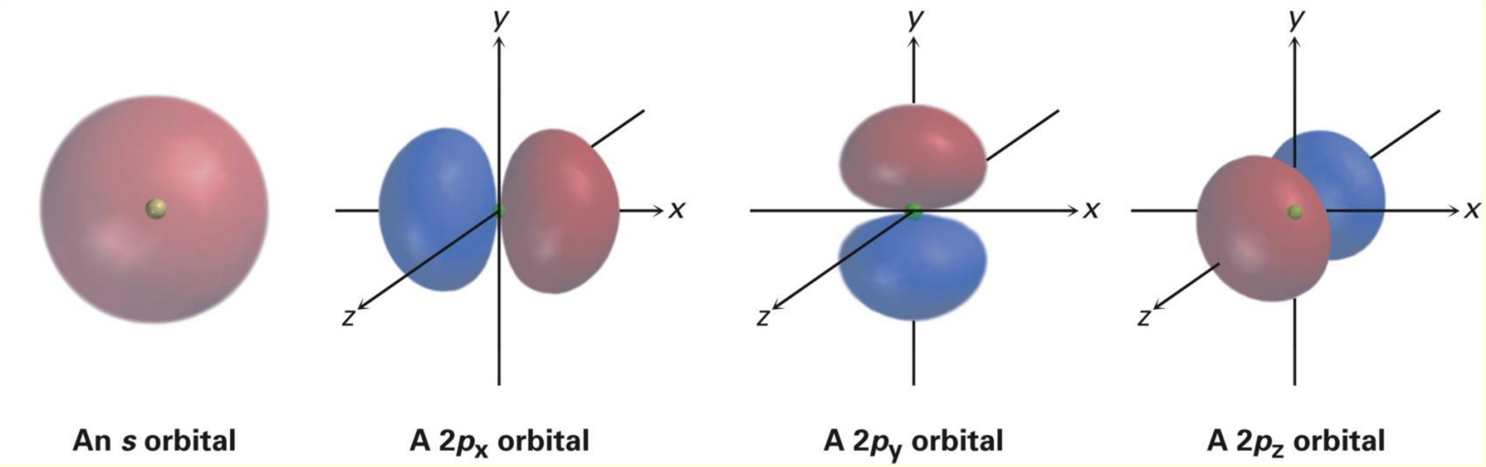
Atomic Structure: Orbitals

- **Quantum mechanics**: describes electron energies and locations by a *wave equation*
  - *Wave function* solution of wave equation
  - Each wave function is an **orbital**,
  - 원자 내의 특정 전자의 행동을 파동 방정식 (wave equation)이라 부르는 수학적 표현으로 기술

- Electron cloud has no specific boundary so we show most probable area

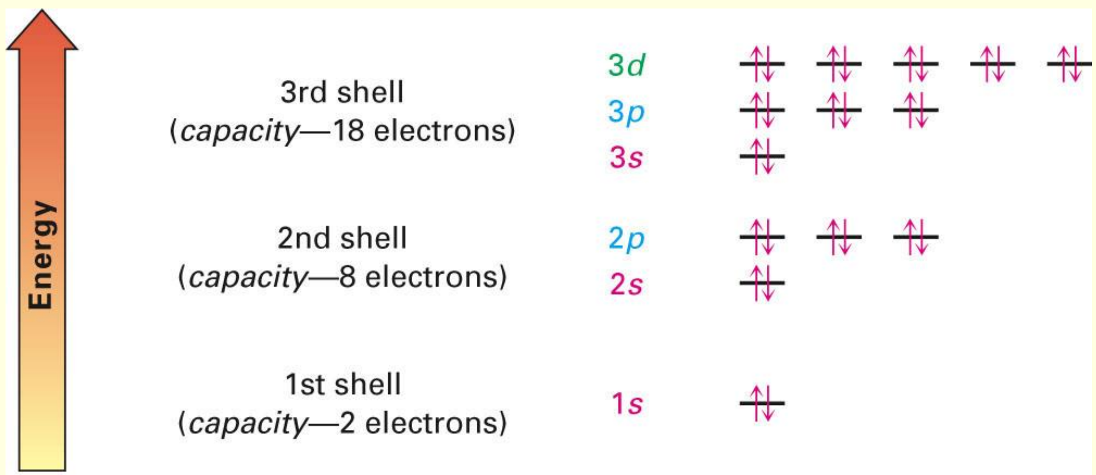
Shapes of Atomic Orbitals for Electrons

- Four different kinds of orbitals for electrons based on those derived for a hydrogen atom
- Denoted *s*, *p*, *d*, and *f*
- *s* and *p* orbitals most important in organic and biological chemistry
- *s* orbitals: spherical, nucleus at center
- *p* orbitals: dumbbell-shaped, nucleus at middle



Orbitals and Shells

- Orbitals are grouped in **shells** of increasing size and energy
- Different shells contain different numbers and kinds of orbitals
- Each orbital can be occupied by two electrons
- First shell contains one *s* orbital, denoted 1*s*, holds only two electrons
- Second shell contains one *s* orbital (2*s*) and three *p* orbitals (2*p*), eight electrons
- Third shell contains an *s* orbital (3*s*), three *p* orbitals (3*p*), and five *d* orbitals (3*d*), 18 electrons

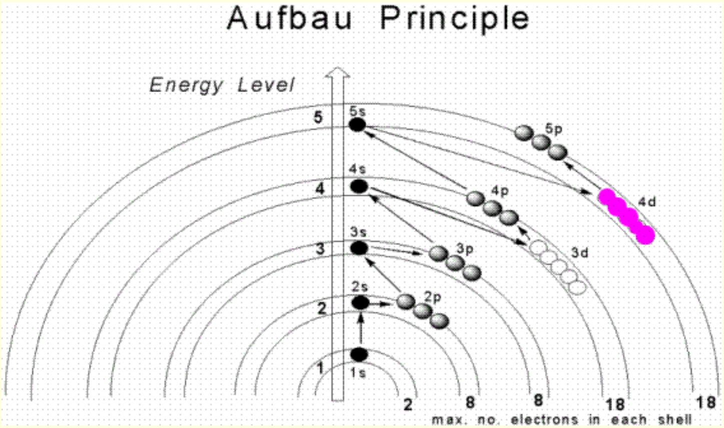


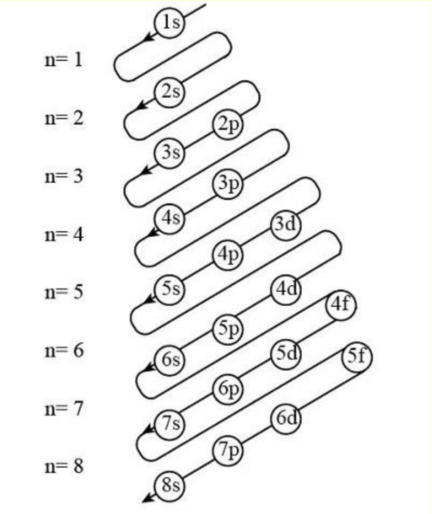
Electron Configuration Chart

s holds up to **2** **p** holds up to **6** **d** holds up to **10**

1.2 Atomic Structure: Electron Configurations

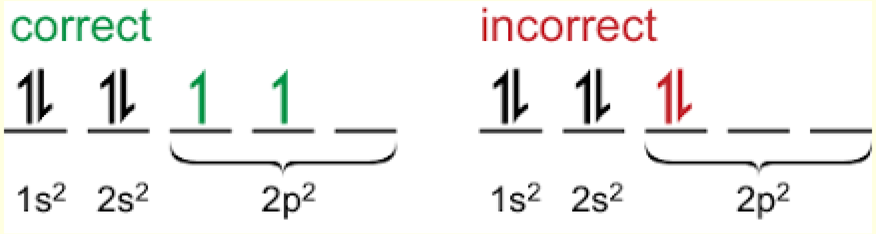
- **Ground-state electron configuration** (lowest energy arrangement) of an atom lists orbitals occupied by its electrons. Rules:
- 1. Lowest-energy orbitals fill first: 1*s* → 2*s* → 2*p* → 3*s* → 3*p* → 4*s* → 3*d* (*Aufbau (*"build-up") principle)
- 2. Electrons act as if they were spinning around an axis. Electron spin can have only two orientations, up ↑ and down ↓. Only two electrons can occupy an orbital, and they must be of opposite spin (*Pauli exclusion principle*) to have unique wave equations
- 3. If two or more empty orbitals of equal energy are available, electrons occupy each with spins parallel until all orbitals have one electron (*Hund's rule*).

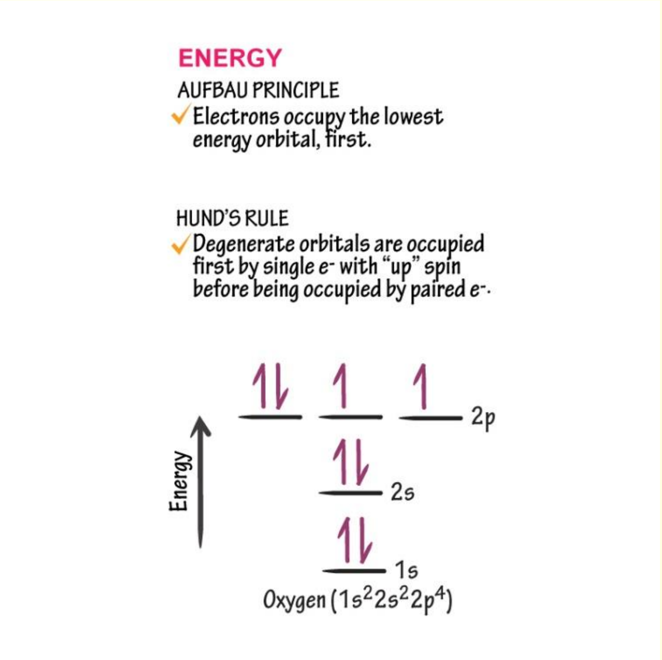




1.2 Atomic Structure: Electron Configurations

- **Ground-state electron configuration** (lowest energy arrangement) of an atom lists orbitals occupied by its electrons. Rules:
- 1. Lowest-energy orbitals fill first: 1*s* → 2*s* → 2*p* → 3*s* → 3*p* → 4*s* → 3*d* (*Aufbau (“*build-up”) principle)
- 2. Electrons act as if they were spinning around an axis. Electron spin can have only two orientations, up ↑ and down ↓. Only two electrons can occupy an orbital, and they must be of opposite spin (*Pauli exclusion principle*) to have unique wave equations
- 3. If two or more empty orbitals of equal energy are available, electrons occupy each with spins parallel until all orbitals have one electron (*Hund's rule*).





1.2 Atomic Structure: Electron Configurations

- **Ground-state electron configuration** (lowest energy arrangement) of an atom lists orbitals occupied by its electrons. Rules:
- 1. Lowest-energy orbitals fill first: 1*s* → 2*s* → 2*p* → 3*s* → 3*p* → 4*s* → 3*d* (*Aufbau (*“build-up”) principle)
- 2. Electrons act as if they were spinning around an axis. Electron spin can have only two orientations, up ↑ and down ↓. Only two electrons can occupy an orbital, and they must be of opposite spin (*Pauli exclusion principle*) to have unique wave equations
- 3. If two or more empty orbitals of equal energy are available, electrons occupy each with spins parallel until all orbitals have one electron (*Hund's rule*).

Table 1.1 Ground-State Electron Configuration of Some Elements

Element	Atomic number	Configuration		Element	Atomic number	Configuration	
Hydrogen	1	1*s*	↑	Phosphorus	15	3*p*	↑ ↑ ↑
Carbon	6	2*p*	↑ ↑ —			3*s*	↑↓
		2*s*	↑↓			2*p*	↑↓ ↑↓ ↑↓
		1*s*	↑↓			2*s*	↑↓
						1*s*	↑↓

Worked Example 1.1

Assigning an Electron Configuration to an Element

Give the ground-state electron configuration of nitrogen.

Worked Example 1.1

Assigning an Electron Configuration to an Element

Give the ground-state electron configuration of nitrogen.

Strategy Find the atomic number of nitrogen to see how many electrons it has, and then apply the three rules to assign electrons into orbitals according to the energy levels given in Figure 1.4.

Solution Nitrogen has atomic number 7 and thus has seven electrons. The first two electrons go into the lowest-energy orbital ($1s^2$), the next two go into the second-lowest-energy orbital ($2s^2$), and the remaining three go into the next-lowest-energy orbitals ($2p^3$), with one electron in each. Thus, the configuration of nitrogen is $1s^2\ 2s^2\ 2p^3$.