

Basic Chemical Concepts and Tables

Second Edition

20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	
38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.91	46 Pd Palladium 106.42	47 Ag Silver 107.87	
56 Ba Barium 137.33	57-71 Lanthanides		72 Hf Hafnium 178.49	73 Ta Tantalum 180.95	74 W Tungsten 183.84	75 Re Rhenium 186.21	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.08	79 Au Gold 196.97
88 Ra Radium	89-103 Actinides		104 Rf Rutherfordium (267)	105 Db Dubnium (268)	106 Sg Seaborgium (269)	107 Bh Bohrium (270)	108 Hs Hassium (277)	109 Mt Meitnerium (278)	110 Ds Darmstadtium (281)	111 Rg Roentgenium (282)
				59 Nd Neodymium	60 Pm Promethium (145)	61 Sm Samarium 150.36	62 Eu Europium 151.96	63 Gd Gadolinium 157.25	64 Tb Terbium 158.93	65 Bk Berkelium (247)

Steven L. Hoenig

Basic Chemical Concepts and Tables

Fully revised and expanded, the second edition of *Basic Chemical Concepts and Tables* is written as a quick reference to the many different concepts and ideas encountered in chemistry. The volume presents important subjects in a concise format that makes it a practical resource for any reader.

Subjects include general chemistry, inorganic chemistry, organic chemistry, and spectral analysis. The new edition includes updated tables that are useful for the interpretation of ultraviolet-visible (UV-Vis), infrared (IR), nuclear magnetic resonance (NMR) and mass spectroscopy (MS) spectra, and expanded sections devoted to the concept of isomers and polymer structures and includes a new chapter on nuclear chemistry. Separate chapters offer physical constants and unit measurements commonly encountered and mathematical concepts needed when reviewing or working with basic chemistry concepts.

Key features:

- Provides chemical information in a concise format, fully illustrated with many graphs and charts, ideal for course review.
- Supplements traditional exam review books, serving undergraduate or graduate students.
- Provides professionals looking for a quick introduction to a topic with a comprehensive ready reference.

Graduate and undergraduate chemistry students, professionals or instructors looking to refresh their understanding of a chemistry topic will find this reference indispensable in their daily work.

Steven L. Hoenig is an instructor at American Public University, where he teaches online Introductory Chemistry classes for non-chemistry majors. He has taught at several universities in which his teaching experience includes both the traditional classroom setting and online courses. He received his Master of Science degree in Chemistry from Long Island University and a Bachelor of Science degree in Chemistry from Polytechnic University. He also recently was an advisor and mentor to scientists in Afghanistan learning the latest analytical techniques. In addition to teaching chemistry, he has also developed a two-semester chemistry course curriculum for a community college. In addition to his current publication, he is also the author of *Basic Training in Chemistry*, *Handbook of Chemical Warfare and Terrorism* and *Compendium of Chemical Warfare Agents*. He is currently a member of the American Chemical Society and a member of the Chemistry and the Law Division and has been listed in Marquis Who's Who on several occasions.



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Second Edition

Steven L. Hoenig
American Public University



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Preface

The second edition of this book's goal still remains as a quick reference to the many different concepts and ideas encountered in chemistry. Most books these days go into a detailed explanation of one subject and go no further. This is simply an attempt to present briefly some of the various subjects that make up the whole of chemistry. The different subjects covered include general chemistry, inorganic chemistry, organic chemistry, spectral analysis, nuclear chemistry, and some mathematical concepts. The material is brief, but hopefully detailed enough to be of use. Keep in mind that the material is written for a reader who is familiar with the subject of chemistry. It has been the author's intention to present in one ready source several disciplines that are used and referred to often.

This book was written not to be a chemistry text unto itself, but rather as a supplement that can be used repeatedly throughout a course of study and thereafter. This does not preclude it from being used by professionals in academia or the chemical industry as a reference source as well.

Having kept this in mind during its preparation, the material is presented in a manner in which the reader should have some knowledge of the material. Only the basics are stated because a detailed explanation was not the goal but rather to present a number of chemical concepts in one source.

The first chapter has been revised to include an expansion in the different chemical bonding theories to include the Lewis Bonding Theory, Valence Bond Theory, and Molecular Orbital Theory. Intermolecular forces are covered as well. Reaction classes and activity series are now located in chapter one. An explanation of chemical formulas and equations has been added as well. The chapter deals with material that is commonly covered in almost every first-year general chemistry course. The concepts are presented in, I hope, a clear and concise manner. No detailed explanation of the origin of the material or problems is presented. Only that which is needed to understand the concept is stated. If more detailed explanation is needed any general chemistry text would suffice. And if examples are of use, any review book could be used.

The second chapter covers inorganic chemistry. Those most commonly encountered concepts are presented, such as, coordination numbers, crystal systems, and ionic crystals. A more detailed explanation of the coordination encountered in bonding of inorganic compounds requires a deeper explanation than this book was intended for.

Chapter 3 consists mostly of organic reactions listed according to their preparation and reactions. The mechanisms of the various reactions are not discussed since there are numerous texts which are devoted to the subject. A section is devoted to the concept of isomers since any treatment of organic chemistry must include an understanding of it. The section on polymer has been expanded to include the different types of polymerizations, structures, molecular forces, and a section on terminology also has been added.

Chapter 4 covers basic nomenclature. It is meant to give the reader a basic idea of how compounds are named and how it relates to the structure. Inorganic nomenclature has been totally revised and is more detailed.

Chapter 5 is intended to present an outline of how wet chemical analysis is done and not a guide for the laboratory.

The sixth chapter covers instrumental analysis. No attempt is made to explain the inner workings of the different instruments or the mechanisms by which various spectra are produced. The material listed is for use by those that are familiar with the different type of spectra encountered in the instrumental analysis of chemical compounds. The tables and charts would be useful for the interpretation of various spectra generated in the course of analyzing a chemical substance. Listed are tables that would be useful for the interpretation of ultraviolet-visible (UV-Vis), infrared (IR), nuclear magnetic resonance (NMR), and mass spectroscopy (MS) spectra.

Chapter 7 now deals with the fundamentals of nuclear chemistry such as radioactivity, types of radiation, half-life, fission, and fusion.

Chapter 8 now consists of physical constants and unit measurements that are commonly encountered throughout the application of chemistry.

Chapter 9 contains certain mathematical concepts that are useful to have when reviewing or working with certain concepts encountered in chemistry. Use of significant figures and their mathematical operations has been added.

An additional appendix, Appendix C, has been added and contains common NMR solvent spectra.

Steven L. Hoenig



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I wish to express my thanks to my oldest and dearest friend Richard Kolodkin, whose friendship has stood the test of time and distance.



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General Chemistry

1

1.1 MATTER

1.1.1 CLASSES OF MATTER

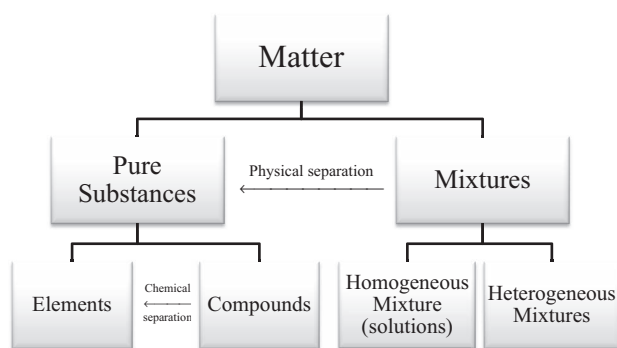


FIGURE 1.1 Organization of Matter.

Matter can exist in different types of forms and can be classified into several distinct categories. Matter can exist either as:

A **pure substance** is a sample of matter that cannot be separated into simpler components without chemical change. Physical changes can alter the state of matter but not the chemical identity of a pure substance. Pure substances have fixed, characteristic elemental compositions and properties. There are two types of pure substances, elements, and compounds. Elements are not chemically decomposable into other elements, and their properties do not vary. Compounds are elements combined chemically in law of definite proportions and their properties do not vary.

A **compound** is a material formed from elements chemically combined in definite proportions by mass. For example, water is formed from chemically bound hydrogen and oxygen. Any pure water sample contains 2 g of hydrogen for every 16 g of oxygen.

An **element** is a substance composed of atoms with identical atomic number. The older definition of element (*an element is a pure substance that can't be decomposed chemically*) was made obsolete by the discovery of isotopes.

When one substance is mixed with another, two types of mixtures are formed—homogeneous and heterogeneous mixtures.

A **homogeneous mixture** is a sample of matter consisting of more than one pure substance with properties that do not vary within the sample. The components are uniformly mixed and have one phase and can also be called a solution.

A **heterogeneous mixture** is a sample of matter consisting of more than one pure substance and more than one phase. Blood, protoplasm, milk, chocolate, smoke, and chicken soup are examples of heterogeneous mixtures. The components are not uniformly mixed and can have more than one phase.

1.1.2 PROPERTIES OF MATTER

Extensive property: A property that changes when the amount of matter in a sample changes. Examples are mass, volume, length, and charge.

Intensive property: A property that does not change when the amount of sample changes. Examples are density, pressure, temperature, and color.

Chemical property: Measurement of a chemical property involves a chemical change. For example, determining the flammability of gasoline involves burning it, producing carbon dioxide and water.

Physical property: Measurement of a physical property may change the arrangement but not the structure of the molecules of a material. Examples of physical properties are density, color, boiling point, volume, temperature, and mass.

1.1.3 STATES OF MATTER

Matter can exist in:

Gas: Matter in a form that has low density, is easily compressible and expandable, and expands spontaneously when placed in a larger container. Molecules in a gas move freely and are relatively far apart. “Vapor” often refers to a gas made of a substance that is usually encountered as a liquid or solid; for example, gaseous H_2O is called “water vapor”.

Liquid: A state of matter that has a high density and is incompressible compared to a gas. Liquids take the shape of their container but do not expand to fill the container as gases do. Liquids diffuse much more slowly than gases.

Solid: A solid is a relatively dense, rigid state of matter, with a definite volume and shape. Molecules in solids are often packed close together in regularly repeating patterns and vibrate around fixed positions.

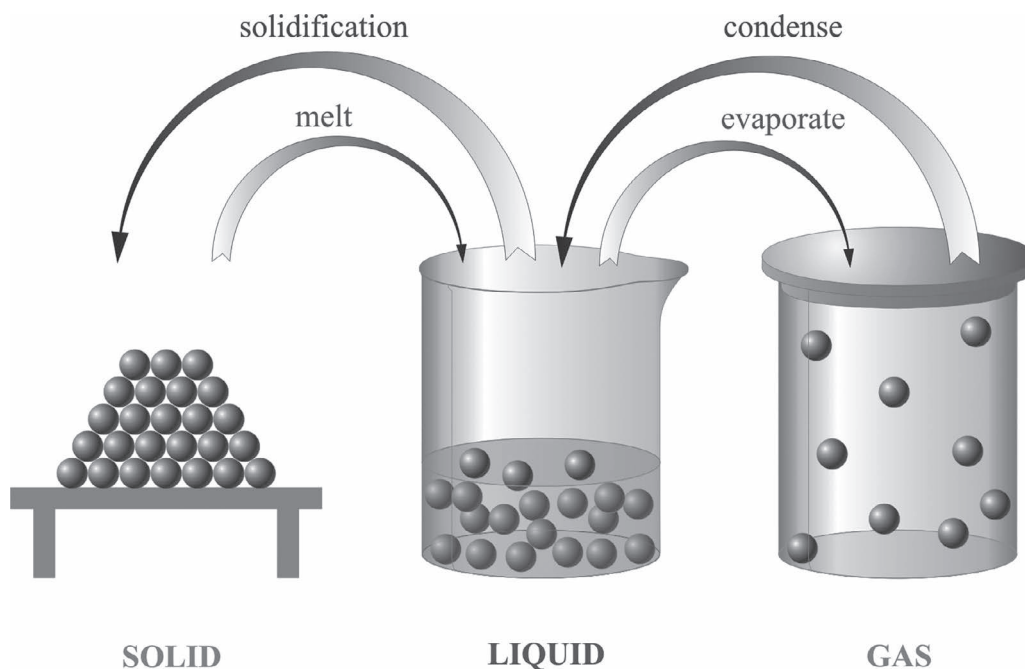


FIGURE 1.2 States of Matter, Generalic, Eni. <https://glossary.periodni.com/glossary.php?en=states+of+matter>.

1.1.4 LAW OF CONSERVATION OF MASS

The Law of Conservation of Mass is the law that states that in a chemical reaction the total mass of the products is equal to the total mass of the reactants.

1.1.5 LAW OF DEFINITE PROPORTIONS

The Law of Definite Proportions is the law that states that every chemical compound contains fixed and constant proportions (by weight) of its constituent elements.

1.1.6 LAW OF MULTIPLE PROPORTIONS

A law proposed by Dalton, which states that when elements combine, they do so in the ratio of small whole numbers. For example, carbon and oxygen react to form CO or CO₂, but not CO_{1.8}.

1.2 ATOMIC STRUCTURE

1.2.1 CONSTITUENTS OF THE ATOM

The atom of any element consists of three basic types of particles . . . the electron (a negatively charged particle), the proton (a positively charged particle), and the neutron (a neutrally charged particle). The protons and neutrons occupy the nucleus while the electrons are outside of the nucleus. The protons and neutrons contribute very little to the total volume but account for the majority of the atom's mass. However, the atom's volume is determined by the electrons, which contribute very little to the mass. Table 1.1 summarizes the properties of these three particles.

TABLE 1.1 Properties of the Proton, Electron, and Neutron

Particle	Symbol	Mass	Unit mass	Electric charge	Unit charge
Proton	p ⁺	1.672×10^{-24} g	1	$+1.602 \times 10^{-19}$ coulomb	+1
Electron	e ⁻	9.108×10^{-28} g	1/1837	-1.602×10^{-19} coulomb	-1
Neutron	n	1.675×10^{-24} g	1	0	0

The **atomic number** (*Z*) of an element is the number of protons within the nucleus of an atom of that element. In a neutral atom, the number of protons and electrons are equal, and the atomic number also indicates the number of electrons.

The **mass number** (*A*) is the sum of the protons and neutrons present in the atom. The number of neutrons can be determined by (*A*−*Z*). The symbol for denoting the atomic number and mass number for an element X is as follows:



Atoms that have the same atomic number (equal number of protons, *Z*) but different atomic masses, *A*, (unequal number of neutrons) are referred to as **isotopes**. For example, hydrogen consists of three isotopes, hydrogen-1, hydrogen-2, and hydrogen-3, also called, respectively, hydrogen, deuterium, and tritium.

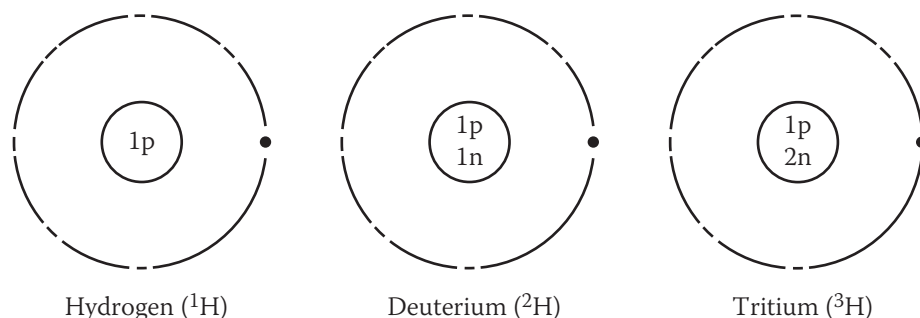


FIGURE 1.3 Isotope of Hydrogen.

1.2.2 ATOMIC MASSES

The **atomic mass unit** (amu) is defined as 1/12 the mass of an atom of carbon-12 isotope. The relative **atomic mass** of an element is the weighted average of all the isotopes relative to 1/12 of the carbon-12 isotope.

For example, the atomic mass of neon is 20.17 amu and is calculated from the following data: neon-19 (amu of 19.99245, natural abundance of 90.92%), neon-20 (amu of 20.99396, natural abundance of 0.260%), and neon-21 (amu of 21.99139, natural abundance of 8.82%):

$$\text{a.m. neon} = (19.99245 \times 0.9092) + (20.99396 \times 0.00260) + (21.99139 \times 0.0882) = 20.17 \text{ amu}$$

The relative **molecular mass** is the sum of the atomic masses for each atom in the molecule.

$$\text{For } \text{H}_2\text{SO}_4 = (1 \times 2) + 32 + (16 \times 4) = 98.$$

TABLE 1.2 Atomic Masses

Name	Symbol	Z	Atomic Mass	Name	Symbol	Z	Atomic Mass
Actinium	Ac	89	227.0278	Mendelevium	Md	101	(258.10)
Aluminum	Al	13	26.9815	Mercury	Hg	80	200.59
Americium	Am	95	(243.0614)	Molybdenum	Mo	42	95.94
Antimony	Sb	51	121.75	Moscovium	Mc	115	(289)
Argon	Ar	18	39.948	Neodymium	Nd	60	144.24
Arsenic	As	33	74.9216	Neon	Ne	10	20.183
Astatine	At	85	(209.9871)	Neptunium	Np	93	237.0482
Barium	Ba	56	137.34	Nickel	Ni	28	58.71
Berkelium	Bk	97	(247.0703)	Nihonium	Nh	113	(285)
Beryllium	Be	4	9.0122	Niobium	Nb	41	92.906
Bismuth	Bi	83	208.980	Nitrogen	N	7	14.0067
Bohrium	Bh	107	(272)	Nobelium	No	102	(259.1009)
Boron	B	5	10.811	Oganesson	Og	118	(294)
Bromine	Br	35	79.909	Osmium	Os	76	190.2
Cadmium	Cd	20	12.401	Oxygen	O	8	15.9994
Calcium	Ca	98	40.08	Palladium	Pd	46	106.4
Californium	Cf	98	(251.0796)	Phosphorus	P	15	30.9738
Carbon	C	6	12.01115	Platinum	Pt	78	195.09
Cerium	Ce	58	140.12	Plutonium	Pu	94	(244.0642)
Cesium	Cs	55	132.905	Polonium	Po	84	(208.9824)
Chlorine	Cl	17	35.453	Potassium	K	19	39.102
Chromium	Cr	24	51.996	Praseodymium	Pr	59	140.907
Cobalt	Co	27	58.9332	Promethium	Pm	61	(144.9127)
Copernicium	Cn	112	(285)	Protactinium	Pa	91	231.0359
Copper	Cu	29	3.546	Radium	Ra	88	226.0254
Curium	Cm	96	(247.0703)	Radon	Rn	86	(222.0176)
Darmstadtium	Ds	110	(281)	Rhenium	Re	75	186.2
Dubnium	Db	105	(268)	Rhodium	Rh	45	102.905
Dysprosium	Dy	66	162.50	Roentgenium	Rg	111	(280)
Einsteinium	Es	99	(252.083)	Rubidium	Rb	37	85.47
Erbium	Er	68	167.26	Ruthenium	Ru	44	101.07
Europium	Eu	63	151.96	Rutherfordium	Rf	104	(267)

Fermium	Fm	100	(257.0951)	Samarium	Sm	62	150.35
Flerovium	Fl	114	(287)	Scandium	Sc	21	44.956
Fluorine	F	9	18.9984	Seaborgium	Sg	106	(271)
Francium	Fr	87	(223.0197)	Selenium	Se	34	78.96
Gadolinium	Gd	64	157.25	Silicon	Si	14	28.086
Gallium	Ga	31	69.72	Silver	Ag	47	107.870
Germanium	Ge	32	72.59	Sodium	Na	11	22.9898
Gold	Au	79	196.967	Strontium	Sr	38	87.62
Hafnium	Hf	72	178.49	Sulfur	S	16	32.064
Hassium	Hs	108	(277)	Tantalum	Ta	73	180.948
Helium	He	2	4.0026	Technetium	Tc	43	98.906
Holmium	Ho	67	164.930	Tellurium	Te	52	127.60
Hydrogen	H	1	1.00797	Tennessee	Ts	117	(294)
Indium	In	49	114.82	Terbium	Tb	65	158.924
Iodine	I	53	126.9044	Thallium	Tl	81	204.37
Iridium	Ir	77	192.2	Thorium	Th	90	232.038
Iron	Fe	26	55.847	Thulium	Tm	69	168.934
Krypton	Kr	36	83.80	Tin	Sn	50	118.69
Lanthanum	La	57	138.905	Titanium	Ti	22	47.88
Lawrencium	Lr	103	(262.11)	Tungsten	W	74	183.85
Lead	Pb	82	207.19	Uranium	U	92	238.03
Lithium	Li	3	6.941	Vanadium	V	23	50.942
Livermorium	Lv	116	(291)	Xenon	Xe	54	131.30
Lutetium	Lu	71	174.97	Ytterbium	Yb	70	173.04
Magnesium	Mg	12	24.305	Yttrium	Y	39	88.905
Manganese	Mn	25	54.9380	Zinc	Zn	30	65.37
Meitnerium	Mt	109	(276)	Zirconium	Zr	40	91.22

1.2.3 THE MOLE

The **mole** (mol) is simply a unit of quantity, it represents a certain amount of material, that is, atoms or molecules. The numerical value of one mole is 6.023×10^{23} and is referred to as **Avogadro's number**. Avogadro's number is derived from his Avogadro's Hypothesis which eventually became Avogadro's Law.

Avogadro's Hypothesis states that two equal volumes of gas, at the same temperature and pressure, contain the same number of molecules.

Avogadro's Law states that at a constant temperature and pressure, the volume of a gas is directly proportional to the number of moles of that gas. Let V_1 and n_1 be a volume and amount of material at the start of an experiment. If the amount is changed to a new value called n_2 , then the volume will change to V_2 . We know this: $V_1 \div n_1 = k$, and we know this: $V_2 \div n_2 = k$.

Since $k = k$, we can conclude that $V_1 \div n_1 = V_2 \div n_2$.

$$\frac{V_1}{n_1} = \frac{V_2}{n_2}$$

The mole is defined as the mass, in grams, equal to the atomic mass of an element or molecule. Therefore, one mole of carbon-12 weighs 12 grams and contains 6.023×10^{23} carbon atoms. The following formula can be used to find the number of moles:

$$\text{moles} = \frac{\text{mass in grams}}{\text{atomic(molecular) mass}}$$

1.2.4 QUANTUM NUMBERS

It has been determined from experimentation that the atom consists of three particles—the proton, the neutron and the electron. It has also been determined that the atom has a center or nucleus that contains the proton and the neutron. As it turns out the nucleus is very small, but it also contains most of the mass of the atom. In fact, for all practical purposes, the mass of the atom is the sum of the masses of the protons and neutrons.

Many of the important topics in chemistry, such as chemical bonding, the shape of molecules, and so on, are based on where the electrons in an atom are located.

To describe how electrons behave in an atom, the quantum mechanical model, a highly mathematical model, is used to represent the structure of the atom. This model is based on *quantum theory*, which says that matter also has properties associated with waves. According to quantum theory, it's impossible to know an electron's exact position and *momentum* (speed and direction, multiplied by mass) at the same time. This is known as the *uncertainty principle*. So, scientists had to develop the concept of *orbitals* (sometimes called *electron clouds*), volumes of space in which an electron is likely present. In other words, certainty was replaced with probability. The quantum mechanical model of the atom uses complex shapes of orbitals. Without resorting to a lot of math, this section shows you some aspects of this model of the atom. Quantum mechanics introduced four numbers, called *quantum numbers*, to describe the characteristics of electrons and their orbitals.

The **principal quantum number**, n , determines the energy of an orbital and has a value of $n = 1, 2, 3, 4, \dots$. The larger the value of n , the higher the energy and the larger the orbital.

The **angular momentum quantum number**, l , determines the “shape” of the orbital and has a value of zero to $(n-1)$ for every value of n . Orbitals that have the same value of n but different values of l are called *subshells*. These subshells are given different letters (see Table 1.3) to help distinguish them from each other.

The **magnetic quantum number**, m_l , determines the orientation of the orbital in space and has a value of $-l$ to $+l$.

The **electron spin quantum number**, m_s , determines the magnetic field generated by the electron and has a value of $-\frac{1}{2}$ or $+\frac{1}{2}$.

Table 1.3 summarizes the quantum number available for the first three energy levels, as well as the number of electrons that are permitted in each energy level and sublevel.

TABLE 1.3 Quantum Numbers and Electron Distribution

Shell	Principal quantum number n	Angular momentum quantum number l	Orbital designation	Magnetic quantum number m_l	Spin quantum number m_s	Total number of electrons per orbital
K	1	0	s	0	$-\frac{1}{2}, +\frac{1}{2}$	2
L	2	1	s	0	$-\frac{1}{2}, +\frac{1}{2}$	2
			p_x	-1	$-\frac{1}{2}, +\frac{1}{2}$	6
			p_y	0	$-\frac{1}{2}, +\frac{1}{2}$	
p_z	+1	$-\frac{1}{2}, +\frac{1}{2}$				
M	3	2	s	0	$-\frac{1}{2}, +\frac{1}{2}$	2
			p_x	-1	$-\frac{1}{2}, +\frac{1}{2}$	6
			p_y	0	$-\frac{1}{2}, +\frac{1}{2}$	
	p_z	+1	$-\frac{1}{2}, +\frac{1}{2}$			
	d_{xy}	-2	$-\frac{1}{2}, +\frac{1}{2}$	10		
	d_{xz}	-1	$-\frac{1}{2}, +\frac{1}{2}$			
	d_{yz}	0	$-\frac{1}{2}, +\frac{1}{2}$			
d_{z^2}	+1	$-\frac{1}{2}, +\frac{1}{2}$				
$d_{x^2-y^2}$	+2	$-\frac{1}{2}, +\frac{1}{2}$				

Table 1.3 also shows that in energy level 1 ($n = 1$), there's only an s orbital. There's no p orbital because an l value of one (p orbital) is not allowed. And notice that there can be only two electrons in that 1s orbital (m_s of $+\frac{1}{2}$ and $-\frac{1}{2}$). In fact, there can be only two electrons in any s orbital, whether it's 1s or 5s.

Each time you move higher in a major energy level, you add another orbital type. So, when you move from energy level one to energy level two ($n = 2$), there can be both s and p orbitals. If you write out the quantum numbers for energy level three, you see s, p, and d orbitals.

There are three subshells (m_l) for the 2p orbital (see Table 1.3) and each holds a maximum of two electrons. The three 2p subshells can hold a maximum of six electrons.

There's an energy difference in the major energy levels (energy level two is higher in energy than energy level one), but there's also a difference in the energies of the different orbitals within an energy level. At energy level two, both s and p orbitals are present. But the 2s is lower in energy than the 2p. The three subshells of the 2p orbital have the same energy.

When placing electrons into orbitals, rather than using quantum numbers a more convenient shorthand representation can be used. There are two common representations for electron distribution. One is the energy level diagram and the other is the electron configuration. Figure 1.4 shows a blank energy diagram that can be used for any particular atom.

Orbitals are represented by dashes in which you can place a maximum of two electrons.

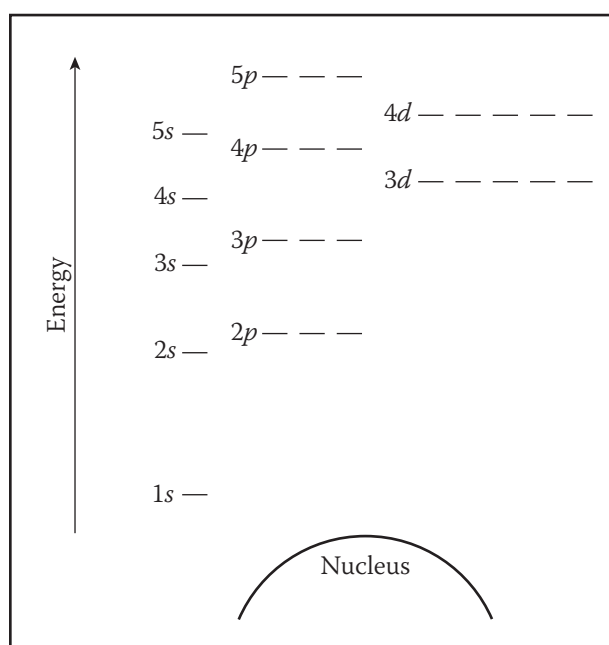


FIGURE 1.4 Energy Level Diagram.

The following is a summary in which the quantum numbers are used to fill the atomic orbitals with electrons:

- No two electrons can have the same four quantum numbers. This is the Pauli exclusion principle.
- Orbitals are filled in the order of increasing energy.
- Each orbital can only be occupied by a maximum of two electrons and must have different spin quantum numbers (opposite spins).
- The most stable arrangement of electrons in orbitals is the one that has the greatest number of equal spin quantum numbers (parallel spins). This is referred to as Hund's rule.

The following diagram (Figure 1.5) shows the completed energy level diagram for oxygen. The arrow notation is used to signify the different spin quantum numbers, m_s , of the electrons in the orbital.

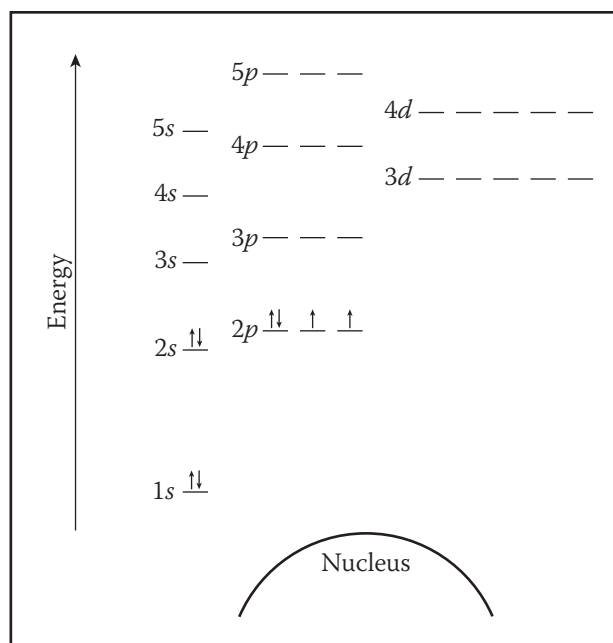


FIGURE 1.5 Energy Level Diagram for Oxygen.

The order that the orbitals get filled does not strictly follow the principal quantum number. The order in which orbitals are filled (the Aufbau principle) is shown in Figure 1.6. Shielding of electrons in one sublevel by electrons in another sublevel accounts for the reason why orbitals are not filled strictly according to the principal quantum number.

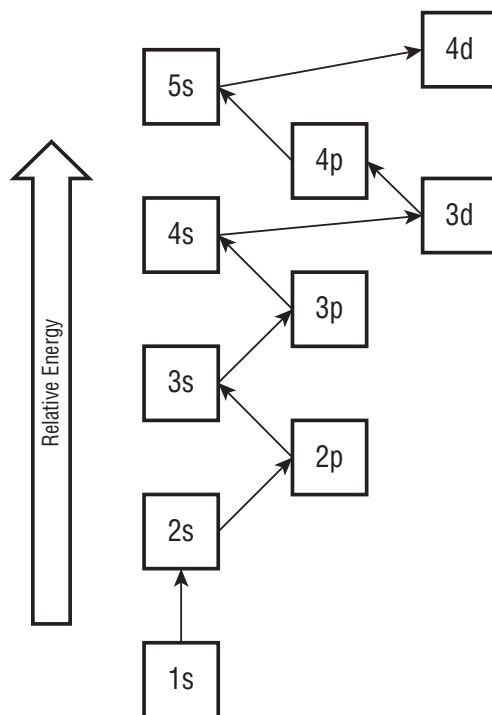


FIGURE 1.6 Filling Order and Relative Energy Levels of Orbitals.

The electron configuration of an atom can be represented in another type of notation. The electron configuration for oxygen is $1s^2 2s^2 2p^4$. Figure 1.7 summarizes the electron notation used.

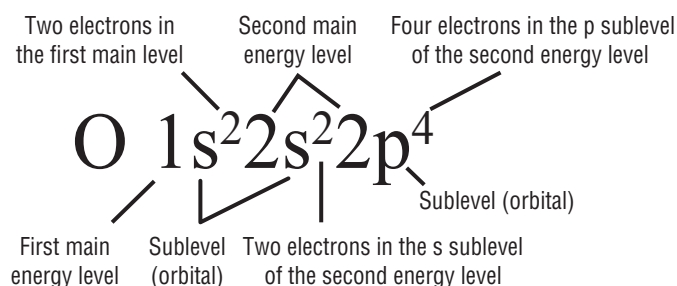


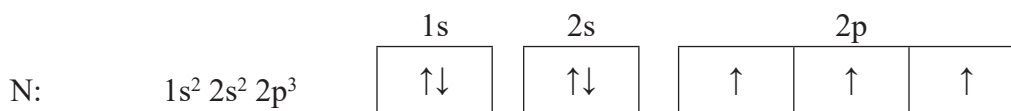
FIGURE 1.7 Electron Configuration for Oxygen.

The ground state orbital configuration for oxygen is $1s^2 2s^2 2p^4$, which can be represented by the following orbital diagram.



Two electrons occupy the 1s orbital, two occupy the 2s orbital, and four occupy the 2p orbitals. Since there are three 2p orbitals with the same energy, the mutually repulsive electrons will occupy separate 2p orbitals. This behavior is summarized by Hund's rule (named for the German physicist F. H. Hund): The lowest energy configuration for an atom is the one having the maximum number of unpaired electrons allowed by the Pauli principle in a particular set of degenerate orbitals. One of the 2p orbitals is now occupied by a pair of electrons with opposite spins, as also required by the Pauli exclusion principle. By convention, the unpaired electrons are represented as having parallel spins (with spin "up").

For nitrogen the three electrons in the 2p orbitals occupy separate orbitals with parallel spins:



For neon the orbitals are completely filled.



1.2.5 ATOMIC ORBITALS

The quantum numbers mentioned earlier were obtained as solutions to a set of wave equations. These wave equations cannot tell precisely where an electron is at any given moment or how fast it is moving. But rather it states the probability of finding the electron at a particular place. An orbital is a region of space where the electron is most likely to be found. An orbital has no definite boundary to it, but can be thought of as a cloud with a specific shape. Also, the orbital is not uniform throughout, but rather densest in the region where the probability of finding the electron is highest.

The shape of an orbital represents 90% of the probability of finding the electron within that space. As the quantum numbers change so do the shapes and direction of the orbitals. Figure 1.8 shows the shapes for principal quantum number $n = 1, 2,$ and $3,$ along with the various sublevels.

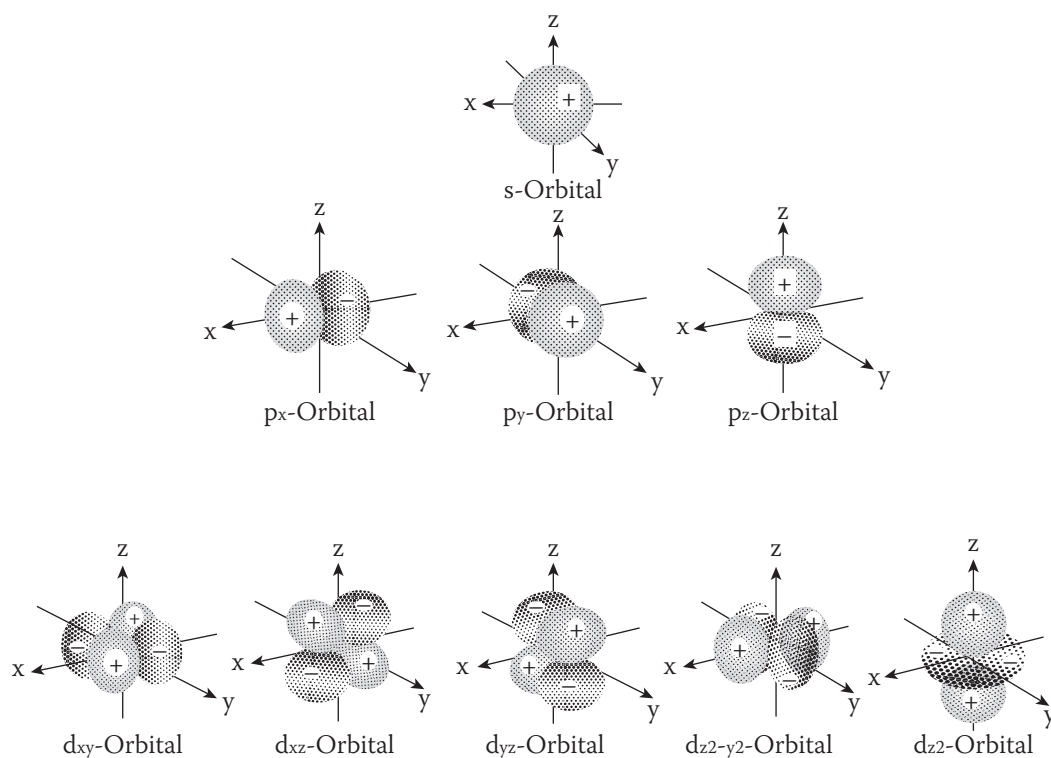


FIGURE 1.8 Representation of Atomic Orbitals.

The s orbital boundary surface is a sphere with the nucleus at its center. The s orbitals are spherically symmetric, which means that the probability of finding an electron at a given distance is the same in all directions. The size of the s orbital is likewise shown to increase as the value of the primary quantum number (n) increases; hence, $4s > 3s > 2s > 1s$. The nodal point is a location where there is no chance of locating the electron.

The p orbitals are formed like dumbbells. The p orbital node is located at the nucleus's center. There are three p orbitals which can occupy a maximum of six electrons. Each p orbital is made up of two parts known as lobes that are located on either side of the plane that runs across the nucleus. The three orbitals are known as degenerate orbitals because they have the same size, shape, and energy. The sole difference between the orbitals is the orientation of the lobes. Because the lobes are orientated along the x -, y -, or z -axis, they are given the names $2p_x$, $2p_y$, and $2p_z$. Similarly to s orbitals, the size and energy of p orbitals rise as the primary quantum number increases ($4p > 3p > 2p$).

For d orbitals, the magnetic orbital quantum number is given as $(-2, -1, 0, 1, 2)$. As a result, we can claim there are five d orbitals. These orbitals are denoted by the symbols d_{xy} , d_{yz} , d_{xz} , $d_{x^2-y^2}$, and d_{z^2} . The forms of the first four d orbitals are similar to each other, which differs from the d_{z^2} orbital, but the energy of all five d orbitals is the same.

1.3 ELECTRON CONFIGURATION AND PERIODIC TRENDS

The electron configurations of atoms play an important role in the physical and chemical properties of the elements and of the compounds that they form. As noted earlier, the electronic configuration follows the Pauli exclusion principle and Aufbau principle when determining the elements electronic configuration. Going across a period, there is a pattern of regular change in these properties from one group to the next. Periodic properties increase or decrease across a period, and then the trend is repeated in each successive period.

Several important properties such as ionization energy, electronegativity, and atomic size are shown.

1.3.1 ELECTRONIC CONFIGURATION OF THE ELEMENTS

TABLE 1.4 Electronic Configuration of the Elements

	Shells	K		L			M			N				O			P			Q
	Sub-Levels	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	5f	6s	6p	6d	6f	7s
1	Hydrogen	1																		
2	Helium	2																		
3	Lithium	2	1																	
4	Beryllium	2	2																	
5	Boron	2	2	1																
6	Carbon	2	2	2																
7	Nitrogen	2	2	3																
8	Oxygen	2	2	4																
9	Fluorine	2	2	5																
10	Neon	2	2	6																
11	Sodium	2	2	6	1															
12	Magnesium	2	2	6	2															
13	Aluminum	2	2	6	2	1														
14	Silicon	2	2	6	2	2														
15	Phosphorus	2	2	6	2	3														
16	Sulfur	2	2	6	2	4														
17	Chlorine	2	2	6	2	5														
18	Argon	2	2	6	2	6														
19	Potassium	2	2	6	2	6				1										
20	Calcium	2	2	6	2	6				2										
21	Scandium	2	2	6	2	6	1		2											
22	Titanium	2	2	6	2	6	2		2											
23	Vanadium	2	2	6	2	6	3		2											
24	Chromium	2	2	6	2	6	5		1											
25	Manganese	2	2	6	2	6	5		2											
26	Iron	2	2	6	2	6	6		2											
27	Cobalt	2	2	6	2	6	7		2											
28	Nickel	2	2	6	2	6	8		2											
29	Copper	2	2	6	2	6	10		1											
30	Zinc	2	2	6	2	6	10		2											
31	Gallium	2	2	6	2	6	10	2	1											
32	Germanium	2	2	6	2	6	10	2	2											
33	Arsenic	2	2	6	2	6	10	2	3											
34	Selenium	2	2	6	2	6	10	2	4											
35	Bromine	2	2	6	2	6	10	2	5											
36	Krypton	2	2	6	2	6	10	2	6											
37	Rubidium	2	2	6	2	6	10	2	6				1							
38	Strontium	2	2	6	2	6	10	2	6				2							
39	Yttrium	2	2	6	2	6	10	2	6	1			2							
40	Zirconium	2	2	6	2	6	10	2	6	2			2							

(Continued)

TABLE 1.4 (Cont.)

	Shells	K			L			M			N				O		P			Q
	Sub-Levels	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	5f	6s	6p	6d	6f	7s
41	Niobium	2	2	6	2	6	10	2	6	4		1								
42	Molybdenum	2	2	6	2	6	10	2	6	5		1								
43	Technetium	2	2	6	2	6	10	2	6	6		1								
44	Ruthenium	2	2	6	2	6	10	2	6	7		1								
45	Rhodium	2	2	6	2	6	10	2	6	8		1								
46	Palladium	2	2	6	2	6	10	2	6	10										
47	Silver	2	2	6	2	6	10	2	6	10		1								
48	Cadmium	2	2	6	2	6	10	2	6	10		2								
49	Indium	2	2	6	2	6	10	2	6	10		1	2							
50	Tin	2	2	6	2	6	10	2	6	10		2	2							
51	Antimony	2	2	6	2	6	10	2	6	10		2	3							
52	Tellurium	2	2	6	2	6	10	2	6	10		2	4							
53	Iodine	2	2	6	2	6	10	2	6	10		2	5							
54	Xenon	2	2	6	2	6	10	2	6	10		2	6							
55	Cesium	2	2	6	2	6	10	2	6	10		2	6			1				
56	Barium	2	2	6	2	6	10	2	6	10		2	6			2				
57	Lanthanum	2	2	6	2	6	10	2	6	10		2	6	1		2				
58	Cerium	2	2	6	2	6	10	2	6	10	2	2	6			2				
59	Praseodymium	2	2	6	2	6	10	2	6	10	3	2	6			2				
60	Neodymium	2	2	6	2	6	10	2	6	10	4	2	6			2				
61	Promethium	2	2	6	2	6	10	2	6	10	5	2	6			2				
62	Samarium	2	2	6	2	6	10	2	6	10	6	2	6			2				
63	Europium	2	2	6	2	6	10	2	6	10	7	2	6			2				
64	Gadolinium	2	2	6	2	6	10	2	6	10	7	2	6	1		2				
65	Terbium	2	2	6	2	6	10	2	6	10	9	2	6			2				
66	Dysprosium	2	2	6	2	6	10	2	6	10	10	2	6			2				
67	Holmium	2	2	6	2	6	10	2	6	10	11	2	6			2				
68	Erbium	2	2	6	2	6	10	2	6	10	12	2	6			2				
69	Thulium	2	2	6	2	6	10	2	6	10	13	2	6			2				
70	Ytterbium	2	2	6	2	6	10	2	6	10	14	2	6			2				
71	Lutetium	2	2	6	2	6	10	2	6	10	14	2	6	1		2				
72	Hafnium	2	2	6	2	6	10	2	6	10	14	2	6	2		2				
73	Tantalum	2	2	6	2	6	10	2	6	10	14	2	6	3		2				
74	Tungsten	2	2	6	2	6	10	2	6	10	14	2	6	4		2				
75	Rhenium	2	2	6	2	6	10	2	6	10	14	2	6	5		2				
76	Osmium	2	2	6	2	6	10	2	6	10	14	2	6	6		2				
77	Iridium	2	2	6	2	6	10	2	6	10	14	2	6	9						
78	Platinum	2	2	6	2	6	10	2	6	10	14	2	6	9		1				
79	Gold	2	2	6	2	6	10	2	6	10	14	2	6	10		1				
80	Mercury	2	2	6	2	6	10	2	6	10	14	2	6	10		2				
81	Thallium	2	2	6	2	6	10	2	6	10	14	2	6	10		2	1			
82	Lead	2	2	6	2	6	10	2	6	10	14	2	6	10		2	2			
83	Bismuth	2	2	6	2	6	10	2	6	10	14	2	6	10		2	3			