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Chemistry to Remember

1.1 Introduction

Wine chemistry is a complex and interesting subject full of mysteries yet to be solved, a bit of a “new frontier.” The first steps toward gaining an understanding of wine chemistry will require a basic comprehension of chemistry fundamentals. This chapter is not a magical shortcut to get around a traditional organic and inorganic chemistry education but as a helpful reminder to the readers who have had some past chemistry education and a learning incentive to those readers who have not.

1.2 Metric System

The metric system is fundamental to all sciences, and wine chemistry is no exception. Serious but common errors made in the laboratory are simply incorrect scientific notations. Misplaced decimal points, incorrect weights, measures, and volumes, and miscalculations contribute to the problem. Correct notation and detailed documentation are the cornerstones of science.

Table 1.1 lists the metric prefixes as they relate to the base units of liter, gram, and meter. Table 1.2 list the metric conversions most frequently used in the wine laboratory and wine cellar. Understanding the metric system and committing it to memory will be a tremendous help to you as you proceed toward your winemaking goal. The Internet has several on-line conversion websites that are very helpful.

1.3 Density and Specific Gravity

Density and specific gravity are physical properties of a substance. Density is defined as the mass per volume of a substance and specific gravity is the *ratio* of the density of a substance measured at a particular temperature to the density of a reference material, often water, also measured at a particular

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TABLE 1.1. Metric prefixes.

mega = 1,000,000 = (10^6) = (number $\div$ 1,000,000) = decimal to the left 6 places 0.002345 megameter (Mm), megaliter (ML), or megagram (Mg)
kilo = 1000 = (10^3) = (number $\div$ 1000) = decimal to the left 3 places 2.345 kilometer (km), kiloliter (kL), or kilogram (kg)
hecto = 100 = (10^2) = (number $\div$ 100) = decimal to the left 2 places 23.45 hectometer (hm), hectoliter (hL), or hectogram (hg)
deka = 10 = (10) = (number $\div$ 10) = decimal to the left 1 place 234.5 dekameter (dam), dekaliter (daL), or dekagram (dag)
deci = 0.1 = (10^{-1}) = $(10 \times \text{number})$ = decimal to the right 1 place 23,450 decimeter (dm), deciliter (dL), or decigram (dg)
centi = 0.01 = (10^{-2}) = $(100 \times \text{number})$ = decimal to the right 2 places 234,500 centimeter (cm), centiliter (cL), or centigram (cg)
milli = 0.001 = (10^{-3}) = $(1000 \times \text{number})$ = decimal to the right 3 places 2,345,000 millimeter (mm), milliliter (mL), or milligram (mg)
micro = 0.000001 = (10^{-6}) = $(1,000,000 \times \text{number})$ = decimal to the right 6 places 2,345,000,000 micrometer (μm), microliter (μL), or microgram (μg)
nano = 0.000000001 = (10^{-9}) = $(1,000,000,000 \times \text{number})$ = decimal to the right 9 places 2,345,000,000,000 nanometer (nm), nanoliter (nL), or nanogram (ng)

Note: Prefixes are combined with basic units (meter, liter, gram). **EXAMPLE:** 2345 meter, liter, or gram expressed in respective prefixes.

temperature (Hägglund, 2004). For the purpose of this text, water will be the reference material when discussing specific gravity.

Density is expressed as grams per cubic centimeter (g/cc). The density of gold is 19.3 g/cc, the density of sulfur is 2.0 g/cc, the density of cork is 0.22 g/cc, the density of salt water is 1.025 g/cc, and the density of water is 1.0 g/cc (Hess, 1955). The difference in density allows cork, which is less dense than water, to float and sulfur, which is denser than water, to sink. The density of water at 20°C is 0.998204 g/cc.

According to Hägglund (2004), specific gravity is the *ratio* of the density of a substance measured at a particular temperature (t_1) to the density of water also measured at a particular temperature (t_2). Temperatures t_1 and t_2 are often the same, but in certain cases, they might be different. To simplify, references to specific gravity in this text will consider t_1 and t_2 to be the same (20°C); therefore, specific gravity compares the density of one substance to the density of water at the same temperature. The specific gravity of water at 20°C is the ratio of 20/20 or the density of water at 20°C (0.998204 g/cc) divided by the density of water at 20°C (0.998204 g/cc), which equals 1.000. Specific gravity has no units.

The specific gravity of wine is less than water. The more alcohol present in the wine, the lower the density and specific gravity, because alcohol has a lower density than water. The more solid and insoluble materials present in wine or juice; the higher the density and specific gravity, because these substances make the wine or juice denser than water.

TABLE 1.2. Metric conversions.

Metric to metric	Metric to english	English to metric	
Capacity			
1 liter (L)			
= 1000 mL	= 1.0567 fluid qt	1 fluid quart (qt)	= 0.9463 liter
= 100 cL	= 0.2642 fluid gal	1 fluid gallon (gal)	= 3.7854 liter
= 0.1 daL	= 4.23 cup		
= 1 × 10 ⁶ μL	= 33.814 fluid oz		
1 milliliter (mL)			
= 0.001 liter	= 0.0338 fluid oz	1 fluid ounce (oz)	= 29.573 mL
		1 teaspoon (t)	= 4.93 mL
		1 tablespoon (T)	= 14.79 mL
		1 cup (c)	= 236.588 mL
		1 gallon (gal)	= 3785.41 mL
1 microliter (μL)			
= 1 × 10 ⁻⁶ liter			
= 0.001 mL			
1 hectoliter (hL)	= 26.418 gal		
Weight			
1 gram (g)			
= 10 dg	=15.43 gr	1 grain (gr)	= 0.0648 g
= 0.001 kg			= 64.80 mg
=1000 mg	= 0.0353 oz	1 ounce (oz)	= 28.35 g
= 1×10 ⁶ μg	= 0.002205 lb	1 pound (lb)	= 453.59 g
1 milligram (mg)			
= 0.001 g	= 3.215 × 10 ⁻⁵ oz		
1 microgram (μg)			
= 1 × 10 ⁻⁶ g			
= 0.001 mg			
1 kilogram (kg)			
= 1000 g	= 2.2046 lb	1 pound (lb)	= 0.4536 kg
	= 0.0011 ton		= 0.0005 ton
Linear Measure			
1 millimeter (mm)	= 0.03937 (in.)	1 inch (in.)	= 25.40 mm
1 centimeter (cm)	= 0.3937 in.	1 inch (in.)	= 2.240 cm
1 meter (m)	= 3.281 ft	1 foot (ft)	= 0.3048 m
	= 39.37 in.		= 30.48 cm
1 hectare	= 2.471 acre		

1.4 Liquid, Solids, and Gases

The physical properties of gases, liquids, and solids are important to understand when working with chemicals and performing analysis. This section will only touch on a few outstanding points.

1.4.1 *Pressure and Temperature*

Pressure is the force exerted on a unit surface, and gas pressure is measured via a barometer. A barometer measures the displacement of a column of mercury by air pressure. Standard pressure is 760 mm of mercury or 1 atmosphere (atm), specifically; the air pressure at sea level supports a column of mercury 760 mm high. Today's technology uses this basic measurement to calibrate an array of fine instruments that can measure the slightest change in barometric pressure and gas pressure electronically.

Temperature is measured by two different scales: degree Fahrenheit ($^{\circ}\text{F}$) and degree Centigrade ($^{\circ}\text{C}$). A thermometer is a column of mercury in a vacuum that expands and contracts depending on the thermometric activity of the substance surrounding it. These thermometric scales have been established using water at sea level. The Fahrenheit scale was developed in 1753 and has 180 degree points; the centigrade scale developed in 1801 uses 100 degree points (Latin for 100 is centi). The freezing point of water is 0°C or 32°F . The boiling point of water at sea level is 100°C or 212°F .

The centigrade scale is used in all sciences and throughout most of the world. Because both temperature scales are used in some form universally, it is important to know the conversion formula: $^{\circ}\text{F} = (9/5)^{\circ}\text{C} + 32$. Absolute zero ($^{\circ}\text{A}$) is the complete absence of heat, the lowest possible theoretical temperature equivalent to -273.15°C or -459.67°F .

The contamination problems associated with mercury have led to improved temperature measurement methods. Mercury thermometers and barometers have been taken off the market for general use but are available for laboratory use. Chapter 2 will cover the handling of mercury and other hazardous material.

1.4.2 *Liquids*

A gas that is cooled or put under pressure, or both, will condense into a vapor as it moves into a liquid state. At room temperature, a liquid has the propensity to vaporize, or evaporate back into the atmosphere. The degree of evaporation is related to the vapor pressure of the liquid. Vapor pressure is the increase in pressure created by a liquid's vapor moving into the atmosphere directly above the liquid. The higher the vapor pressure of a liquid, the greater amount of vapor that will move into the atmosphere, or evaporate.

The boiling point of a liquid is the temperature at which the liquid's vapor pressure equals the pressure of the atmosphere about it. The freezing point is the temperature at which a liquid moves into a solid state.

The gravitational attraction of molecules to one another in a liquid (cohesion) exerts a force in all directions. At the surface of a liquid, the molecules are not surrounded, creating an imbalance of attractive force. The surface molecules are pulled back into the liquid as the molecules below exert a

greater attractive force, creating an encasing film on the surface; this is known as surface tension.

Adhesion is the attraction between liquid molecules and the molecules of the liquid's container. Capillary action is the rise or fall of a liquid's surface when a small-diameter tube penetrates the liquid's surface. The degree of capillary action depends on the adhesion of liquid and tube.

1.4.3 Gases

Boyle's Law, Charles's Law, and Dalton's Law of Partial Pressure explain the physical properties and propensities of gases:

Boyle's Law: The volume occupied by a gas is inversely proportional to the pressure at a given temperature: $P_1 V_1 = P_2 V_2$.

Charles' Law: The volume occupied by a gas is directly proportional to the absolute temperature of the gas at a given pressure: $V_1/T_1 = V_2/T_2$.

Combined Gas Law: $P_1 V_1 \div T_1 = P_2 V_2 \div T_2$.

Dalton's Law of Partial Pressure: The total pressure of a gas mixture is the sum of the partial pressure of each gas: $P_{\text{total}} = P_1 + P_2 + P_3 + \dots P_n$.

Wineries utilize gases such as carbon dioxide (CO_2) and nitrogen (N_2) to displace oxygen in storage containers. Sulfur dioxide (SO_2) gas is used as a microbial agent and an antioxidant. A variety of wine laboratory analyses might require the use of compressed gas or liquid gases. Understanding the gas laws is important when working with any gas.

1.5 Chemistry Fundamentals

We have looked at some of the physical properties of substances; now we move on to chemical properties. Chemical properties describe the ability of one substance to form a new substance via chemical reaction and the circumstances of that reaction.

1.5.1 Matter

Matter is made up of mixtures and substances. Mixtures are made up of substances held together by physical means that retain their individual properties and can be separated back into those individual substances by physical change. Substances are comprised of compounds or pure elements. Compounds are chemically combined elements that form unique substances. Compounds can only be decomposed into their individual elements by chemical change. Elements are the basis of all matter—the simplest form.

Combination, replacement, double displacement, and decomposition are the principal types of chemical reaction. Two or more simple substances or compounds that join to form a more complex compound are called a combination

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reaction. Replacement reaction involves compounds that replace one element for another. Two compounds reacting and exchanging substances is a double-displacement reaction and a decomposition reaction is the breakdown of a complex compound into a simpler compound or its elements.

Some reactions require a catalyst to change the speed of the reaction. Reactions will have a change in energy by absorbing or emitting energy in a variety of forms. You will remember the famous Einstein equation $E=mc^2$, where E represents energy, m equals mass, and c is the velocity of light. Energy cannot be created or destroyed.

1.5.2 Structure

The atom is the smallest particle of an element that maintains the properties of the element. The atom is made up of electrically charged particles: protons, neutrons, and electrons. Protons possess a positive charge and neutrons have no electrical charge. Protons and neutrons are contained within the nucleus of the atom and exert a positive charge. Negatively charged electrons orbit the nucleus at different levels called shells, held in orbit by their attraction to the positive nucleus. There are never more than eight electrons in the outermost shell. Atoms are electrically neutral and have an equal number of electrons orbiting the nucleus as there are protons in the nucleus.

The atomic number of an element is the number of electrons orbiting the nucleus. Atomic weight is the *sum* of the relative weights of protons and neutrons. There are a few elements that contain atoms with different atomic weights; these are termed *isotopes*. The atomic weight of an element represents the average weight of the isotopes of the element.

Chemical reaction involves electrons in the outermost shell and, occasionally, electrons in the second outermost shell. Elements with a full outer shell (eight electrons) are termed *inert elements*; they have no chemistry and they combine with nothing.

1.5.3 Periodic Table

Studying the structure of elements will allow the reader to understand the formation of compounds, write formulas, solve equations, and anticipate the outcome of reactions. The periodic table (Fig. 1.1) is an arrangement of elements according to their atomic number. Figure 1.1 includes the number of electrons in the element's outermost shell, valence numbers, and number of shells.

1.5.4 Compounds

An element's valence number is the number of electrons involved in forming a compound through a shift of electronic charge. A valence number of an element can be positive or negative, but the total of all element valences in a compound must equal zero.

Compounds add, subtract, and share electrons to achieve a neutral state. Electrovalence is the transferring of electrons to form a compound and the creation of ions that are electrically charged particles with properties totally different from the atom from which they came. Covalence is sharing pairs of electrons via a single, double, or triple bond.

Radicals are clusters of elements held together by covalent bonds that behave as if they were a single element. There exists a surplus or deficit of electrons; thus, the radical is a complex ion and will combine as a unit with other ions to form electrovalent compounds. Table 1.3 lists the common radicals.

Molecular weight is the sum of all the atomic weights of the elements present in a compound. A mole is a quantity of the compound equal in weight to its molecular weight.

The ratio of the number of atoms of each element present in a compound is a chemical formula, and a chemical equation is an account of the chemical change taking place. Equations must balance with an equal number of each type of atom on either side of the equation. Coefficients are used to balance the number of atoms in an equation (Fig. 1.2).

A pure compound always contains the same elements in the same proportions by mass; this is the Law of Definite Proportions. Based on the Law of Conservation of Matter and Definite Proportions, we are able to mathematically formulate a chemical change and solve problems. Table 1.4 lists several useful equations to express concentration, composition, and proportions.

1.5.5 Solutions

Solutions are mixtures of the solute (the substance dissolved) and the solvent (the dissolving medium). The solute is dispersed into molecules or ions consistently throughout the solution. Any given unit volume of solution will have an equal amount of solute molecules or ions. The amount of solute per unit volume of solvent is the concentration of the solution and can be expressed as molarity, normality, molality, or as a percentage (Table 1.4).

TABLE 1.3. List of radicals.

Valence +1	Valence -1	Valence -2	Valence -3
Ammonium NH_4	Acetate $\text{C}_2\text{H}_3\text{O}_2$	Carbonate CO_3	Phosphate PO_4
	Bicarbonate HCO_3	Chromate CrO_4	
	Chlorate ClO_3	Dichromate Cr_2O_7	
	Hydroxide OH	Sulfite SO_3	
	Cyanide CN	Sulfate SO_4	
	Nitrite NO_2		
	Nitrate NO_3		
	Permanganate MnO_4		

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VALENCE NUMBER	+1	+2												
Group	1	2	3	4	5	6	7	8						
	1 electron in outermost shell ↓	2 electrons in outermost shell ↓												
▼ Period = number of shells														
1 shell	1 HYDROGEN H 1.008													
			1 HYDROGEN H 1.008		ATOMIC NUMBER NAME ATOMIC SYMBOL ATOMIC WEIGHT									
2 shells	3 LITHIUM Li 6.941	4 BERYLLIUM Be 9.012												
3 shells	11 SODIUM Na 22.990	12 MAGNESIUM Mg 24.305	TRANSITION ELEMENTS											
4 shells	19 POTASSIUM K 39.098	20 CALCIUM Ca 40.078	21 SCANDIUM Sc 44.956	22 TITANIUM Ti 47.867	23 VANADIUM V 50.942	24 CHROMIUM Cr 51.996	25 MANGANESE Mn 54.938	26 IRON Fe 55.845						
5 shells	37 RUBIDIUM Rb 85.468	38 STRONTIUM Sr 87.620	39 YTTRIUM Y 88.906	40 ZIRCONIUM Zr 91.224	41 NIOBIUM Nb 92.906	42 MOLYBDENUM Mo 95.940	43 TECHNETIUM Tc 98.000	44 RUTHENIUM Ru 101.070						
6 shells	55 CESIUM Cs 132.910	56 BARIUM Ba 137.330	71 LUTETIUM Lu 174.970	72 HAFNIUM Hf 178.490	73 TANTALUM Ta 180.950	74 TUNGSTEN W 183.840	75 RHENIUM Re 188.210	76 OSMIUM Os 190.230						
7 shells	87 FRANCIUM Fr [223]	88 RADIUM Ra [226]	103 LAWRENCIUM Lr [262]	104 RUTHERFORDIUM Rf [261]	105 DUBNIUM Db [262]	106 SEABORGIUM Sg [266]	107 BOHRIUM Bh [264]	108 HASSIUM Hs [269]						
Atomic mases in parentheses are those of the most stable or commom isotope.														
*Lanthanoids			57 LANTHANUM La 138.910	58 CERIUM Ce 140.120	59 PRASEODYMIUM Pr 140.910	60 NEODYMIUM Nd 144.240	61 PROMETHIUM Pm [145]	62 SAMARIUM Sm 150.360						
**Actinoids			89 ACTINIUM Ac [227]	90 THORIUM Th 232.040	91 PROTACTINIUM Pa 231.040	92 URANIUM U 238.030	93 NEPTUNIUM Np [237]	94 PLUTONIUM Pu [244]						

FIGURE 1.1. Periodic table depicting groups, periods, valence numbers, and the number of electrons in the outermost shell. Elements in italics are the more recently discovered elements.

Molarity is the number of moles of solute per liter of solution. Normality is the number of equivalents of solute per liter of solution. Molality is the number of moles of solute per 1000 g of solvent. The percentage composition is expressed by weight when solids are dissolved in liquids or by volume when liquids are dissolved in liquids or gases are dissolved in gases.

A standard solution is a solution with a precisely known concentration. Standard solutions can be diluted and the new concentration calculated using the equation in Table 1.4.

Solubility is the maximum amount of solute that can be dissolved in a given volume of solvent. Factors such as temperature and pressure will affect

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				+3	± 4	-3	-2	-1	INERT
9	10	11	12	13	14	15	16	17	18
PERIODIC TABLE				3 electrons in outermost shell ↓	4 electrons in outermost shell ↓	5 electrons in outermost shell ↓	6 electrons in outermost shell ↓	7 electrons in outermost shell ↓	8 electrons in outermost shell ↓
									2 HELIUM H 4.003
				5 BORON B 10.811	6 CARBON C 12.011	7 NITROGEN N 14.007	8 OXYGEN O 15.999	9 FLUORINE F 18.998	10 NEON Ne 20.180
				13 ALUMINUM Al 26.982	14 SILICON Si 28.086	15 PHOSPHORUS P 30.974	16 SULFUR S 32.065	17 CHLORINE Cl 35.453	18 ARGON Ar 39.948
27 COBALT Co 58.933	28 NICKEL Ni 58.693	29 COPPER Cu 63.546	30 ZINC Zn 65.390	31 GALLIUM Ga 69.723	32 GERMANIUM Ge 72.610	33 ARSENIC As 74.992	34 SELENIUM Se 78.960	35 BROMINE Br 79.904	36 KRYPTON Kr 83.800
45 RHODIUM Rh 102.910	46 PALLADIUM Pd 106.420	47 SILVER Ag 107.870	48 CADMIUM Cd 112.410	49 INDIUM In 114.820	50 TIN Sn 118.710	51 ANTIMONY Sb 121.760	52 TELLURIUM Te 127.600	53 IODINE I 126.900	54 XENON Xe 131.290
77 IRIDIUM Ir 192.220	78 PLATINUM Pt 195.080	79 GOLD Au 196.970	80 MERCURY Hg 200.590	81 THALLIUM Tl 204.380	82 LEAD Pb 207.200	83 BISMUTH Bi 208.980	84 POLONIUM Po [209]	85 ASTATINE At [210]	86 RADON Rn [222]
109 MEITNERIUM Mt [268]	110 DARMSTADIUM Ds [271]	111 UNUNUNIUM Uuu [272]	112 UNUNBIUM Uub [277]	113	114 Uuq [296]	115	116 Uuh [298]	117	118 Uuo [?]
63 EUROPIUM Eu 151.960	64 GADOLINIUM Gd 157.250	65 TERBIUM Tb 158.930	66 DYSPROSIUM Dy 162.500	67 HOLMIUM Ho 164.930	68 ERBIUM Er 167.260	69 THULIUM Tm 168.930	70 YTTERBIUM Yb 173.040		
95 AMERICIUM Am [243]	96 CURIUM Cm [247]	97 BERKELIUM Bk [247]	98 CALIFORNIUM Cf [251]	99 EINSTEINIUM Es [252]	100 FERMIUM Fm [257]	101 MENDELEVIUM Md [258]	102 NOBELIUM No [259]		

FIGURE 1.1. (Continued)

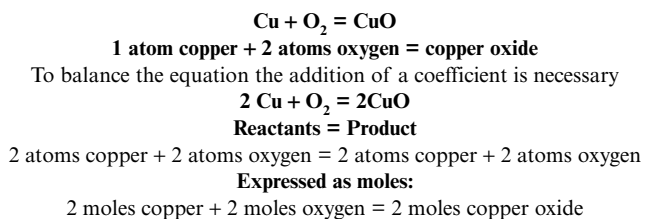


FIGURE 1.2. Balancing an equation.

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TABLE 1.4. Useful calculations.

Percentage by weight of elements in a compound

$$= \frac{\text{Total wt. of element present}}{\text{Molecular wt. of compound}} = \% \text{ of element}$$

Weight of one substance in a compound

$$= \frac{\text{Actual wt. of one substance}}{\text{Its equation wt.}} = \frac{\text{Unknown actual wt.}}{\text{Its equation wt.}}$$

Equivalent weight of a compound

$$= \frac{\text{Molecular wt.}}{\text{Net positive valence}}$$

Number of equivalents of a compound

$$= \frac{\text{Actual wt. of compound}}{\text{Equivalent wt. of compound}}$$

Normality

$$= \frac{\text{No. of equivalents of solute}}{\text{Volume of solution in liters}}$$

Number of moles

$$= \frac{\text{Actual wt. of compound}}{\text{Atomic wt. of elements in compound (molecular wt.)}}$$

Molarity

$$= \frac{\text{Actual wt./Molecular wt.}}{\text{Volume (in liters)}}$$

Molality

$$= \frac{\text{Actual wt. of solute/1000 g of solvent}}{\text{Molecular wt. of solute}}$$

Dilution of a more concentrated solution

$$C_1 V_1 = C_2 V_2$$

where C_1 = concentration of initial solution, V_1 = volume of initial solution, C_2 = concentration of final solution, and V_2 = volume of final solution

Note: Weight(wt.) is expressed in grams.

the solubility of a substance. The degree that a substance will dissolve into a solvent is dependent on the polarity (amount of electrical activity) and structure of the molecules involved. Water is very polar and is used more as a solvent than any other compound. The more similar the substances, the more likely they will dissolve one another. When a solution can hold no more solute, it is *saturated* and, conversely, a solution that has the ability to hold more solute in solution is termed *unsaturated*.

A solute that dissolves by absorbing moisture from the air is a *desiccant*.

1.5.6 *Electrolyte Solutions*

An electrolyte solution is a solution that conducts an electric current. The electrolyte is the solute, which when dissolved in water, creates the electrically conductive solution. Both electrolyte and nonelectrolyte solutions can change the properties of solvents, but the electrolyte solutions do so to a greater extent. In solution, electrolytes separate into positive and negative ions and these ions are responsible for the conductivity of the solution (Fig. 1.3).

Electrolytes are broken down into three categories:

Acids produce hydrogen ions (H^+).

Bases produce hydroxide ions also known as hydroxyl ions (HO^-).

Salts produce other ions.

Strong electrolytes ionize 100%, whereas weak electrolytes ionize only to some extent. Strong and weak refer *only* to the ionization of electrolytes and do not refer to the concentration of a solution (water is a weak electrolyte):

Strong acids Hydrochloric acid (HCl)

 Nitric acid (HNO_3)

 Sulfuric acid (H_2SO_4)

Strong bases Potassium hydroxide (KOH)

 Sodium hydroxide (NaOH)

 Hydroxides of groups 1 and 2 on the periodic table
(Fig. 1.1)

Ions in solution usually react with each other in three ways:

Forming a weak electrolyte

Forming an insoluble substance

Oxidation (reduction) of molecules

IONIZATION

Sodium Chloride

NaCl dissociates in water = Na^+ and Cl^- ions

Acetic Acid

$HC_2H_3O_2$ dissociates in water = H^+ and $C_2H_3O_2^-$ ions

NEUTRALIZATION

Hydrochloric Acid and Sodium Hydroxide in water:

HCl ionizes = H^+ and Cl^-

NaOH ionizes = Na^+ and OH^-

The ionic formula:

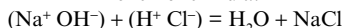


FIGURE 1.3. Electrolytes are solutes that when dissolved in water dissociate into ions creating a solution that conducts electricity. Neutralization is the reaction of an acid and base combined in the presence of water to form water and a salt.

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An acid or base mixed with water will disassociate into their constituent ions. Mixing these acid and base solutions creates a neutralizing reaction forming water, heat, and a salt (Fig. 1.3). The degree of neutralization is dependent on the ionization ability of the acid and base (strong or weak) and the concentration used. The salts produced can be of a strong acid and base, a strong acid and a weak base, a weak acid and a strong base, or a weak acid and base. These salts might have ions that can react with the water the salt is dissolved in to form weak electrolytes. This reaction is called *hydrolysis*.

1.5.7 pH

Hydrogen ions in a water solution are responsible for the acid properties of that solution and hydroxide ions in a water solution are responsible for the base properties of that solution.

Water ionizes slightly, 0.00001% (Hess, 1955). The molar concentration of free H^+ in water is very small (1×10^{-7}). In dilute acid solutions, the amount of H^+ is also very small. The pH scale was developed as a tool to indicate very small quantities of free H^+ in a solution containing water.

The pH is defined as the logarithm of the *reciprocal* of the molar concentration of the hydrogen ion, $[pH = \log (1/H^+)$; more simply, $pH = -\log(H^+)$]. Hydroxide is expressed as $pOH = \log [1/(OH^-)]$ or, more simply, $pOH = -\log(OH^-)$.

In pure water, $(OH^-) = (H^+)$. Using the equations for pH and pOH, you will find that $pH + pOH = 14$ (Law of Mass Action). This tells us the pOH is 7 and the pH of pure water is 7. The calculation is

$$\begin{aligned} pH &= \log (1/1 \times 10^{-7}) \\ &= \log 1 \times 10^7 / \log 1 \\ &= \log 10^7 - \log 1 \\ &= 7 - 0 \\ &= 7.0 \end{aligned}$$

Solutions with a pH less than 7.0 have *more* H^+ than water and exhibit acidic properties. Conversely, solutions with a pH greater than 7.0 have *less* H^+ than water and exhibit basic properties.

The pH scale has a range of 0.0–14.0. A slight change in a solution's pH indicates a much greater change in the concentration of free H^+ . The pH of juice and wine are normally in the acidic range pH 3.0–4.0.

1.5.8 Oxidation: Reduction and Electrolysis

Oxidation–reduction reactions are commonly referred to as “redox” reactions. The reaction is one of gaining and losing electrons (i.e., a change in positive valence). The oxidation side of a reaction is the process of losing the electrons and increasing the valence number. The reduction side of the reaction is the process of gaining the electrons and reducing the valence number. The number of electrons lost and gained in the reaction must be equal.

Oxidizing agents gain electrons via reduction and the reducing agents lose electrons via oxidation. It is just a bit confusing, but remember that we are looking at the flow of electrons, or electric current, from one substance to another. Passing an electric current through an electrolyte solution will create a redox type reaction *at the electrodes*. This breakdown of the electrolyte by an external electric current is called *electrolysis*.

1.5.9 Halogens

Elements that tend to form salts are called *halogens*. The four primary non-metal halogens are fluorine, chlorine, bromine, and iodine. Fluorine is the most active halogen and forms very stable compounds. Going down the list, iodine is the least active and forms less stable compounds. All halogens are poisonous.

Hydrogen halides are halogens combined covalently with hydrogen. Hydrogen halides are very soluble in water and disassociate into ions similar to electrolytes. They will fume in moist air as they combine with the moisture and then condense, forming drops of acid solution. When hydrogen halides are in a water solution, they are known as hydrohalic acids. The acids produced are hydrofluoric acid, hydrobromic acid, hydrochloric acid, and hydriodic acid.

1.5.10 Sulfur

Sulfur is used throughout wineries and vineyards as an antimicrobial agent and antioxidant. Sulfur compounds are used in laboratories as acids and oxidizing agents in chemical assays. The significant roll of sulfur in winemaking will be discussed in upcoming chapters.

Sulfur combined with heat and a metal forms a *sulfide*. Sulfides react with HCl to form hydrogen sulfide (H_2S).

Sulfur dioxide dissolved in water forms sulfurous acid (H_2SO_3 , hydrogen *sulfite*). Salts of sulfurous acid are sulfites. Sodium sulfite (Na_2SO_3) plus sulfur equals sodium thiosulfate ($\text{Na}_2\text{S}_2\text{O}_3$), a common reducing agent used in the wine laboratory.

Sulfuric acid (H_2SO_4 , hydrogen *sulfate*) when mixed with water liberates a tremendous amount of heat, creating a dangerous scenario of boiling water and spattering. Dilution of concentrated sulfuric acid requires small amounts of the acid added to the water while stirring constantly to dissipate the heat (Chapter 2).

1.6 Organic Chemistry

Organic chemistry is the study of compounds containing hydrogen and carbon bonds (hydrocarbons). There are approximately 8 million compounds

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known to date, with 300,000 new compounds found each year (Petrik Laboratories Inc., 2003).

All living things fall under the realm of organic chemistry; we are truly “carbon-based units.” Carbon has a valence of 4 and forms covalent bonds with atoms of hydrogen, nitrogen, oxygen, sulfur, halogens, and additional carbon atoms.

Carbon and hydrogen are readily available in our world, thus allowing simple compounds to build on each other to create long carbon chains or rings of carbon atoms with a variety of single, double, and triple bonds. Single bonds are the least active and triple bonds are more volatile. Some compounds contain literally thousand of carbon atoms.

Compounds are divided into two classes: aromatic and aliphatic. Aromatic compounds contain rings of carbon atoms with alternating double bonds (benzene ring) and aliphatic compounds have an array of carbon chains in different configurations. The longest unbroken chain of carbon atoms in a compound is designated with a root name to assist in identification (Table 1.5).

Organic compounds are identified by six different methods. I will use ethanoic acid as an example:

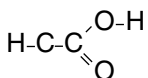
1. **Name** is based on accepted nomenclature.
Example: $\text{CH}_3\text{CO}_2\text{H}$ is called ethanoic acid.
2. **Molecular formula** is the actual number of atoms of each element.
Example: $\text{C}_2\text{H}_4\text{O}_2$
3. **Empirical formula** is the simplest whole-number ratio of atoms of each element.
Example: CH_2O
4. **Structural formula** shows how the atoms are arranged.
Example: CH_3CO_2

TABLE 1.5. Root name of a compound.

Carbon atoms	Root term
1	meth-
2	eth-
3	prop-
4	but-
5	pent-
6	hex-
7	hept-
8	oct-
9	non-
10	dec-
11	undec-
12	dodec-

5. **Graphical formula** demonstrates how the atoms are spaced and the type of covalent bond.

Example:



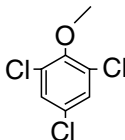
6. **Skeletal formula** is an abbreviated form of the graphical formula with an understanding that the lines have a carbon atom at each end.

Example:



Aromatic hydrocarbons contain benzene rings that bond to each other or other functional groups. The names of compounds containing benzene rings give the position on the benzene ring containing the functional group.

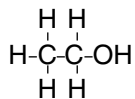
Example:



2,4,6-Trichloroanisole

Trillions of compounds have the same molecular formula but entirely different structural formulas; they are called *isomers*. Figure 1.4 illustrates the different molecular and graphical formulas of simple hydrocarbon compounds

ETHANOL $\text{C}_2\text{H}_6\text{O}$
Single bonds



DIMETHYL ETHER $\text{C}_2\text{H}_6\text{O}$

NOTE: The molecular formula is identical to ETHANOL but the structural formula is different this is called an isomer

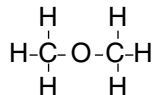


FIGURE 1.4. Structural and molecular formulas of selected organic compounds.
(continued)

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BENZENE C_6H_6

Single and double bonds in a ring formation

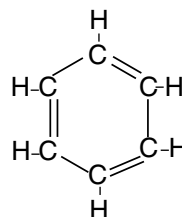
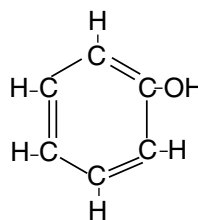
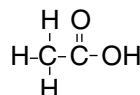
PHENOL C_6H_6O ACETIC ACID $C_2H_4O_2$ 

FIGURE 1.4. (Continued)

A functional group is made up of an atom or group of atoms that together have their own characteristic properties. Table 1.6 lists the various functional groups of organic compounds. In the wine laboratory, we are very interested in the aromatic hydrocarbons, carbonyl compounds, alcohols, organic acids, amines, and esters. Further study of these groups will be beneficial in understanding wine chemistry.

TABLE 1.6. Homologous series of common organic compounds with their corresponding functional group suffix and typical structure and bonds.

Name	Suffix	Structure
Alkanes (alkyl)	-ane	Single bond
Alkenes (alkyl)	-ene	Carbon to carbon double
Alkynes (alkyl)	-yne	Carbon to carbon triple
Esters	-oate	
Carboxylic acids (organic acids)	-oic acid	

TABLE 1.6. (Continued)

Name	Suffix	Structure
Acid halides	-oyl halide	
Amides	-amide	involved 
Nitriles	-nitrile	Carbon to nitrogen triple
Aldehydes (carbonyl compounds)	-al	
Ketones	-one	
Alcohols	-ol	-OH
Amines	-amine	-NH ₂

Note: Open-ended lines indicate that a carbon atom or carbon chain is attached.