The Study of Ions and Salts in Chemistry



Rose Marie O. Mendoza

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Arcler Press

224 Shoreacres Road Burlington, ON L7L 2H2 Canada www.arclerpress.com Email: orders@arclereducation.com

e-book Edition 2023

ISBN: 978-1-77469-696-5 (e-book)

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ISBN: 978-1-77469-432-9 (Hardcover)

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LIST OF ABBREVIATIONS

ADP	adenosine diphosphate			
AIDS	acquired immunodeficiency syndrome			
AMP	adenosine 5'monophoshate			
AN	acetonitrile			
APIs	active pharmaceutical ingredients			
ATP	adenosine triphosphate			
CNTs	carbon nanotubes			
CO ₃ ²	carbonate			
COPD	chronic obstructive pulmonary disease			
CVD	cardiovascular disease			
DEME	N, N-diethyl-N-methyl-N-(2-methoxyethyl) ammonium			
DSC	differential scanning calorimetry			
EC	European Commission			
ED	electrodialysis			
EIA	environmental impact assessment			
FAO	Food and Agriculture Organization			
FDF	food and drink federation			
FSA	Food Standards Agency			
GCS	Gouy-Chapman-stern			
GI	gastrointestinal			
H_2SO_4	hydrosulfuric acid			
H ₃ P	hytransferhosphoric acid			
HCl	hydrochloric acid			
HHS	health and human services			
HKF	Helgeson, Kirkham, and flowers			
IBSA	Institut Biochimique SA			
IM	intramuscular			

IR	infrared		
IUPAC	International Union of Pure and Applied Chemistry		
IV	intravenously		
MSA	mean spherical approximation		
MSG	monosodium glutamate		
NF	nanofiltration		
NH_4^+	ammonium		
NHANES	National Health and Nutrition Examination Survey		
NMR	nuclear magnetic resonance		
OH	hydroxide		
PC	propylene carbonate		
PD	pharmacodynamics		
РК	pharmacokinetics		
PPIs	proton pump inhibitors		
PZC	zero charge potential		
RO	reverse osmosis		
SACN	scientific advisory committee on nutrition		
SDS	sodium dodecyl sulfate		
SFs	salt forms		
${\rm SO}_4^{\ 2-}$	sulfate ion		
SR	sustained-release		
UF	ultrafiltration		
US FDA	US Food and Drug Administration		
USDA	United States Department of Agriculture		
WHC	water holding capacity		

PREFACE

Positive and negative ions are bound together by ionic bonding in most of the compounds that make up the Earth's crust. An ionic compound is one that contains both negative and positive ions and is electrically neutral. W.H. Bragg and W.L. Bragg discovered the crystalline structure of sodium chloride salt in 1913. This revealed that each atom had six equidistant closest neighbors, indicating that the components were not organized in molecules or limited aggregates, but rather as a networked structure with the long-range crystalline organization. More inorganic compounds were discovered that share structural similarities. These compounds were quickly identified as containing ions rather than neutral atoms, but verification of this theory did not come until the late 1920s, when X-ray tests (which determine the density of electrons) were carried out.

Max Born, Alfred Landé, Fritz Haber, Erwin Madelung, Kazimierz Fajans, and Paul Peter Ewald were known major contributors to the creation of a theoretical explanation of ionic crystal formations. Max Born projected crystallization energies based on the idea of ionic components, which matched thermochemical data well, confirming the hypothesis.

Precipitation, evaporation, or freezing can form ionic compounds (including salts) from their constituent ions. Reactive metals, such as alkali metals can generate an ionic product by reacting directly with strongly electronegative halogen gasses. They can also be made as a result of a high-temperature solid-solid reaction.

This book contains detailed information about ions, ionic compounds, different types of salts, and their applications. There are eight chapters in the book. The book is mainly divided into two parts. The first part consists of the initial four chapters, which deal with the properties, classifications, and applications of ions and ionic compounds. The second part introduces the readers with the fundamentals of different types of salts and their applications.

Chapter 1 introduces the readers with the fundamentals of ions and ionic compounds with emphasis on ionic bonding and classifications of ions. Chapter 2 deals with the salient features of ions and ionic compounds. Chapter 3 contains information regarding the basics of ion extraction and ion mobility. Chapter 4 introduces the readers with novel concepts of ionic liquids and their applications.

Chapter 5 explains the key concepts of salt chemistry and aqueous solutions. Chapter 6 illustrates the role of salts in public health and food sciences. Chapter 7 contains information about the saline environment and the use of saline water and salts in agriculture. Finally, Chapter 8 describes the fundamental concepts of salts and their uses in pharmaceutical industries.

This book is primarily written for chemistry students who wish to learn more about the connections between atomic structure and bonding, as well as the macroscopic features of ionic compounds and salts. Similarly, the book aims to help teachers and educators to substantiate their lessons through a simple and informative manner of explaining the chemistry of ions and salts.

-Author

CHAPTER

INTRODUCTION TO IONS AND IONIC COMPOUNDS

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1.1. INTRODUCTION

By definition, an atom is considered neutral because the total number of electrons (charged negatively) is the same as the total number of protons (positively charged particle). Since the number of negatively charged particles is equivalent to the number of the positively charged patricles, the total charge on the atom is zero (0). However, this one-to-one charge ratio is not the most frequent condition for a large number of elements. Disorders, therefore, in ratio result in the formation of charged particles termed ions (Koppenol, 2002; Poulsen, 2010; Ball et al., 2011). Across nature, highenergy objects flow to lesser-energy positions.. These lesser energy variables are exemplified as noble gas components in terms of atoms. These elements from their electron configuration have filled energy sublevels which makes them inert. While by principle that lower energy sublevels are filled first before the higher levels, they are in a lesser energy state and have the ability to remain in that condition (Bewick, 1969; Hirschhorn et al., 2001; Bernhoft, 2012) unless external force or energy is supplied to disturb or excite electrons tightly held in the sublevels.

1.1.1. Octet Rule

Elements other than the noble gases has several degrees of incompleteness in their lowest sublevels, making them unstable as matched to noble gases. That instability pushes these elements to achieve the filling to completeness their lower energy levels to achieve the stability of the nearby noble gases in the periodic table. The outermost energy states in these lower energy levels include eight electrons (an "octet"). The "Octet Rule" refers to an atom's preference to have 8 electrons in the outermost sublevel to achieve stability (Gillespie and Silvi, 2002; Saito et al., 2009).

An atom lacking an octet of electrons in the outermost shell can gain an octa in valance shell in one of two ways. One method is to transfer electrons from one atom to another till both have octets. There is no net change in the number of electrons since a few atoms will transfer electrons and the other atoms will accept electrons; nonetheless, along with the transport of energy, the distinct atoms gain other than zero charges (Lever, 1972; Schleyer et al.,

1982). The tendency of the atom to transfer or accept atoms is indicated by its charges or valence. An atom with a valance of +1 means that it has the ability to transfer 1 electron to be stable. When this atom transfers the said available electron to another atom, it means that it already has a stable lower sublevel. On the other hand, an atom with a valence of -1 indicates their ability to accept an electron to achieve octet or make their last energy level filled (Linnett, 1961; Noury et al., 2002). transferWhen the release of electron of one atom was accepted by another atom, a chemical bond is created kanown as *ionic bonds*. Furthermore, the positive and negative charges approach one other as opposing charges attract (and comparable charges repel), in a type of attraction driven by electrostatic forces between atoms. The resultant chemicals are ionic compounds (Gillespie and Robinson, 2007; Quayle et al., 2015). For an ionic bond to form, the transfer and acceptance of electrons must be between metallic and non-metallic atoms, respectively.

Another way the atom might acquire the octa of electrons is by sharing electrons with another atom. On the contrary, sharing of electrons usually takes place between two non-metallic atoms. Upon sharing of electrons, the lowest sublevel of the two atoms overlaps for electron pairing, allowing both atoms to achieve an octet or filled sublevels. Those paired electrons fill the outermost shells of these two atoms at the same time. When electrons are shared, a *covalent bond* is formed (Joki and Aksela, 2018).

1.1.2. Electron Dot Symbols in Periodic Table

The number of electrons present in the outermost shell of an atom or the *valence* (number) of an atom can be readily identified through their location in the periodic table. The periodic table separates into two groups: transition elements and main group elements. Elements that belog to Group A designated by the letters IA through VIIIA, also indicates their valence number (Figure 1.1). For instance, the halogen familyis designated as Group VIIA. This means that all halogens contain seven electrons in its outermost shell. The valence shells of all transition and inner transition elements contain two or more (up to 4) total electrons (Railsback, 2003; Jena, 2013).



Figure 1.1: Elements periodic table. The components of the main group, transition, and inner transition are shown.

Though that is quite simple as for a specific quantity of outer shells electron, a graphical presentation is generally useful. An Electron-Dot Symbol is the graphic representation for the valence electrons an atom holds. This can be done by drawing the number of valence electrons using dots around the symbol of the atom or element. For instance, halogens or elements belonging to Group VIIA, as discussed have 7 valence electrons, thus there should be 7 electrons around the element symbol. Remember that the Lewis Dot symbols must represent electrons to be in pairs (Fontani et al., 2015; Kwatra, 2017). Students frequently need to arbitrarily position those electron dots about element, but then again it is helpful to utilize the four basic directions like a guidance (top-bottom-left-right) in distributing the electrons around the element symbol. Occupy single electrons in every of 4 basic places surrounding the atom till all valence electrons are represneted(Lengler and Eppler, 2007; Farooq et al., 2020). It should be noted that noble gases contain full octets as well and will have eight electrons in the outermost shell (Figure 1.2).



Figure 1.2: Electron Dot Symbols of electrons.

Note: Before electrons are coupled with another electron (see Carbon with a valence of 4, one electron would position at every one of 4 basic directions.

Overall, the periodic table may be utilized to find the number of outer electrons in every element (Figure 1.3).



Figure 1.3: Electron dot symbols place on above of every group or family of elements, with x as any element within that family or group.

Source: https://wou.edu/chemistry/files/2017/01/sodium-ion.jpg.

1.2. IONS AND THE PERIODIC TABLE

Non-metals at the right side of periodic table accept electrons needed to achieve an electron configuration as that of the closest noble gas. Metals at

the left side of periodic table transfer electrons required for attaining a stable electronic configuration as that of the closest noble gas. On the other hand, transition elements might differ in their approach to stabilize their lower energy configurations (Richens, 1997; Silver and Phung, 2005).

1.2.1. Common Cations

Ions with a charge of +1 are formed by elements in Group IA. When ionized, they lose one electron and revert to the configuration of electrons of preceding noble gas. As illustrated in Figure 1.4, while a (Na) sodium atom is ionized, from its 11 electrons, one electron is lost, resulting in a Na⁺ (sodium ion) with electronic configuration of preceding noble gas, i.e., neon. Because sodium ion is one less electron than protons, it has a singular positive (+1) electrical charge and is considered as a *cation*.



Figure 1.4: Sodium-ion formation.

Note: It should be noted that sodium is capable to transfer its outermost shell electrons in the third shell at the time of the creation of an ionic bond. It now contains the electron configuration of neon and does have a complete octa in the second shell. It is important to notice that this ion still contains the similar number of protons (11) like an actual sodium atom and keeps its sodium character. Conversely, the electron cloud now has only 10 electrons, resulting in an overall positive (+1) charge (Nadeau et al., 1997; Pyykkö, 2011).

Source: https://www.gcsescience.com/a4-sodium-ion.htm.

The sodium ion possesses an octet of electrons at the second major energy state as a result of losing that electron. The sodium ion's electron configuration is becoming identical to that of the noble gas neon. The ion and atom of separate atom (or two distinct ions) with a similar electronic configuration are referred to be *isoelectronic*. The sodium ion and a neon atom are, therefore, isoelectronic.

To attain the electron configuration of the noble gas succeeding ions/ atoms at the periodic table, say, Group IA elements must surrender and transfer one electron during ionic bonding. It is worth noting that the atom's nucleus stays constant, and so the identity of the atom as an ion remains unchanged. The electronic configuration of a sodium ion is similar to that of neon, only in terms of the neutron-proton configuration. Likewise, Group IIA elements transfers their two outer electrons to produce +2 ions; Group IIIA elements transfers their outermost 3 electrons to generate +3 ions (Vinogradov et al., 2003; Chen et al., 2018).

On the other hand, there are elements that served to be an exception to the octet rule, and one of them is hydrogen. Though hydrogen is located in the leftmost part of the periodic table along where metals are located, it is not considered as a metal and does not chemically behave as a metal either. This is due to the fact that hydrogen is extremely tiny and can only hold a total of two electrons before becoming full. As a result, rather than obeying the octet rule, hydrogen achieves stability by accumulating 2 electrons in its shell, or a "duet" by associating with some other atoms. Based on the element with which it interacts, hydrogen could create both ionic and covalent bonds. When hydrogen forms ionic bonds, it usually loses an electron, generating cation with a charge of +1. Since hydrogen contains a single electron to start with, while it transfers one electron in its ionic form, there is just one proton remaining in a atom's nucleus. As a result, when hydrogen is ionized to H⁺, this is commonly known as a proton. This may also be ionized, resulting in the formation of a -1 ion or an *anion*. In this scenario, the hydride ion is formed by naming the H⁻ion according to conventional procedures. The H⁺ state is much more prevalent during hydrogen ionization than the H⁻ form. Furthermore, the H⁺ ion is crucial in the acidic chemistry. In aqueous solutions, acids are substances known to give H⁺ ions. Cations, on the other hand are simply named by putting the word "ion" after the element name, like sodium ions for Na⁺.

1.2.2. Common Anions

Non-metals, on the other hand, tends to accept electrons to achieve a steady electronconfiguration as that of the noble gases in the preceding *period*. A *period* is the horizontal arrangement of the periodic table, read from left to right. At the extreme right of the periodic table are the halogens and the noble gases.

Ionized Group VIIA elements, therefore, need to acquire an electron and bears a negative charge. When chloride (Cl) is charged, it gains one electron, enabling it to achieve the electrical configuration of the noble gas argon. as shown in Figure 1.5, the a single negative charge then turns it into the chloride ion (Cl⁻); notice the little variation in suffix -ide which later becomes -ine as its anion name.



Figure 1.5: The creation of chloride ion.

Note: On the left, the chlorine atom had 17 electrons. A chloride ion then gains one electron (to the right), changing the munber of electron from 17 to 18 electrons and acquiring a -1 charge. The chloride ion's outer energy level is now completely filled and thus, have eight electrons, according to the octet rule.

Source: https://chem.libretexts.org/Courses/can/health/03%3A_Ionic_Bonding_and_Simple_Ionic_Compounds/3.3%3A_Ions.

Similarly, when elements of Group VIA are ionized, they acquire two electrons, resulting in a charge of -2 and achieving an electron configuration that corresponds to the electron configurations of the noble gases in the preceding periodic. On the other hand, elements of Group VA receive three electrons, giving it a -3 charge and resembling the electron configurations of noble gases.

This is critical just not to mistake an idea of isoelectronic substances. Isoelectronic substances only reflect similarities in the electronic properties of the number of neutron and protons but not on the characteristics and chemical properties of the involved substances. Since the nuclei of a sodium ion and a neon atom have different amounts of protons, they are quite different. One is an important ion found in table salt, whereas the other is an inert gas found in very minute amounts in the environment. Similarly, sodium ions differ significantly from fluoride ions, magnesium ions, and other all the components of neon isoelectronic series (Mg²⁺, N₃, Ne, O₂, Al³⁺, Na⁺, F) (Figure 1.6).



Figure 1.6: Isoelectric atoms contain distinct features.

Note. Neon atoms (A) and the Sodium ions (B) are isoelectronic. Neon is like a colorless, nonreactive gas that emits an unusual red-orange tint when discharged via the gas discharge tube. Sodium ions are often present in salt crystals, like sodium chloride, commonly used as table salt.

Source: https://www.ck12.org/chemistry/anion-formation/lesson/Anion-Formation-CHEM/.

1.2.3. Ions of Transition and Inner Transition Metals

The transition and inner transition metals, are just as important as well as the previously discussed substances and falls into a more complex category of elements to study. These elements have variable electron distribution designs that do not always obey the electron filling principles as discussed in the Aufbau principle. The formation of ions by transition and inner transition metals also falls in a more complex process and needs to be evaluated further to check is it does represent the actual substance. To identify the ionic forms of transition and inner transition elements, beginners are recommended to closely look again into the the general ion representation of the periodic table as illustrated in Figure 1.7.



Figure 1.7: The Periodic Table in Elemental ionic states.

Note: . The ionic states of the transition and inner transition metals indicated the valence states of the elements. Some transition and inner transition metals are "multi-valent" of having 2 or more valences based on their ability to transfer electrons to be stable.

Source: https://wou.edu/chemistry/courses/online-chemistry-textbooks/3890–2/ ch104-chapter-3-ions-and-ionic-compounds/.

1.3. IONIC BONDING

The majority of minerals and rocks that comprise the crust of Earth are made up of positively charged and negatively charged ions that bond with each other through ionic bonding. An ionic compound is a chemical substance that is electrically neutral. Among the several popular ionic compounds to name is sodium chloride (NaCl). A sodium chloride particle is made up of equal parts positive charged sodium ions (Na⁺) as well as negatively charged chloride ion (Cl⁻).

To establish an ionic bond, the charges of anions and cations are fundamentally opposite. As such, an ionic bond can be formed whenever a cation and an anion are pulled together by electrostatic attraction. An ionic compound is made up of two or more ions that are held together by electrostatic attraction. Binary ionic compounds are the simplest ionic compounds because they are literally made up of a cation and an anion (Taber, 1997; Coll et al., 2003). On the other hand, there are ternary ionic compounds that are composed of a group of cations or group of anions behaving as one unit. These are ionic compounds made up of *radicals* or polyatomic substances behaving as a cation or an anion. For this section, we shall first concentrate on creation of the binary ionic compounds(Mendoza, 2016).

As discussed earlier, one of the most popular ionic substances is sodium chloride (NaCl) or table salt. In the formation of sodium chloride, an electron released by sodium is transferred to chlorine, resulting in the formation of the chloride ion. The chloride ion has the tendency to receive one electron thus, it has a negative charge while the sodium ion has a tendency to remove from itself and transfer 1 eeletron so has a +1 charge. The transfer and acceptance of electrons from sodium to chlorine creates an electrostatic attraction between two substances, forming a new substance in the form of NaCl. It is critical to understand that electrons could not be "lost" somewhere; they constantly finish up going to the other molecule or atom. Ionic processes may be shown using electron dot and curved arrow diagrams to illustrate the movement of electrons from sodium ions to chlorine as shown below for NaCl (Schäfer et al., 1973; Di Girolamo et al., 1977) (Figure 1.8).

$$Na \cdot : CI: \rightarrow Na^+: CI:$$

Figure 1.8: Ionic bonding of sodium chloride.

Source: https://chem.libretexts.org/Bookshelves/Environmental_Chemistry/Green_Chemistry_and_the_Ten_Commandments_of_Sustainability_(Manahan)/04%3A_Compounds-_Safer_Materials_for_a_Safer_ World/4.03%3A_Sodium_Chloride_and_Ionic_Bonds.

The electrostatic attraction is what causes the Na^+ ion's affinity for the Cl^- ion. To emphasize that the original energy level holding the outermost electron has been depleted, the cationic particle is often shown without dots from around the symbol. The anion now has a complete octet of electrons. In NaCl, it is worth noticing that both ions are displayed, despite the fact that their charges aren't (Skomski et al., 2012; Vladušić et al., 2016). This is because the total charge on the molecule within ionic compounds remains zero, which means that the charge levels of anion(s) and cation(s) included in the bond must always be in a way that the number of positive charges

equates the number of negative charges. Thus, the total charge of any ionic compound must be equal to zero. The total charge of the compound is calculated based as the summation of the number of atoms of each entity present, multiplied by their valance or oxidation number. On the other hand, in the symbol of the cation is followed by the symbol of the anion when ionic compounds and written by chemical formula (Reed and Schleyer, 1990; Kang et al., 2017).

On the other hand, the process is a bit complex in the case of magnesium chloride. Due to the fact that magnesium possesses two outermost electrons, it must transfer both electrons to obtain the noble gas configuration. As a result, there should be two chlorine atoms present to accept the electrons (Figure 1.9).



Figure 1.9.1: Magnesium chloride ionic connection.

 $MgCl_2$ now is the chemical formula for magnesium chloride. The subscript (2) adjacent to chloride ion shows that each magnesium cation is linked with two chloride ions. From the final formula $MgCl_2$, the total charge is represented by the calculation {[1(+2) + (2)(1)] =0}, where +2 is the charge of Mg ions and -1 is the charge of chlorine ions. The coefficients 1 indicates the presence of 1 atom of Mg and 2 for 2 atoms of chlorine in the compound (Taber et al., 2012; Luxford and Bretz, 2014).

For another example, assume we need to create the chemical formula for molecule with Fe⁺³ as a cation and Cl⁻ as an anion. To keep track of the number of ions used, their charges, and the overall negatively and positively charged number on the molecule. For beginners, though there are some versions of the periodic table that indicates the net charge of an ion, or the valence or oxidation numbers of the element, it is recommended that you start by constructing the electron dot symbols of each ions involved to determine the net charge on each ion. An illustration of a basic charge box is as follows (Ruddick and Parrill, 2012).

Then determine how so many cation and anion atoms are necessary to balance the total positively and negatively charged on the final molecule. Notice that for one atom of Fe has 3 available electrons to transfer, thus it needs 3 chlorine atoms to maintain the nest charges to zero. So, you put 1 in the number of cation (Fe) atoms and 3 for the anion (Cl). Compute the overall ion charge of the anion(s) and cation(s) found by multiplying each ion charge by the number of atoms, and then adding these numbers collectively determine the overall charge on complex:

$$\left(1 \operatorname{atom of Fe} x \xrightarrow{+3}_{atom of Fe}\right) + \left(3 \operatorname{atom of Cl} x \xrightarrow{-1}_{atom of Cl}\right) = 0$$

Or simply: (1)(+3) + (3)(-1) = 0

It will almost always lead to a stable ionic formula with an overall neutral charge of zero (Bent, 1953; Zhou et al., 2011).



• Valence electron of Fe is 5 and Cl is 7 as represented by the Lewis Dot Structure

• Remove the paired electrons to avoid confusion and retain the unpaired ones. This will show that Fe has a charge of +3 and Cl has a charge of -1

• Transfer electrons of the metallic element to the non-metal, you can add multiple non-metals until all electrons are transferred. Now you know that it takes 3 chlorine atoms to balance out the +3 electrons of Fe. The charge of the compound now is 0.

Figure 1.9.2: Formation of ferric chloride and calculation of total ionic charge.

1.4. PRACTICE WRITING CORRECT IONIC FORMULAS

To approximate and record suitable chemical formulas, first step is to be familiar with the charge of the atom or its oxidation or ionic state, then check for the neutrality of the compounds-its total charge must be equal to zero, and finally, write the chemical formulas with the symbol of the cation first, then the anion. The charge or the cation becomes the subscript of the anion and vice versa. Note that the formula must be written with the subscripts representing the smallest ratio of the anions and cations (Pauling, 1933; Dehmer and Fano, 1970).

Always remember that ionic bonding happens when an anion (electron acceptor) and a cation (electron donor) come together to produce a molecule with a neutral net charge. Ionic bonds are most commonly formed between metals and nonmetals. Once we know of covalent bond formation (which happens most typically amongst two nonmetals or between a nonmetal and a semimetal/metalloid), this will make it easier to detect ionic compounds.

To write the formula of an ionic compound, write each ion (cation and anion) with their. For instance, in the case of magnesium (+2) and chlorine (-1) combining:

Mg⁺² Cl⁻¹

The charge or superscript of the cations becomes the subscript of the anion and viceversa. Thus, when magnesium (+2) and chlorine (-1) combine to form an ionic compound Magnesium Chloride, it is written as:

MgCl,

Notice that the subscript 1 is not written in the formula.

In FeCl_3 is formed by combining three atoms of chlorine (Cl) with one atom of iron (Fe). The subscripts from the number of atoms column are then used to generate the right ionic formula.

This process can be done mentally, once you were able to determine the right ionic charges and the basics in writing chemical compounds.. Say,what is the right ionic formula for aluminum sulfide, for instance? From the periodic table, the charge of Aluminum is +3 and Sulfur is -2, Al_2S_3 is the right representation for the ionic compound formed.. So, remembering the simple process discussed earlier,

 $Al^{+3} S^{-2} \rightarrow Al_2 S_3$

On cations and anions with the same ionic charges like NaCl, this is from Na^{+1} and Cl^{-1} , which theoretically Na_1Cl_1 , but a basic rule we do not write 1 as subscript in writing chemical formulas so we write it as NaCl.

Similarly, we do not write in the chemical formula, subscripts that are numerically identical for all combining elements. Say FeS, is the combination of ions Fe^{+2} S⁻², and writing it using our basic process will give:

 $Fe_2S_2 \rightarrow FeS$

This substance, basically falls under 2 rules, one is that identical numerical subscripts for all combining ions are nor written, and that all subscripts must be reduced to its simplest ratio. This can be viewed ion the combination of Pb^{+4} and S^{-2} , which is written correctly as PbS_2 :

 $Pb^{+4} S^{-2} \rightarrow Pb_2S_4$ (the subscripts when both divided by 2) $Pb_{2/2}S_{4/2} \rightarrow Pb_1S_2 \rightarrow PbS_2$

1.5. NAMING IONS AND IONIC COMPOUNDS

Majority of the substances have 2 sets of names. Its common name and its IUPAC name. Classic example is water (H₂O), in which water is a name that does not describe the chemical make-up of the substance. Thus, a common name is usually a name that was popularized by people to call it easier rather than identifying first what chemical element comprises it. On the other hand, the IUPAC name is the name of "any" chemical compound which is based on the substances that comprises it. In general, common names are for popular and simple chemistry substances, while IUPAC may have both for popular and unpopular, as well as simple and complicated substances since IUPAC adopts an internationally accepted system of naming for both nature of substances. This book will mostly use the International Union of Pure and Applied Chemistry (IUPAC) name system for this chapter. In addition to the IUPAC system, there is an earlier and much more system for archaic (-ous and -ic) naming. In certain cases, the earlier name scheme is still widely used. These departures from of the IUPAC system would be acknowledged throughout the book, as this older terminology is still widely used in chemical labs and the health sciences (Wirtz et al., 2006; Kavak, 2012).

The name of cations adheres to a straightforward convention. It's as easy as adding 'ion' to an end of an element name. The term sodium ion refers to a sodium atom that has transferred an electron (Na⁺). This indicates that the sodium would have a +1 positive electrical charge, as compared to its elemental state (which has similar number of electrons and protons and is neutral in charge). When referring to ions, it is critical to utilize the ion naming system other than the element names of atoms, since the sensitivity of an ion vs. the elemental form of material might be pretty different. For instance, if you add the sodium ion in the form of NaCl (or table salt) to a glass of drinking water, you'll get a salty, pleasant drink. However, if you put elemental sodium in your glass full of water, it will burst in your face since elemental sodium is very reactive with water!

To distinguish the many ionic forms in cations with more than one charge phase, the symbol of the atom or of the element is accompanied by a roman number that represents it ionic charge or oxidation state. For instance, iron exists in two primary ionic forms: Fe^{2+} and Fe^{3+} . As a consequence, the first ion can be written as Fe (II), while the second is is written as Fe (III) (Baker and Ollis, 1957; Lind, 1992).

Anions are on the other hand is a bit complex than the cations. Several letters in the end of its name is frequently removed and replaced with -ide. Cl⁻, for example, can also be called chloride other than the usual term, chlorine ion. In this scenario, the '-ine' end of chlorine is substituted with the 'ide' end. To create the sulfide ion, the '-ur' ending is removed and substituted with 'ide.' Phosphorus is then transformed to phosphide ion, nitrogen to nitride ion, and oxygen to oxide ion in the same manner (Goodenough et al., 1961; Churchman and Carr, 1975). The '-ide' ending is significant as it benefits the reader and listeners to rapidly differentiate among the two kinds of ions being named (the cation, that recollects the element label, and an anion, that adds the '-ide' ending).

The word "ion" is then omitted when identifying ionic compounds, and the names of the anions and cations are combined, with cation always stated first then the anion mentioned last.. Remember that roman numerals are only used when talking about metals that has more than potential ionic state/ oxidation number or charge.

Whenever the Na⁺ and Cl⁻ atoms combine to form NaCl, the resultant chemical is known as sodium chloride. When Mg^{2+} and Cl⁻ combine to form $MgCl_2$, the resultant chemical is known as magnesium chloride. This follows the formula: Name of the metallic substance (cation) then the name of the non-metallic substance (anion) with its ending changed to -ide.

When the metal component in an ionic bond contain more than one ionic charge/state, the roman numerical value representing its actual ionic charge is employed to determine that that specific ion is involved in the bond. For instance, if Fe_3^+ and Cl^- react to generate $FeCl_3$, we'll have to differentiate it from Fe_2^+ and Cl^- reacting to generate $FeCl_2$. This indicate that $FeCl_3$ in another sense be written as Fe (III) Chloride, while $FeCl_2$ is alternatively written as Fe (II) Chloride (Wulfsberg et al., 2006; Thong et al., 2015).

While it arises to naming ionic compounds, the most significant thing to recall is that you'll be capable of drawing the shape from the name and build the term from the structure. Let's put our skills to the test!

Practice Exercise 1

- Name the formula of the compound when the following ions combine: (a) zinc and sulfur, (b) aluminun and oxygen, (c) Lead (+4) and chlorine, (d) mercury and fluorine, (e) Chromium (+6) and sulfur
- Write the name of the following compound both in IUPAC and roman numeral system (for cations with multiple charges): (a) arsenic chloride, (b) Chromium (III) fluoride, (c) arsenic (V) nitride, (d) potassium bromide, (e) Barium oxide

1.6. POLYATOMIC IONS

Till recently, we have focused on compounds containing monoatomic ions, or ions formed by a single atom. Though, a few regularly occurring ions are made of several atoms which are joined together by electron sharing or covalent bonds. These ions function identically as monatomic ions, possessing a single overall charge and reacting with some other ions and molecules either as cations or but mostly as anions. Due to the fact that these ions are composed of many atoms, they are referred to as polyatomic ions or radicals. Negatively charged polyatomic ions are more prevalent than positively charged polyatomic ions. The chart below illustrates some of the more often found radicals (Cooks et al., 1990; Shvartsburg and Jarrold, 1996).

Common Polyatomic Ions					
C ₂ H ₃ O ₂	acetate	OH_	hydroxide		
NH4 ⁺	ammonium	C10 ⁻	hypochlorite		
co ₃ 2-	carbonate	NO3	nitrate		
C103	chlorate	$N02^{-}$	nitrite		
C102 ⁻	chlorite	C ₂ O ₄ ²⁻	oxalate		
Cr04 ²⁻	chromate	C104	perchlorate		
CN ⁻	cyanide	Mn04	permanganate		
Cr ₂ 07 ²⁻	dichromate	P04 ³⁻	phosphate		
HCO3-	bicarbonate	\$04 ²⁻	sulfate		
HS04	bisulfate	\$03 ²⁻	sulfite		
HSO3	bisulfite				

Table 1.1: Frequently Used Polyatomic Ions

Source: https://cpanhd.sitehost.iu.edu/C101webnotes/chemical-nomenclature/polyatomsalts.html.

Polyatomic ions or radicals are identical to monoatomic ions in that they are ionized by acquiring or releasing electrons to acquire a charge. They will form an anion if they receive electrons, and a cation if they release electrons. A polyatomic ion's charge is indicated by a superscript located at the ion's top righthand edge. For instance, the chemical formula for the phosphate ion is PO_4^{3-} . This means the whole PO_4 molecule has a -3 charge, and thus when it is used to produce an ionic compound, the whole PO_4^{3-} ion moves and is considered as a single unit. Let us begin by attempting to synthesize a few molecules utilizing phosphate as an illustration. To begin, let us construct a sodium phosphate molecule. Take note that when asked to create compounds based on their names, you can frequently tell when you do have a polyatomic ion. Remember that monoatomic anions are suffixed with '-ide.' Therefore, when you come across a distinct suffix ending, including such '-ate' or '-ite,' you should be aware that you are dealing with radical and check the Table 1.1 to identify and verify the exact ion formula to use. When the charge of the reacting substances are finalized, the formula of the ionic substance comprising of a radical is written as if you are writing the basic binary ionic compound since the radical behaves as one atom (either as cations or anions). For sodium phosphate, this is primarily a compound composed of sodim and phosphate ions. In this case, sodium is a positively charged cation, then it follows that the phosphate is a negatively charged anion (Bates, 1986; Miller et al., 1997). Sodium is Na⁺¹ and from Table 1.1, phosphate ions is written as PO_4^{-3} , thus:

 $Na^{+1}PO_4^{-3} \rightarrow Na_3(PO_4)_1 \rightarrow Na_3PO_4$

The -3 charge of the phosphate ions becomes the subscript of sodium while the phosphate ion will have a charge of -1. As a rule, we do not write -1 as a subscript thus, we write sodium phosphate as Na_3PO_4 .

The chemical formula Na_3PO_4 means that there are three (3) sodium atoms and one phosphate molecule in the structure.. Take note that the resultant molecule is named identically to that of other ionic compounds. The cation's name is given first (in roman numeric where necessary), followed by the anion's name (in this phosphate case). Sodium is a monovalent atom (has only 1 valence or charge, so there is no need to worry about its roman numeral formula.

Let's consider now magnesium phosphate. Magnesium is written as Mg^{2+} ion (Houk and Praphairaksit, 2001; Sakata and Kawabata, 1994), while again phosphate is PO_4^{-3} .

Utilizing the existing process we employ to write chemical formulas (Patil et al., 2020):

 $Mg^{+2}PO_4^{-3} \rightarrow Mg_3(PO_4)_2 \rightarrow Mg_3(PO_4)_2$ Notice that in the final formula, we retain the parenthesis on the phosphate ion since the subscript is greater than 1. The structural diagram of that molecule is presented in Figure 1.10. Keep in mind that each straight line in the phosphate ion represents a covalent link. Each straight line indicates the sharing of pair of electrons between two atoms. Chapter 4 will discuss covalent bonding in greater depth. For the time being, it is significant to realize the radicals behave in unison by the atoms sharing electrons essentially and maintain closeness to one another. The (-) and (+) symbols denote the ionic bonding. The Magnesium phosphate forms a total of six ionic bonds (Lifshitz, 1983) (Figure 1.10).


Figure 1.10: Ionic bonding in magnesium phosphate.

Source: https://www.softschools.com/formulas/chemistry/magnesium_phos-phate_formula/573/.

Another example is mercury (I) chloride since formation of this compound deviates from to the standard bonding procedures. In mercury (I) chloride (Hg(I) Cl or HgCl, it is assumed that based on charge possibilities, it is known that chloride ion have a charge of -1 while mercury (I) is supposed to hold a charge of +1. On the other hand, Mercury is unique in that its single ionized oxidation configuration, mercury(I), is seen as a dimeric cation, Hg₂²⁺, in which two mercury atoms are covalently bound to form a polyatomic ion. Every mercury atom in the bond pair is in the positive charge state. This results in a +2 state for the total ion, as seen below (Wyttenbach et al., 2013) (Figure 1.11):

+Hg—Hg+

Mercury (I) Ion

Figure 1.11: Mercury ions in the Hg-Hg bond.

Source: https://wou.edu/chemistry/courses/online-chemistry-textbooks/3890–2/ch104-chapter-3-ions-and-ionic-compounds/.

This substance lacks a distinctive name which differentiates it from conventional monoatomic cations. As a result, this can be recognized as a diatomic element. For a theoretical chemical formula of Hg_2Cl_2 , the complete chemical formula of mercury (I) chloride requires two chloride ions to stabilize both ions (Figure 1.12).

Cl⁻ + Hg—Hg⁺⁻Cl

Mercury (I) Chloride

Figure 1.12: Bonding of mercury chloride.

Source: https://www.softschools.com/formulas/chemistry/mercury_ii_chlo-ride_formula/463/.

Although mercury (I) chloride is uncommon, it was widely utilized in the 1800s and 1900s as a medication for treating infectious disorders such as yellow fever and syphilis. Additionally, it was taken as a common tonic to induce regurgitation and cleanse the body of 'impurities.' Calomel caused serious negative impacts and cytotoxicity during its medicinal usage, resulting in hair and tooth loss. Indeed, calomel was a popular component in teething powders in the United Kingdom until 1954, resulting in a large amount of mercury poisoning within type of pink illness, which had a fatality rate of one in 10 at the time.. In the United States, the use of calomel declined in the late 1800s as more effective therapies became available, such as Alexander Flemming's late-19th-century discovery of penicillin (Patterson, 1972).

1.6.1. Abraham Lincoln and "Blue Mass"

In the Civil War era, "blue mass," a drug composed of elemental mercury and different additions, was widely utilized to treat a variety of conditions. While mercury was the recognized highly toxic, this was a common component of medical treatment for "hypochondriasis," an illness which encompassed a variety of what we now refer to as mood disorders, as well as digestive system difficulties. Abraham Lincoln was found to suffer from hypochondriasis and was prescribed blue mass medicine. Interestingly, colleagues, and acquaintances reported that he suffered from sleeplessness and mood swings, and there is some indication that he had further neurological problems. These are mercury poisoning symptoms. Within the body, uncharged elemental mercury is converted to mercuric mercury (Hg²⁺), that has a +2 charge. This type of mercury is extremely toxic to a variety of physiological systems, resulting in malfunction that may have contributed to Abraham Lincoln's symptoms. Due to lack of full knowledge on the medicine itself, there is no clear assurance that the therapies have mattered to his recovery or his death.

1.6.2. Naming Polyatomic Ions

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Table 1.1 presents several radicals or polyatomic ions with their charges/ oxidation states. Radicals containing oxygen are generally termed as *oxyanions*. Oxyanions are substances that have one or more oxygen ions. The basic rule on oxyanion nomenclature is that the one with the lesser oxygen atoms usually ends in "-ite" while those having the greater number of oxygen atom usually ends in "-ate". This is usually illustrated by oxyanions that has 2 and/or 3 oxygen atoms in it. Nitrogen and sulfur oxyanions being are excellent examples as shown below:

NO₃¹⁻ is nitrate while NO₂¹⁻ is nitrite;

 SO_3^{2-} is sulfite while SO_4^{2-} is sulfate.

In situations there will only be one oxygen atom is present, the prefix 'hypo-' is utilized ending the name with '-ite'. For four (4) oxygen atoms in the oxyanions, the prefix 'per-' is used then ending it with '-ate'. The chlorinated family of ions is indeed a good illustration of when these prefixes as illustrated in the example below.

- ClO⁻ is referred to as hypochlorite.
- ClO_2^{-} is also known as chlorite.
- ClO_3^{-} is referred to as chlorate.
- Perchlorate is the chemical formula for ClO_4^-

There will be oxyanions that is in combination with hydrogen.

You may come across a "bi-" prefix on occasion. This is an ancient prefix that signifies the chemical may both pick up and losing a proton (H⁺). The IUPAC nomenclature would utilize hydrogen in the name, but the earlier nomenclature would use the "bi-" as a prefix. In both instances, the oxyanion will also have a hydrogen atom in it, reducing its charge by one. When Carbonate (CO_3^{2-}) is combined with Hydrogen to form another radical, it is then names as Hydrogen carbonate (HCO_3^{-}) or simply bicarbonate, thus, Hydrogen carbonate is also known as bicarbonate (Kollman et al., 1975).

Another prefix found to accompany names of oxyanions is "thio-" which is used when the oxygen in an oxyanion is replaced with sulfur.. This is illustrated by Cyanate or OCN⁻, of which, replacing O with S becomes SCN⁻ or thiocyanate.

Ionic compounds containing polyatomic ions are named in a similar manner extras that of the binary ionic compounds. Similarly, the cation name goes first (with roman numerals when required), followed by the name of the anion or the radical (Yoder, 2006).

1.7. PROPERTIES AND FORMATION OF IONIC COMPOUNDS

Electrostatic forces caused by the pull of positive charge cations and negative charges anions hold ionic compounds together. These can be simple ions, such as chloride (Cl) and sodium (Na⁺) or polyatomic species, such as carbonate (CO_3^{2-}) and ammonium (NH_4^+) ions in ammonium carbonate. Ions in an ionic compound typically are in optimum distances from each otehr, forming part of a continuous three-dimensional structure or lattice, which is frequently crystalline (Goodenough et al., 1961; Patil et al., 2016) (Figure 1.13).



Figure 1.13: (A) NaCl Crystal Lattice.) A common ionic compound, sodium chloride, NaCl, has a crystal structure. The purple spheres are sodium cations (Na^+) , whereas the green spheres are chloride anions (Cl). (B) Evaporation of salty water results in the formation of halite, the crystalline form of sodium chloride.

Source: https://en.wikipedia.org/wiki/Ionic_compound.

Salts is another term denoted for binary ionic compounds. Any substance that is made up of a metal and a non-metal atom held together by electrostatic or ionic bonds can be classified as a "salt". In short, NaCl, MgCl₂, FeCl₃, even Na₂SO₄ and FeNO₃ all falls under one classification, which is, they are all salts. Salts and ionic substances, in general, are often hard and brittle, having high boiling and melting points. They are normally electrically insulated

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as solids, but when dissolved or melted, the ions become mobilized and exceedingly conductive. Electrolytes are ions that have been mobilized in a solution and have the ability to conduct electricity (Baker et al., 1949; 1950; Butts and Smith, 1987).

1.8. ARRHENIUS ACIDS AND BASES AND THEIR ROLE IN SALT FORMATION

Acids are ionic substances that contain hydrogen ions (H⁺), while bases include oxide (O_2)⁼ or hydroxide (OH⁻) ions. Arrhenius acids and bases are some of the most important actors in acid-base chemistry and salt formation. An Arrhenius acid, is a substance that raises the amount of hydrogen (H⁺) in aqueous medium. Thus, acids are compounds which, when dissolved in water, releases hydrogen ions in the solution. On the other hand, an Arrhenius base is a substance which when dissolved in water, releases hydroxide ions (OH⁻). Many bases are ionic compounds with hydroxide as an anion (Anderson et al., 2005; Tarhan and Sesen, 2012; Zhang et al., 2019).

The strongest bases are those hydroxides of that contain alkali and stronger alkaline earth metals (Kolb, 1978; Hawkes, 1992).

STRONG BASES			
Name	Structure		
Group 1A metal hydroxides	LiOH, NaOH, KOH, RbOH, CsOH		
Heavy Group 2A metal hydroxides	Ca(OH) ₂ , Sr(OH) ₂ , Ba(OH) ₂		

When an Arrhenius acid and Arrhenius base reacts, the process is generally called neutralization, which gives way to the formation of salt and water. Thus, on way to produce salts is by neutralization process. On the other hand, slats formed out of neutralization process are classified as weak salts or salts that tend to be dissolved easily or separated as ions through ordinary chemical reactions. Arrhenius acids' structures may include either binary compounds or polyatomic anions, their naming system is a bit more difficult. When distinguishing acids from binary compounds, the prefix 'hydro-' is being considered to designate the cation H⁺, while the suffix '-ic' plus the term acid indicates that it is an acidic form. The element name of the anion may be used directly, as Hydrobromic acid or HBr, or it can be modified by omitting the '-ine,' '-ous,' or '-ogen' suffix and substituting '-ic acid,' as in hydrochloric acid (HCl), Hydrocyanic acid acid (HCN), and hydrofluoric acid (HF).

Acids comprising of oxyanions on the other hand does not require prefixes.. Instead, the ending is just changed to -ic for higher oxygen atomcontaining substand and it should end with -ous for the lesser oxygen atom-containing substance, then added by the word "acid". As implied by the name, nitric acid (HNO₃) and sulfuric acid (H_2SO_4) is attributed the presence of polyatomic anions nitrate and sulfate in combination with hydrogen.. In another example, is denoted by HNO₂, while carbonic acid is denoted by HCO₃. The prefixes 'hypo-' and 'per-' are also restored in the acid nomenclature for elements having many oxyanion states. For example, the chlorine-containing oxyanions may create the following acids (de Vos and Pilot, 2001; Ouertatani et al., 2007):

- Chlorinated water (HClO₃); chloric acid
- Hydrochloric acid (HClO₂); hypochloric acid
- (HClO_{4}) perchloric acid
- (HClO) hypochlorous acid

They are all distinct from binary chlorinated acids. HCl is an abbreviation for hydrochloric acid. Acidic solutions are those that totally degrade into their ionic states in solution. Table 1.2 is a list of common strong acids (Drechsler and Schmidt, 2005; Paik, 2015).

Table 1.2: Strong Acids and Their Structures (Brønsted, 2013; Munjal andSingh, 2020)

STRONG ACIDS		
Name	Structure	
Perchloric Acid	HCIO ₄	
Chloric Acid	HCIO ₃	
Hydrochloric Acid	HCI	
Hydrobromic Acid	HBr	
Hydroiodic Acid	HI	
Nitric Acid	HNO ₃	
Sulfuric Acid	H ₂ SO ₄	

1.9. IONS, NEURONS, AND NEURON IMPULSES

Ions have a variety of critical roles in living organisms, including cellular metabolism, muscle contraction, and ATP energy synthesis, but one of the most critical is probably in brain function. The brain is a very complex structure made up of billions of microscopic neurons. A neuron, also known as a nerve cell, is an excitable (electrically charged) cell that receives, analyzes, and sends information through chemical and electrical impulses. These impulses are sent between neurons through synapses, which are specialized connections. Neurons may link to build incredibly complex pathways in the brain and circuits (Mahowald and Douglas, 1991; Spitzer, 1991). Neurons are the basic building blocks of the central and peripheral nervous systems (brain and spinal cord) (autonomic nervous system and somatic nervous system).

Some neurons may be divided into different types depending on their form, location, or function (see Figure 1.14). Sensory neurons respond to particular stimuli such as light, touch, and see sound, or any other stimuli that impact sensory organ cells, and convert them into electrical impulses that are subsequently sent to the spinal cord or brain through transduction. Motor neurons take information from the brain and spinal cord and use it to control a wide range of actions, from muscle contraction to glandular production. In neural networks, interneurons link neurons in the same area of the spinal cord or brain (Nicholls and Kuffler, 1964; Viana et al., 2002).



Figure 1.14: Illustrations of various forms of neurons.

Note: (a) Olfactory neurons have become so termed because of their role in the sensation of smell. (b) In the cerebellum, the Purkinje cell is named for the person who discovered it. (c) Pyramidal neurons are multipolar cells with a cell body that resembles a pyramid. They are present in the cerebral cortex.

Source: https://www.pinterest.com/pin/42573158966224457/.

A neuron is made up of an axon, (soma)cell body, and dendrites (see Figure 1.15). The term neurite can refer to just an axon, or dendrite especially when it is in undifferentiated phase. Dendrites are microscopic frameworks that develop from the cell body, typically reaching hundreds of micrometers in length and branching several times to create a complex "dendritic tree." An axon (alternatively called a nerve fiber) is a form of cellular extension (procedure) that originates from the cell body at a site called an axon hillock and extends up to one meter in humans and much beyond in other species. The dendrites of the majority of neurons receive signals and convey them along their axons. Before an impulse may be carried down the axon, the dendrites must always gather and provide a threshold signal to the axon hillock. If the signal is sufficiently strong at the axon hillock, a single all or none neuron impulse is sent down the axon, resulting in the release of neurotransmitters into the synaptic cleft (see Figure 1.16) (Krishnan et al., 2009).



Figure 1.15: Neuron anatomy.

Note: The neuron is seen in the figure, along with axon extensions, typical dendrite, and its core cell body (soma). Outside signals are normally received by a neuron's dendrites, and the axon is utilized to deliver the chemical pathway to later target cells in the communication route.

Source: https://askabiologist.asu.edu/neuron-anatomy.



Figure 1.16: Neuronal signaling.

Note: Figure 1.16 illustrates how neurons communicate with one another following the discharge of the working potential all along axon of a presynaptic neuron. Secretory vesicles carrying neurotransmitters including like serotonin and dopamine are released from the axon terminal into a synaptic cleft, wherever they connect along sensors on the soma or dendrite of the post-synaptic neuron.

Source: https://slideplayer.com/slide/9765217/.

Numerous axons are frequently bundled together to form fascicles, which generate the nerves of the peripheral nervous system (such as strands of wire makes cables). Tracts are packets of axons located in the central nervous system. A neuron's cell body usually produces many dendrites but not more than an axon, despite the fact that the axon might split numerous times before terminating. The most of synapses transmit signals from one neuron's axon to another's dendrites. There are, however, several alternatives to these rules: neurons might be devoid of dendrites or axons, and synapses can link a dendrite or an axon or to another axon or dendrite (Orkand et al., 1966; Yogeeswari et al., 2004).

Neurons develop a resting negative potential inside their cells in order to become excitable cells capable of transmitting an electric signal. This is performed by isolating cations and anions at various amounts within (intracwlluar) or outside the cell (extracellular). That results in a resting state of -70 mV within the cell. As a result, the cell is polarized or negatively charged. The neuron generates this resting negative potential mostly via the Potassium (K⁺)/ Sodium (Na⁺) ATPase Protein. That protein is anchored in all neurons' plasma membranes, where it acts as a pump. Protein pumps utilize energy to actually transport molecules from all over plasma membrane in opposition to their concentration gradient. Adenosine triphosphate (ATP) is the energy source for this activity. Three sodium ions are pushed out of the cell and two potassium ions are injected into it for each ATP molecule that is degraded into adenosine diphosphate (ADP) (Figure 1.17). This results in an electrochemical gradient between the outside and interior of the cell, with a high amount of sodium ions on the outside and a higher proportion of potassium ions on the inside. Calcium ions, meanwhile, collect on the neuron's surface. Additionally, the interior of the cell contains many organic anions and phosphate anions, which contribute to the cell's significant resting negative potential of -70 mV (Somjen et al., 2008). These phenomenon inside highly specific in terms of location and process. The pumping of sodium and potassium inside and outside the cells takes place in what is termed as "sodium-potassium channels" which are utilized by sodium and potassium only. Same with calcium receptors that are only found within the neuron's surface.

All neurons express the Na⁺/K⁺ ATPase pump, which is always trying to retain this gradient. Indeed, it's one of the primary energy consumers in the body, accounting for over 20% of total energy consumed each day. The establishment of this gradient of concentration enables neurons to connect with downstream specific cells by transmitting electric pulses down the cell axon. This allows us to understand, functionate our muscles, and experience our environment via touch, hearing, smell, and sight.



Figure 1.17: The sodium-potassium ATPase pump is depicted. The Na^+/K^+ ATPase pump utilizes the energy contained in ATP to pump three Na^+ out of the cell and two K^+ into it. These gradient permits neurons to maintain an internal resting potential of -70 mV.

Source: https://wou.edu/chemistry/files/2018/12/atpase-pump.png.

A neuron must have a wave of positive current flowing down its axon in order to create a neuron impulse. When it reaches the axon's terminal, it signals the release of neurotransmitters such as dopamine, serotonin, or glutamate into the synaptic cleft. These tiny chemical messengers are employed to connect with the muscle cell or neuron in the downstream direction. Ion channels serve a critical part in the generation of the neuron impulse within the neuron. Ion pathways are proteins implanted in the neuron's plasma membrane that generate a pore big enough to permit the passage of certain ions. Ion states do not require energy and can just promote the movement of ions along their gradient of concentration from a region as of higher concentration to a region of lower concentration (Falk et al., 1997; Ryan and Herrington, 2014).

Two types of ion channels are necessary for the production of a neuron impulse: receptor/ligand-activated gateways and voltage-gated channels. Again, in the case of a receptor/ligand-activated gate, a small chemical messenger (often referred to as a ligand) connects to the receptor and produces a shape change in the receptors, hence going to open an ion channel. These receptors are often found on a receiving cell's dendrite, where they communicate with neurotransmitters. Once bound to a neurotransmitter, the receptor opens a calcium channel, allowing calcium ions to enter cells fast, thereby lowering the negative charge in the immediate vicinity. When the charge inside the neuron approaches zero (or becomes more neutral), a depolarization event happens (Champion et al., 1967; Friedrich and Kreutz, 2020).

If powerful enough, this localized depolarization event can activate nearby sodium channels of voltage gate (Figure 1.18). When the charge in the adjacent area is transferred, these channels open in response to the neuron's charge state. At this point, the voltage-gated sodium channels will undergo a structural change, enabling sodium ions to move into the cell faster and along the concentration gradient. This leads the neuron to deprotonate even more, causing other voltage-gated sodium channels to open nearby. When the charge potential of the neuron reaches neutrality and becomes positive (approximately +30 mV) on the inside, the sodium channels of voltage-gated sodium channels undergo another conformational change, closing the channels and inhibiting sodium ion intake. At this point, the voltage-gated potassium channels are open, enabling potassium ions to exit the cell across a concentration gradient (Nagaoka et al., 1994; Muráth et al., 2018) (Figure 1.19).





Note: (A) Neurotransmitters sent from of the axons into the synapse bind to the receptor, causing the receptor to alter the conformation and activate the calcium ion medium. Ca^{2+} enters the cell through its concentration gradient, resulting in localized depolarization. (B) At the time of resting position of the cell, a receptor is in the closed conformation. Outside the cell, the calcium ion concentration is high, but inside the cell, the anion concentrations cause a -70 mV resting condition.

Source: https://wou.edu/chemistry/files/2018/12/ Receptor-activated-channel. png.



Figure 1.19: Voltage-gated ion channels.

Note: (A) Whenever the neuron is at rest, the voltage-gated sodium channels are closed. The cellular depolarization caused by neurotransmitter activation induces the voltage-gated sodium channels to experience a change in conformation, activating the sodium channel and enabling Na^+ to enter the cell. The voltage-gated Na^+ channels shut owing to an extra conformation change whenever the cell charge goes to positive (about +30 mV) and enter a refractory phase when they cannot be reopened. The protein structure is restored to its resting state when the charge level inside the neuron is reduced to -70 mV. (B) At the time of the state of the rest of the neuron, the voltage-gated potassium channel is closed, and it is not active until the cell polarity switches to roughly +30 mV. Potassium ions flow off to the cell, along concentration gradient, and return the neuron's resting potential to -70 mV after activation.

Source: https://www.news-medical.net/health/Importance-of-Ion-Channels-in-the-Body.aspx.

The voltage-gated potassium channels open, restoring the neuron's negatively resting potential. An ion gradients, though, are out of proportion at this moment, by high sodium states within cell and high potassium states out of the cell. This results in a time of total refractoriness, during which the neuron could not be awakened. After the potassium channels reopen and the

neuron's negative potential is recovered, the neuron undergoes a relative refractory phase in which eliciting a new function potential is difficult but not impossible (Liu et al., 2018; Zhang et al., 2019). The pumped of Na⁺/ K⁺ ATPase repairs the ion gradient during this period, causing sodium to be pushed out of the cells and potassium to be driven back in. The neuron has been restored and is fully responsive to receive another signal at this moment. The working potential depolarization event may be connected with the opening and closure of certain ion networks, which can be shown visually in terms of voltage over time. Within 4–5 milliseconds, the whole impulse can be completed (mS) (Figure 1.20).



Figure 1.20: Graphic illustration of a nerve impulse.

Note: A neuron's resting state potential is -70 mV. Whenever a cutoff of -55 mV is reached on the axon hillock, the neuron impulse is transmitted down the axon. This opens the voltage-gated sodium channels all along the axon, allowing neurotransmitters to be released from the axon terminal. Whenever the cell potential rises to +30 mV, the voltage-gated sodium channels closes and becomes refractory. This also causes the voltage-gated potassium channels to open, reestablishing the neuron's resting state potential. At the time of relative refractory phase, the Na⁺/K⁺ ATPase Pump recovers the K⁺ and Na⁺ gradients inside the neuron, allowing the neuron to completely recover and fire one other neuron impulse (Zhang et al., 2018; Mohsin, 2000).

Source: https://www.researchgate.net/figure/Generation-of-nerve-impulse-2_fig6_269168110.

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The refractory time at one region in the neuron also permits the depolarization event to go from the neuron's dendrites to the cell body in a directed manner. If the signal is significant enough just to instigate depolarization of the neuron, then the neuron impulse will be generated and delivered down the neuron's axon. The discharge of neurotransmitters to the synaptic cleft signifies the stimulation of downstream neuron or target cell (Sawatzky et al., 1976; Guo et al., 2014).

It's significant to mention that these are just two cases of how ion channels might be controlled. Cell's physical movement, like that of hair cells in the inner ear, or other chemical changes, such as phosphorylation, can also activate certain ion channels. Several ion channels are weak and always open, allowing ions to travel slowly and continuously across the membrane. This regulates osmotic pressure and prevents it from rising to unsafe levels, akin to having an overflowing gate on your bathtub to prevent the water from rising too high and overflowing (Rode and Foster, 1962; Haaland et al., 2000).

1.10. CHAPTER SUMMARY

When an atom gain one or so more electrons, it becomes a negatively charged anion. When an atom loses one or more than one electron, it becomes a cation, which is positive charge particle. Cations are formed by metals, while anions are formed by nonmetals. These positive and negative charges approach one other, creating ionic bonds, since opposite charges are attracted (while like charges repel). Ionic chemicals are the consequence of this process. Binary ionic compounds, or those with only two atoms, one functioning as the cation and one acting as the anion, are the simplest ionic compounds (Bosman and Havinga, 1963; Duchateau et al., 1991).

The "Octet Rule" refers to an atom's inclination to form a state in which it has eight valence electrons. An ion of a separate atom (or two separate ions) which have the similar electronic configuration are referred to be isoelectronic. Of becoming isoelectronic with noble gas as in preceding row (period) just on chart, cations release electrons. With noble gas in the same line as the anion, anions gain electrons and become isoelectronic. The periodic table could be used to forecast the elements' common ion states (Bidlingmeyer, 1980; Sato et al., 2016).

Electron dot drawings is used to depict electron motions during the creation of ionic bonds. Ionic compounds that are stable have a balance charge state, meaning that the charge on the entire molecule is zero. The cation is usually first in chemical formulations, whereas the anion has always been last. Chemical formulae for stable compounds must be stated in such a way that the entire compound has full neutral charge (that is, the entire positive charge equals the entire negative charge). Subscripts are being used to indicate the number of atoms in ionic formula. Chemical formulae are always simplified to reflect the smallest number of cations and anions necessary for the formation of a single compound (Pauling, 1928; Sherman, 1932).

The element name is followed by the term 'ion' to designate cations. If a cation has much more than one ionic form, Roman numbers are appended after the element name. Anions are given their names by substituting the last section of the element name with suffix '-ide' preceded by the word 'ion.' While name an ionic compound, the cation name comes firstly, preceded by the anion name (adding roman numerals if necessary). Polyatomic ions are ions which are made up of many covalently linked atoms. When it comes to ionic bonding, polyatomic ions are named in the same manner as binary ionic compounds are named. The cation's name appears first (with roman numerals if required), followed by the anion's name (Wagner, 1972; Naah and Sanger, 2012).

Solid ionic compounds, rather than individual molecules, create a complete three-dimensional net or lattice, generally in a crystalline structure. Ionic compounds are often rigid and brittle, with high and boiling and melting temperatures. They are usually electrically insulating as solids, but then when melted or dissolved, the ions are mobilized, and they become extremely conductive. Electrolytes are ions that have been mobilized in a solution (Benedetto et al., 2014).

Ionic materials containing hydrogen ions (H⁺) are categorized as acids, whereas those containing hydroxide (OH) or oxide (O₂) ions are classified as bases, according to the Arrhenius criteria. Salts are all other ionic substances that do not include these ions. Basic ionic compounds and salts are named according to conventional ionic nomenclature principles. For acids that does not their bonds are considered to be covalent, where a very week electrostatic force exist due to the varying electronegativities of the combining ions, thus they can be named in a synonymous as that of ionic substances. The prefix 'hydro-' is used to denote the cation H⁺ in labeling acids from binary compounds, while the suffix '-ic' acid is being used to show that it is an acidic form. When a polyatomic ion is present in an acidthe radical/anion's

name that ends in "ate" is changed into "-ic" then the word "acid, while the radical/anion's name that ends in "ite" is changed ""-ous" adding again the word "acid" as the acid last name. For radicals with multiple oxyanion states, the prefixes 'hypo-' and 'per-' are also kept in the acid nomenclature (Politzer et al., 2010).

Neurons are excitable (electrical) cells that create nerve impulses termed neuron impulses via ion gradients. Ion gradients are established within the neuron via ion pumps such Na⁺/K⁺ ATPase Protein. Ion pumps move ions through the cell membrane as against with a concentration gradient using energy. This results in a -70 mV rest membrane voltage within the neuron, as well as a state where Na⁺ is abundant outside cell and K⁺ abundant inside the cell. Facilitated diffusion is used by ion channel proteins to move ions from across plasma membrane and down respective concentration gradient. Neurotransmitters bind to receptor/ligand ion pathways in dendrites of a neuron, causing depolarization of the targeted area. Na⁺ can enter into the cell and produce additional depolarization when voltage-gated sodium receptors are activated. The neuron impulse is produced at the axon terminal, and neurotransmitters are released if a cell depolarizes to -55 mV just at axon hillock. The activation of potassium channels of voltage-gated resets the neuron's resting potential. The Na⁺/K⁺ ATPase pump will then be used to readjust the ion gradients in the neuron, preparing it for the next signaling event. The entire procedure takes about 4-5 milliseconds. In humans, brain signaling accounts for around 20% of overall energy use (Butts and Smith, 1987).

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2

CHARACTERISTICS OF IONS AND IONIC COMPOUNDS

CHAPTER

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2.1. INTRODUCTION

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The term ion derives from the Greek word ion, the neuter present participle of ienai "to go," which comes from the *pie* root *ei⁻ "to go." A cation is anything that goes downward, while an anion is something that moves upward. The name comes from the fact that ions gravitate toward the electrode with the opposite charge. Michael Faraday, an English physicist, and chemist used the term electromotive force in 1834 to describe an unidentified species that travel from one electrode to the other across an aqueous medium. Faraday was unaware of the nature of these species. Still, he was aware that, because at one electrode, metals dispersed into and goes into a solution, and at the other electrode, new metal emerged from a solution, that substance had moved across the solution in the form of a current at that electrode (Suni et al., 2008). This is the method of transporting stuff from one location to another. He also invented the terms cation and anion to refer to ions attracted to and repealing the corresponding electrodes.

Ions are charged particles that take electrical charges; however, in concentrated phases, they occur as electrically neutral sequences of negatively and positively charged particles known as anions and cations. Cations and anions are positively and negatively charged particles that carry electrical charges. Even though water is the most common solvent, ions may be found in a variety of different environments, including mixed and nonaqueous solvents, as well as condensed phases devoid of any solvents, such as molten salts and ionic liquids (Miyasaka et al., 2010).

An electrolyte is a chemical substance with a neutral combination that is proficient in dissociating (almost entirely) into its fundamental ions when exposed to the appropriate conditions. The subscript 2 denotes a quantity referring to an electrolyte, I denote a quantity concerning an ion, and Iz denotes a quantity about a generalized ion.

2.2. ISOLATED IONS

Isolated ions live in a perfect gaseous state, with no interaction with their environment or with one another. They have numerous charges of the fundamental units $e = 1.60218 \times 10^{-19}$ C, denoted by the symbol zI. The mass of ions mIis commonly described in Avogadro's number NA = 6.02214 $\times 10^{23}$ mol⁻¹ (a mole) of ions, atoms or particles. When it comes to shape and form, monatomic isolated ions, are characteristically round or spherical (Jain

et al., 2015 ions that are composed of multiple atoms, the shape can vary based on the elongations brought about by the interaction of the electron clouds. The most common and frequent molecular shapes are tetrahedral (NH_4^+) , planar (NO_3^-) , while some are elongated such as $(SCN^-, \text{ octahedral } (Fe(CN)_{4_-}^6))$, or more irregular $(CH_3CO_2^-)$. Since its outer electrons spread in a random manner, it is impossible to determine an isolated ion's size (radius) (Figure 2.1).





Figure 2.1: Isolated transition metal ions.

Source: https://www.sciencedirect.com/science/article/abs/pii/ S0021951702001070 (Marcus, 2012).

The standard molar Gibbs energy and formation enthalpy, fG(Iz,g) and fH(Iz,g), from the elements in their standard states, as well as their standard molar entropy and constant pressure heat capacity, S(Iz,g) and CP(Iz,g), all at $T = 298.15^{\circ}$ K, are all reflective of its stable state. The ionization potential, denoted by the symbol Ip, is the energy necessary to convert a neutral particle into a cation. There have also been reports of these energies in electron-volt units (1 eV/particle = 96.483 kJ mol⁻¹), obtained for many different types of ions (Marcus, 2012).

The vast majority of ions are diamagnetic, and their molar magnetic vulnerabilities, Im, range from a few to several 100 times the value of -10^{-12} mol⁻¹. Because paramagnetic ions contain unpaired electrons, their molar magnetic sensitivities are $1.676n(n + 2) \times 10^{-9}$ m³ mol⁻¹ at 298.15°K. To acquire the molar refractivity of a neutral species, the polarizability of

an ion I = $(3/4NA)RI = 3.964 \times 10^{-25}$ RI is measured experimentally and the polarizability of an ion I = $(3/4NA)RI = 3.964 \times 10^{-25}$ RI is derived empirically from the refractive index nD of neutral species. Each of the constituent ions has an additive effect, and the individual ionic values are calculated using the random amount of Na⁺ ions: $0.65 \times 10^{-6}m^3$ mol⁻¹ is a unit of volumetric concentration (Wasserscheid and Keim, 2000).

2.3. DISSOLVED IONS

It is possible to achieve the effect of infinite dilution by combining an insignificant amount of electrolyte with a limited amount of solvent. In this state, the ions are separated from one another and merely encircled by the individual ion, and solvent amounts are consequently additive to one another. They are weighted in the electrolyte based on their stoichiometric coefficients: cations Cz+ and anions Az-, where cations Cz⁺ = anions Az⁻ and anions Az⁻ = cations Cz⁺ (Kang et al., 2014) (Figure 2.2).



Figure 2.2: A classic example of dissolved ions.

Source: https://socratic.org/questions/52f1151702bf34733dc14e7e.

Because the water molecules in aqueous solution are orientated toward the cations, tiny multivalent cations, for instance, transition metal cations and Mg^{2+} form coordinate bonds in the first hydration shell, which is particularly important for transition metal cations (Hem and Minear, 2012). These water molecules create hydrogen bonds with molecules in the surrounding environment in a second hydration shell. For other cations, for example, alkali metal cations and the Ca²⁺, the number of coordinated water molecules is not a fixed quantity but rather a random dispersal with a small average number of water molecules.

Anions have hydrogen atoms drawn to them by the water molecules in aqueous solutions, resulting in hydrogen bonds. Multivalent anions, for example, CO_3^{2-} , are particularly well hydrated due to water molecules. Additionally, anions, $H_2PO_4^-$ or HSO_4^- can contribute hydrogen bonds to neighboring water molecules (Mansfeld and Gilman, 1970).

Although $(C_6H_5)_4B$ - and other ions and hydrophobic groups in their perimeter surrounding a hidden charge are normally only moderately hydrated, their presence in the water structure improves it.

2.4. SIZES OF IONS

In crystals, the interionic distances, which are on the order of 0.2–1.0 nm, are assessed with an accuracy of 0.0001 nm by diffraction of x-rays and neutrons and are rather regularly preservative in the sizes of the ions in the crystal. The separation of interionic lengths into ionic radii rI is dependent on the geometry and coordination number while geometry itself is dependent on the coordination number (Marcus, 2012). A "chosen" set of ionic radii, rI, for those coordination numbers that correlate to the hydration of ions has been supplied for those coordination numbers (Marcus, 2012). The radius of polyatomic ions that deviate significantly from a globular form is a subject of debate (Figure 2.3).



Figure 2.3: Sizes of different ions in picometer.

Source: https://en.wikipedia.org/wiki/Ionic_radius.

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Aqueous salt solutions have also been studied using diffraction techniques, which have been used to determine the distances dI-O among the center of anions and the center of the oxygen atoms of nearby water molecules. They have got a 0.002 nm mean uncertainty, and if the length of a water molecule, rW = 0.138 nm, is subtracted from the dI-O values, the results are consistent with the rI set for the "bare" ions, as highlighted by Marcus (1988) and the findings are quite consistent with the rI set for the "bare" ions.

In a solution of volume V, the real volume to be ascribed to an electrolyte in solution is its partial molar volume, which is $V_2 = V_2 + m_2(V_2/m_2)T$, where $V_2 = (V - n_1V_1^*)/n_2$ is its apparent molar volume in a solution of volume V made up of n_2 mol of electrolyte and n_1 mol of water, and $m_2(V_2/m_2)T$. Assuming that the solute has a density of M_2 and that the molality of the solution is m_2 , $V_2 = M_2 + 1,000(-1)/m_2$, where M_2 is the molar mass of the solute and 1* is the density of pure water. $V_2 = V_2$ when the extrapolation is made to infinite dilution; the contributions of the anions and cations, V(Iz, aq), are additive when this is done (Seredych et al., 2008). To divide the observed V_2 into such components, at 298.15°K, the value V(H⁺, aq) = 5.4 cm³ mol⁻¹ has been acknowledged as an acceptable, plausible approximation. According to the authors, the ionic values stated have an uncertainty of a minimum of 0.2zI cm³ mol⁻¹. It should be noted that the values of V(Iz, aq) for multivalent cations and some cations are negative; as a result, such cations induce significant electrostriction (Marcus, 2012).

2.5. PROPERTIES SHARED BY IONIC COMPOUNDS

When negative and positive ions attract each other in an ionic bond, the characteristics of ionic compounds are determined by how strongly the ions attract each other. The following characteristics are also seen in ionic compounds (Goodenough et al., 1961).:

2.5.1. They Form Crystals

Ionic chemicals, as opposed to amorphous solids, crystallize into lattice structures. Even though molecular compounds may crystallize, they commonly do so in various ways, and molecular crystals are generally softer than ionic crystals in their structure. Ionic crystals are regular structures at the atomic level, with the anion and cation varying and generating a 3-D structure based mostly on the smaller ion filling in the spaces among the bigger ion in an even and consistent manner (FJ et al., 1993).

2.5.2. They Have High Boiling Points and High Melting Points

It is necessary to heat ionic compounds to high temperatures to reduce the attraction between the negative and positive ions. As a result, a significant amount of energy is required to melt or bring ionic substances to a boil (Zhang et al., 2019).

2.5.3. They're Brittle and Hard

It is difficult to separate negative and positive ions in ionic crystals because they are strongly attracted to each other. Ions with identical charges may be pushed closer when pressure is applied to an ionic crystal. The electrostatic repulsion between atoms and molecules can be sufficient to fracture a crystal, which is why ionic solids are also fragile (Shamshina et al., 2015).

2.5.4. They Conduct Electricity When They Are Dissolved in Water

Dissociated ions, when ionic substances are dispersed in water, are free to carry electric charge via the solution. It is also possible for molten ionic compounds to conduct electricity.

2.5.5. They're Good Insulators

Ionic solids do not conduct electricity well, even though they conduct well in molten form or in aqueous solution. This is because the ions are closely bonded to one another.

2.5.6. A Conventional Household Example of Ionic Compound

Table salt, also known as sodium chloride, is a common example of an ionic substance. Salt has a melting point of 800°C, which is quite high. Saline solutions conduct electricity far more readily than a salt crystal, which acts as an electrical insulator. Molten salt has the additional property of becoming a conductor. If you look closely at salt crystals under a microscope, you can see the regular cubic shape that results from the crystal matrix. Salt crystals are hard and fragile; it is simple to break a salt crystal. Solid salt does not have a discernible flavor, even though it has a small vapor pressure and does not emit any odor (Sarmiento et al., 2013).

Sugar, on the other hand, is a covalent complex. It has a melting point that is lower than that of salt. It disperses in water but does not dissociate into ions, resulting in a solution that does not conduct electricity. Sugar crystallizes, and its sweetness may be detected due to its high vapor pressure as compared to other substances (Gorter et al., 1970).

2.6. PHYSICAL PROPERTIES OF IONIC COMPOUNDS

2.6.1. Melting Points

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Ionic crystal lattices are extremely electrostatically strong due to many simultaneous interactions between anions and cations during the formation process. It is necessary to apply considerable amounts of energy to the melting process of an ionic compound to completely break all the ionic bonds present in the crystal structure. For instance, the melting point of sodium chloride is around 800°C. In comparison, the ice melts at 0°C (Deetlefs et al., 2006).

2.6.2. Shattering

Ionic compounds are hard yet fragile in general. Why? A substantial amount of mechanical force is required to induce one layer of ions to move comparatively to its neighbor, such as smashing a crystal with a hammer. However, when this happens, it draws together ions with the same charge (see Figure 2.4). The crystal shatters due to the repulsive interactions between like-charged ions. Due to the regular layout of the ions, when an ionic crystal fractures, it prefers to do so alongside smooth surfaces (Zhang et al., 2018).



Figure 2.4: (A) The crystal of sodium chloride is demonstrated in two dimensions. (B) When a hammer strikes a crystal, the negatively charged chloride ions are pushed close to one other, causing the crystal to break due to the repulsive force.

Source: https://flexbooks.ck12.org/cbook/ck-12-chemistry-flexbook-2.0/section/8.9/primary/lesson/physical-properties-of-ionic-compounds-chem/.

2.6.3. Conductivity

The electrical conductivity of ionic compounds is another unique attribute that distinguishes them from covalent compounds. Figure 2.5 depicts three tests wherein two electrodes attached to a light bulb are put in beakers holding three distinct chemicals, each connected to a different light bulb.



Figure 2.5: (A) Water that has been distilled does not conduct electricity. (B) A solid ionic substance does not carry electricity either. (C) An ionic compound dissolved in water conducts electricity effectively.

Source: https://encyclonetcultuland.blogspot.com/2018/11/ion.html.

The distilled water in the first beaker does did not conduct electricity, thus, does not carry a current because it is not a conductor of electricity, in the first place. It is made up of molecules of water that is theoretically neutral. Similarly, solid sodium chloride does not carry out a current in the second beaker, because the ions are still strongly bonded with each other. Even though the ions are ionic and therefore made of charged particles, the solid crystal lattice prevents the ions from moving among the electrodes and vice versa. In the 3rd setup, solid sodium chloride was dissolved in water which dissociates the compound into Na⁺ ions and Cl⁻ ions and are completely dispersed in water(Fumino et al., 2011). The dissociation of table salt into positive and negative ions disrupts the crystal lattice and what we now have
is a stream of distinct negative and positive ions are free to wander about in space. When a load, say a lightbulb was connected into the solution, the positive and the negative terminal of the lightbulb becomes an electrode that interacts directly to the positive and negative ions in the solution. When ions interact with electrodes electrons are travel from one terminal to another generating electricity. When ions migrate within the solution, electrons flow from one electrode to another, causing a potential difference. (Figure 2.6).



Figure 2.6: The A⁺ ions move towards the negative electrode in an ionic solution, while the B ions migrate towards the positive electrode.

Source: https://encyclonetcultuland.blogspot.com/2018/11/ion.html.

2.6.4. Characteristics

In the case of charged objects, opposite charges attract while like charges repel.. These phenomena can be well represented by the trajectories deflected by the magnetic field when in motion (Rogers, 2007).

Atoms and molecules with loose electrons are smaller in size than those without looseelectrons because electrons have a lesser mass and, as a result, have greater space-filling characteristics as matter waves. Consequently, anions are bigger than the parental atom or molecule since the surplus electron(s) resist each other and contribute to the physical size of the ion, which is defined by the electron cloud around it. Because of the reduced size of the cations, the electron cloud is significantly smaller than their equivalent

parent atoms or molecules. When it comes to hydrogen, one cation (that of hydrogen) does not contain any loose electrons. The electrons of hydrogen are paired in the energy level where it is located so its radii is more intact and smaller and thus is composed solely of a single proton, which is much lesser than the paternal hydrogen atom (Maksimov et al., 2004).

2.7. CATIONS AND ANIONS

"Anion" is a misnomer. It's not to be associated with Anyon, a quasiparticle (Figure 2.7).



Figure 2.7: Ionic properties of hydrogen.

Note: The hydrogen atom comprises a single electron and a single proton. Thus, it is the most basic element. The removal of electron results in a cation (on the left), while the accumulation of an electron results in an anion (on the right) (right). With its lightly maintained two-electron cloud, the radius of the hydrogen anion is significantly bigger than the radius of the neutral atom, which is significantly larger than the radius of the naked proton of the cation (Zhang et al., 2019).

Source: https://en-academic.com/dic.nsf/enwiki/10982658.

An anion (/na.n/ ANN-eye-n, from the Greek word v (án), which means "up") is an ion that has more electrons than protons, resulting in a net negative charge. An anion (/na.n/ ANN-eye-n). As the name suggests, a cation (/ ktai.n/ KAT-eye-n, from the Greek word (káto), which means "down") is an ion that has more protons than electrons, giving it a positive charge.

A variety of different names refers to ions having numerous charges. For instance, an ion with a negative charge is referred to as a dianion, whereas an ion with a positive charge is a dictation. A neutral molecule is a zwitterion with negative and positive charges at various positions throughout the molecule's structure (Zhao, 2003). Anions and cations are distinguished by their ionic radius, which varies according to their relative size: Cations are tiny, with most of them having a radius of less than 1010 m (1008 cm). However, most anions are big, including oxygen, the most prevalent anion on Earth. It is clear from this fact that the anion takes up most of the space in a crystal, with the cations fitting into the crevices among the anion and the crystal (Baker and Ollis, 1957). Cation and anion were first used in electrolysis in 1834 and were joined by Michael Faraday.

2.7.1. Natural Occurrences

We see ions all around us, and they are responsible for a wide range of events, ranging from the luminescent character of our Sun to the presence of the Earth's ionosphere. Atoms in an ionic form may have a diverse hue from neutral atoms, and hence the color of gemstones is determined by the amount of light absorbed by metal ions. The interface of ions and water is extremely important in both organic and inorganic chemistry; for example, the energy required to drive the break of adenosine triphosphate is extremely important (ATP). The settings in which ions are prominent are described in the following sections: They reduce physical length-scale order, from solar to microscopic (Baker and Ollis, 1957).

2.7.2. Related Technology

Ions can be created non-chemically by employing a variety of ion sources, which are often characterized by high voltage or temperature. A wide variety of instruments, including optical emission spectrometers, mass spectrometers, particle acceleration chambers, ion engines, and ion implanters, rely on these materials for the operation (Konarev et al., 2012).

In addition to being employed in air purification through disrupting microbes, they are also used in domestic items, such as, smoke detectors, because of their reactive charge. Cell death is caused by the loss of an ionic gradient across membranes, which controls signaling and metabolism in these species. This is a general mechanism used by synthetic and natural biocides, such as the ion channels amphotericin and gramicidin, to kill bacteria and viruses. Dissolved ions in water are as total dissolved solids (TDS) a wellrecognized indication of water quality (Sawatzky et al., 1976). TDS when in large amounts cause the water to get turbid.

2.7.3. Detection of Ionizing Radiation

Detecting radiation like X-rays, beta, gamma, and alpha on gas by measuring the ionizing effect of radiation is a common application for some instruments. Initially, in these devices, the first ionization event outcomes in producing an "ion pair." Consisting of a positively charged ion and an uncharged free electron on gas molecules because of ion impact by radiation. The chamber of ionization is the most basic of these detectors. It is responsible for collecting all the charges generated through direct ionization inside the gas because of the usage of an electric field (Nacham et al., 2015) (Figures 2.8 and 2.9).



Figure 2.8: An ion chamber with ions drifting across it is seen in this diagram. Because electrons have a lot of lesser mass than positive ions, they wander much more quickly.

Source: https://www.fulviofrisone.com/attachments/article/444/Radiation%20 Detection%20and%20Measurement,%203rd%20ed%20-%20Glenn%20F.%20 Knoll%20(Wiley,%202000).pdf.



Figure 2.9: Between the two electrodes, there is an avalanche effect. The first ionization event releases one electron, and every successive collision releases more electrons, resulting in a total of two electrons emerging from every collision: The ionizing electron and the released electron, as shown in the diagram.

Source: https://en.wikipedia.org/wiki/Ion#cite_note-knoll-4.

2.7.4. The Basics of Chemistry

Whenever you write the chemical formula for an ion, the net charge of the ion is put in superscript directly following the chemical structure of the atom (Kahn, 1985). With the magnitude, the net charge is written preceding the sign; for example, a doubly charged cation is written as 2+ rather than +2 to indicate that it is doubly charged. It is not necessary to specify the amount of charge when dealing with separately charged atoms; for instance, the sodium cation is denoted by the letter + instead of the letter 1+ (Figure 2.10).



Figure 2.10: Ferrous is a term used to describe a Fe atom (iron) that has lost two electrons and is hence described too as ferrous.

Source: https://www.shutterstock.com/image-vector/equivalent-notationsiron-atom-fe-that-2071818731. In addition to indicating actual number reflective of the ion charge, another appropriate method of representing an atom with several charges is to draw out the specific charge several times. This is commonly seen through transition metals. When chemists circle the sign, it is only for decorative purposes and does not affect the chemical interpretation of the sign (Didchenko and Gortsema, 1963) (Figure 2.10).



Figure 2.11: The uranyl ion is represented by Roman numerals and charge notations.

Note: The uranyl ion is represented by Roman numerals and charge notations. Superscripted Roman numerals represent the oxidation state of the metal. Still, the charge of the whole facility is represented by the angle symbol, which is also represented by the sign and magnitude of the total net charge (Sanz et al., 2001).

Source: https://commons.wikimedia.org/wiki/File:Ions_notation2.svg.

Another method is to used roman numbers in denoting atomic charges, especially in spectroscopy; for instance, the Fe^{2+} ion in the previous example is discussed as FeII or Fe(II). An element's formal oxidation state is represented by a Roman numeral, whereas the net charge is represented by Indo-Arabic numerals superscripted on the Roman numeral. When it comes to monatomic ions, the two notations can be interchanged, but the Roman numerals cannot be used when it comes to polyatomic ions. However, as demonstrated by the uranyl ion example, combining the data for the specific metal centers with those for a polyatomic compound is feasible (Suski, 1979).

2.7.5. Sub-Classes

A radical is an ion that includes unpaired electrons and is formed when an ion possesses unpaired electrons. In the same way that uncharged radicals are highly reactive, radical ions are also highly reactive. Oxyanions are polyatomic ions that include oxygen, like carbonate and sulfate, and are classified as such. Organic ions have at least one carbon-to-hydrogen link and are composed of carbon and hydrogen atoms. If the charge in an organic ion is formally centered on carbon, the ion is referred to as a carbanion or carbocation (Li et al., 1991).

2.7.6. Formation

2.7.6.1. Monatomic Ions

Monatomic ions are generated by an atom when it gains or loses electrons from the valence shell. As a result, electrons in the inner shells of an atom are strongly linked to the positively charged atomic nucleus. They are unable to engage in this type of chemical interaction (Yamada, 1988).

Atoms can be ionized by being bombarded with radiation, however the most common ionization mechanism observed in chemistry is the transport of electrons among molecules or atoms. This transport is typically triggered by the achievement of stable electronic structures (also known as "closed shells"). Atoms will acquire or lose electrons based on whatever activity requires the minimum energy to complete (Buschow and Sherwood, 1978).

Example: The sodium (Na) atom comprises two stables, packed inner shells of two and eight electrons, with a single electron in the valence shell encircling them. To achieve this stable configuration, an additional electron on a sodium atom is likely to be lost and achieve this stable configuration, resulting in the formation of a sodium cation in the process.

 $Na \rightarrow Na^+ + e^ Cl + e^- \rightarrow Cl^-$

However, the chlorine atom has only 7 electrons in its valence shell, which is one electron short of the stable configuration, full shell with 8 electrons found in an oxygen atom. A chlorine atom will tend to add an extra electron and eventually achieve a stable 8-electron configuration, resulting in the formation of a chloride anion in the process (Kandpal et al., 2007) (Figure 2.12).

 $Na^+ + Cl^- \rightarrow NaCl$



Figure 2.12: A representation of the nitrate ion's electrostatic potential map (NO_3^{-}) . A 3-dimensional shell represents a single subjective isopotential in three dimensions.

Source: https://en.wikipedia.org/wiki/Ion.

2.7.6.2. Polyatomic Ions

In neutral molecules, molecular, and polyatomic ions are frequently produced because of the gain or loss of a proton, H^+ , or other protons (Franse and Radwański, 1993). For instance, when the ammonium ion, NH_3 , absorbs a proton, H^+ , the ammonium ion, NH_4^+ , is produced in a process known as protonation. Ammonium and ammonia have a similar number of electrons, thus, theythe same electron configuration. Still, ammonium has an extra proton, which results in a net positive charge of (4+) compared to the other two combining elements in the periodic table.

Ammonia may also receive a positive charge by losing an electron, resulting in the ion NH_3 . However, since it has an inadequate valence shell surrounding the nitrogen atom, this ion is unstable, and as a result, it is a very reactive radical ion (Coey et al., 1990).

Rather than losing or gaining electrons, molecular, and polyatomic ions are typically produced by losing or gaining protons or elemental ions like H^+ making radicals very unstable and reactive. In this way, the molecule can maintain its stable electronic structure even simultaneously gaining an electrical charge (Shimizu et al., 1984).

2.7.6.3. Ionization Potential

The ionization potential, often called the ionization energy, is the amount of energy required to remove an electron from a molecule or an atom. As 64

electrons are transported or transferred from one atom to another, there should be an adequate amount of energy that must be supplied to the system for the process to proceed. That adequate amount of energy to remove an electron from the valence shell is the ionization energy. The amount of energy needs to remove the first electron from the valence shell us termed as first ionization energy, the followed by the second ionization energy and so on. (Shimizu et al., 1984).

The first ionization energy is characteristically the highest of all the ionization energies. When the electrons in any specific block of atomic orbitals are depleted, the shell where it came from can be more or less stable. It becomes less stable when it needs to remove more to achieve the more stable sublevel configuration. Atoms or elements with a charge of +1 indicates that one electron can leave the shell for it to achieve the more stable configuration. Similarly, atoms with more than 2 charges such as Fe²⁺ requires the transfer of the first electron, followed by the second. As the first electron is transferred, the 2^{nd} ionization energy is lower, indicating that it is easier for the 2nd electron to be removed or transferred from the orbital. thus, making that atom less stable or more reactive. When the 2nd electron is transferred, what is left is the next energy sublevel filled to its capacity, making that atom stable and soon will stop moving or transferring electrons. As a result, ions are more likely to form in a fashion that leaves them with complete orbital blocks (Li, 2016). Because sodium has only one valence electron in its outer shells, it is usually seen ionized with one electron lost, denoted by the symbol Na⁺. Chlorine has seven valence electrons on the other side of the periodic table. It is often encountered in the ionized state with one acquired electron, denoted by the symbol Cl. Cesium possesses the lowest observed ionization energy of all the elements, whereas helium possesses the highest ionization energy. According to general principles, metals have significantly lower ionization energies than nonmetallic materials. As a result, metals lose electrons to produce positively charged ions, whereas nonmetallic materials gain electrons to produce negatively charged ions (Gignoux and Schmitt, 1995).

2.8. IONIC BONDING

Ionic bonding is a chemical bonding that occurs because of the electrostatic attraction of ions that have opposite charges. Ions with similar charges repel each other. Thus, ions do not normally exist independently; instead, they form crystal lattices when they meet ions of opposite charge. A compound

formed by this reaction is known as an ionic compound, and it is kept together by ionic bonding. It is possible to determine the ionic radius and spatial extension of individual ions in ionic compounds by measuring the characteristic distances between ion neighbors in the compound (Taber, 1997).

The most frequent ionic bonding is found in compounds that is formed between nonmetals and metals. Metals are distinguished by the presence of a tiny number of electrons more than the amount required for a stable, closed-shell electronic state. Because of this, they tend to remove these excess electrons to achieve a more stable state. Electropositivity is the term used to describe this feature. Alternatively, nonmetals are defined by having an electron structure that is only a few electrons away from a stable form (Coll and Treagust, 2003) (Figure 2.13).



Figure 2.13: Ionic bonding mechanism.

Source: https://socratic.org/questions/what-are-similarities-of-covalent-and-ionic-bonding.

Consequently, non metals tend to gain additional electrons to achieve the more stable arrangement of atoms and molecules. The tendency of the material to attract electrons towards itself is referred to as electronegativity. Thus, nonmetals' reactivity is reflected by its electronegivity. Whenever a strongly electronegative nonmetal and a highly electropositive metal are joined, the excess electrons from the metal atoms are transmitted to the electron-scarce nonmetal atoms. This reaction results in nonmetal anions and metal cations, which are attracted to one another and combine to form a salt (Schäfer et al., 1973).

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3

ION EXTRACTION AND ION MOBILITIES

CHAPTER

CONTENTS

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3.1. INTRODUCTION

When charged particles (such as protons or electrons) travel across a material because of an electric field dragging them, this is referred to as electrical mobility. Spectrometry in the gas phase and electrophoresis in the liquid phase need to separate ions to confirm its presence in an analyte or a sample, this separation in spectrometry is referred to as ion mobility because ions are separated according to their mobility in the gas phase or any mobile phase (Mutelet et al., 2005).

Either indirectly or directly, the ion movement of its constituents affects the properties of electrolyte solutions. This item is concerned with the mobility of ions in both nonaqueous and aqueous systems. In the liquid phase, the mobile phase is a solvent where the ions can be observed to move freely. Each ion has unique mobility with reference to a mobile phase.

Ion extraction is a process that involves extracting one or many ions from a liquid phase, which is commonly water and transporting them to another phase, which can be either liquid or solid. Overall, the goal is to either extract ions from concentrates or native solution. The phrase "ion separation" is used when distinct types of ions must be removed from a mixture, i.e., when it is necessary to execute a selective extraction of each individual ion (Aki et al., 2001).

The development of new technology, as well as the expansion of innovation together with the world's population, have both had a significant impact on the market for metal resources. Several metals today are branded to have geopolitical issues because of its unequal distribution worldwide. On the other hand, governments will be forced to impose restrictions due to the limited availability of mental resources and fossil fuels, which will surely result in the reduction of exports that automatically corresponds to an increase in the price. Furthermore, the extraction of metal ions from ores results in the production of hazardous wastes, the disposal of which is becoming increasingly expensive due to the proliferation of environmental protection rules. It is estimated that most of these wastes are categorized as hazardous and poisonous, owing to the presence of various metals like chromium, cadmium, arsenic, and lead. There will be an increasing demand for the progress of more effective and environmentally friendly recycling systems centered on the ion extraction method to prevent the future mining of subsurface resources because of this trend (Stolte et al., 2007). Ion extraction will be discussed in the latter part of this chapter.

3.1.1. Charge Flow in an External Electric Field

Ions in an electrolyte solution in random motion disperse until it reaches homogeneity, and because of this, the electric field of the system is not in equilibrium with the ions; it is subjected to generalized forces that might cause irreversible events like relaxation or transport to occur. As the source of such a force, we can look to a gradient in the chemical potential of the ions under consideration, which produces a particle movement that guides to diffusion and electric conductance. The flow of ion *i* is described by the following equation when activity coefficients are ignored.

$$\vec{J}_i = \underbrace{-D_i \text{grad} c_i}_{\text{diffusion}} + \underbrace{D_i \frac{c_i z_i F}{RT}}_{\text{migration}} \vec{E}$$
(1)

With $c_i D_i z_i$ and as the concentration, diffusion coefficient and charge number, of the ion, respectively. is the applied electric field strength, and F and R are Faraday and gas constant, respectively. The ionic mobility u_i is the velocity v_i of an ion i under the unit electric field ($u_i = v_i/E$) and is related to the single ion conductivity λ_i via Faraday constant (Dupont et al., 2000).

$$\lambda_i = u_i F \tag{2}$$

The following relationship between diffusion coefficient Di and single ion conductivity may be inferred from the migration component of Eqn. (1) and Ohm's law:

$$\lambda_i = D_i \frac{|z_i|F^2}{RT} \tag{3}$$

Eqn. (3) establishes a critical relationship between the corresponding limiting values l_i and D_i , which are distinctive ionic transport parameters that are not disturbed by ionic contact (infinite dilution). Table 3.1 contains examples of several solvents that have been used (Sugden and Wilkins, 1929).

In Ref, a wide range of l_i -values in nonaqueous and aqueous solutions are provided for practical application (Sugden and Wilkins, 1929).

Three contributions can be used to express conductivity:

$$\lambda_i = \lambda_i^\infty - \lambda_i^{el} - \lambda_i^{rel} \tag{4}$$

There are two concentration-dependent factors coupled with the ionic conductivity λ_i that diminish ionic mobility in addition to the ion movement under unperturbed conditions at infinite dilution. While the electrophoretic term l_i^{el} represents the average effect of the hydrodynamic interactions of

solvent and solute, the relaxation term l_i^{rel} represents the relaxation of the deflection of the ionic cloud around the central solute. The above dependence on ionic strength I is obtained by expanding the appropriate formulas in series:

$$\lambda_{i} = \lambda_{i}^{\infty} - S_{i}\sqrt{I} + E_{i} I \ln I + J_{1i}I - J_{2i}I^{3/2},$$

$$I = \frac{1}{2}\sum_{i} z_{i}^{2}c_{i}$$
(5)

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Table 3.1: Restrictive Ionic Conductivities at 25°C

$\lambda_i^\infty \cdot 10^4 / (\mathrm{m}^2 \Omega^{-1} \mathrm{mol}^{-1})$						
Ion	Water	Ethanol	PC	Sulfolane (30°C)	Nitromethane	
K^+	73.5	23.4	11.1	4.1	58.1	
$\mathrm{H}^{\scriptscriptstyle +}$	350.0	-	-	_	_	
Li+	38.8	17.1	7.1	4.3	53.9	
Cl-	76.3	23.7	18.7	9.3	62.5	
$Bu_4^{}N^+$	19.3	19.8	9.0	2.8	34.1	

In the case of symmetrical electrolytes, full expressions for the coefficients of t4his equation may be observed in Sugden and Wilkins (1929), while in the case of unsymmetrical electrolytes, they can be found in Gorman (2001). As an illustration, Figure 3.1 depicts experimental single ion conductivities of thiocyanate and potassium ions in methanol as a function of concentration. A theoretical curve is represented by a line, which was derived with the aid of Eqn. (5).



Figure 3.1: Single ion conductivities of potassium thiocyanate in methanol (1: K⁺, 2: SCN) (Sugden & Wilkins, 1929).

Source: https://www.worldcat.org/title/electrolyte-data-collection/ oclc/946201132.

It is separate from any counter-ions that appear in the solution when the single ion conductivity reaches its limit for a particular solvent, and it is this value that characterizes and distinguishes the solvated single ion conductivity. Consequently, for a binary electrolyte, the limiting equivalency conductance (L1) of the electrolyte may be simply computed from the ion conductivities, which is a simple calculation.

$$\Lambda^{\infty} = \lambda_{+}^{\infty} + \lambda_{-}^{\infty} \tag{6}$$

3.1.2. Future Directions

Ionic transport qualities such as ion mobilities and the corresponding conductivities l_i and diffusion coefficients D_i are quantities that allow for the formulation of useful assumptions and information in electrolyte solution theories. At low and moderate concentrations, the models now in use are quite satisfactory; however, at high concentrations, they still require considerable refinement to be satisfactory. Despite this, the application of the mean spherical approximation (MSA) theory to transport systems has yielded some promising findings (Keskin et al., 2007).

3.2. ION EXTRACTION BASICS

In most cases, aqueous chemistry is used in metals from ores, recycled or leftover materials, and recovery of materials from wastes. Overall, one of the areas responsible for this processes is hydrometallurgy. The process may be broken down into three broad categories (Swatloski et al., 2004):

- Leaching is a process in which metals are converted into soluble salts in aqueous form;
- Purification and concentration of solutions are accomplished using ion extraction methods; and
- Metal recovery from the filtered solution is accomplished using several complex processes, one of which for example, is by electrolysis.

This section attempts to provide a succinct summary of the most significant ion extraction procedures, which include solvent extraction, cloud point extraction, ion flotation, ion exchange, membrane separation, and precipitation, among others. All these strategies are usually directed on the identification of ions with chemical or physical occurrences in the environment. This recognition might come from a variety of sources, depending on the technique:

- This includes ion-pairing characteristics, surface effects such as polarizabilities and charge density of the species, and other electrostatic properties; and
- Physical effects, such as shape and size recognition.

In a porous structure, steric hindrance has the potential to have a significant impact on ion selectivity. Aside from that, the bulk physicochemical characteristics of the ions in water may be of critical importance during the process of ion extraction and separation. One such instance is the fact that numerous ion effects in solution are known to be caused by the process of "ion-hydration," which is defined by the entropy and the heat produced during the process of "hydration."

Solvent extraction is a word that refers to the dispersion of a solute among two unmixable liquid phases that are in contact with one another, often water and oil, which is also referred to as "diluent" in hydrometallurgy (Welton, 1999). When contemporaneous solutes in organic phase have distinct distribution ratios (D), are defined as the ratio between the solute concentration and the solute concentration in the aqueous phase, as shown in Eqn. (1), it is possible to separate these solutes. Temperature, concentration, pressure, and other thermodynamic parameters of the system influence D. It is possible to link D to the Gibbs free energy of the extraction process by utilizing the Gibbs free energy of the system (DG).

$$D_M = \frac{\left[\overline{\mathbf{M}}\right]_{t,org}}{\left[\mathbf{M}\right]_{t,aq}} \quad \Delta G = -RT \ln D_M \quad (7)$$

The total concentrations of the metal species in either their aqueous media or their complexed organic form are represented by the symbol (Mt).

Turbulent stirring of the two liquid phases is commonly used to promote surface contact between the oil and the water to achieve quick dispersion of the solute in the mixture. It is also necessary to settle the two liquid phases, which must be done as quickly and efficiently as possible to be suitable for industrial purposes (Short, 2006) (Figure 3.2).



Figure 3.2: An ion extraction system in the water/oil contact interface is depicted in this diagram. Ions from the aqueous phase are transported to the organic phase via extractant reverse micelles.

Source: https://link.springer.com/referenceworkentry/10.1007% 2F978-1-4419-6996-5 13.

As a result, metal ions are often totally dehydrated in the extractant reverse micelles when used in extraction.

There are many distinct types of ions extractants available, and they may be categorized into the following categories based on how they extract their ions (Short, 2006):

- Extraction by cation exchange, for example, with an acidic function, as in HDEHP;
- Extraction via solvation, for example, with a neutral function, as in TBP;
- Extraction is accomplished by the creation of ion pairs, e.g., amine salts such as TOA;
- Increased U(IV) extraction by connecting an acidic extractant with a neutral extractant, for example, is an example of complicated synergistic effects in extraction.

In solution, the chemical performance of these four classes of extractant molecules determines the mechanism of ion transfer into the organic phase: classes 1 and 3 depend on the molecule's ionizability and thus on the electrostatic attraction with the metal ion, while class 2 depends on the extractant's competition with the metal ion's first solvation shell, which once swapped enable the transfer of the hydrophobic ion compound into an organic phase.

3.2.1. Ion Exchange

Ion exchange, along with solvent extraction, is the most widely used method of ion extraction. It depends on a process of aggressive adsorption that occurs at a charged solid in the middle of two ions' surfaces. This method is reversible; the ion exchanger may be regenerated or reloaded by washing with the proper ions after it has been depleted (Sugden and Wilkins, 1929).

Materials employed as ion exchangers can have a variety of chemical properties, including gel polymers or functionalized porous known as clays, zeolites, ion-exchange resins, and soil humus, among others. When it comes to separating cations, anions, or both from a solution, ion exchangers are classified as amphoteric, cationic, or anionic, depending on the situation. However, the amphoteric exchange is more efficient when done in mixed beds with a mix of cation and anion exchangers or when the treated solution is passed across multiple distinct ion-exchange materials (Sugden and Wilkins, 1929). Zeolites are all-inorganic microporous minerals that are commonly employed in the extraction of ions from solutions. Their porous structure allows them to contain a broad range of cations and exhibit ion selectivity based on the cation and pore size combinations. Porous support structures, generally in the form of tiny beads (1-2 mm), composed of an insoluble organic polymer substrate serve as ion exchange resins. The holes on the surface are utilized to readily catch and release ions, making it possible to trap and release ions quickly. Ion trapping occurs only when other ions are released at the same time as the ions being trapped.

The functional groups of the four main types of ion-exchange resins are as follows: strongly acidic, strongly basic, weakly acidic, and weakly basic; there are also specialty resin varieties available that incorporate chelating agents. Ion exchangers can be non-ion-specific or exhibit binding selectivity for specific ions or classes of ions, depending on the type of the functional group (Wilkes et al., 1982; Gorman, 2001).

3.2.2. Ion Flotation

It is possible to concentrate ionic species existing in a dilute aqueous solution using ion flotation (also known as foam fractionation) as an extraction/ separation method (Wilkes et al., 1982). There are several applications for this simple and cost-effective approach, including the concentration of valued materials or the elimination of harmful elements from extremely large volumes of extremely dilute solutions which makes it an excellent choice for waste-water treatment (Fannin et al., 1984). A subgroup of the larger flotation process, often known as froth flotation, ion flotation is a type of ionization. Solid-liquid separation is a technique for splitting solid minerals from gangue that makes use of variations in their hydrophobicity. Hydrophobicity disparities between waste gangue and precious minerals are widened by the application of surfactants to the mineral surface, which adsorb on the mineral surface. Processing complicated ores become economically possible due to the selective separation of the minerals used in the process (Figure 3.3).

Ion flotation is the process of adding an ionic surfactant to a solution comprising ions of opposing charge to separate them. After then, gas bubbles up into the solution. In response to the rising bubbles, the surfactant molecule, which is composed of a charged hydrophilic head group and a hydrophobic tail group, adsorbs to the surface of the bubble, causing the surface of the bubble to become negatively charged. At the bubble surface, ions in the solution adsorb, where they are exchanged with the surfactant counter ion, resulting in an ion-exchange process (Renner, 2001):



Figure 3.3: An ion flotation lab setting is depicted schematically.

Source: https://link.springer.com/referenceworkentry/10.1007% 2F978-1-4419-6996-5 13.

Because of the huge surface area to liquid volume ratio of the foam, the liquid that follows the breakdown of the foam is significantly richer in the ion than the initial solution. The selectivity of the charged surfactant boundary for the ion in the existence of multiple counter-ions is critical to the success of ion extraction and separation in the laboratory (Shariati and Peters, 2005).

3.2.3. Cloud Point Extraction

When compared to liquid-liquid extraction, CPE is an analytic tool that is sometimes existing as a solvent-free substitute. It is useful as a preconcentration method for analytical purposes because it has numerous advantages, including low costs, safety, and ease of use. It is also quick to perform and has a high capacity for concentrating a wide variety of analytes.

Extraction from the initial solution is possible for any species that has an interaction with the micellar system. For ion extraction to occur, it is necessary to incorporate a suitable hydrophobic ligand or extractant into the non-ionic surfactant micelles, which are solubilized in the surfactant micelles. Recently, a method that relies on the use of a surfactant that has been functionalized by a complexing component has been proposed (Brennecke and Maginn, 2001).

The CPE procedure is separated into three stages (Welton, 1999; Short, 2006): the analytes' solubilization in micellar aggregates, clouding caused by rising temperature, and phase separation. A surfactant's cloud point causes a phase separation in a solution, resulting in two phases: one surfactant-rich phase that includes the ion-extractant complex, and the other water-rich phase that includes the surface-active agent at a concentration less than or equivalent to the critical micelle concentration.

3.2.4. Precipitation

Chemical precipitation is a common method for removing heavy metals from inorganic waste and it is also effective (Renner, 2001). To achieve basic conditions (pH >9), it is necessary to modify the dispersed metal ion speciation and then change the metal ions on an insoluble solid phase by using a precipitant agent such as lime as the primary chemical reaction catalyst (Figure 3.4).



Figure 3.4: Ion elimination by precipitation is depicted schematically.

Source: https://link.springer.com/article/10.1007/s11270-020-04863-w.

As a rule, because of a general reaction defined by the following equation, the metal occurs out of solution in its hydroxide state:

$$M_{aqu.}^{n+} + nOH_{aqu.}^{-} \rightleftharpoons M(OH)_n$$
 (8)

The metal ions (Mn^+) and precipitant (OH) are represented by their respective symbols, whereas M(OH)n is the insoluble metal hydroxide symbolized by its symbol.

Also proposed was the selective metal ion precipitation (liquid-solid extraction) from acidic aqueous waste solutions, which may be used to separate actinides in a straightforward manner, for example, by utilizing cationic surfactant as a precipitant (Seddon, 1995; Yang and Dionysiou, 2004). It is possible that this procedure will have some noteworthy benefits over solvent extraction because some stages are eliminated, such as stripping of the isolated species and solvent washing. Furthermore, because no polluted organic solvent is created, the amount of trash generated is significantly reduced.

3.2.5. Membrane Filtration

It is possible to remove not just suspended solids or organic chemicals but similarly inorganic substances like heavy metal ions using membrane filtration. Reverse osmosis (RO), nanofiltration (NF), and Ultrafiltration (UF) are three separate methods that can be used to treat inorganic compounds, depending on the type of the inorganic component.

In ultrafiltration (UF), permeable membranes with membrane weights of 1,000–100,000 Da and holes of 5–20 nm are used to allow for the flow of low molecular weight particles and water even as retaining macromolecules with sizes larger than the pores are retained. Membranes are made of many materials such as polyamide, cellulose acetate, alumina, and silica, amongst others (Figure 3.5).





Source: https://www.sciencedirect.com/science/article/abs/pii/ S0376738820306815.

It is necessary to separate ions of various elements and elements like cobalt II, nickel II, zinc II, copper III, and cadmium (II). In some cases, with metal concentrations ranging from 10 to 112 mg/L, it is possible to attain > 90% removal efficiency depending on the membrane parameters. A surfactant like sodium dodecyl sulfate (SDS) to generate water-borne polymer or micelle-like chitosan to complexions might theoretically improve separation by increasing the size of the micelles formed. However, the issues associated with membrane fouling have prevented this approach from being used in a broader range of industrial waste-water treatment applications (Lagrost et al., 2003).

NF is characterized by the presence of electrical and steric effects. The attraction of NF membranes rests in their tiny pore size (1 nm) and high surface charge, which permits charged solutes lesser than the membrane pores to be rejected together with salts and larger neutral solutes, hence increasing the efficiency of the membrane. Organic or inorganic membranes, such as polyvinyl alcohol or titanium dioxide, can be used. Chelating compounds like HEDTA, EDTA, and DTPA can aid in the separation of actinides (III)

from lanthanides (III), for example, in the actinides (III) separation (Lagrost et al., 2003).

Water can travel via the membrane in the RO process. However, heavy metals are trapped by the membrane. Hydrostatic pressure can be used to remove cationic chemicals from the water that is greater than the osmotic pressure of the feeding solution in a closed system. RO is the most successful membrane separation technology for the removal of metal ions from inorganic solutions, with refusal rates ranging from 97% to 200% for metal concentrations ranging from 21 to 200 milligrams per liter. RO can operate in an extensive pH range (3-11) and at pressures ranging from 4.5 to 15 bars (depending on the features of the membrane). The membranes are composed of sulfonated polysulfide or polyamide, depending on the application. There are several advantages of using the RO: The pressure applied to the membrane, the biological stability, and the chemical, thermal, and high flux rate of the membrane all influence the effectiveness of metal removal. The clogging of the microscopic pores, which may be permanent, and the high energy utilization of RO are the two most significant constraints of the technology (Shariati et al., 2005).

The method of electrodialysis (ED), in addition to these other approaches, is classified as either an electrochemical or electrically driven membrane technique (Shariati et al., 2005). It is employed to move ions from one solution to another solution under the impact of an applied electric potential bypassing the ions via an ion exchange membrane in the first solution. The membranes are constructed of thin layers of polymer polymers that have either cationic or anionic characteristics, depending on the application. ED is carried out in an ED cell, which is comprised of 3 major compartments, the (1) feed compartment, the (2) diluate compartment, and the (3) concentrate compartment. The separation of ions takes place inside an ED stack which is composed of a single or multiple pair of selective cationic and anionic membranes arranged alternately two electrodes (Mendoza et al., 2014; Mendoza et al., 2018. The process yields two products namely the diluate, which is product water that is free from ions and the concentrate which is product water enriched with ions. This takes place due to the presence of an applied potential that drives ions through the membranes. Cationic membranes only allow passage of cations while anionic membranes only allow passage of anions. This makes two streams on each membrane, an ion deficient stream (diluate) and the ion enriched stream (concentrate). Depending on the beneficial use of water, the process is optimized to yield desired materials. In water treatment, particularly desalination of brackish

water or saltwater, ED is used in the generation of clean and ultrapure water by collecting the diluate stream while in the production of lactic acid, the concentrate stream of the ED process becomes the major product of consideration (Zhao et al., 2005; Mendoza et al., 2018). Variation of the ED process is called Reverse Eletrodialysis (RED or EDR in some books) where the pola

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CHAPTER

4

FUNDAMENTAL CONCEPTS OF IONIC LIQUIDS

CONTENTS

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4.1. INTRODUCTION

The chemical industry's broad use of hazardous and volatile solvents results in significant environmental harm to the environment. Consequently, in the chemical and pharmaceutical sectors, there is a great need to develop a viable substitute for these environmentally friendly solvents that has the characteristics of conventional solvents. For example, Ionic Liquids and supercritical carbon dioxide are two new types of solvents that may be used as both solvents and green catalysts. Ionic liquids are formed entirely of ions and include organic substances that are all comprised of ions. A recent class of chemicals, ILs (ionic liquids), has gained a great deal of interest in recent years due to their unique properties. This class of chemicals is utilized as environmentally friendly solvents in a wide range of chemical processes, as well as in the production of innovative materials. There are broad descriptions of ILs and historical background provided in this chapter; the structure of ILs, the anion and cation types, and synthesis techniques in the associated literature are all covered in the next section. The key application areas, as well as the fundamental applications, are also explored in-depth (Holade et al., 2015).

The term "ionic liquid (IL)" was developed just recently to refer to liquid salts that may be stored at room temperature, and the concept has since been the subject of significant debate and some change. It is most beneficial to adopt the following definition of an IL in practice: "A liquid that is totally composed of ions." We can go a bit more into this subject. Is an IL different from a molten salt according to this definition? Yes and no. The phrase "molten salt" refers to the liquid phase of crystalline salt, such as sodium chloride (NaCl). In addition, the term "ionic liquid" has a far wider spectrum of potential applications. Consider a combination of the two salts Sodium Bis(fluorosulfonyl)imide (fsi) and Alkylmethylpyrrolidinium (Cnmpyr) Bis(trifluoromethanesulfonyl)imide(Cnmpyr)Bis(trifluoromethanesulfonyl) imide (Cnmpyr) Bis(trifluoromethanesulfonyl)imide (Cnmpyr (NTF2) (Ruiz et al., 2001). At room temperature, this mixture of salts is a liquid, and it is legitimately referred to as an IL according to our definition. Indeed, an IL may contain a very high number of distinctions at the same time. It should be noted that the phrase 'molten salt' has evolved to refer to a variety of salt combinations in popular usage, despite the fact that the term itself clearly refers to a single compound. It is a matter of principle (and, in fact, a crucial thermodynamic principle) that the IL generated by combining Na(fsi) and Alkylmethylpyrrolidinium is identical to that formed by mixing

the right amounts of Na(NTf2) and Alkylmethylpyrrolidinium. When defining the IL, the origins of the ions are unimportant; just the amounts of the individual ions present are taken into consideration. As it turns out, ILs containing extremely high concentrations of Na or Li salts are proving to be quite successful as electrolytes for both Na and Li batteries (Hirosawa et al., 2017). It is common for some definitions of IL to include a temperature range, such as "below 100°C," but this is not required. In fact, doing so can be restricted since it can distort our perception of which substances or mixes may be appropriate for specific purposes. As a matter of fact, there are numerous and quite beneficial uses of ILs at temperatures exceeding 100°C, such as the synthesis of MnOx water oxidation catalysts by electrodeposition at 130°C (Gutfleisch, 2000). The most important prerequisite for this is that the IL be a liquid at 130°C. For this use, it is preferable if the compound is likewise liquid at room temperature, although this is not required, and compounds with melting temperatures more than 100°C should not be ruled out entirely. Furthermore, a definition that includes "a salt with a melting point below 100°C" (or any other value, such as room temperature) is an unnecessary limitation since, in certain circumstances, it may be difficult to identify and test the melting point because of practical difficulties. Liquids can be supercooled to temperatures below their equilibrium melting points, and in certain situations, the liquid becomes so viscous that the crystalline phase does not form on a timeframe that is useful for practical purposes. Due to the fact that the melting points of individual compounds are typically significantly lowered in combinations, this is especially true of salt mixtures, which we have acknowledged are perfectly OK IL (Goya et al., 2003).

Ionic liquids are chemicals that have had a significant impact on the scientific community and the chemical industry recently. These complexes, which are found in green chemicals such as solvents, play a critical role in minimizing the usage of hazardous, poisonous, and ecologically detrimental substances. Ionic liquids are organic molecules formed up of ions that are liquid at 100°C, according to current knowledge. One of the factors driving the current flurry of research into ionic fluids is the desire of scientists to find an appropriate replacement for volatile solvents in the industrial setting (Dempsey et al., 2007; Contreras et al., 2017). When it comes to environmental contamination in the chemical and pharmaceutical industries, volatile organic solvents are by far the most significant cause. Obviously, this does not imply that all ionic liquids are environmentally friendly solvents; in fact, some of them are quite poisonous. Because of its distinctive features, this novel chemical group has the potential to minimize
the usage of harmful and polluting organic solvents while also participating in a variety of innovative syntheses. At room temperature, ILs are salts that are liquid, as opposed to molten salts, which are molten at very high temperatures. Studies noted that there were just a few copyright applications for ILs in 1980, but by 2000, the number of copyright applications had climbed to 100, and by 2004, the number had increased to more than 800, according to the authors (Gajbhiye et al., 2008; Ningthoujam and Gajbhiye, 2010). This is an unequivocal indicator of the great level of interest in the ILs36–48 among academics and businesses.

According to popular belief, Paul Walden was the one who invented the protic ionic liquid which is the first IL to be discovered at room temperature (Das et al., 2005). He created ethyl ammonium nitrate, which is the first protic ionic liquid (a kind of IL detailed further below). He realized that the low melting point $(13-14^{\circ}C)$ was due to the bigger organic cation, which reduces the degree of ion association when compared to an inorganic salt, and that this was the cause of the low melting point. In addition, it is possible that liquid organic salts were identified as a source of irritation by organic chemists long before Walden, when they were most likely classified as 'intractable oils' and disposed of.

One of the most commonly mentioned characteristics of ILs is their 'tunability.' Understanding that we may employ massive charge-diffuse ions to lower the melting point of high-temperature molten salts leads to the realization that there is an unusually vast number of ions from which to choose when creating our IL. To put it another way, if we know what qualities the various ions will create, we can 'tune' the IL to meet our application needs. This nomenclature refers to the usage of functionalized alkyl groups to promote the partitioning of certain metal ions into the IL phase from water, but it has now broadened in scope to include other types of ionic liquids as well (Ruiz et al., 2001; Ohno et al., 2002).

The use of IL mixes to attain the desired characteristics adds a new level of flexibility to the process (Figure 4.1).



Figure 4.1: The anions and cations represent the general factor group.

Source: https://www.researchgate.net/figure/The-cations-and-anions-representing-the-common-factor-group-22_fig1_346413647.

4.2. STRUCTURE OF IONIC LIQUIDS

Ionic liquids have a molecular structure that is composed of a variety of cations and anion species. The cation is often represented as a big organic molecule, whereas the anions are significantly lesser in volume than the cations, and their composition is inorganic (in contrast to organic compounds). Ionic liquids are characterized by a weak link between their two components, which is because of the size difference between cations and anions. The structure of ionic liquid is related to that of ionic liquid. Ionic liquids are capable of operating at temperatures in excess of 100°C.

Those that are liquid at temperatures greater than 100°C are referred to as molten liquids, and those that are liquid at temperatures lower than this are referred to as ionic liquids. Some ionic liquids, referred to as RTILs, are liquid at room temperature (Stoner and Wohlfarth, 1948).

Ionic liquids are complexes that are comprised of the pyridinium and chemical molecules imidazole, which are both cations of the compound pyridine with the formula C_5H_5N . Figure 4.2 depicts the organizational structures of both groupings. Ionic liquids are created by reacting to various cations and anions together. There is a large range of ionic liquids available, each with a specialized use or increased physical-chemical capabilities. Anions such as BF_4^- , BF_6^- , Br^- , Cl^- , and so on are commonly seen (McFadden et al., 1999).





Source: https://pubs.acs.org/doi/10.1021/ie0488061.

The following are the most significant advantages of ionic liquids (Stoner & Wohlfarth, 1948; McFadden et al., 1999):

- They are highly polar;
- They are non-volatile and have a low vapor pressure;
- They are normally stable and heat resistant up to 300°C;
- They are liquid at a wide temperature range, up to 200°C;
- These chemicals have a high electrical conductivity;
- Several common organic solvents are incompatible with these substances.

4.3. PROPERTIES IONIC LIQUIDS

4.3.1. Properties of Ionic Liquids with Solvent Use

When it comes to the chemical business, the existence of volatile and poisonous solvents, which are frequently employed, is the most significant environmental hazard in these industries. To discover a viable replacement for volatile solvents, researchers have looked at a variety of options. The subsequent materials have recently been recognized as being appropriate for this application. Simultaneously, each of the options listed below has its own set of advantages, restrictions, and issues (Stoner and Wohlfarth, 1948).

- Supercritical CO₂;
- Fluorinated solvents;
- Ionic liquids.

In the initial scenario, CO_2 gas is heated to a supercritical pressure and temperature high enough to cause it to turn into a liquid, retaining both the qualities of a gas and a liquid at the same time. Carbon dioxide gas has a critical temperature of 31°C and a supercritical pressure of 74 bar at its supercritical temperature. Hyper volatile carbon dioxide is an environmentally friendly solvent, but it has two significant drawbacks. To utilize this solvent needs the requisite equipment to employ supercritical pressure. Furthermore, the breadth of solubility in this solvent is relatively limited. Fluoride solvents are another class of other solvents that have drawbacks, such as being costly and emitting harmful compounds as a result of the heat generated. A family of chemicals known as ionic liquids has emerged as the most effective substitute for volatile solvents in many applications. Aside from being environmentally friendly, ionic fluids have the ability to dissolve a wide range of organic, inorganic, and metalorganic substances, as well as essential metal ions and molecules (Tartaj et al., 2003).

4.3.2. Purity Ionic Liquids

The chemical and physical characteristics of ionic liquids can be altered by the existence of contaminants in the solution. This makes the filtration of ionic liquids absolutely necessary. Organic and water-based substrates, as well as halides, are the most significant ionic liquid pollutants, and they are often derived from unreacted materials. Given the high moisture absorption capacity of ionic liquids, it is no surprise that hydrophobic ionic liquids also have high moisture absorption capacities. Heat and vacuum are used to dry ionic liquids, although it is complicated to totally remove water from these liquids in most cases. The existence of water decreases the viscosity and density of a substance, as well as alters its chemical characteristics (Stoner and Wohlfarth, 1948).

4.4. DIFFERENT GENERATIONS OF IONIC LIQUIDS

4.4.1. First-Generation

Ionic liquids are chemicals that are commonly employed as solvents because of their ionic properties. These complexes have distinct physical characteristics that can be improved by altering the anions or cations in their composition. These ionic liquids are shown in Figure 4.3 as the first generation of ionic liquids (Bedanta et al., 2009).



Figure 4.3: The 1st generation of ionic liquids with biological, chemical, and physical properties.

Source: https://pubs.acs.org/doi/10.1021/ie048806l.

4.4.2. Second Generation

As a result of the increasing popularity of these complexes, a class of ionic liquids called ionic liquids with particular chemical applications was developed. There are one or more particular functional groups on the cation of these compounds, which allow them to play and interact with a specific chemical role. For instance, they are utilized as complex ligands and lubricants in a variety of applications. These compounds, which are called the 2nd generation of ionic liquids, have a variety of chemical properties, including the physical properties already mentioned. As depicted in Figure 4.4, these ionic liquids are the 2nd generation of the material (Stoner and Wohlfarth, 1948).



Figure 4.4: The 2nd generation of ionic liquids with biological, chemical, and physical properties.

Source: https://ojs.wiserpub.com/index.php/FCE/article/view/693.

4.4.3. Third Generation

The toxicity of several active pharmaceutical compounds with structures similar to ours, which contain classical ionic units, has been examined. These active pharmaceutical compounds are physiologically active and have low toxicity. The third generation of ionic liquids, which are based on these medications, has been introduced as a result of the use of these pharmaceuticals. These chemicals are extremely low in toxicity, and their physical characteristics are similar to those of ionic liquids. This suggests that our ionic ions have the potential to be employed as pharmaceuticals. These ionic liquids are depicted in Figure 4.5 as the third generation of ionic liquids.



Figure 4.5: The 3rd generation of ionic liquids with biological, chemical, and physical properties.

Source: https://www.researchgate.net/figure/The-third-generation-of-ionic-liquids-with-physical-chemical-and-biological-properties_fig4_346413647.

4.5. APPLICATIONS OF IONIC LIQUIDS

Ionic liquids are now generally employed in a wide range of scientific and technological fields. The most significant application of ionic liquids is as a green solvent, which may be used in place of volatile solvents. Ionic liquids are now used for a variety of diverse applications, a few of which are concisely discussed here (Stoner and Wohlfarth, 1948).

4.5.1. Catalytic Reactions

The Friedel-Crafts reaction, which was discovered 20 years ago, was the first time that ion fluids were utilized as a catalyst. As a two-phase catalyst or substrate for other catalysts, ionic liquids have a variety of applications. Using ionic liquids, it is feasible to recycle the catalyst after it has been used once. Figure 4.6 depicts the overall condition of the reaction in its entirety.



Figure 4.6: Friedel-crafts reaction.

Source: https://en.wikipedia.org/wiki/Friedel%E2%80%93Crafts_reaction.

4.5.2. Stability of Nanocatalysts in an Ionic Liquid Medium

Organic processes are frequently aided by metal nanocatalysts like palladium, platinum, gold, ruthenium, and rhodium, among others. The difficulty with nanocatalysts is that they tend to cluster together in reaction settings, which reduces their overall activity significantly, as previously stated. A number of ionic solutions are employed to keep this from happening. For example, nanocatalyst rhodium (Rh) is more active in the ionic liquids indicated in the hydrogenation process of alkenes and rainfall than conventional catalysts (Stoner and Wohlfarth, 1948).

4.5.3. Solvent

As previously stated, the primary application of UV liquids is as a solvent. One of the most significant advantages of employing ionic liquids is that they accelerate reactions and improve orientation when compared to conventional solvents, which are both beneficial.

4.5.4. Electrochemistry

It was more than two decades ago when electrochemists discovered the application of molten salts and ionic fluids in power systems. In electrochemical devices, for example, fuel cells, power storage, electric hydration systems, and solar cells, several ionic fluids were shown to be the most effective materials. This is owing to the extremely high conductivity, high electrochemical stability, and extensive temperature performing range that this material demonstrates. In response to the increasing need for highcapacity batteries for a variety of applications, researchers began looking for non-aqueous electrolytic solutions. The ionic liquid looks to be a promising electrolyte for rechargeable lithium batteries, according to preliminary findings. The electrode is unable to regenerate or oxidize due to the vast range of electrochemical potential available to them. Ionic liquids have a voltage range of more than 4.5 volts, whereas blue electrolytes have a voltage range of 1.2 volts. Further to this, ionic liquids exhibit greater thermal stability as well as greater conductivity and solubility than traditional electrolytes. Examples include the fact that in lithium batteries, their conductivity is five times greater than that of mixed and lithium salts in non-aqueous solvents (Stoner and Wohlfarth, 1948).

4.6. IONIC LIQUIDS FOR SUPERCAPACITORS

Supercapacitors, in contrast to typical electrochemical power sources such as batteries, contain an electrolyte that restricts the energy density of a cell by restricting the operating voltage and specific capacitance of a cell. As shown in the following equation, the specific capacitance C of a supercapacitor cell U is dictated by its working voltage V and the energy density of the cell U:

U 1/4 ð1=2ÞCV²

It is determined by the number of ions accumulating on the surface of a unit mass of porous electrode, which determines the specific capacitance of a capacitor cell. Instead, the operating voltage of a capacitor cell is significantly determined by the cathodic and anodic decomposition potential limitations of electrolytes. For effective energy storage technologies, safety concern is also required to be considered. In this perspective, the range of nonflammable components is vital to increase inherent safety (Wilson et al., 1997).

In the development of commercial supercapacitors, both non-aqueous and aqueous electrolyte solutions have been used. The operating voltage of cells in aqueous electrolytes is limited to 1 V, which causes them to malfunction. Organic solvents, on the other hand, are very flammable, which poses a significant barrier to the production of non-aqueous electrolytes in the laboratory. For high-energy applications, an electrolyte with nonflammability and a large electrochemical window is desired (Figure 4.7).



Figure 4.7: Ionic liquids in supercapacitors.

Source: https://link.springer.com/article/10.1007/s41061-017-0150-7.

Researchers from a wide range of fields have been drawn to the study of ionic liquids, which are defined as molten salts at room temperature. This is due to their "ionic" nature, which distinguishes them from both nonaqueous and aqueous "molecular" media, and the fact that most ionic liquids are composed of anions and cations with organic structures, which allow the properties of ionic liquids to be controlled (Hirosawa et al., 2017). To be used in electrochemistry, ionic liquids have a number of benefits over other materials, including strong conductivity, nonflammability, and broad electrochemical windows (Gutfleisch, 2000). Some studies have concentrated on the electrochemical stability of organic solvent electrolytes because they believe that the electrochemical breakdown of organic solvent electrolytes is triggered by the solvent species. In the subsequent sections, the several types of ionic liquids that may be used as supercapacitor electrolytes, as well as their features, will be briefly discussed. First and foremost, the peculiar structure of the double layer generated in ionic liquids is described in detail. Specifically, their use in double-layer capacitors (EDLCs) is discussed in detail in the next section.

4.6.1. Double Layer Formed in Ionic Liquid

Because the solvent in the Gouy-Chapman-Stern (GCS) hypothesis of double-layer production is absent in ionic liquids, it is plausible to suppose that the electric double layer designed is different from that formed in normal aqueous or organic solvent electrolytes. An alternate theoretical model for the interface between ionic liquid electrolyte and electrode has been presented based on the mean-field approach and the assumption of the limiting of local ion densities at the double-layer area (Sarma and Chandra, 2021). Differential capacitance, according to the theory, has a potential dependence that differs from the GCS model, namely, a bell-like or camellike potential dependence with local minimum or maximum at zero charge potential (PZC). Whereas experimental data on the potential requirement of double-layer capacitances in various ionic liquids do not fit this model, it can explain some unexpected behavior like the parabolic and hump curves (Nakamura et al., 2013). Recent spectroscopic or electrochemical attempts to corroborate the structure of the double layer in ionic liquids have been intriguing. There have also been proposed models for the structure of the double layer in pores (Gutfleisch et al., 2006).

4.6.2. Ionic Liquids for the Use in Double-Layer Capacitors

When used in high-energy EDLC, ionic liquid electrolytes must have high thermal stability, high conductivity, and a wide electrochemical window to ensure the cell's safety. Several attempts to use different ionic liquids for EDLC have been attempted (Raisigel et al., 2006). Figure 4.7 depicts some of the most often studied anions and cations for double-layer capacitors. The characteristics of ionic liquid, which are regulated by cation and anion species as explained below, determine the performance of a capacitor cell. Ionic liquids containing the 1-alkyl-3-methyl imidazolium cation have high conductivity and low viscosity, but their low cathodic stability limits their energy density (Zimm et al., 1998; Contreras et al., 2017). The employment of those with quaternary ammonium cations, on the other hand, improves stability toward the negative electrode at the expense of fluidity.

Because it is difficult to immerse high-viscosity ionic liquid in the pores of a porous carbon electrode in ionic liquid electrolytes, in ionic liquid electrolytes, the specific capacitances of traditional porous carbon electrodes are frequently low, and the capacitances suffer severe degradation under high-rate discharge (Tishin and Spichkin, 2003). As a result, several papers on EDLC with ionic liquid electrolyte use temperatures as high as 60°C or the ionic liquid is blended with varying amounts of organic solvents such as propylene carbonate (PC) or acetonitrile (AN) (Brück et al., 2008). For ionic liquids, the degree to which viscosity decreases as temperature rises is important. As a result, the high-temperature operation seems to be sufficient for devices using the ionic liquid electrolyte. The dissolving of liquid salt into the organic solvent is comparable to the mixing of ionic liquid with the organic solvent. The use of ionic liquid as an electrolytic salt has several advantages, including increasing salt concentration, preventing hunger, and ensuring low-temperature functioning. Nisshinbo Co.'s appealing contribution, dubbed "N's CAP," is a marketed example of this approach. For this, they first made ionic liquids containing the N, N-diethyl-N-methyl-N-(2-methoxyethyl) ammonium (DEME) cation. These ionic liquids have good fluidity and a great electrochemical window, as shown in Table 4.1. Four types of capacitor modules with operating voltages of 15, 100, 200, and 400 V are listed on their website. The 15 V cell has a capacitance of 200 F, the internal resistance of 8 mO, and a maximum current of 600 A. They claim that even at 40°C, their test cell holds over 95% of its roomtemperature capacitance (Ohno et al., 2002).

4.6.3. Future Research Directions

With viscous ionic liquid electrolyte, it is expected that an appropriate EDLC setting will be achieved to merge porous electrodes to ensure facile ion transfer (Brück, 2005). One such candidate is the CNT (carbon nanotube), which provides "open" mesopores from interfibrous spaces when inserted into the interfibrous space. Ions in ionic liquid are easily available to the electrode surface when they are contained within open pores. Vertically aligned carbon nanotubes (CNTs) in particular have a particularly accessible structure for viscous ionic liquids. It has been demonstrated that the pattern of ionic liquid electrolyte and CNT electrodes can achieve excellent high-rate performance (Holade et al., 2015). The studies on graphene demonstrate that recent progress in the nanoscale design of carbon materials has been anomalous. As a result of the development of novel nano carbons, it is expected that useful high-performance EDLCs, including neat ionic liquid electrolytes, will become a reality in the near future (Ruiz et al., 2001).

Although a small number of research have been conducted in which an ionic liquid electrolyte has been used in a redox capacitor system, this is likely owing to difficulties in reproducing in ionic liquid media the pseudo-capacitive reaction. However, even as the notion of pseudocapacitance of conductive polymer electrodes allows for the use of ionic liquid electrolytes, the high viscosity of the ionic liquid and the presence of ions that are "inactive" may cause the pseudo-capacitive reaction to being slow. It is anticipated that the employment of a nanostructured conductive polymer electrode in combination with an ionic liquid electrolyte will be successful (Gajbhiye et al., 2008). When it comes to transition metal-based redox capacitors, where the proton is regularly involved in the reaction mechanisms, using ionic liquids is much more difficult. A number of anions, including thiocyanate, have been shown to increase the pseudo-capacitance of manganese oxide (Ningthoujam and Gajbhiye, 2010). In order for hydrous ruthenium oxide to have pseudo-capacitance, the proton must be adsorbed on the electrode surface, which means that there must be a proton present in the electrolyte. As a result, researchers have attempted to use proton-containing ionic liquids in conjunction with a ruthenium oxide electrode (Goya et al., 2003). According to a recent report, 1,3-substituted imidazolium cations, for example, EMI, support the pseudo-capacitive reaction of ruthenium oxide. This is particularly interesting from the standpoint of the formation of the pseudo-capacitive system on the basis of the chemical nature of ionic liquids, which is currently under investigation (Barbeta et al., 2010).

4.6.4. Liquid-Liquid Extraction

Liquid-liquid extraction is one of the separation techniques that are employed. Because of its high energy efficiency, this method is widely used in the industrial sector. Specifically, two non-mixed phases, namely the blue and organic phases, are employed in this procedure. The vast majority of solvents utilized in chloroform's organic phase are volatile solvents, which means they evaporate quickly. Aqueous ionic liquids are a good substitute for the organic phase in many applications. Ionic liquids are primarily employed in the extraction of precious metal ions like actinides, lanthanides, and gold, as well as the separation of harmful metal ions such as mercury and cadmium from drinking water sources. Table 4.1 contains a list of the ionic liquids that were employed in the metal ion extraction method.

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	Substances	Metal Chelator/ Ligand/Extract- ant	IL
Alkali metals	K ⁺ , Na ⁺ , Li ⁺ , Cs ⁺ , Rb ⁺	DC18C6	(CnMIM)(PF6) (n = 4–9)
Heavy and radioactive metals	Pb ²⁺	DC18C6	(CnMIM)(PF6) (n = 4–9)
Alkaline earth metals	$\frac{Mg_{2^{+},}}{Ba^{2^{+}}}Ca^{2^{+}}, Sr^{2^{+}},$	DC18C6	(CnMIM)(PF6) (n = 4–9)

Table 4.1: Various Ionic Liquids with the Solvent Employed in the Metal Ion

 Extraction Process

4.7. METHODS FOR THE SYNTHESIS OF IONIC LIQUIDS

4.7.1. Alkylation

Several ammonium-, phosphonium, pyridinium-, and imidazole-based ionic liquids contain alkyl cations, which are formed by reacting a proper precursor with an alkylating agent like d-alkyl sulk or haloalkane. Taking the example of alkyl imidazole, which is one of the fundamental building blocks of imidazole-based ionic liquids, alkalizing imidazole is a straightforward procedure to follow. In a similar vein, halogens of alkanes are employed to alkaline pyridine and to yield alkyl salts of pyrimidine, which are both useful compounds. Asymmetric halides, such as phosphorus tetrachloride asymmetric, are typically formed by growing the nucleus bond of the 3rd type of phosphine to haloalkanes, as in phosphorus tetrachloride asymmetric (Stoner and Wohlfarth, 1948; McFadden et al., 1999).

4.7.2. Anion Exchange

Several ionic liquids utilized in typical investigations, like the hexafluorophosphate and tetrafluoroborate ionic liquids, are generated in a two-step method employing imidazole diacetyl cations. Primary, the halide salt is generated by reacting the alkyl with the appropriate cation. The anion halide is then shifted by a twofold alternate with the required anion. In this method, an anion of an elemental salt is changed by a mineral anion, like silver salt or metal salt group (Brück, 2005; Brück et al., 2008).

4.7.3. Solvent-Free Synthesis

In general, there are two processes involved in the synthesis of non-alcoholic ionic liquids. In the process of double anion exchange, the employment of a haloalkane as an alkylating agent result in the creation of undesirable halide salts that must be removed. It should be observed that haloalkanes, particularly those with high boiling temperatures, are hard to separate from the result once this reaction has been completed. Another important factor to consider is that halide salts, which are formed through a double substitution reaction, have a major impact on the physical properties of ions. With the aid of intermediary metals, halide salt impurities can produce inactivation or poisoning of catalysts in which ionic liquid serves as the solvent for an accelerated reaction involving a catalyst (Shiroishi et al., 2009).

4.7.4. Synthesis of Chiral

Asymmetric synthesis is made possible by the use of crystal ionic fluids as a catalyst and a solvent, respectively. It is possible to obtain these compounds from chiral sources, which include a diverse range of pre-crystal precursors, such as amino acids and synthetic enantiomers, chiral compounds, terpenes, and sugars. Others are naturally obtained from plants and animals. Ionic liquids are often produced by alkalinizing a pre-crystal precursor and then exchanging anionic ions with the precursor (Stoner and Wohlfarth, 1948).

4.7.5. Synthesis of Ionic Liquids with a Distinct Performance

Ionic liquids are used in a variety of applications where large-scale cations or anions are present. The use of functional ionic liquids, or more specifically, ionic liquids with unique performance, in chemical synthesis, catalyst production, and the production of products such as pharmaceutically active compounds, missile propulsion systems, and lubricants is becoming increasingly common. Because of this, there has been an increasing trend in the study into the manufacturing of these materials in recent years. Several methods for the manufacture of ionic liquids with exceptional performance have been published in the literature. Ionic fluids containing the causative agent's pyridinium, phosphonium, and imidazolium are created by reacting a commonly active haloalkane with the causative agents. It was in the early 1900s when the creation of immunosuppressive ionic liquids was first reported, and it was centered on the removal of metal ions from aqueous solutions. Because of anionic exchange with commercial acids and alkaline

salts, it is possible to generate a variety of ionic liquids using an ionized agent (Stoner and Wohlfarth, 1948).

There are alternative methods of sterilizing anion, such as using interesting fiction. An ionic liquid containing a functionalized alkyl sulfates anion has been constructed using this approach, which has been proposed for the first time.

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5

CHEMISTRY OF SALTS AND AQUEOUS SOLUTIONS

CHAPTER

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5.1. INTRODUCTION

In chemistry, a salt is defined as a chemical substance that is made up of an ionic assembly of cations and anions, which is defined as follows: As a rule, salts are constituted of a similar number of cations and anions, resulting in a product that is characterized as electrically neutral by the scientific community (without any net charge) (Ladd, 1994). They can be organic, such as acetate (CH₃CO₂), or inorganic, such as chloride (Cl); they can be monatomic, like fluoride or polyatomic, like sulfate (SO²⁻⁴), or a combination of the two types. CuCl₂, NaCl, and other forms of salt are presented as examples:

 $Acid + Base \rightarrow Salt + Water$

Because of its broad use on a daily basis, NaCl is the most well-known salt, and it is the one salt that practically everyone refers to Kunz (2010). Let us have a look at the many varieties of salt that are described in subsections.

5.1.1. Acidic Salt

Acidic salt refers to the salt that is generated as a result of the partial neutralization of a polyprotic or diprotic acid solution. These salts have ionizable H+ ions as well as another cation in addition to the ionizable ions. The ionizable hydrogen ion (H+) is classified as an anion for the most part. In baking, a few acid salts can be used to add flavor. Examples are KH_2PO_4 , NaHSO₄, and others.

		1		
Acid		Salt		
Carbonic acid	H ₂ CO ₃	Carbonate salts	Iron(ll) carbonate Calcium carbonate	FeCO ₃ CaCO ₃
Nitric acid	HNO ₃	Nitrate salts	Potassium nitrate Aluminum nitrate	KNO ₃ Al(NO ₃) ₃
Hydrochloric acid	HCl	Chloride salts	Sodium chloride Ammonium chloride	NaCl NH ₃ Cl
Ethanoic acid	CH ₃ COOH	Ethanoate salts	Lead(ll) ethanoate Copper(ll) ethanoate	$\frac{\text{Pb(CH}_{3}\text{COO)}_{2}}{\text{Cu(CH}_{3}\text{COO)}_{2}}$
Phosphoric acid	H ₃ PO ₄	Phosphate salts	Iron(ll) phosphate Ammonium phosphate	FePO ₄ (NH ₄) ₃ PO ₄
Sulfuric acid	H ₂ SO ₄	Sulfate salts	Ammonium sulfate Magnesium sulfate	$(\mathrm{NH}_4)_2\mathrm{SO}_4$ MgSO ₄

H.SO.	+ NaOH ·	\rightarrow NaHSO	+ H.O
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5.1.2. Alkali or Basic Salt

A basic salt is a salt that is generated as a result of the partial neutralization of a strong base through a weak acid. Basic salts are found in nature. These salts undergo hydrolysis, resulting in the formation of a basic solution. Due to the fact that when the hydrolysis of a basic salt happens in solution, the conjugate base of the weak acid is formed in the solution (D'Ans, 1933) for instance, white lead.

5.1.3. Mixed Salts

Mixed salt is a type of salt that contains a fixed percentage of two salts and which frequently shares either a common anion or cation with the other salts—for example, CaOCl₂.

5.2. HISTORY OF SALT

Salt is composed of two elements: sodium and chloride, with sodium accounting for up to 40% of the molecule's total weight. The salt and chloride requirements of the human body must be met by dietary sources. Salt, in conjunction with fermentation and dehydration (by air or sunlight), are traditional ways of food preservation that date back to prehistoric times. When the Chinese discovered that soaking meat or fish in salt solutions permitted for long-term preservation, they applied this approach to a wide variety of foods. Because boiling food, in particular, would have eliminated the salt naturally present in the food, it is possible that the use of salt in the diet began soon after man began cooking food. Over the course of centuries, salt rose to become one of the most traded commodities on the planet, as well as one of the most heavily taxed (Euliss et al., 2003) commodities. As a way of putting a monetary value on slaves in ancient Greece, the statement "not worth his salt" arose. In Roman times, salt rations, known as "Salarium Argentum," were given to Roman troops, from whence the English word "salary" was formed. Indeed, salt became so highly prized as a food preservative during the Classical and Medieval periods that it was employed as a type of currency to exchange products and services (Voigt, 2001).

The mineral salt occurs naturally in seawater and rock salt deposits when an region of seawater is enclosed and the water evaporates as a result of the heat from the sun. Other than that, salt may also be found in conjunction with other ingredients in specific rocks, or it may dissolve in natural brines originating from porous rock or flowing from salt springs beneath the surface of the earth where it can be found dissolved. The salt may be buried beneath layers of other sediments that have accumulated over millions of years, leaving only the rock salt beneath the surface. Over 100 countries throughout the world have facilities for generating white salt. These range from rudimentary sun evaporation facilities to modern multistage evaporation processes in purpose-built salt refineries (Freyer and Voigt, 2004).

5.3. PROPERTIES OF SALT

5.3.1. Color

When it comes to solid salts, transparency is usually preferred, as seen by the sodium chloride molecule. When it comes to monocrystals, the apparent opacity or transparency is only connected to the size difference between the individual monocrystals in most circumstances. Because light imitates from the grain boundaries, the bigger crystals appear to be transparent, whereas the polycrystalline aggregates appear to be white powders because light reflects from the grain boundaries (Garrett, 2004).

5.3.2. Odor

Strong salts are non-volatile and often odorless, but weak salts may smell like the component ions' conjugate acid or conjugate base.

5.3.3. Taste

Bitter, sweet, salty, sour, and umami or savory are all flavors that can be elicited by different types of salts.

5.3.4. Conductivity

Salts are known for their ability to behave as insulators. Electricity is conducted by molten salts or salt solutions. As a result, liquified (molten) salts, as well as solutions containing dissolved salts, are mentioned to as electrolytes in scientific literature.

5.3.5. Melting Point

Salts are known for having high melting points due to their chemical composition. At a temperature of 801°C, assume that sodium chloride melts.

Some salts with low lattice energies are liquid at or near room temperature, but the majority are solid. In this category, you'll find melted salts, which are typically combinations of salts and ionic liquids, which are typically cations that have been organically modified. These liquids have peculiar qualities, such as solvents, and should be avoided.

5.4. IDENTIFICATION OF SALTS

In chemistry, if a chemical is formed by the reaction of either an anion or a cation, it is referred to as a salt by definition.

In their most basic form, salts are compounds formed when one sort of metal cation reacts with one type of non-metal anion. When we notice at the periodic chart, we can see that there is a dark and stair-step line over on the right side. The atoms that occur to the left of it are referred to as metals, and those that exist to the right of it are referred to as non-metals. A handful of the atoms that exist on the steps are referred to as metalloids or semi-metals.

Salts can be compounds that contain a polyatomic anion and a metal cation in addition to the metal cation. Salts are also compounds that contain both a polyatomic cation and an anion, and they are found in a variety of forms (Steiger and Asmussen, 2008).

5.5. DIFFERENTIATION BETWEEN ACIDIC AND BASIC SALT

A basic salt is a compound that holds the conjugate base of a weak acid. As a result, acetate is referred to as the conjugate base of acetic acid, which is a weak acid. As a result, sodium acetate is a basic compound.

The conjugate acid of a weak base is contained within an acidic salt. As a result, the ammonium ion is referred to as the conjugate acid of the weak basic ammonia. As a result, ammonium chloride would be considered the acidic salt.

NaCl and other neutral salts are produced by the conjugate bases of strong acids and the conjugate acids of strong bases, which are both designated as neutral.

5.6. SALTS IN AQUEOUS SOLUTIONS

Salts are a very vast and essential group of chemical substances that are found in nature. The solubility process and chemistry of salts in aqueous solutions,

particularly in multi-ion systems, are critical to the natural occurrence of salts as well as industrial methods for their recovery, conversion, purification, and application. In wide T-p-x ranges, it is necessary to have information of the properties of aqueous salt solutions in order to model these processes and design new ones. This information includes a rising number of components in solutions as well as a knowledge of their properties. Using thermodynamic records of solids and aqueous species in combination with a suitable ioninteraction model to achieve equilibrium calculations for species distributions in phase equilibria and solution is the generally accepted methodology, at least for the thermodynamic properties. The current status in terms of existing thermodynamic prototypes and data for their parameterization is examined in detail with respect to a few representative situations. There is a greater emphasis placed on the accuracy with which phase equilibrium data are determined experimentally for the purpose of deriving model parameters as a result of this. Also concluded is that experimental investigations should be carried out in accordance with a chemical systematic. Physical models or quantum chemical calculations are unable to forecast unknown quantities in databases with adequate precision when using simple physical models or quantum chemical calculations (Möhlmann and Thomsen, 2011).

Finally, the effects of elevated temperatures on solubility changes in saltwater systems are examined. As protic ionic liquids, systems that can be termed molten hydrates exhibit fascinating phase behavior and chemical reactivity that distinguish them from other types of liquids. The latter can be used in chemical syntheses to replace mixes of intense acids such as HNO_3/H_2SO_4 with simple salts such as ferric nitrate, which are less concentrated.

A resurgence of chemical directed basic analyzes of water–salt systems would be beneficial for gaining a better knowledge of the chemical and phase behavior of water–salt systems in terms of structure-property relationships (Königsberger et al., 2009).

When it comes to the chemistry of salts in aqueous solutions, it is primarily concerned with the processes of their dissolution and crystallization, as well as hydrolysis and the production of complicated ions in solution. Metal cations combined with inorganic anions such as halide, sulfate, nitrate, phosphate, and other common elements result in a huge number of compounds having salt-like characteristics, which are defined as those characterized by the dominance of ions. The class of salts encompasses a vast range of substances, ranging from sodium chloride (NaCl) to gypsum (CaSO₄2H₂O), anhydrite (CaSO₄), saltpeter (NaNO₃), and cryolite (Na₃AlF₆), as well as salts of heavy metals and noble metals. Solubility of salts is a topic that is addressed in many

fields, including geology, environmental science, medicine, and industrial operations. The answer to this question is the ion combination that will result in the formation of a solid salt from an aqueous solution of a specific composition and temperature. Common and organic chemistry textbooks characterize salts as ionic substances that crystallize in ionic lattices with a particular lattice energy, which is a property of ionic lattices. The process of ionic hydration is required in order to dissolve these salts in water because the lattice energy must be overcome. It is then possible to utilize these two values to explain trends in the solubility of simple salts, such as alkaline metal halides or alkaline earth metal sulfates, which are frequently related to the Haber–Born cycle (Debye, 1923). This illustration is only suitable for gaining a general understanding of factors such as ion charge/radius ratio that have an impact on the solubility of salts. Aside from the fundamental qualities of the solids, there are other considerations (lattice enthalpy, entropy) The interactions between ions and water, as well as between ions and other ions, determine the solubility of salts in water or in solutions surrounding other ions. Concentration, composition, and temperature all have a significant effect on these interactions, which change very quickly. Even with the use of definitive structural models, chemistry is still unable to provide a quantitative response at this time. Solubility relationships of different salts in mixed ionic solutions serve as the foundation for insight into their existence and stability in contact with aqueous solutions, which is important for many applications (Guggenheim, 1936).

Van't Hoff, the first person to win a Nobel Prize in chemistry in 1901 (Figure 5.1), was responsible for carrying out the first systematic inquiry of this kind. In 2011, we commemorated the 100th anniversary of his death. By employing state-of-the-art theory of chemical equilibrium and thermodynamics, he and his coworkers were able to develop inside 12 years of research an almost complete scheme of the composition and temperature conditions for the creation of the numerous salt phases from aqueous solutions of the oceanic system, which contains the ions K⁺, Na⁺, Mg²⁺, Ca^{2+} , Cl^{-} , and SO_4^{2-}). Investigating the circumstances of the development of oceanic salt deposits, particularly of the stassfurt deposit, was a wellknown book that compiled the findings of the 52 pieces published in the journal science. Additionally, this was the first systematic examination of a multi-component saltwater system, which was critically required at the time for a more successful discovery of potash resources and recovery of potash for use in the production of potash fertilizer. Following van't Hoff's work, D'Ans (D'Ans, 1933) carried on the work, which has been carried on to

the present day (Guggenheim and Turgeon, 1955). More than a century of research into this salt system has progressively enhanced technology in the recovery of mineral fertilizers, the knowledge of salt deposit formation, and the production of simple chemicals as part of the prolonged oceanic system, counting carbonates, OH^- and H^+ , among other things.



Figure 5.1: Jacobus Henricus van't Hoff and the Swedish Academy of Science document bestowing the Nobel Prize in Chemistry to him.

5.7. SALT–WATER SYSTEMS IN MODERN APPLICATIONS

Storage of nuclear waste in biological salt formations, such as in northern USA or New Mexico, Germany, in old salt mines stowage of inorganic toxic waste, CO_2 sequestration in highly saline aquifers of great depths, and exploitation of geothermal brines, are all new aspects of applications that require detailed knowledge of solubility. These additional duties need an understanding of phase behavior and solution characteristics over a wide range of temperatures and pressures, as well as the addition of more complex components such as CO_2 , Li⁺, actinides, bases, and acids, and heavy metals (Lu and Maurer, 1993) (Figure 5.2).



Figure 5.2: Thermal desalination system containing saltwater.

Source: https://www.researchgate.net/figure/Thermal-Desalination-Systemsource-https-studycom_fig1_330180828.

The latter ion has recently emerged as a critical issue in the recovery of lithium salts through brines of lakes and salt flats in Asia and South America, in order to confirm a sufficient supply of Li_2CO_3 for use in large lithium batteries for automotive and other applications in both the United States and China. The brines found in the salt crusts include between 300 and 4000 parts per million (ppm) Li⁺. The concentration is increased as a result of solar evaporation. While this is going on, massive quantities of additional salts must be crystallized (Scatchard et al., 1970) and separated by taking advantage of the multicomponent solubility equilibria (Figure 5.3).

Another topic to discuss is the weathering of antique and contemporary structures. It is frequently regulated by the crystallization and dissolution of salts in response to changes in the relative humidity of the surrounding atmosphere. These procedures require thorough information on phase diagrams and characteristics of alkaline earth metal chlorides and alkaline, nitrates, and sulfates (Reilly et al., 1971).



Figure 5.3: The intergranular brine under the salt surface in the Salar de Uyuni has an average lithium level of 500–600 ppm Li⁺/L. Inset: major ions in solution with quantities of salts to be crystallized for the manufacture of 1 t of Li_2CO_3 in a brine cavity 40 cm below the surface.

In addition to interplanetary science, the chemistry of saltwater systems is requested for a topic in environmental chemistry. New findings from Mars missions have revealed that aqueous salt solutions can survive at extremely low temperatures (180–250°K), according to the researchers. The concerns emerge as to what cryotectic water–salt mixes can be created at temperatures as low as 200°K, what features can be expected from these solutions, and whether or not they could be a suitable habitat for life. A significant number of saltwater systems must be investigated in order to provide answers to these problems.

Today's applications, of course, include any and all hydrometallurgical processes used in the purification and recovery of zinc, aluminum, and heavy metals such as cobalt, nickel, copper, and other elements. In order to better regulate leaching and solid-liquid separation processes, it is necessary to have a more accurate understanding of phase and chemical equilibrium as well as the kinetics that lead to these equilibria (Puigdomenech and Plyasunov, 1997).

To take full advantage of the sensitivity and precision of modern concentration monitoring methods, environmental sciences require more accurate equilibrium data than is currently available.

5.8. SOLUTION MODELS AND THERMODYNAMIC DATABASES

The physical explanation of long-range ion-ion interactions was the focus of additional study in the theory of salt solutions, or more generally electrolyte solutions, beginning with van't Hoff (Debye, 1923). In conjunction with ion-limited, short-range interface factors, equations for the concentration dependency of osmotic coefficients, activity coefficients of salt elements, or more generally the extra Gibbs energy of mixing have been derived. As of this writing, Pitzer's ion interaction model is the most widely used method for the thermodynamic treatment of concentrated electrolyte solutions (Puigdomenech and Plyasunov, 1997). On virial equations a number of essential considerations for electrolyte solutions, a limitation to the second and third virial coefficients, and a carefully chosen mathematical form for the ionic strength dependency all serve to support this conclusion. In this way, when model constraints are calculated from appropriate ternary and binary saltwater systems, the model can accurately explain the thermodynamic properties of electrolyte solutions up to ionic strengths of around 6-10 mol/ kg H₂O, depending on the ionic strength. Using a particular temperature and a typical system like the one described above, three parameters for every binary system and two additional empirical parameters for the ternary system are required; in this example, there are a total of eight parameters. All interactions in higher-component systems are estimated solely from the parameters of the corresponding binary and ternary systems, with no further parameters used. A similar study has been conducted for the oceanic salts for the most relevant 35 salt phases. When used in conjunction with proper equilibrium calculation codes, Pitzer solubility factors and parameters produce a data set that may be kept in a thermodynamic database (Bea et al., 2010).

It is fully dependent on the model parameters' temperature dependency that Pitzer's theory is applied, and so only empirical equations are employed. There are up to 8 temperature coefficients required for each Pitzer parameter over the temperature range 0 to about 200°C. In the case of solubility constants, the same holds true. Databases including such temperature-dependent data allow for the calculation of enthalpic effects as well as other impacts. The predictive power of the Pitzer model, on the other hand, is restricted for those solutions which contain more than 6 molar ionic strength (Haghtalab et al., 2011).

Personal computers and laptops have adequate computing capability to execute equilibrium calculations with phases in seconds and hundreds of species, thanks to advances in-memory technology. For this reason, in order to research geochemical and industrial procedures, thermodynamic modeling and simulation are used in conjunction with a suitable database and software code. It is being attempted to link equilibrium calculations with transportation codes (Voigt et al., 2007). Computing time for the equilibrium states develops extremely important in this situation (Ge and Wang, 2009).

Such data are only accessible for a small number of ternary systems at a single temperature, and the situation is significantly worse when temperature ranges are taken into consideration. There has recently been a study of database projects (Xu and Macedo, 2003), which collect existing data from the literature and use it to extract model parameters.

As a result, ongoing efforts are devoted toward the development of models with a fewer number of configurable variables. However, only binary saltwater systems (Pazuki and Arabgol, 2005) have been extensively studied for their application. One general strategy is to combine standard nonelectrolyte models like the UNIFAC, UNIQUAC, or NRTL models with an expanded Debye–Hückel term (Haghtalab and Joda, 2007), which is a method that has been used in the past.

In their paper (Jaretun and Aly, 2000), Iliuta, and Thomsen provide massive explanations for the implementation of an extensive NRTL model for saltwater systems. Because temperature-dependent models are taken into consideration, the advantage of having an apparent reduced number of factors in the solution model is frequently outweighed by the fact that the solubility constant has an abnormally large number of temperature coefficients. Despite the fact that the presence range of a double salt or salt hydrate is frequently < 15° K, the solubility constant can be approximated using five temperature coefficients (Lu et al., 1996). Some additional types of models make use of physical reference models, such as MSA, integral equation method, or others, which are discussed by Lu et al. (1996).

It is also possible to obtain missing interaction coefficients in a Pitzer model by using "quasi-experimental" data generated by mixing methods such as those proposed by Zdanovskii or Young (Iliuta et al., 2002), for example.

The information is provided on the thermodynamic standard-state properties of ions in water at 298°C (Kuramochi et al., 2007). The correlation from Helgeson, Kirkham, and Flowers (HKF model) is frequently used for prolonged temperatures and pressures, and the values provided by the HKF standard can be conveniently retrieved because of the software program SUPCR92. It is also possible to estimate standard data for high temperatures using more straightforward correlations such as those suggested by Cobble and colleagues or the coulombic advantage principle (Yan et al., 1999).

These data are frequently available in online databases, making them easily accessible (Li et al., 2005). However, it is the user's responsibility to guarantee that standard data, speciation, and activity models are along with one another and with other databases (Barthel et al., 1998). However, in spite of consistency challenges and ambiguities in the validity varieties of model parameters, among other things, the community of users who consistently deploy packages involving of a solution model, calculation algorithms, and databases to deal with aqueous chemistry difficulties is constantly expanding. There is a great emphasis on expanding the databases as well as improving the codes and their user interfaces (Wang, 2009).

5.9. DATA SOURCES AND EXPERIMENTS

The essential forms of experiments from which constraints for thermodynamic models are expected are (Marcus, 1991; Königsberger et al., 2008):

- Vapor pressure measurements;
- Isopiestic measurements;
- Galvanic cells in dilute aqueous solutions;
- Measurements of heat capacities and heat of dilution or dissolution;
- Determination of solid-liquid equilibria (solubilities); and
- pH, spectrophotometric measurements, NMR, and Raman spectroscopy for speciation equilibria (Chase, 1998).

Experiments of categories a–e are often carried out in undersaturated solutions, with the results revealing just the properties of the solution. Using the results of solid-liquid equilibrium determinations, it is possible to derive the thermodynamic quantities of the solid phases (Wagman et al., 1992).
In principle (and at the most fundamental level), the latter information can be acquired from measurements of the enthalpy of dissolution of the solid phase and the heat capacity at low temperatures. The majority of the formation data would be wrong if the solubility data were not accurate as well (Haas et al., 1995).

Especially in the case of solubility determinations, it is frequently necessary to review extremely old works, since in aqueous salt systems, the study of solubility is not considered to be of scientific interest in contemporary chemistry, save in few cases (Johnson et al., 1992). One realworld example is the solubility equilibria of polyhalite, a triple salt mineral with the chemical formula K₂SO₄. MgSO₄.2CaSO₄.2H₂O that is widely distributed in rock salt formations. Van't Hoff (Harvie et al., 1984) is the only authors who have published data at the standard temperature of 298°K. Apart from the solubility product of polyhalite itself, it is necessary to know the Pitzer parameters for the Mg²⁺–Ca²⁺ and Mg²⁺–SO4^{2–}–Ca²⁺ interactions at high concentrations of MgSO4 in order to develop a thermodynamic model to define the structures of solutions in which polyhalite can be in equilibrium. The latter can be determined most accurately by measuring the solubilities of gypsum in MgSO₄ solutions. At a temperature of 298°K, Harvie, Möller, and Weare constructed the Pitzer equation-based seawater model that is well-known in the geochemical world (Djamali and Cobble, 2010). For the description of the Mg^{2+} - $SO4^{2-}$ -Ca²⁺ interaction, they had to depend on Cameron solubility determinations of gypsum from the year 1906, which they had to use in their data compilation process. The determination of Ca²⁺ contents in highly concentrated magnesium salt solutions was not possible at the time due to a lack of suitable analytical methods. Illustration of the difference between the new and old data is shown in Figure 5.4. Using the example of polyhalite in potassium and magnesium sulfate solutions at 298°K, the implications of the new results are demonstrated. It is estimated for the presence of polyhalite at 298°K using the revised Pitzer version of the hexary oceanic salt system, which incorporates a significantly greater composition range than the previous model. This has implications for the interpretation of brine analyzes based on geochemical data (Fernandez-Prini, 1991) (Figure 5.5).



Figure 5.4: Solubility of gypsum as per Cameron 1906 (\circ), Wollmann, and Kolosov 2010, error bars.

Source: https://www.degruyter.com/document/doi/10.1351/PAC-CON-11-01-07/html.



Figure 5.5: Crystallization field of polyhalite (Ph) in the system K_2SO_4 -MgSO₄-CaSO₄-H₂O at 298°K; thin lines = calc. With Pitzer model depend on new solubility data, Stars = presence triangle for polyhalite according to Van Klooster's tests, thick-lined polygon = polyhalite field calculated with HMW's model.

Source: https://tubaf.qucosa.de/landing-page/?tx_ dlf[id]=https%3A%2F%2Ftubaf.qucosa.de%2Fapi%2Fqucosa%253A22719 %2Fmets. Furthermore, we find that Polyhalite in combination with solution can have a lower formation temperature than 286°K, contrary to what van't Hoff anticipated and which has never been changed till the current day (Rard et al., 1991). Drillings in the Salar de Uyuni, where temperatures are far lower than 286°C, have revealed the presence of polyhalite, which appears to support this conclusion (Apelblat and Korin, 2001).

5.10. FORMATION OF SALT HYDRATES AND DOUBLE SALTS

Long-standing problems in crystallization field prediction have arisen from the study of distinct hydrate forms of a salt or double salt. In the past, the direct phase equilibrium experiment was the chosen method of investigation. In order to investigate the equilibrium phases of a specific type of salts or their mixtures, the phases in equilibrium were isolated and chemically examined. The contrast of a sequence of systems and their phase diagrams, directed by some associations of chemical parameters such as softness, chemical hardness, and ionic radius (Gruszkiewicz and Simonson, 2005) or ligand field stabilization energies, directed to inferences about the possible presence of double salts in analogous systems that had not been investigated previously. Certainly, connections of this nature were almost qualitative in nature. In the previous two decades, the situation has radically transformed. It has been made possible by advancements in X-ray crystal structure research tools to uncover a huge number of novel crystal phases both naturally occurring and artificially created (Rard et al., 1991). Often, the composition of known salts can be determined with more precision, as was the case for the "MgSO₄.12H₂O," which is now known as meridianite, MgSO₄.11H₂O, and for kainite and loeweite, among others. As a result, hundreds of double salt phases have been identified architecturally, but no thermodynamic data on their creation or crystallization have been discovered, and the conditions under which they formed or crystallized remain a mystery. For ionic hydrates, for example, numerous estimating approaches have been proposed by Jenkins and Glasser to close the data gaps in thermodynamic databases (Hamer, 1935). The authors usually make use of linear relations of the type:

{ $\Delta f H^{\circ}$ hydrate, $\Delta f G^{\circ}$ hydrate} = { $\Delta f H^{\circ}$ anhydrate, $\Delta f G^{\circ}$ anhydrate} + a $n H_2 O$ (1)

where, fH° and fG° signify the Gibbs energies of formation and standard enthalpies; nH_2O denotes the number of moles of water in the hydrate; and the slope "a" denotes the increase per mol of water added to the mixture. Inside a scatter of 25 kJ/mol, the data are consistent with the equation. As a result, this strategy produces only very rough estimations. Because difference rules of this sort do not take into account the structural characteristics of the solids, and because the formation amounts are linear, hydrates with any quantity of nH_2O would be projected to be stable for a given salt (Giordano et al., 1977).

Using Eqn. (2), another recently published (but not actually new) strategy is to estimate the solubility constants of double salts, KL(DS), from their single component salts using their single component salts (Shi-Yang and Shu-Ping, 2003).

 $K_{\rm L}({\rm DS}) = K_{\rm L}(1)K_{\rm L}(2)$ (2)

Since relation (3) is valid Eqn. (2) suggests the additivity rule of the Gibbs energies of:

 $-RT\ln[K_{I}(i)] = \Delta_{I}G^{\circ}(i) (3)$

A process in which the constituent salts are formed this, on the other hand, indicates the lack of a driving force for the formation of the double salt. By comparing predicted and experimentally determined solution concentrations, it appears that this "law" has been confirmed. This appears to be due to the shape of various solubility diagrams, as illustrated in Figure 5.6, along with the accuracy of chemical analysis (Lourenço et al., 2006). For type A solutions, the composition of solution in equilibrium with the double salt is not significantly different from the composition of solution of a combination of the single salts, and the "rule" appears to be applicable in this situation as well. This is not the case in the cases of types B and C, where the production of the double salt reduces the overall salt concentration by a significant amount in comparison to the inferred single salt areas in the diagram (Schroedle et al., 2010).



Figure 5.6: Types of solubility isotherms of systems MX–NX–H₂O with double salt formation MXNX.

Note: The thick line represents the crystallization branch of the double salt, while the thin lines represent the crystallization branches of the single salts MX and NX.

Source: https://www.researchgate.net/figure/Types-of-solubility-isotherms-ofsystems-MX-NX-H-2-O-with-double-salt-formation-MXNX fig5 270560194.

Tutton's salts, which are double salt hydrates of the type M_2SO_4 . M'SO_4.6H₂O, are among the most thoroughly explored of the double salt hydrates. From aqueous, the Gibbs energy of formation ions could be estimated using one of the aforementioned programs and solution models, and then the crystallization branches of probable double salts could be computed using one of the aforementioned programs and solution models (Smith-Magowan, 1981). On the right-hand side of Figure 5.7(a), the known Gibbs energies of production for M = K are shown to be connected with the ion's radius M'2+ and its location in the periodic table (7a) (7b). Based on the graphs for Mn²⁺, V²⁺, and Cr²⁺, it is clear that the correlation would result in negative Gibbs energy of formation; nevertheless, there is a small uncertainty of approximately 3 kJ/mol in the results. Figure 5.8 shows the effect of a variance of fG°(DS) of this magnitude on the concentration of $M'^{2+} = Mg^{2+}$ (Jones et al., 2007). In addition, other phases for instance leonite join in the field of uncertainty as a result of the abrupt changes in the solubility isotherms. Furthermore, there have been attempts to employ quantum chemistry approaches to anticipate the presence of solid phases. However, they are far too incorrect when it comes to double salt estimates (Hakin et al., 2005).



Figure 5.7: At 298°K, the conventional Gibbs energies of production of picromerite, K_2SO_4 . $MSO_4.6H_2O$, from aqueous ions are correlated, and M = Mn is predicted. The radius of an ion with a coordination number of 6 is called an ionic radius.

Source: https://www.researchgate.net/figure/Correlation-of-the-standard-Gibbs-energies-of-formation-of-picromerite-K-2-SO-4-MSO-4-6H_ fig6_270560194.



Figure 5.8: At 298°K, the effect of a 3 kJ/mol uncertainty in the Gibbs energy of production of picromerite on the solubility curve.

Note: Open circles represent the picromerite's solubility, stars represent the measured picromerite's solubility with increased or reduced Gibbs energy of formation, and open rectangles represent the solubility of leonite; picromerite is represented by the formula K_2SO_4 . $MgSO_4$. $6H_2O$, and leonite is represented by the formula K_2SO_4 . $MgSO_4$. $6H_2O$, and leonite is represented by the formula K_2SO_4 . $MgSO_4$. $6H_2O$, and leonite is represented by the formula K_2SO_4 . $MgSO_4$. $6H_2O$.

Source: https://www.researchgate.net/figure/Effect-of-an-uncertainty-of-3-kJ-mol-in-the-Gibbs-energy-of-formation-of-picromerite-on_fig7_270560194.

In order to forecast the solubility of unknown double salts, substantially more accurate data on $fG^{\circ}(DS)$ are required. The estimating approaches that are now available are not adequate for this reason. Table 5.1 contains all of the famous double salts of the type $M_2SO_4M'SO_46H_2O$ that have been discovered. Until now, the K–Mn combination has not been possible to prepare. At 298 and 313°K, our own examination of the system K_2SO_4 –MnSO₄–H₂O revealed the synthesis of the double salts K_2SO_4 .3MnSO₄.5H₂O, K_2SO_4 . MnSO₄.2H₂O, K_2SO_4 .MnSO₄.1.5H₂O, K_2SO_4 .MnSO₄.4H₂O, and K_2SO_4 .2MnSO₄ (Chen et al., 1996), however no Tutton's type was discovered. Perhaps the latter can be discovered at lower temperatures; nevertheless, even at ambient temperatures, equilibration times of 1–2 months were required to get the equilibrium solid phases in order to obtain the equilibrium liquid phase (Polya et al., 2001).

Table5.1: Evidence to Support the Existence of Tutton's salts $M_2SO_4M'SO_4.6H_2O$; Number of PDF Entries, "No Success" Implies no Successful Preparation Efforts, "No Info" Means no Information at All

M'+ M ²⁺	Cs	Tl	Rb	К	\mathbf{NH}_4
Ni	2	1	2	3	7
Ru	no info	no info	no info	1	no info
Cu	2	2	2	2	6
Mg	2	1	2	2	5
Zn	2	1	2	3	5
Со	2	1	2	4	4
V	no info	no info	no info	no info	2
Fe	2	1	2	1	2
Cr	no info	no info	no info	no info	1
Mn	2	1	1	no success	2
Cd	no info		no info	no success	2

5.11. AT ENHANCED TEMPERATURES THE PROPERTIES OF SALT SOLUTIONS

When the temperature is raised, the solubility of salts can either rise or reduce; in the case of $MgSO_4$, both effects can be observed as illustrated in

Figure 5.9. $MgSO_4$ becomes a sparingly soluble salt at temperatures close to 200°C, where it is equivalent to $CaSO_4$. Ion hydration and association are significantly reduced at low temperatures, resulting in a negative temperature coefficient of solubility. If the concentrations of another electrolyte are high enough, the negative temperature coefficient can be converted to a positive temperature coefficient by adding more electrolytes (Del Re et al., 1990).



Figure 5.9: Temperature dependence of the solubility of MgSO₄, symbols: experimental data.

Source: https://www.semanticscholar.org/paper/Chemistry-of-salts-in-aqueous-solutions%3A-and-theory-Voigt/db41b28103b8d1e7912149209dff5a9ad6a5380c.

Valyashko (2003) provided an in-depth discussion of this subject. It was recently discovered that the solubility of $CaSO_4$, anhydrite, in solutions of NaCl at elevated temperatures can be validated by this phenomenon, which is particularly noticeable at 7.0 mol/kg H₂O, where the crossing point of the solubility isotherms occurs (see Figure 5.10) (Öhman, 1998).



Figure 5.10: Anhydrite solubility isotherms at 373, 423, and 473°K as a function of NaCl concentration; huge symbols: arrows: data, temperature coefficient of solubility in one direction.

Source: https://www.researchgate.net/publication/301294445_'The_System_ NiOH2-NiCl2-H2O_at_25C_and_200C_-_and_relations_between_basic_ nickel_and_magnesium_chlorides.

Because of the coordination rivalry between cations for water and anions at very high concentrations in mixed salt solutions, unusual behavior can occur, as seen in Figure 5.11 for the system KCl–MgCl₂–H₂O. As the concentration of MgCl₂ increases, the course of KCl solubility isotherms approaches a minimum, which occurs in the region of molten hydrates at extremely high MgCl₂ concentration (Szilágyi et al., 2009).



Figure 5.11: Solubility isotherms in the system KCl–MgCl₂–H₂O at 160°C (*), 170°C (\circ), and 180°C (\bullet) (Szilágyi et al., 2009).

Note: At point A, when water is add up to a saturated solution, the supersaturation of KCl is indicated by the arrow and hatching region. Solids other than water: $M1 = MgCl_2 + 4H_2O$, M2 = solid solution; C = carnallite, $KCl - MgCl_2 - 6H_2O$; $M1 = MgCl_2 + 4H_2O$; $M2 = solid solution KCL - KCl - MgCl_2 + 2H_2O$, M3 = KCl. *MgCl*₂.2*H*₂*O*, *M*4 = 1.5 *KCl.MgCl*₂.2*H*₂*O*, *M*3 = *KCl.MgCl*₂.2*H*₂*O* (*Bebie et al.*, 1998).

Source: https://onlinelibrary.wiley.com/doi/abs/10.1002/zaac.19895760112.

The action of KCl as a chloride ion donor for MgCl₂, which results in the formation of chlorocomplexes, causes solubility to increase once more (Brugger et al., 2001). When the temperature is below 160°C and the concentration of magnesium chloride is greater than 130 mol/1000 mol H₂O, a very soluble salt like KCl can be crystallized by the addition of water (Figure 5.11), which is extremely remarkable (Gajda et al., 2009).

The modified Brunauer–Emmett–Teller (BET) model (Sipos et al., 2006) has been effectively used to characterize the thermodynamic properties of molten salt hydrates in the range of temperatures. Every salt component is represented by only two parameters in this model. In many cases, a linear or quadratic function can adequately characterize the temperature dependency of these parameters. It is not possible to utilize the simple BET model when the salt–salt interfaces are significant (Valyashko et al., 2003) (Figure 5.12).



Figure 5.12: Using a reaction chain model, simultaneously describe the phase diagram of the system $\text{KCl}-\text{MgCl}_2-\text{H}_2\text{O}$ (A) between 373–523°K and the thermodynamic characteristics of the anhydrous molten system $\text{KCl}-\text{MgCl}_2$ at 1073°K (Valyashko et al., 2003).

Source: http://publications.iupac.org/pac/83/5/1015/references/index.html.

The acidity and reactivity of molten salt hydrates are two further characteristics that distinguish them. By decreasing the molar water/salt ratio to less than 6 (Harvie et al., 1984), the acidity of simple solutions like

zinc chloride and aluminum chloride becomes comparable to the acidity of powerful mineral acids like hydrochloric acid. Noble metals such as gold can be dissolved at temperatures lower than 100°C in these liquids (Wollmann, 2010). To put it another way, molten salt hydrates are protic ionic liquids, the reactivity of which may be regulated by the amount of water present and the exact anion–cation mixture used. Figure 5.13 depicts the structural state and resultant reactivity of molten ferric nitrate pentahydrate, and it can be used to get a better understanding of the issue. In this state, the water molecules are strongly polarized among nearest-neighbor cations and anions, allowing proton transfer to occur more easily and the formation of an activity of HNO₂ (Balarew and Duhlev, 1984).



Figure 5.13: The nitrating action of liquid ferric nitrate pentahydrate might be explained by the structural state in the molten ferric nitrate pentahydrate.

Source: https://www.semanticscholar.org/paper/Chemistry-of-salts-in-aqueous-solutions%3A-and-theory-Voigt/db41b28103b8d1e7912149209dff5a9ad6a5380c.

Direct coordination of NO^{3-} at Fe^{3+} can result in a scenario that is analogous to the production of a nitryl cation in some cases. The nitrating ability of this molten hydrate is unquestionably due to the effects of the aforementioned processes. Toluene can be nitrated in this medium to form dinitro- and mono-toluene (Peterson and Wang, 2006)., a consequence for which strong sulfuric and nitric acid mixes are often required.

5.12. SUMMARY

Precision property data of aqueous salt solutions over a wide range of temperature, pressure, and composition are required by modern research and technology. At the same time, there is an increasing number of ionic constituents that must be taken into consideration. The computing capability PC is adequate to calculate speciation equilibria and complex solubility of multicomponent water-salt systems using current equilibrium calculation codes, which are available on the market. The results, on the other hand, are constrained by the limitations of the underlying thermodynamic databases and the limitations of solution models. The constraints concern:

- The precision with which experimental data is described is important;
- The coefficients of the numerous ion-ion interactions that are currently accessible in the model;
- Data on solid salts, notably double salts and hydrates, that are considered standard; and
- The limits of pressure and temperature.

Present physical models, particularly for solid phases such as double salts and hydrates, are unable to forecast missing data with the accuracy required. Simple mixing rules, like, Young's rules or Zdanovskii's, should be favored over extrapolation of validity ranges of more sophisticated models for extrapolation of mixed solution characteristics toward higher concentrations when extrapolating mixed solution properties toward higher concentrations.

Application-oriented experimental programs are being developed in order to fill up some of the gaps in the data. An acceleration in the creation of structure–property-related models suitable for prediction would occur in parallel with a revival in systematic physicochemical investigations of electrolyte systems, which would occur concurrently.

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CHAPTER

6

ROLE OF SALT IN PUBLIC HEALTH AND FOOD SCIENCE

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6.1. INTRODUCTION

In food preparation since the beginning, salt has been a staple ingredient, and it is still commonly employed in recent food processing procedures. Salt can be included during cooking; however, processed foods account for a considerable proportion of dietary salt. High salt consumption is closely associated with elevated blood pressure (hypertension), which predisposes persons to the development of cardiovascular disease (CVD), which is the primary reason for death in advanced countries (Hester and Diamond, 1955; Brandsma, 2006) (Figure 6.1).



Figure 6.1: Percentage of salts in different dietary sources.

Source: https://www.mdpi.com/2072-6643/9/9/933/htm.

The growth of kidney illness, the aggravation of asthma symptoms, and the start of osteoporosis have all been linked to excessive dietary salt intake, according to research. Results from a vast number of human research have led to the implementation of international programs aimed at lowering present stages of salt consumption. As a result, there is a critical need to minimize excessive dietary salt intake, which is particularly prevalent in processed foods (Akgun et al., 2018; Shohan et al., 2019). When compared to the current daily consumption numbers, which might range from 10–12 g NaCl daily, an intake of 4 g salt daily is enough. Several public health organizations around the world have set a target reduction of 6 g of sugar per day as their goal. An incremental decrease in the salt content of foods seems to be the most effective technique for lowering blood pressure levels in the general population. In processed foods, any reduction in salt level, on the other hand, must not have an adverse effect on sensory quality or product

safety. Several public health characteristics of salt consumption are discussed in this chapter. Furthermore, in foods, the technological consequences of salt reduction are examined, as is the potential for replacing salt with salt substitutes, spices, herbs, and further culinary additives to retain product quality while reducing sodium intake (Betts et al., 2007).

6.2. SALT IN FOOD MANUFACTURING

In food manufacturing, the role of salt is derived from its functions in preservation as well as its influences on flavor, color, and texture in foods. Salt serves as a preservative by reducing the aw content to levels below those required for bacterial growth. The ratio of the vapor pressure of water in a portion of food to the vapor pressure of pure water at room temperature is known as the vapor pressure ratio. Aw serves as a measure of the water available for enzyme reactions, metabolism, and microbial development. A minimum aw exists for each microbial species below which it cannot grow (Betts et al., 2007). High-perishable foods with an aw of 0.950, such as fish, meat, cooked sausages, milk, vegetables, and bread, as well as foods containing around 4 oz (w/w) sucrose or 7% NaCl, allow the growth of bacteria such as Escherichia coli, Pseudomonas, Klebsiella, Shigella, Proteus, Clostridium perfringens, Bacillus, and several types of bacteria, including Vibrio parahemolyticus, Salmonella, Clostridium botulinum, Pediococcus, Lactobacillus, Serratia, and some molds, can grow in foods with an aw of less than 0.910, including some fruit juice concentrates, cured meats, some cheeses, and foods that contain 55% (w/w) the fermentation of dry cheeses, sponge cakes, sausage, margarine, and meals comprising 65% (w/w) sucrose or 15% NaCl, as well as the growth of several yeasts and Micrococcus, are all possible in foods with an aw of less than 0.870. Foods with an aw of less than 0.800, such as chocolate syrup, sweetened condensed milk, fruit juice concentrates, fruit, and maple syrups, pulses, rice, flour containing 15–17% moisture, high sugar cakes, and fruit cake, support the growth of most molds, Staphylococcus aureus, and furthermost Saccharomyces species, among others. Foods consuming an aw of ~ 0.750 like marzipan, marmalade, jam, marshmallows, and glacé fruits let the growth of highly halophilic bacteria, mycotoxigenic aspergilli. Foods as low as 0.600, such as dried fruits with 15-20% moisture, honey, caramels, and toffees, allow the formation of Xerophilic molds and Saccharomyces. There is usually no microbial growth for aw values below 0.500 (Beuchat, 1983) (Figure 6.2).



How salt is used

Figure 6.2: Use of Salt in the food industry.

Source: https://www.mitsui.com/jp/en/innovation/business/salt/index.html.

The process of salt-induced microbial growth inhibition seems to be connected to plasmolysis or the loss of water from the cell. In response to salt addition, bacteria experience osmotic shock and plasmolysis, which results in the loss of turgor, then to the cessation of growth, death, or the establishment of a latent state. It is necessary for aw to return to values that allow cells to recuperate for growth to restart (Wood, 1999; Davidson et al., 2012). To redevise turgor, microbial cells raise aw by accumulating and up-taking solutes that are compatible with their environment (Roebler and Müller, 2001). Compatible solutes are small organic molecules that are highly soluble in water and do not affect metabolism, even when amassed in high quantities. These molecules include sugars and polyols as well as amino acids. It is possible that salting meals will result in a prolonged lag phase, during which bacteria must adjust to their new environment before entering the exponential phase (Vibhakara et al., 2006; Detkova and Boltyanskaya, 2007).

Salt, in addition to its preservation properties, enhances the flavor, texture, and mouthfeel of a variety of items, particularly processed meals. If it is added to food products, it imparts both its own specific flavor and an enhancement of the flavor of other ingredients, as well as a reduction in

bitterness in certain products (Hutton, 2002). It is also one of the four basic flavors associated with foods, and it is one of the four basic flavors associated with foods (salty, acidic, bitter). Sodium and lithium are the only two anions that have a sodium-related transduction process that does not happen with the other anions. In this mechanism, an electrical signal is carried across the nervous system to detect the taste of salt, which is unique to sodium and lithium (McCaughey, 2019). Salt can be employed to impart flavor to sweet products such as chocolate, even though it is more generally associated with savory dishes. Salinity is a critical component in cheese manufacture, and it is included to produce levels in the end products that range from 0.7% (weighted average) in Swiss-type cheese to 6% (weighted average) in an Egyptian variant called Domiati cheese. During the cheesemaking process, the amount of aggregation, or para-casein hydration, occurs, which in turn affects the amount of water-binding capacity of the casein matrix, its inclination for syneresis, and the cooking, textural, and rheological features of the finished cheese (Guinee, 2004). Salt regulates the acidification activity of starting cultures and has an impact on the activity of a variety of ripening enzymes. When it comes to cheese kinds such as Cheddar, the contribution of salt to the whole flavor profile can be determined by the fact that low salt cheese is often considered to be 'insipid' or without flavor (Guinee and Fox, 1993).

When it comes to the production of meat products and meat, salt has a variety of functional qualities, including the activation of proteins to increase water binding capacity and hydration; improving the binding properties of proteins to improve texture; and increasing the viscosity of meat, which allows for the development of a stable batter (Desmond, 2006). It is also employed in the maintenance of color. When sodium nitrite is combined with salt in cured meats, the meat gets a reddish color that eventually turns pink. To produce these color changes, nitrite combines with the myoglobin in the meat. First, it converts to nitroso myoglobin (a brilliant red pigment), and then, when heated, it converts to nitrosohemochrome (Kilcast and Angus, 2007). The ability of myofibrils to surge in the existence of salt (3-9%) has also been shown to have a tenderizing impact on meat, resulting in increased water holding capacity (WHC) of the meat. It is likely that these salt concentrations are like those found in comminuted meats in general. Salt concentrations at or above this level result in a significant rise in the quantity of protein extracted from meat products, which results in the formation of a salt and protein complex that holds pieces of meat together. Salt also modifies the ionic environment and the pH, which aids in the construction

of this consistent structure. It is also required in the production of ready-toeat sliced meats, burgers, and sausages and is used in the manufacturing of ready-to-eat sliced meats, burgers, and sausages (Kicast and Angus, 2007). Salt is essential in the production of bread because it increases the stability of wheat gluten and makes it less extendable, reducing the sticky texture of the finished product. It accomplishes this by forcing the dough to become tighter or more tightly bound. The sodium ions are assumed to be the cause of this because they compete for hydrogen binding sites in the gluten protein molecule (Stanton et al., 2001; Kicast and Angus, 2007), which is thought to be the case. Salt also influences the rate of fermentation in bread by limiting the quantity of gas produced, as indicated by the fact that insufficient salt levels can result in excessive yeast fermentation, which results in poor loaf structure. Fermented vegetables such as sauerkraut and pickles, among other things, rely substantially on the addition of salt to their production. Salt regulates microbial growth by permitting the proliferation of valuable cultures in the vegetable substrate, which in turn creates the circumstances necessary for a safe fermentation to take place. The subsequent buildup of acidity promotes the growth of acid-resistant bacteria like Lactobacillus plantarum, which is responsible for the conversion of carbohydrates to lactic acid. The amount of salt used in pickled onions can also alter the texture of the product, as unbrined pickling onions contain high levels of acetic acid, which can cause a haze to build around the product. The addition of salt may be effective in preventing the establishment of this layer. Salt can also help to avoid the pinking of onions that appears when they are acidified prior to bringing. Since acid-tolerant spoiling species are not generally Salttolerant, salt addition may also help to prevent the decomposition of acidpreserved products. Salt is utilized in a variety of industries, including food processing, soap production, and glass production (Desmond et al., 2002; McClure, 2005).

6.3. EFFECTS OF SALT ON BACTERIA

Salinity improves the flavor, texture, and mouthfeel of a range of foods, particularly processed foods, in addition to its preservation capabilities. In food goods, it adds both its own distinct flavor and an augmentation of the flavor of other components while also reducing the bitterness of certain products. It is also used to make cosmetic products more appealing. It is also one of the four basic flavors associated with foods, and it is one of the four basic flavors associated with. It is also one of the four basic flavors associated with and it is one of the four basic flavors associated with foods. Except for lithium, sodium, and lithium are the only

two anions that have a sodium-related transduction process that does not occur with the rest of them. This technique involves the transmission of an electrical signal across the nervous system to recognize the taste of salt, which is unique to sodium and lithium (Faleiro et al., 2003; Hamon et al., 2006). Even though salt is generally linked with savory dishes, it can be employed to enhance the flavor of sweet products such as chocolate. A crucial module of cheese production, salinity, is included to produce levels in the finished product that range from 0.7% (weighted average) in Swiss-type cheese to 6% (weighted average) in an Egyptian version known as Domiati cheese. As the cheesemaking process progresses, the amount of para-casein hydration or aggregation takes place, which has an impact on the amount of water-binding capacity of the casein matrix, its proclivity for syneresis, and the cooking, textural, and rheological characteristics of the finished cheese. It is known that salt governs the acidification activity of beginning cultures and that it influences the activity of several ripening enzymes. Cheddar, for example, is known for its salt content, which may be ascertained by the fact that low-salt cheese is frequently referred to be 'insipid' (Sneath et al., 1986; Jenkins et al., 1990).

When it comes to the manufacturing of meat and meat products, there are a variety of options. Its functional capabilities include activating proteins to boost their hydration and water-binding capacity, improving the binding properties of proteins to improve texture, and increasing the viscosity of meat, which allows for the production and stabilization of a stable batter. Aside from that, it is also used in the preservation of color. In preserved meats, when sodium nitrite is coupled with salt, the meat takes on a reddish hue that finally turns pink. For these color changes to occur, nitrite must combine with the myoglobin found in animal tissues (Browne and Dowds, 2001; Kicast and Angus, 2007). First, when heated, it converts to nitroso myoglobin (a brilliant red pigment), and then when heated again, it transforms into nitrosohemochrome. It has also been demonstrated that the ability of myofibrils to expand in the existence of salt has a tenderizing effect on meat, resulting in an increase in the WHC of the meat. It is likely that the salt concentrations in these comminuted meats are comparable to those observed in other comminuted meats. At or above this concentration, salt causes a considerable increase in the amount of protein extracted from meat products, resulting in the creation of a protein complex and salt that keeps pieces of meat together in a cohesive manner. Salt also changes the ionic environment and pH, which contributes to the formation of this cohesive structure. The creation of ready-to-eat sliced meats, burgers, and sausages

(Kicast and Angus, 2007), as well as the manufacturing of sausages, burgers, and ready-to-eat sliced meats (Kicast and Angus, 2007), are all dependent on the availability of this ingredient. When it comes to baking bread, salt is crucial because it promotes the stability of wheat gluten and makes it less extensible, which reduces the sticky texture of the completed product (see Figure 6.3). When the dough is forced to grow tighter or more securely bonded, it achieves this result. Due to their competition for hydrogen binding sites in the gluten protein molecule (Pichereau et al., 2000; Kicast and Angus, 2007), sodium ions are suggested to be responsible for this phenomenon. According to the fact that insufficient salt levels can guide to too much yeast fermentation, which results in a poor loaf structure, salt also influences the rate of fermentation of bread by reducing the amount of gas produced. Sauerkraut and pickles, among other fermented vegetables, rely heavily on the addition of salt to their manufacturing processes to get their desired results. Microbial growth is controlled by salt, which allows beneficial cultures to flourish and proliferate in the vegetable substrate. This allows for the safe fermentation of food to take place under the right conditions (Rodriguez-Romo et al., 2005; Kicast and Angus, 2007). The resulting accumulation of acidity encourages the growth of acid-resistant bacteria like Lactobacillus Plantarum, which is responsible for the conversion of carbohydrates to lactic acid during the fermentation process. When it comes to pickled onions, the amount of salt used can also affect the texture of the result. This is because unbrined pickling onions have significant levels of acetic acid, which causes a haze to accumulate around the product. It is possible that the addition of salt will be effective in avoiding the formation of this layer. Aside from that, salt can aid in preventing the pinking of onions that occurs when onions are acidified prior to brining. Aside from the fact that acid-tolerant spoiling species are not typically salt-tolerant, the addition of salt to acid-preserved products may also aid in avoiding the decomposition of the products. Food processing, soap manufacturing, and glass manufacturing are just a few of the businesses that rely on salt for their operations (Conner et al., 1986; Ryser and Marth, 1999) (Figure 6.3).



Figure 6.3: Effect of salts on bacteria and plant growth.

Source: https://www.sciencedirect.com/science/article/pii/ S0944501317312806.

In studies of the stress protection responses of Lb. Acidophilus, researchers discovered that incubation in the presence of 2% salt resulted in an increase in population, but incubation in the pore solution ranging from 4 to 18% resulted in a drop in population (Kim et al., 2001). Unlike Listeria and Bacillus species, Lactobacilli do not produce the same osmo protectant proteins as those produced by these bacteria (Sutherland et al., 1996; Boziaris et al., 2007).

6.4. PUBLIC HEALTH CHARACTERISTICS OF SALT INTAKE

Extreme salt consumption by consumers has been linked to the growth of hypertension and, as a result, the increased risk of developing CVD, particularly in sub-groups like hypertensives, the elderly, and people of color (Thompson et al., 1994; Allender et al., 2007). As early as the 18th

century, the Chinese recognized that a "hard pulse," showing high blood pressure, related to large consumption of salt, and they related this "hard pulse" with an increased risk of stroke. Nevertheless, it was not till 1904 that the Western world recognized the link between excessive salt consumption and high blood pressure (Fodor, 2000). As per the Irish Heart Foundation, CVD is the leading cause of mortality in Ireland, accounting for more than 10,000 fatalities each year and accounting for 37% of all deaths, with 24% of all premature deaths in those under the age of 65 (Edwards et al., 2005; Harrington, 2006). In the United Kingdom, the percentages are comparable, with CVD accounting for approximately 40% of all deaths and approximately 40% of those aged 55 to 64 exhibiting signs of heart disease (Edwards et al., 2005; Harrington, 2006) (Figure 6.4).



Figure 6.4: Health effects of excessive salt intake.

Source: https://www.amjmed.com/article/S0002-9343(11)00949-1/fulltext.

Hypertension, often known as high blood pressure, is relatively frequent in industrialized countries like the United Kingdom and the United States. During a person's life, their blood pressure is measured in millimeters of mercury. The force of blood pressing compared to the walls of their arteries while their heart pumps blood throughout their body is referred to as blood pressure (Timotijevic et al., 2013). Normal blood pressure as defined during the Joint National Committee on Prevention, Treatment, Evaluation, and Detection of High Blood Pressure (2003), was expressed as systolic pressure over diaphragm pressure, with the systolic pressure being the pressure experienced during cardiac muscle contraction, and the diaphragm pressure

being pressure experienced during diaphragm contraction. Hypertension, or high blood pressure, is defined as having a systolic blood pressure of 140 mmHg or higher and a diastolic blood pressure of 90 mmHg or higher. A new term, "prehypertension," was also coined during the Joint National Committee VII, which refers to those who have blood pressures varying from 120-139 mmHg systolic (Lenfant et al., 2003) blood pressure. The condition for the kidneys to defecate or preserve adequate sodium to provide appropriate sodium content and blood volume regulates blood pressure in the body. As a result, excess sodium is expelled in most cases. The presence of excess salt causes an increase in blood volume, which raises glomerular filtration rate, arterial pressure, and renal perfusion, resulting in an increase in sodium excretion and water. Excessive salt can cause enhanced water retention, which, if it surpasses water excretion, can result in hypertension and tissue damage. Excess salt may also cause increased water retention if it exceeds water excretion (Lenfant et al., 2003). A target of 5 mm Hg for average systolic blood pressure has been set in the United Kingdom, according to the COMA report "The Health of the Nation." Reduced alcohol intake, obesity, and excessive salt consumption are all considered to be issues that must be handled to reach this goal. In blood pressure, the COMA report emphasized the importance of achieving a gradual reduction across the entire community rather than aiming for a big reduction in blood pressure in certain groups, such as hypertensive persons, as recommended by the American Heart Association. The justification for using this approach is that it has the potential to result in a bigger overall reduction in illness rates. In the United States, the DASH (Dietary Approaches to Stop hypertension) program looks to be the most effective dietary method for lowering blood pressure and cholesterol. The DASH studies were conducted on 412 randomly selected adults who were assigned to one of two diets: a standard American diet or a diet rich in low-fat dairy products, vegetables, and fruits. Individuals in every dietary group were kept at one of three different daily salt consumption levels, which were 4, 6, or 8 g (He and MacGregor, 2008). Persons following the DASH diet experienced an overall drop in blood pressure, with the biggest reductions reported in individuals following the DASH diet that comprised the lowest daily salt intake of the group (4 g).

Aside from kidney stones and kidney disease, other disorders associated with excessive salt consumption include kidney failure and renal failurerelated death. It has also been discovered that people who consume a lot of salt have a higher risk of developing stomach cancer and that excessive salt consumption can make asthma worse. Additionally, dietary salt has a considerable impact on calcium excretion and is thought to be a key contribution to the development of osteoporosis (Cohen and Roe, 2000; Harsha et al., 2004). Several researchers have already established that a rise of 100 mmol sodium daily induces an increase in urinary calcium secretion of 0.6 mmol calcium daily in both young women and men. Because calcium and phosphorus account for approximately one-third of the skeleton's composition, chronic significant calcium losses can result in decreased bone density,the National Osteoporosis Society in the United Kingdom recommended that those who may be impacted by osteoporosis avoid adding salt to their diet (Cattaneo et al., 2019; Li et al., 2020).

6.5. SALT INTAKE AND DIET

Through its role in managing fluid balance, sodium is a vital component of the human body. It also plays a role in the transmission of nerve impulses, the relaxation and contraction of muscles, and the transport of nutrients into cells. Most of the sodium in our diet comes in the form of sodium chloride (salt) and 1 g of sodium (Street, 2005; Al-Otaibi and Wilbey, 2006). Prior to the invention of agriculture, humans' diets were thought to be low in salt, with an estimated daily sodium consumption of 768 mg, which is comparable to 1.92 g of salt (Eaton and Konner, 1997). Nevertheless, the actual salt consumption for the average adult is far greater, averaging roughly 10 g daily in Ireland and the United Kingdom and reaching as high as 12 g per day in some European nations, according to some studies. The National Diet and Nutrition Survey in the United Kingdom, which was conducted on persons aged 19 to 64 years, discovered that males had a mean daily intake of salt that was approximately 3 grams more than that of females (Henderson et al., 2003). 2.3 grams of sodium or 5.75 grams of salt per day for adults is advised by the Department of Health and Human Services (HHS) and the United States Department of Agriculture (USDA) in a report published in the United States in 2010. Middle-aged and older persons, black people, Individuals with hypertension, and those with kidney disease were advised to consume no more than 1.5 grams of sodium or 3.75 grams of salt per day (Johnson and Kimlin, 2006; Allison and Fouladkhah, 2018) (Figure 6.5).





Source: https://www.who.int/news-room/fact-sheets/detail/salt-reduction.

Through its role in managing fluid balance, sodium is a vital component of the human body. It also plays a role in the transmission of nerve impulses, the relaxation and contraction of muscles, and the transport of nutrients into cells (Pollard et al., 2002; Tobin et al., 2013). For babies and children, the recommended daily limit (RDA) for salt is significantly lower than it is for adults. An article published by the Scientific Advisory Committee on Nutrition (SACN) in the United Kingdom suggests that the recommended daily salt intake for children should be in the range of 0.6 grams per day for newborns, 1.8 grams per day for children aged 4–6 years, and 4.08 grams per day for children aged 11–14 years (McCarron, 2000; Appel, 2006).

6.6. HUMAN STUDIES

The first human investigations into the negative consequences of excessive salt consumption on health were conducted in the 1970s. The effects of short-term adjustments of NaCl consumption over the physiologic range in both hypertensive and normotensive patients were investigated in one such study. Salt was identified as a clear source of high blood pressure in a report

published by the Surgeon General during the same decade. These findings cleared the path for the implementation of National Health Policies (Dyer et al., 1990). Most of this research, on the other hand, was only focused on the role of salt in blood pressure management. In 1988, the findings of a much larger, thorough, and well-organized multinational investigation were published. An example of this research is the Intersalt study (Chrysant, (2000), which entailed measuring electrolyte excretion in human beings from around the world and determining how this was connected to blood pressure. The Intersalt study was supported by the National Blood, Lung, and Heart Institute (USA). The findings revealed a significant variation in sodium excretion, with values ranging from 0-2 mmol/24 h to 242 mmol/24 h. According to the findings of this study, in communities with a daily salt intake of less than 50 mmol, there was also a direct association between 24-hour blood pressure and urine sodium excretion in such populations. In general, populations with limited sodium excretion had low occurrences of hypertension, with blood pressure increasing at a slow rate with age in these populations. Similarly, a large investigation, the National Health and Nutrition Examination Survey (NHANES I), revealed that salt excretion in the urine was associated with a higher proportion of cardiovascular fatalities in a large population of monitored people (Kotchen and McCarron, 1998). However, the DASH research, which was also conducted in the United States, is the definitive clinical trial in this field. As previously noted, this study discovered that participants following the DASH diet with a low salt intake (4 g) experienced the highest reductions in blood pressure (Dolan, 2010). He and MacGregor (2007) describe the results of migration studies that were conducted. This study examined the mobility of a Kenyan population from a rural to an urban context, as well as the reasons behind their migration. It was shown that the quick increase in blood pressure that occurred after the migration was mostly caused by an increase in dietary salt consumption. Because of the findings of these studies, international measures to limit the amount of dietary salt consumed have been developed. These activities involve consumer education as well as reductions in salt added through food manufacturing.

6.7. WORLDWIDE INITIATIVES TO DECREASE SALT CONSUMPTION

Governments around the world are increasingly launching programs to decrease the average daily salt consumption of the public. In the United

Kingdom and Ireland, local authorities, food agencies, national health agencies, and food industries are working together to implement government policies to reduce salt consumption to target intakes. Most of the time, these campaigns involve alerting the public about the consequences of excessive salt intake and how they might reduce their sodium intake by making dietary changes. Pressure is also being applied to the manufacturers of processed foods, which are the primary source of dietary salt, to lower the amount of salt included in their goods. Food enterprises and their representative organizations are now participating in this voluntary salt reduction program (Coles et al., 2003). These businesses are engaged in the manufacturing of meat products, cereals, bread, savory sauces, confectionery, and snack foods. As well as excessive levels of sodium in new goods or recipes, CASH points out that the average salt content of supermarket-ready meals has decreased by 45% since 2003. So, the Food Standards Agency's (FSAs) goal of decreasing salt levels in processed foods by 2010 appears to be within reach. There are 85 types of processed foods covered by the targets, including staples such as bread and bacon, and ham as well as convenience items like savory snacks, ready meals, pizza, and pastries and cakes. According to CASH, if a new daily salt intake restriction of 3 g for individuals could be achieved, a one-third decrease in fatal strokes and a quarter reduction in mortality from heart disease may be accomplished. This figure of 3G is not implausible, as the National Blood, Lung, and Heart Institute of the United States has suggested an average daily intake of 3.75 g of fiber. The Food and Drink Federation (FDF) in the United Kingdom asserts that the country is at the forefront of the global push to reduce salt consumption (Coles et al., 2003; Li et al., 2020).

6.8. LABELING OF SODIUM CONTENTS OR SALT IN FOODS

Unavoidable difficulty in relation to public health salt reduction initiatives is the classification of sodium and salt concentrations in goods. This is especially true for pre-packaged items, such as chilled or frozen ready meals and snacks, soups, and pizzas. In the European Union, nutritional classification is not required except a nutritional claim is being prepared for the food being labeled with. When a nutritional privilege is made on a food product, cataloging is required and must include the following information: the amount of protein, energy value, carbs, fat, saturated fat, sodium, fiber, and sugar (Cowburn and Stockley, 2005); and A label containing a list

of ingredients as well as other important information is required for prepackaged foods in Ireland (Bertino et al., 1982; Radwan et al., 2015) (Figure 6.6).

Nutrition Facts Serving Size 1/2 cup (130g) Servings Per Container 31/2				Nut Serving Si Servings F	ritic ize 1/2 c Per Con	on Facts cup (130g) ntainer 31/2		
Amount P	er Servi	ng		Amount P	er Servi	ng		
Calories	25	Calories from	Fat 0	Calories 2	25	Calories from Fa	t 0	
		% Daily	Value*			% Daily V	alue*	
Total Fat	0g		0%	Total Fat	0g		0%	
Saturated Fat Og 0%			Saturate	ed Fat Og	9	0%		
Trans Fa	at Og	-		Trans Fa	at Og		_	
Cholester	ol Oma		0%	Cholester	ol Oma		0%	
Sodium 10	Omg		1%	Sodium 15	50mg		6%	
Potassiun	n 270mg		8%	Potassium	1 2 30 mg		6%	
Total Carbohydrate 5g 2%			Total Carbohydrate 5g 29					
Dietary	Fiber 1g		4%	Dietary	Fiber 1g	d.	4%	
Sugar 3	g			Sugar 3	g		_	
Protein 1g]			Protein 1g)			
Vitamin A Calcium	5% 4%	Vitamin C Iron	30% 4%	Vitamin A Calcium	5% 4%	Vitamin C Iron	20% 6%	
"Percent Da diet.	ily Values	are based on a 2,00	0 calorie	*Percent Dai diet.	ily Values	are based on a 2,000 c	alorie	

Figure 6.6: Labels indicating content of different elements.

Source: https://daradirhan.wordpress.com/2011/11/11/blood-pressure-5-read-ing-a-food-label-for-sodium-content/.

Customers are more inclined to read ingredient lists and nutritional labeling on items, particularly pre-packaged processed foods, as they become more aware of the health consequences of eating a healthy diet as their awareness grows. In today's world, many food labels and statements can be confusing to consumers and determining the real amount of salt in a product can be challenging. The amount of salt or sodium in certain foods is listed in grams, while others are listed in grams per 100 g, and others are listed in grams per serving, which can be around 375–400 g. Although current EU regulation specifies that only sodium content must be labeled, many food manufacturers declare the amount of salt in their products to comply with the law (Bussell and Hunt, 2007).

In the United Kingdom, the FSA has advocated a "traffic light" labeling system, which would allow consumers to rapidly determine whether a food item contains high, medium, or low amounts of fat, saturated fat, carbohydrates, and salt by simply looking at the label. A red label indicates that the food contains high amounts of a certain nutrient, an amber label signifies medium levels, and a green label shows that the food includes low levels of a specific nutrient (Sharp, 2004; Fellendorfa et al., 2016). Since its inception, the European Commission (EC) has refused to support this kind of labeling, claiming that it "oversimplifies" the problem by providing a narrow picture of a single food and failing to educate consumers about the advantages of a balanced, nutritious diet. The EC, on the other hand, has proposed legislation that would require pre-packaged meals to clearly show nutritional information on the front of the package. Information such as energy values, lipid content, carbohydrate content per 100 mL or 100 g or per portion, with specific reference to sugar and salt contents, will be included as per legislation (Watson, 2008). The suggested improvements in labeling should assist customers in making informed dietary decisions, particularly in connection to overweightness and excessive salt consumption (Cheftel, 2005). In Australasia, producers pay a fee for the right to show the "Pickthe-Tick" mark, which signifies a healthier alternative, providing that the products meet the requirements of the National Heart Foundation (Sharp, 2004). It appears that this strategy has been highly successful, as evidenced by the elimination of 33 tons of salt from food products in a single year in New Zealand, where it was implemented. The FSA has also established a fundamental labeling system that will immediately inform customers whether a food has a low or high salt content, defined as more than 1.5 g salt per 100 g or less than 0.3 g salt per 100 g, respectively (Cattaneo, 2019).

The sodium/salt content of a food product must be less than 0.12 grams per serving for the product to be labeled as "low in sodium/salt." To make the claim that a product has a very low sodium/salt content, the product must contain less than 0.04 g of sodium per 100 g of body weight. Sodium-free or salt-free claims can only be made on products that include no >0.005 g of sodium in accordance with European Union Directive 80/777/EEC (salt-free claim). It is necessary for a product to claim to be salt/sodium-reduced to do so. The sodium or salt equivalent value must be 25% less than the sodium or salt equivalent value in a related product under the EU Directive 90/496/EEC (Durack et al., 2012).
6.9. REPLACEMENT OR REDUCTION OF SALT IN FOODS

As previously said, salt is essential in delivering typical organoleptic and textural features in a variety of foods, and as a result, its removal and/ or substitution may have significant consequences for the quality and processing of the food. Salt enhancers and salt replacers are the two main alternatives to salt that are accessible to food technologists, respectively. Salt trimmings are compounds that increase the sense of saltiness, or the taste of a salt-tasting compound deprived of having any saltiness themselves in their composition. Lysine, glycerine monoethyl ester, Glycine, mycoscent, trehalose, lactates, L-argine, O-aminoacyl sugars, L-ornithine, glutamates, and alapyridaine like monosodium glutamate (MSG) are examples of such compounds (Kilcast and Angus, 2007). When it comes to salt enhancers, one of the most used is MSG, which contains high levels of glutamic acid and imparts a distinct "umami" flavor to savory foods. MSG includes high levels of glutamic acid and imparts a distinct "umami" flavor to improve the acceptability and palatability of savory foods (Yamaguchi and Ninomiya, 2000). Umami is a Japanese phrase that refers to a flavor note that is savory, meaty, or broth-like in nature. Using MSG to replace salt in dishes has several advantages, the most important of which is that it includes just one-third of the sodium found in salt (Samuels, 1999). MSG use, on the other hand, has been linked to a condition known as 'Chinese Restaurant Syndrome,' which can result in headaches, edema, and weakness.

Ingredients in which the sodium cation has been replaced by ions like lithium, calcium, or potassium are referred to as salt replacers. KCl is one of the most extensively employed salt substitutes in the food business, and its use allows for a substantial reduction in the amount of salt used in recipes. Salt reduction is commonly achieved by substituting 25–30% potassium for sodium, and as up to 50% potassium substitution may be attained in some food products, the inclusion of KCl above this level of inclusion may result in the formation of metallic or bitter off-flavors (Champagne et al., 1993). According to Colmenero et al. (2005), potassium has the opposite impact of sodium on the body, reducing blood pressure. In addition to decreasing systolic blood pressure, it has been proven that a high-potassium diet can reduce the development of kidney impairment in laboratory rats. Humans with hypercalciuria (abnormally high amounts of calcium in the urine) should increase their potassium intake to reduce the chance of kidney stone formation, and this is especially true in the elderly. Potassium chloride, on

the other hand, has been documented to be detrimental to those who have specific medical disorders (Gao et al., 2006). It was discovered that the addition of KCl produced an aw reduction comparable to that achieved by salt addition. A range of NaCl and KCl concentrations from 0 to 1.4 mol was used, and in both cases, aw was reduced from 0.999 to 0.950. Another class of salt substitutes that have been employed is potassium salts such as metal ions, magnesium sulfate, and calcium chloride (Gimeno et al., 1998; 2001). In dry fermented sausages, replacing NaCl with a mixture of chloride salts improved the amount of solubilization and binding capability of the meat proteins. When bitter compounds are present, blocker additives can be employed in conjunction with salt replacement to conceal the bitterness. Adenosine 5' monophoshate (AMP) is an example of a blocker component since it decreases the activation of taste cells by bitter compounds (Portillo-Ruiz et al., 2005; McGregor, 2007).

Some food manufacturers reduce the amount of salt in their products without substituting it with an alternative. Human salt-taste receptors are said to be undetectable by a 10-20% transfer in sodium levels, according to CASH (Ainsworth and Plunkett, 2007). Another approach for lowering the amount of salt in foods is to use herbs and spices as salt replacements. Numerous advantages can be gained from the use of certain food items. First and foremost, they are widely recognized to have antibacterial qualities from a microbiological standpoint, and studies documenting these capabilities have been conducted for a variety of spices and their important oils, such as thyme, oregano, cinnamon, garlic, and clove (Arora and Kaur, 1999). Aside from imparting desirable flavor, color, and texture to the completed product, herbs, and spices can also help to mitigate any flavor deficits that may occur because of salt reduction. This clearly demonstrates that processed food makers must explore these components' applications in greater depth and include them into their product formulations as part of a comprehensive plan to reduce sodium intake in processed foods (Ankri and Mirelman, 1999; Shim and Kyung, 1999).

6.10. SUMMARY

Extensive global public health research continues to demonstrate the detrimental effects of a high-salt diet on several population groups, including children, the aged, men, and women, and people of different ethnic and ethnic backgrounds. Consequently, health and government organizations have recognized that a reduction in the amount of daily dietary salt is immediately

needed. In the processed food industry, such a reduction is especially beneficial, where it is well acknowledged that processed foods contribute more to dietary salt intake than any other food group in the diet. As a result, it is critical that food manufacturers maintain their efforts to minimize or change the salt in these food goods in their products (Bajaj et al., 2006). The important functional responsibilities of salt in food manufacturing have been detailed in this review, which includes the addition of flavor notes, the development and preservation of texture, the preservation of color, and the prevention of spoilage and harmful microbe growth. As a result, salt reduction is not a simple procedure for food technologists, and it must be supported by research to identify the consequences of a sodium/salt reduction strategy on product safety and quality. Reduced dietary salt intake should result in lower rates of hypertension, stroke, CVD, and other kidney-related diseases, which will benefit the public by lowering the load on public health services. The continuation of government measures to educate the public about the levels of salt and sodium in various foods is therefore critical to enable educated dietary choices among the public in the future. The issue for food manufacturers is to give consumers with low- or reduced-sodium product options high-quality, particularly in the case of processed meals (Moorillon, 2005).

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CHAPTER

7

USE OF DIFFERENT SALT COMPOUNDS IN SALINE AGRICULTURE

CONTENTS

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7.1. INTRODUCTION

The demand for freshwater, fuel, and food is growing every day as the world's population continues to rise. As a result, there is a pressing need to conceive, design, and practice a new style of agriculture that is both environmentally maintainable and soil-appropriate. The increment in soil salinity is the most significant stress in plant agriculture around the world. This is especially evident in emerging countries, which have the maximum rates of population expansion and, consequently, soil deterioration occurs at enormous rates. As a result, plants of soil tolerance are a viable option for several emerging countries. These plants may grow in areas with little land and water for conventional crops that generate essential oils, pharmaceuticals, food, fuel, fiber, fodder, and resin. They can be utilized for soil rehabilitation and reintegration of landscape at the same time, in addition to their potential for production. This chapter will discuss essential topics such as halophyte's crop capacity and saline agriculture to manage food requirements using salt-contaminated resources (Borlaug, 2007) (Figure 7.1).



Figure 7.1: Graphic representation for the consumption of saline water in growing plants.

Source: https://wle.cgiar.org/news/making-case-reusing-saline-water-and-re-storing-salt-affected-agricultural-lands.

In November 2011, it was believed that humanity had achieved a population of 7 billion people, with the United States (2008) forecasting a rise in population to 8.01 billion people by 2025. In approximately 50

years, the human population will have doubled. As a result, among the most crucial issues in the 21st century is developing agriculture techniques that feed everyone. There is significant economic and demographic pressure to expand agricultural production by around 50% in the next four decades in a responsible manner that satisfies global food demands (Borlaug, 2007; Guillon et al., 2012). Other factors contribute to the exacerbation of this desire, including (a) the issues created by the emergence of rare severe climatic circumstances, especially natural disasters, which are frequently attributed to "climate change events," (b) increased land use for biofuel production, diverting arable land away from food crops, (c) a few imbalances in soil pressure caused by post-green revolution processes, and (d) soil depletion and/or soil degradation and/or soil soils are increasing rapidly, reducing arable land (Prins et al., 2011). "Our capacity to fulfill the global demand for food, fiber, and fuel while maintaining a landscape capable of delivering a complete range of environmental services is contingent upon our capacity to create more energy on less land. This demand is especially strong in emerging nations. Rudel et al. (2009) encapsulated humanity's food supply dilemma.

Agriculture is the world's earliest human practice and the most prevalent use of land (Galvani, 2006). Agriculture is defined as "artificial manipulation of agricultural land to maximize its food value" and is "the country's most significant land use" (Howden et al., 2007). Increasing yields and cropping intensity, genetic alteration, which may include convergent germplasm and seed protection and improvement strategies, and/or creating means for reusing polluted or dry soils, which have been neglected as completely unproductive at the same time, are some developing strategies for improving food production (Bruce, 2012).

This trend is especially noticeable in developing countries, which have the fastest rates of population increase and, consequently, the highest percentage of soil depletion (Central Asia, Mediterranean Basin, Australia, and the North and Middle East of Africa). This requirement is so critical that it is included with the United Nations' Millennium Development Goals (Silva, 2008). In 2004, the United Nations Food and Agriculture Organization (FAO) projected as 852 million people were undernourished worldwide in 2000–2002, with Southern Asia and Sub-Saharan Africa being the most affected regions. However, the FAO pointed out in 2004 that, in most cases, hunger difficulties are caused by a shortage of food and poor farming techniques. This issue, on the other hand, is the confluence of more

complicated difficulties (Galvani, 2006). This is demonstrated by statistics data indicating that nearly 9 million people are hungry in industrialized countries where there is, in theory, no shortage of food (Toledo and Burlingame, 2006). FAO predicted a 20% increase in developed country food demand and a 60% increase in developing country food requirements in 2008.

As a result, it is widely acknowledged that food demand is outpacing crop supply, and experts and policymakers are increasingly emphasizing the critical requirement for improved alternative agriculture approaches (Yamaguchi and Blumwald, 2005; Singh, 2015). To put it another way, to increase production and enhance quality, it is critical to invest in new technology. While also developing methods that contribute to sustainable cultivation without depleting lands and natural assets (Galvani, 2006).

Despite these growing food challenges, the FAO issued a report in 2011 emphasizing the losses throughout the food chain, indicating that roughly one-third of all food produced in the world is lost, amounting to roughly billion tons annually. FAO found that far more food is lost in developed countries than in emerging countries, with Food waste per capita is projected to be 95–115 kg/year in Europe and North America, contrasted to 6–11 kg/ year in South/Southeast Asia and Sub-Saharan Africa.

Food waste and loss are primarily the result of budgetary, administrative, and technical constraints in harvesting procedures, storing, and cooling capabilities under severe in low-income countries, weather conditions, infrastructure, packaging, and marketing strategies in low-income countries, weather conditions, marketing strategies, packaging, and infrastructure, all play a role. Food is wasted to a large amount during a phase of utilization n mid and high countries, implying that it is rejected while being fit for human consumption.

In this approach, the FAO emphasizes that at initial steps in meeting global food demands is to encourage food waste minimization, that has a significant ability to raise the quality of the entire chain of food (Ertek et al., 2014). It is essential to highlight which decreasing food wastage is a priority that should not be ignored.

Agriculture must also examine the kind of water and land available while improving and adapting to 21st-century issues (Khan and Duke, 2001; Singh, 2015).

Between the 1960s and the 1980s, irrigated area rose dramatically. Irrigation projects comprise only 15% of the world's agricultural area, but they account for two-thirds of global food output (Munns, 2002). Irrigation is also thought to be limiting productivity on 600,000 acres of "potentially suitable agricultural land" (Singh, 2015). When these data are combined, it is important to be cautious when anticipating agricultural quantity and quality improvements. However, some fascinating work employing halophytes to supplement agriculture demands has been done (Bernstein, 1975).

In developing countries, it is anticipated that an increment in agricultural production will necessitate approximately 202,106 ha of arable land, while only about 93,106 ha appear to be accessible (Khan and Duke, 2001). Contrary to what would be predicted if true improved agricultural methods predominated, these statistics indicate the need to establish sustainable agriculture policies. Every year, Agricultural land on millions of hectares is devastated, the majority of which occurred during the last 50–60 years of agricultural production (e.g., because of excessive use of fertilizers, unsustainable irrigation practices, soil contamination, climate changes, urban pressure). The Agriculture Organization of the United States handled this issue effectively, estimating that nearly 10 million hectares of arable land are lost each year around the world (Boström and Klintman, 2006).

Fortunately, the number of countries adhering to social sustainability and addressing the Millennium Development Goals is rising, and therefore the emphasis on sustainable measures (e.g., soils and water conservation) is increasing, despite enhancing food supply and urbanization challenges.

7.2. INSUFFICIENT FRESHWATER, SALT CONTAMINATION, AND SOIL DEGRADATION

Due to its global distribution, most of the world's largest arid and semiarid areas are located in developing nations (Rasouli et al., 2012). Arid parts of the world are usually found in the States of America, Australia, Israel, and the Mediterranean Basin have a long history of preventing soil degradation through agricultural use of the land (Setia et al., 2012). For instance, in the United States, a significant amount of wasteland is utilized to grow biodiesel plants. However, in Australia, a massive issue with dryland salinity has developed as lead to rising water levels caused by the destruction of indigenous flora as a result of different plant population types (Munns, 2002). Other nations, such as Israel, have agricultural production systems that use atypical irrigation water sources, and the use of saline water deserves special scrutiny. Additionally, substantial study has been undertaken in Tunisia on this subject, and agricultural approaches based on alternative plant species have been developed, the most of which would be halophytes able of enduring extreme heat and/or water scarcity (Lakhdar et al., 2009).

Salinity is among the most prevalent mechanisms of soil degradation on the world. Around 1 to 3 million hectares in Europe, particularly in Mediterranean nations, are affected by soil salinization. It is often regarded as the major cause of desertification and hence a severe form of soil loss, with salinization and solidification being two of the most significant degradation processes influencing the possible use of European soils. In Spain, for instance, 3% of the 3.5 million hectares of irrigated land is severely damaged, considerably reducing agricultural ability, while another 15% is gravely endangered.

Other areas of Europe with saline soil include the Caspian Basin in Ukraine and the Carpathian Basin in Hungary (Gruiz, 2015).

The availability of fresh water is a key limitation for sustainable agriculture. Water scarcity is a problem in these rising regions, where population pressure is increasing, reducing the amount of usable land and food yield available to these people. According to Galvani (2006), significant adjustments in alternate agriculture are required in extreme environments such as deserts and semiarid regions (Bueno and Kismödi, 2012).

Irrigated agriculture is especially important in this sense since it produces larger yields and is less susceptible to weather fluctuations. Expansion of irrigated agriculture might make a significant contribution to satisfying and stabilizing food and fiber demand. However, increased water supplies are insufficient to support such expansion. Agriculture that is irrigated is already the major use of established water resources. In the meantime, drainage return from irrigated farmland is one of the primary reasons of waterlogging (typically in low-lying areas) and water pollution (according to salts, nitrates, agricultural chemicals, and certain natural, potentially toxic trace elements).

For irrigation, water availability could be increased by making wise and appropriate recycling saline water and usage of drain waters. Significant quantities of that kind of water are present in several locations around the globe including Egypt, the former Soviet Union, India, Australia, Pakistan, Israel, the United States, and Waters that are usually seen as inappropriate for irrigation can, by the way, be efficiently utilized to cultivate crops without causing longstanding harm to soils or crops better management and farming practices are used. The production of crops with higher salt tolerance, as well as implementation of water management and new crop approaches, will improve and simplify the usage of saline waters for irrigation and agricultural production, while preventing soil salinity from being excess. The reusing of drain waters for irrigation will as well as use to preserve water and reduce harmful impacts of irrigation on the ecology and environment (Epstein et al., 1980).

The establishment of suitable methods for using saline waters irrigate needs a thorough understanding of how salts affect water, plants, and soils. However, the stability of permanent irrigated and productive agriculture, particularly with the use of saline irrigation fluids, necessitates considerably more. It necessitates the deployment of proper management measures to control salinity, not only in an irrigated region, even within geohydrologic structures and irrigation systems. This is critical to remember since the bulk of present waterlogging and salinity issues in big irrigation projects worldwide are a result of the use of "high-quality" irrigation water. As a consequence, it can be concluded that the principal sources of salinity problems now seen in ordinary irrigation projects must first be eliminated. If irrigation with more salty than typical waters is effective, this entrain a water salinity within allowable range to bring forth benefit so, such usage will not raise the probability of salinity issues in a specific crop. Contrary to this, reusing drainage waters for irrigation can assist in reducing drains, floods, and salt-loading issues that come, particularly at project or river basin scales, resulting in a total reduction in irrigation-induced and salinityrelated issues, including environmental pollution. In any case, it is crucial to regard management techniques for regulating water and soil salinity at such scales as a major component of the management needs for irrigation with saline waters. This needs the following (Glenn et al., 1997):

- This, the gravity of environmental issues related to salts, as well as the susceptibility of irrigated areas to waterlogging and salination, be identified;
- Understanding of the mechanisms that contribute to these difficulties, as well as the impacts of salts on plants and soils;
- That the values of salinity as well as variations of irrigated fields as well as related water sources be frequently monitored utilizing suitable monitoring and controlling methods that give expressive and appropriate data.
- Those issues related to salinity be identified and treated utilizing suitable values; that future water and soil salinity conditions be sufficiently forecasted utilizing appropriate prognostic methods;

• And that the legitimacy of agricultural production and related water resources be maintained through appropriate long-term control rule.

7.3. SOIL SALINITY

Salinization of soils is a famous issue that is frequently attributed to both anthropogenic and climate change-related reasons. Salinity poses a significant risk to the availability of agricultural goods. The growth in population in current years includes a rise in agriculture and, as a result, an increment in water use, utilizing this resource to the utmost possible extent (Borlaug, 2007). Agricultural practices (i.e., fertilizer use, inadequate irrigation projects) have resulted in saline soil conditions and degraded water quality (2). Salinity stress has an effect on seedling growth, seed germination, root, and shoot lengths, leaf size, shoot fresh weight, shoot dry weight, spikelet number, proportion of sterile florets, and productivity tillers per plant, and flowering stage (Rudel et al., 2009; Prins et al., 2011) (Figure 7.2).



Figure 7.2: Procedure of soil salinization.

Source: https://sites.google.com/site/102beetwo/salinity/causes.

Salt-tolerant crops may perform much better on salty soils (Choukr and Hamdy, 1993). Numerous characteristics, including ion exclusions, osmotic tolerance, and tissue tolerance, can be exploited to boost crop salt resistance (Toledo and Burlingame, 2006). Saline tolerance in plants is characterized by the involvement of structural and functional adjustments including such plant growth promotion, osmotic adjustment, variations in water ability, mineral nutrition changes, and hormone balance, all of which can mitigate the negative effects of these stresses (Yamaguchi and Blumwald, 2005). Growth inhibition is a frequently used technique for testing a plant's tolerance for salty irrigation water. However, when it comes to beautiful plants, it's critical to inspect the foliage quality, as salt stress can result in leaf loss, reducing their market value. Understanding how Na+ is sensed and transferred in stressed plants will aid in the creation of salt-tolerant agricultural species. Halophytes have been investigated for their possible uses in phytoremediation, desalination, secondary metabolite generation, food, and saline agriculture, and harvested halophytes may have commercial value, with regenerated soil being utilized for agricultural purposes (Shekhawat et al., 2006).

The usage of saline water to recover and use soil of salt-affected for agriculture as well as landscaping applications is becoming increasingly popular. Spinach (Spinacia oleracea L. Matador) growing in pots was treated with saline solutions of six various salinities. The salinity of the soil increased in a linear relationship with the salinity of irrigation water (Boström and Klintman, 2006). As demand for high-quality water becomes more intense, saline water can be used to irrigate salt-tolerant ornamentals. Spite of the significance of ornamental shrubs in Mediterranean locations, little attention has been paid to their salt tolerance. The use of recycled irrigation water is one of the methods that increase soil salinization. In locations where freshwater is short, saline water is widely being used for agricultural cultivation (Bchini et al., 2010). Continuous irrigation with saline water, on the other hand, has a negative impact on the system of soil-crop. The most important factors affecting crop yields and agricultural production is irrigation water. Saline water's most basic agricultural purpose is to give water for plant absorption (Bueno and Kismödi, 2012).

Tetragonia tetragonioides (New Zealand spinach) is a perennial salad plant that flourishes in hotter climates and tolerates salt. Medicinal uses have been reported for New Zealand spinach. Greenhouse farming is known for its high mineral uptake, stable environmental conditions, lack of natural precipitation, and salt control (Epstein et al., 1980). Approaches for the nutrient availability and salinity condition of the substrate and soil have been established in the greenhouse sector (Glenn et al., 1995).

Knowing the processes of crop plant tolerance to high NaCl concentrations in soils may eventually aid in enhancing production on saline areas. In spite of the fact that most plants collect significant concentrations

of both chloride (Cl) and sodium (Na+) ions in their shoot tissues at the time of growing in saline soils, most salt tolerance research in perennial crops has concentrated on the harmful effects of Na+ accumulation. The most prevalent salt that creates salinity stress is sodium chloride (NaCl). The quantity, quality, and rate of water applications, as well as the kind of salt, soil, and climatic circumstances, crop classes, and the amount, value, and occurrence of irrigation, all affect salinity risks (Aslam et al., 2009).

7.4. SOIL AND WATER AVAILABILITY

The usage of salted soils and salted water in a system known as saline agriculture is a unique method for increasing land and water availability. In the last 30 years, the usage of seawater for agricultural production in coastal deserts has been proposed (Glenn et al., 1995).

Beneficial and enhanced agricultural practices are utilizing saline land and saline irrigation water with the goal of improving production through the integrated and sustainable use of genetic sources (plants, animals, fish, insects, and microorganisms) while preventing costly soil recovery measures (Aslam et al., 2009). Salt-contaminated phreatic sheets, Seawater, brackish water (from, for example, estuaries), drainage water from those other plantations irrigation, drainage water from humanized areas, such as sewage, and sometimes even water resulting from fish farming waste are all instances of saline water that can be used to irrigate halophyte crops. Almost 50% of irrigation systems are believed to be at risk of salt pollution or waterlogging as a result of low water quality, leaching, and rising water tables (Szabolcs, 1994). In view of population pressures, technological improvements, the increase of salinized soils, and the shrinking arable land available for traditional agriculture, it is evident that utilizing salt affected soils in alternate agriculture might be regarded as a strategy of meeting food demand (Shekhawat et al., 2006).

7.5. SALINE AGRICULTURE: AN OPPORTUNITY FOR SALINE SOILS USE

Globally, soil salinization has been identified as one of the most serious challenges affecting crop output in arid and semi-arid countries. As mentioned previously, some developing areas are at risk of increased soil salinization, including Central Asia, the Mediterranean Basin, the Middle East, Australia, and Northern Africa (Murugan and Sathish, 2005).

Soil salinization occurs for a variety of reasons, including natural causes such as microscopic salt crystals present in wind from the oceans, or as previously noted, some anthropogenic causes (secondary salinization), among the most significant of which is in terms of irrigation water quality.

Utilizing salinized land such as through irrigation without using highquality water, but rather some salinized water, may thus be the solution, but it will need more research into the potential of halophytes to establish as different crops and a shift in human behaviors to introduce these new crops into daily diets (Bueno and Kismödi, 2012).

Additional research is needed to determine the potential utility of halophytes in saline agriculture, as well as utilization and assimilation into the diets of users. Additionally, sufficient conditions for boosting halophyte species development to industrial levels (e.g., physiological research, organoleptic, nutritional qualities, etc.), demand increased attention. As Koyro et al. (2008) indicate, several criteria must be met in order to pick tolerant plants with capable yields and traits which make them ideal as crops in saline agriculture: (a) sifting through the literature in search of their native environments, and so on; (b) estimating the salinity threshold after selecting the species (Munns, 2002).

7.6. WHICH HALOPHYTE CROPS CAN WE USE?

The possibility for halophytes to be used in saline agriculture has been investigated throughout the last few years. While the usage of halophytes in industrial cultures or its exploration is currently limited, certain species are already being cultivated/exploited commercially. Additionally, the Seawater Foundation's "Greening Eritrea" initiative demonstrates how to transform a decertified region into useable soil (Prior et al., 2015).

Halophytes can be modified to produce new salt-resistant crops or utilized as a source of genes to be transferred into existing crop species whose economic viability generally declines as soil salinity increases. We will address the potential for halophytic plants to be employed as emerging or established crops in arid and semiarid settings, with an eye toward environmental sustainability. Halophytes can be used sustainably for a variety of objectives, including promoting productive ecosystems and regreening degraded regions. Around 2,600 halophytic species have been identified, but only a few have been thoroughly researched for their agricultural and biological potential as source materials of oils, gums, resins, flavors, pharmaceuticals, and fibers, or for their environmental potential for ecosystem conservation and protection (e.g., modification of soil structure and fertility, habitat for wildlife, source of biomass for biodiesel production) (Xue et al., 2017) (Figure 7.3).



Figure 7.3: Features of halophyte plants.

Source: https://www.frontiersin.org/articles/10.3389/fmicb.2018.00148/full.

7.6.1. Food Yielding Halophytes

Aster trifolium (other names: Sea Aster or Sea Spinach) is a perennial herbaceous plant belonging to the Asteraceae family (Compositae). This Northern European plant, which grows in marshlands and estuaries, is exceedingly hardy and maybe cut several times, with fresh branches regrowing every three to four weeks. That is a well-known plant in the Netherlands, as it was once utilized as a famine meal and has developed into a staple today. According to Piernik et al. (2015), Aster tripolium grows naturally in temperate areas, mainly in salt meadows along the ocean. Additionally, some exciting studies are being conducted on the response of *Puccinellia maritima* and Aster tripolium to increased atmospheric carbon dioxide, as well as their correlations with floods and salinity (Lenssen et al., 1995).

Salicornia bigelovii (Chenopodiaceae) is a well-studied genus. As is the case with common halophyte, it is a succulent (CAM metabolism) plant that is cultivated for its seeds (for animal and human use) and straw. The residual seed meal is high in protein (about 33–34% crude protein). This

oilseed halophyte develops seeds that are equivalent to soybeans through productivity and quality, yielding 2 tons of seed per hectare with a protein content of 31% and a fat content of 28% (Glenn et al., 1999). Indeed, field trials with *Salicornia bigelovii* in Puerto Penasco, Mexico (a coastal desert environment) revealed an 18 t/ha biomass output and 2 t/ha seed production throughout a 200-day life cycle with the seed having 28% oil and 31% protein-rich in polyunsaturated fatty acids (being the linoleic acid 74% of the total). *Salicornia bigelovii*-fed animals develop at a similar pace to those fed typical forages such as wheat bran and alfalfa in equivalent amounts (Glenn et al., 1992) (Figure 7.4).



Figure 7.4: Rules of biochemical and physiological procedure in halophytes.

Source: https://www.researchgate.net/figure/Regulation-of-physiological-and-biochemical-process-in-halophytes-through-ionic_fig2_342550015.

7.6.2. Oilseeds

Arthrocnemum macrostachyum, S. brachiata, Suaeda fruticosa, Haloxylon stocksii, Salicornia bigelovii, Halogeton glomeratus, and Kochia scoparia, seeds have a substantial amount of good condition eatable oil with unsaturation varying as 70–80%. S. persica and Salvadora oleoides seeds include 40–50% fat and are a better resource of lauric acid, making them the viable alternative for coconut oil.

Also, *Diplotaxis tenuifolia* is the suitable class for saline agriculture since that grows organically at the salty/dry habitats or under the effects of the sea. It (plant) has the ability to be used for both forage and food (salads). *Diplotaxis tenuifolia* exhibited halophyte-like behavior when exposed to salt, comparable to those of recognized halophyte plants like fodder beet or *Cakile maritima* (Debez et al., 2006). Guerra et al. (1998) showed that Diplotaxis plants maintained, developed, and restore in all salinities to the range of 300 mM NaCl, instead a little growth drop in the greater proportion, with better growth values at 100 mM and no waste of nutritional value. This shows that class has a strong ability for large-scale saltwater/soil manufacture.

The *Diplotaxis* L. (DC.) genus originated in the Mediterranean Basin on nutrient-rich, sandy, and dry soil while being widely spread nowadays (Bianco, 1995; Hanson, 2004). It can be grown on sands and roadsides along with extra halophytes such as *Cakile maritima*, frequently close to the sea. A few research has been conducted along with this class, for instance, in Portugal and the Netherlands. This former has a coast with different features, the possible utilization, high rates development of this and additional halophytes, and the progress of opportunities in a rising market.

7.6.3. Fuel Wood and Timber

In poor nations, over a billion people depend on wood for cooking and heating. Most frequently, fuel of wood is extracted from shrubs and trees of salt-tolerant, such as *Salsola, Prosopis, Capparis, Tamarix, Acacia, Pithecellobium, Kochia, Suaeda, Casuarina, Salvadora*, and *Parkinsonia*. Furthermore, *Pongamia pinnata, Dalbergia sissoo, Tamarix* spp, and *Populus euphratica*, may yield high-quality wood. *Aegiceras* mangrove *Avicennia, Ceriops*, and *Rhizophora* classes are excellent fuel woods as well as help in charcoal formation in coastal locations.

Contrary to this, agricultural applications of biofuels to meet global energy demands have increased in recent years, as high oil prices have created new value of agricultural goods which can be utilized as feedstock for the production of biofuel. Thus, biofuels are positioned as a means of achieving a variety of policy objectives, including increased energy security in terms of liquid fuels, increased country incomes, reduced economic possibilities, and greenhouse gas emissions, for developing nations (Heffer and Prud'homme, 2008). Biofuels like biodiesel can be produced from a variety of biomass sources, including wood chips and cow manure. The benefit of creating biofuel from the halophytes over other kinds of biomass is that plants of saltwater do not need freshwater, which is becoming limited, and may be irrigated with abundant seawater.

The Sahara Desert, Western Australia, the Southwest United States, sections of the Middle East, and areas of Peru are all suitable regions for cultivating halophytes. According to scientists, a region less than the size of the Sahara Desert may produce sufficient biomass to meet the fossil fuel demand worldwide. Additionally, because halophyte production occurs in the desert, it results in a wetter, cooler land surface, that may result in rainfall in the world places at where moisture is unusual (O'leary and Glenn, 1994; Khanna et al., 2009).

In this way, the growth and invention of biofuels, as well as debates over sustainable growth of conservative crops used like feedstock of biofuel, will probably benefit halophytes gain more attention and benefit, as the majority of presently used biofuel resources are standard crops such as corn, palm oil rapeseed, and sugar cane, which do not encounter the majority of sustainable criteria. Bioethanol, which is produced from starch and sugar crops, and biodiesel, which is produced from animal fats, vegetable oils, and other recyclable greases, are two specific examples.

Factors like competition with land use, food, pressure energy efficiency on other critical resources like fresh water and rain forest, and in some circumstances political uncertainty are all points of contention in the debate over conventional biofuels, which can raise the prices of food (Harvey and Pilgrim, 2011).

7.6.4. Source of Chemicals

Salsola, Suaeda, Haloxylon, and *Salicornia* species produce the type of soda that is utilized in soap manufacturing and the glass industry in huge numbers. Annona glabra seeds contain pesticides (Khan et al., 2006). *Suaeda* and *Salsola*, is strongly indicative of an ancient origin. Resistance in these plants relies heavily on methods of removing the salt once it has been transported to the leaves. Similarly, Al accumulators, containing more than 1 mg Al g⁻¹ shoot fresh weight, tend to be primitive on taxonomic grounds, suggesting that tissue abscission, a physiologically crude method of excretion, is in evolutionary terms a first attempt.

It is likely that the more sophisticated mechanisms have evolved more recently, in particular, the combinations of resistance mechanisms that characterize most specialist toxicity-resistant species. Resistance to toxic ions can be multilayered, involving an exclusion mechanism at the root surface which reduces the degree of stress, and localization within the tissues of those ions which do penetrate these defenses.

7.6.5. Ornamenta

Several halophytes are ornamental plants; examples include, *Sesuvium portulacastrum, Tamarix nilotica, Aster tripolium, Noronhia emarginata, Limoniastrum monopetalum, Batis maritima, Tamarix amnicola, Cistanche fistulosum,* and *Atriplex halimus* (Khan et al., 2006).

There are about 54 species of *Tamarix* which is a specie of shrubbed and low trees (family Tamaricaceae) that, with false tamarisk (*Myricaria, 10 species*), thrive in salt deserts and highly saline soils, by shores in mountainous areas and other semi-arid areas from the Mediterranean region, to central Asia and Northern China. China. Many have been introduced into North America. They have deep-ranging roots and long, slender branches with numerous small, gray-green, scalelike leaves. Clusters of small pink flowers, hanging at the ends of branches or from the trunks, give the plants a feathery appearance. Each flower has 4 or 5 free sepals, 4 or 5 petals, and from 4 to 10 stamens. The petals and stamens arise from a fleshy disk. In *Tamarix* the stamens are separate; in *Myricaria* they are united. The fruit is a capsule with numerous seeds; each seed has a long tuft of hairs at one end.

7.6.6. Environmental Protection

A few halophyte classes, including *Spartina alterniflora*, *Avicennia marina* and *Spartina maritime*, can make significant contributions to the safety and conservation of seaside ecosystems (Callaway and Zedler, 2004).

Spartina alterniflora is the plant that may environmental and marine scientist view to address the natural coastal soil erosion problems. *S. alterniflora* is a rhizomatous perennial grass that grows 0.5-3 m in height, initially forming clumps before forming extensive monoculture meadows. It has dense root/rhizome systems that binds coastal mud, and its sturdy stem decreases wave action allowing silt deposition, causing elevation of the mudbank, assisting in land reclamation. Because of this attributes, it was widely planted at coastal sites throughout the UK, Northern Europe, Australia, New Zealand, China and USA, where it has naturally colonized

(via seed or vegetative fragments) large areas of tidal mudflats, becoming an invasive species (CABI, 2019).

Avicennia germinans (black mangrove) and other avicennia species is being researched for its ability to restore back-barrier salt and coastal marshes by utilizing the vast root system and plant's structure of wood, which provide stability and habitat (Alleman and Hester, 2011). Members of the genus are among the most salt-tolerant mangroves and are often the first to colonise new deposits of sediment. The sap is salty, and excess salt is secreted through the leaves. These species of plants have the ability to shift substrates because of their spreading root systems. Their pneumatophores or "vertical or pencil roots" because it project from the mud (upwards) like pencils pierced into the surface outwards which allows them to exchange gas from the atmosphere, since there is very little oxygen in the mud.

The embryos exhibit crypto vivipary, a process where they start to develop before the seed is shed, but do not break through the outside of the fruit capsule.^[4]

7.7. ENVIRONMENTAL AND ECONOMIC IMPACT OF SALINE AGRICULTURE

The economics of irrigation of saline water are divided into three categories: (i) consistent consumption of saline water for irrigation; (ii) the recycling of drain water for drainage and irrigation installations; and (iii) regeneration of salty and sodic soils prior to cultivation (Arons et al., 2020).

The influence on the economy and ecology was proved in a government statement on the "Saline agricultural farmer participation progress project in Pakistan" conducted from 2002 to 2008.

Plantations of trees are stable resources of materials for a range of businesses, including, panel products, pulp, and matchmaking, paper, saw wood, sporting goods, furniture lumber, plywood, fuelwood, and fiberboard, to name a few. Using fuelwood from crops and fertilizing agricultural areas can save a lot of dung (Aslam et al., 2009).

In terms of environmental management, trees can be a valuable asset in the recovery of salt-affected land. Due to huge infiltration and lesser rise in water capillary, vegetation over saline soils helps in lowering the concentration of topsoil salt. With the use of trees, farmers can gain quick commercial revenues by cultivating field crops, as well as direct economic advantages from wasteland of saline. Because it is less expensive and lasts longer, such planting is favored over various luxurious engineering procedures. The importance of trees in terms of microclimate, soil erosion, and flooding is well understood. Furthermore, huge crops provide more favorable rainfall circumstances.

The potential of trees to work as scavengers of pollutants by eliminating condensation of water nuclear units and lowering fog having gases hazardous to life is also illustrated in this research, as the leaves, stems, and branches precipitate and filter dust (brought by the wind) (Aslam et al., 2009) (Figure 7.5).



Figure 7.5. Diagram of methods in the developed and the developing world.

Note: Approaches used in poor countries have mainly failed (red), while others are inconsistent (orange). Ways that have been effectively applied in the developed world (green) as well as emergent approaches (brown) are promise for possible implementation in poor nations to reduce the impact of salinity on sustainable development.

Source: https://www.mdpi.com/2071-1050/11/17/4558/htm.

In degraded salt-affected locations, saline agriculture could be a viable technique for lowering CO_2 levels in the atmosphere. Other research

suggests using halophyte crops to restore saline soils, because these plants can decrease soil salt content over time (Keiffer and Ungar, 1997).

The "discovery of major genetic factors of stress tolerance," according to Yamaguchi and Blumwald (2005), is a prerequisite for expanding knowledge on salt-tolerant crops. These same authors look at two different genetic approaches: the first is the use of marker-assisted breeding to exploit natural genetic differences, and the second is the development of transgenic plants, which is a major topic among scientists right now. In fact, to adapt our conventional food crops to rising temperatures, reduced water availability in some places and flooding in others, rising salinity, and changing pathogen and insect threats. The usage and improvement of traditional and molecule stuffing (but also molecular genetic modification—GM) are being studied by researchers. Because nitrogenous compounds in fertilizers are the primary source of waterway eutrophication and greenhouse gas emissions, improving crop nitrogen absorption and use efficiency is a critical environmental advantage of such research. (Gregory et al., 2009).

7.8. ASSESSING THE SUITABILITY OF SALINE WATER FOR CROP PRODUCTION

It is necessary to determine the feasibility of a water source for irrigation using parameters that indicate its propensity to cause soil conditions that are harmful to the growth of crops and, as a result, to animals or humans that consume those crops. The following are the most important parameters for determining the quality of irrigation water in view of the possible crop growth threats: Tilth and permeability The salinity of the water. Toxicology and nutritional deficiency. The sodium adsorption ratio and Electrical conductivity (ECiw) forecast to happen on the topsoil after irrigation (SAR) are used to assess permeability and crusting hazards, with Border tolerances (allowable ratios of ECi and SAR) according to the specific soil or, in the absence of special knowledge, a reasonable relation. SAR is estimated to use a computer model (such as Watsuit, which is used in that article) or, in the absence of a computer, by calculating the SAR value of the irrigation water (SARiw). Toxicity salinity, and nutritional problems are defined by determining the levels of soil water salinity, toxic-ion concentrations, and Ca/Mg ratios predicted to occur in the root zone of the soil following irrigation with appropriate salinity, toxic-ion concentrations, and Ca/Mg ratios for the specific crop(s) in question (using Watsuit). Tables showing tolerated salty and toxic-ion concentrations are available on a wide range

of crops and plants. Without considering salt precipitation and dissolving processes, forecasts of soil salinity following irrigate with a specific saline water may also be generated without using a computer (Pessarakli, 2008). The technique's accuracy and precision are restricted by uncertainty in model forecasts and a dearth of knowledge concerning soil and crop responses to salts and harmful ions (Krüger and Peinemann, 1996).

7.9. ENVIRONMENTAL ASPECTS OF IRRIGATION

Irrigated agriculture has caused serious environmental problems in a number of nations, including waterlogging and salinization, depletion, and contamination of water supplies, particularly groundwaters, and improved health hazards. Improper irrigation development and practices have also harmed the recreational, esthetic, and habitat values of many water systems and agricultural landscapes. Excessive irrigation water use caused by inefficient irrigation distribution systems and poor on-farm management practices, inefficient drains monitoring, and release of "spent" drainage water in greater water stores has resulted in the majority of secondary salinization and waterlogging problems in lands of irrigation, as well as related pollution of water. These concerns have developed even when less salinity water has been used for irrigation. That may cause one to achieve that irrigation with saltwater exacerbates these problems. That is not always the case, though. With good management, watering with salty waters in the levels given below will not result in severe saline soils or waterlogging. Indeed, the ability to intercept drain waters percolating beneath rootzones and repurpose them for irrigation mitigates soil degradation processes common in irrigated lands, such as excessive deep percolation, salt mobilization, waterlogging, and secondary salinization, as well as associated water pollution challenges associated with their release into high-quality water supplies (Kopec et al., 2006). Consider the following when considering the use of saline water for irrigation and selecting appropriate management practices to ensure water quality: the total volume of a saline water supply cannot be usefully utilized for irrigation or crop yields, and the greater the salinity, the less it can be used before the salt concentration becomes limiting. Blending or diluting extremely salty waters with rising quality of water sources should be carried out only after a comprehensive examination of the effect on linked and independent supplies of consumable water. Combining or diluting drainage fluids with clean water in order to improve water supply or meet discharge restrictions may be inefficient in some circumstances. It is often feasible to

gain a greater crop yield from the overall water supply by isolating the water components (Raman and Mohr, 2014) (Figure 7.6).



Figure 7.6: Effects of irrigation of saline water.

Source: https://www.sciencedirect.com/science/article/abs/pii/ S0378377498001206.

Separating saline drainage fluids from "good quality" water supplies is a priority, even more so when the latter are to be used to irrigate salt-sensitive crops. Saline drainage fluids can be more efficiently used by substituting "excellent quality" water for irrigation of rotational crops following seedling establishment.

7.10. CONCLUSION AND FUTURE PERSPECTIVES

The growing need for nutrients by a rich society, along with the diminishing quantity of arable land and freshwater, creates the issue of agriculture's sustainable development. With these viewpoints in mind, saline agriculture is gaining traction as a potential role.

This agricultural sector may become extremely important in the future for Mediterranean countries as a result of rising soil degradation in some areas and their geographic and climatic characteristics (Guerra et al., 1998).

Without a significant and long plan that is adaptable to present social, economic, edaphic, climatic, and hydrogeological conditions, it is considered that future issues associated with irrigated agriculture employing low-quality water would be impossible to overcome.

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8

USE OF SALTS IN THE PHARMACEUTICAL INDUSTRY

CHAPTER

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8.1. INTRODUCTION

The salt formulations of active pharmaceutical ingredients (APIs) have a significant impact on their biological and physicochemical characteristics. A variety of factors influence the salt formulation, including API chemistry, planned dose form, pharmacodynamics (PD), and pharmacokinetics (PK). The right salt may help an API's ultimate therapeutic and pharmacological benefits. The wrong salt form, on the other hand, might have the inverse impact and be highly harmful to ultimate drug formation. The impact of salt formulations on the pharmacological characteristics of APIs are discussed in this chapter, as well as many parameters for selecting the right salt formulations. This chapter provides detailed background on the salt selection methods as well as a complete examination of the selection parameters (Figure 8.1).



Figure 8.1: Kinds of salts in the pharmaceutical sector.

Source: https://www.intechopen.com/chapters/42078.

To obtain acceptable formulation qualities, particular salts of active pharmaceutical ingredients (APIs) are produced. While among the most prevalent motivations for using salt production is to address low water solubility, pharmaceutical firms often utilize salt production to address other biological and physicochemical problems like poor absorption, toxicity, stability, and production process challenges. The importance of salts is evidenced by the fact that around half of all active pharmaceutical ingredients approved by the US Food and Drug Administration (US FDA) are in salt form (Paulekuhn et al., 2007). Pharmaceutical salts also make about half of the top 200 prescribed medications in the United States (Prohotsky and Zhao, 2012). Several factors influence the type of salt that should be used. The development of a possible commercial salt necessitates coordinated efforts and a detailed understanding of the physical and chemical properties of the APIs and counter ions utilized. For the most cost-effective choice of the finest salt, a rational decision tree technique must be used. Moreover, to reduce mistakes, all relevant testing must be carried out within the initial stages of the drug production procedure. Salts may drastically modify the chemical/physical characteristics of an API, allowing the drug production procedure to be sped up.

The chemical and physical features of the API impact its eligibility for salt choice; alternative counter ions may be used to remedy one or more of the APIs inadequacies. An important study field is the estimation of a salt's quantitative and/or qualitative characteristics depending on the counter ion utilized. A relationship between salt characteristics and the counter ions utilized has been discovered in many kinds of research (Gould, 1986; Thomas and Rubino, 1996). Although it is possible to make some accurate predictions, there is no efficient method to examine salt characteristics depending upon the counter ion utilized. For the preparation of API salts, a broad range of approved counter ions is now accessible (Table 8.1) (Wiedmann and Naqwi, 2016). Employing compounds that have already been utilized in FDA-approved medications and are thus usually regarded as secure (GRAS) is a crucial factor in the selection of counter ions (Gould, 1986).

That article would go through numerous factors in choosing salt formulations, along with appropriate examples for every genre. Because that's beyond the focus of this research to have all of the instances for every criterion, just a few typical examples are presented. It must be noticed that several textbooks have been written on API salt types; most of the material focuses on improving API solubility via salt formulation. This study is unusual because it strives to provide a concise report on salt choosing criteria depending upon pharmacological, chemical, biological, and cost-effective uses of various salt forms (SFs). **Table 8.1:** A List of the Counterions that are Currently Accessible for Salt Production (Wiedmann and Naqwi, 2016)

Chemistry (Type of Ion)	Examples of Counter Ions		
Cations	Aluminum	Lysine	
	Arginine	Magnesium	
	Benzathine	Histidine	
	Chloroprocaine choline	Meglumine	
	Ethanolamine	Procaine	
	Diethanolamine	Potassium	
	Ethylenediamine	Triethylamine zinc	
	Calcium	Lithium	
Anions	Acetate	Malate	
	Aspartate	Lactobionate	
	Isethionate lactate	Maleate	
	Benzoate	Mesylate	
	Benzenesulfonate	Mandelate	
	Besylate	Mucate	
	Bitartrate	Methylsulfate	
	Bicarbonate	Napsylate nitrate	
	Camsylate	Oleate	
	Bromide	Octanoate	
	Carbonate	Pamoate	
	Citrate	Phosphate	
	Chloride	Pantothenate	
	Decanoate	Polygalacturonate	
	Estate	Salicylate	
	Edetate	Propionate	
	Fumarate	Acetate	
	Gluconate	Stearate	
	Glucophage	Sulfate	
	Glutamate	Succinate	
	Hexanoate	Tartrate	
	Glycolate	Tosylate	
	Iodide	Template	
	Hydroxynaphthoate	-	

8.2. DRUG CHEMISTRY CONSIDERATIONS

8.2.1. API Functional Groups

The existence of basic or acidic functional groups is a necessary condition for salt production. Because they are usually weakly basic or mildly acidic, most of the APIs found are great choices for salt production during medication synthesis. The characterization of basic or acidic functional groups is the first step in salt testing. A suitable counterion may be chosen based on the existence of such groups and pharmacological requirements. Acids and Bases having a low molecular weight are more likely to be a liquid with a lower melting temperature to increase their melting temperatures and transform and sustain the solid-state, a salt synthesis can be utilized. For instance, compound NBI-75043, an experimental molecule for the treatment of insomnia, was described by Gross et al. (2007) as a crystalline, free base with a lower melting temperature (64°C). The development of salt with a high melting temperature was one of the most essential medicinal criteria for this compound. Weak basic pharmaceuticals require acidic counterions to create ionic bonds, hence 14 acids were chosen as possibilities. Because this drug's lower melting temperature was a problem, researchers used differential scanning calorimetry (DSC) to describe salt formulations. DSC is a useful method for detecting the melting temperature, solvates, crystallinity, and the existence or lack of polymorphs. They were able to locate the salt formulation of NBI-75043 by concentrating on the medication's chemistry (Gross et al., 2007).

8.2.2. pK_a of the Drug

The pK_a rule is used to choose a counterion, and it takes into consideration the degree of ionization of the basic or acidic functional groups in the drug (Cruz-Cabeza, 2012 Salt production is predicted by the pK_a rule whenever the pK_a difference between a base and an acid is bigger than 2 or 3 (Stahl and Skinner, 2011). Generally, the pK_a of a basic medicine must be at least 2 pH units greater than the pK_a of the counterion, whereas the pK_a of an acidic drug will be at least 2 pH units less than the pK_a of the counterion. This difference maintains high binding energy among the opposing ionic species, preventing the complexes from dissolving into specific species when they are no longer needed. Phenytoin, for example, is a well-known acidic medication with a pK_a value of 8.4 but has poor solubility. Improving the drug's water solubility was an essential pharmaceutical feature that required to be fixed. Basic counterions with pK_a values >10.4 were more likely to generate pharmaceutical formulations salts due to the acidic quality of the medication. To create a suitable phenytoin salt, a strongly basic counterion like NaOH was required. Weak basic counterions will be unable to synthesize salts with phenytoin due to their inability to increase the pH beyond the requisite pH_{max} value of 11 (Serajuddin and Jarowski, 1993).

8.2.3. Lipophilicity

The synthesis of salts is a process that is often used to improve the solubility of medicine in water. However, increasing the lipophilicity of a pharmacological molecule by the use of hydrophobic salts has been proposed (Miller et al., 2010). To improve chemical stability, it is sometimes necessary to reduce aqueous solubility. This is especially true at higher temperatures and higher humidity. A good example is the synthesis of sulfate and hydrophobic salts of xilobam, both of which are toxic. Because of this, the sulfate salt of this medication is completely ionized. Aryl groups were discovered in the sulfate counterion for this medicine, which prevented the base from being easily hydrolyzed in the existence of higher temperature and higher humidity, according to the findings. Pharmaceutical firms can create more persistent medications without decreasing their bioavailability due to the creation of hydrophobic salts (Walkling et al., 1983). As a result of the neutralization of the total electrostatically charge due to salt production, the lipophilicity of hydrophilic or water-loving molecules increases, which in turn increases the membrane permeability of hydriphilic molecules. The impact of numerous ibuprofen counterions on log P value and membrane permeability was investigated by Sarveiya et al. (2004) as seen in Table 8.2, and it was proven that the impacts of the various counterions on such parameters were distinct.

Table 8.2: Ibuprofen Counterions, as Well as Their Associated Membrane Absorption Values and Log P Values

Ibuprofen Counterion	Intestinal Flux (µg·cm ⁻¹ ·h ⁻¹)	Log P
Ethylamine	5.42	0.97
Triethylamine	48.4	1.18
Sodium	3.09	0.92
Diethylamine	7.91	1.12
Ethylenediamine	15.31	1.11

8.2.4. Hygroscopicity

The capacity of a substance to acquire and hold moisture at different humidity and temperatures levels are known as hygroscopicity. Drugs with low hygroscopicity are recommended because moisture content has a substantial impact on persistence. APIs are characterized as non-hygroscopic, mildly hygroscopic, or hygroscopic solids depending upon the amount of water absorption (Visalakshi et al., 2005). A non-hygroscopic material may absorb moisture from a humid environment, influencing the physical and solubility characteristics of the material and hence the drug's effectiveness. Because of the case of moisture and pH changes in the salt's microenvironment, easily hydrolyzable medicines are more rapidly destroyed. When synthesizing a salt version of a medicine, hygroscopicity must be properly managed. Mineral acid salts, for example, are extremely polar, resulting in enhanced hygroscopicity and a lower microenvironmental pH. Because of the increased rate of hydrolysis, such variables may influence the stability of certain medications (Carstensen, 1988).

8.2.5. Water of Hydration

A hydrate type of salt is defined as salt with crystallization water as an accompanying liquid. Such APIs include water molecule(s) in the crystalline structure of the crystalline structure. Hydrate types of APIs are relatively frequent; it is predicted that roughly one-third of APIs may form hydrates if subjected to circumstances suitable to hydrate synthesis (Suzuki et al., 2012). Pharmaceutical hydrates are generated when an API comes into contact with liquid among the processing steps of crystallization, aqueous film coating, wet granulation, lyophilization, storage, and spray drying (Li et al., 2008). The water of crystallization may be lost when subjected to a dry area, resulting in the formation of a reduced level of hydration or a dry type in the hydrate. The interchange of water with pharmaceuticals and excipients like starch or cellulose may have an impact on the mechanical and solubility characteristics of a medicinal product (Etter et al., 1990). In pharmaceutical hydrates, the presence of water molecules has an impact on internal energy, dissolution rate, thermodynamic activity, hygroscopicity, stability, and solubility (Khankari and Grant, 1995). To further comprehend such characteristics and to solve serious difficulties if they develop, it is essential to first understand how they exist in their hydrated state.

8.2.6. Polymorphism

Polymorphism refers to a solid compound's capability to exist in several crystalline forms. Several medications have many crystalline formulations or structural polymorphisms. The presence of a viable polymorph or a viable pseudo-polymorph must be developed for a chemical to evolve into a viable medication. The chemical stability of drug polymorphs (or pseudo-polymorphs) varies; usually, a much more thermodynamically viable polymorph is more chemically viable than a metastable polymorph. The optimal alignment of molecules, non-hydrogen bonds, and hydrogen bonds in the crystalline structure is critical for crystal structure thermodynamical stability. Even little alterations in crystal packing may cause considerable chemical reactivity discrepancies between 2 polymorphs of the similar medication (Singhal and Curatolo, 2004) (Figure 8.2).



Figure 8.2: Mechanism of drug polymorphism.

Source: https://curiaglobal.com/insights/drug-polymorphism-a-key-consideration-for-api-development/.

Owing to the unavailability of a 3D crystal structure, free volume, and increased molecule mobility, the amorphous version of the similar medication is lower viable than the crystalline state. Penicillin G in its amorphous state was found to be lower viable than the crystalline potassium and sodium salts (Macek, 1996). There have been a lot of instances of drug polymorphism's impact on the medication's pharmacological destiny. To cover all of the

cases would be beyond the scope of this research. Furthermore, it's worth mentioning the ritonavir (Norvir®) polymorphism, which was discovered like a wake-up call for pharmaceutical corporations. Ritonavir is an antibiotic medication that was first commercialized in 1996 by Abbott Laboratories as semisolid gel pills to cure acquired immunodeficiency syndrome (AIDS) (Bučar et al., 2015). Form I, the unique known crystal state, was found during the synthesis phase and was included in the capsules. In 1998, although, a novel and substantially lower soluble polymorph of ritonavir precipitated in semisolid gel capsules, dubbed Form II (Chemburkar et al., 2000). In hydroalcoholic solutions, this form was shown to be substantially less soluble than the marketed Form I (Chemburkar et al., 2000). The formulation of ritonavir semisolid capsules consisted of a hydroalcoholic solution of the medicine that was discovered to be saturated with Form II during testing. The abrupt development and domination of such lower soluble form rendered the formulation un-manufacturable, and it also had an impact on the storage of Norvir® oral solution at refrigeration temperatures, as fewer storage temperatures caused Form II to crystallize (Bauer et al., 2015). Abbot Laboratories withdrew the medicine due to such concerns, as well as a lack of inventory, leaving tens of thousands of AIDSs patients lacking treatment throughout the world. Before being released on the market, ritonavir was modified and authorized in 1999, costing Abbott nearly 250 million dollars in income (Bučar et al., 2015). Identifying salt formulas and their relationship to polymorphism initially in the medication development phase is therefore critical to reducing therapeutic failures later on.

8.2.7. Chemical Stability

Liquid dose formulations containing basic or acidic counterions may have their pH altered by these counterions. A shift in acid-base balance can affect the interaction of APIs with excipients, resulting in either better stability or deterioration of the API, depending on the circumstances. The presence of unfavorable contacts may result in the presence of considerable contaminants in a therapeutic product (Narang et al., 2015).

For instance, amlodipine is a neutral base that was first selected for use in the development of a maleate salt formulation. Furthermore, the existence of maleic acid altered the microenvironment of the medicinal products, and this change resulted in the production of the aspartic acid derivative (UK-57269) via Michael addition as a result of the maleic acid addition. This breakdown product was discovered to contain a variety of biological functions, and as a result, amlodipine maleate was determined to be inappropriate for further research at this time. Although these reactions might be prevented via the appropriate choice of excipients and the avoidance of alkaline environments besylate (benzenesulfonate) was selected as the most acceptable salt form since it caused substantially fewer issues (Gupta et al., 2018). It is demonstrated in this example how the stability of medicine might be significantly affected if the counterion is not properly chosen (Figure 8.3).



Figure 8.3: In the vicinity of maleic acid, amlodipine undergoes a degradation reaction.

Source: https://www.mdpi.com/1420-3049/23/7/1719/htm.

8.2.8. Solubility and Dissolution Rate

Approaches involving salt production have been frequently used to improve a drug's solubility and, consequently, the rate at which it dissolves. It is among the most often used techniques for increasing the solubility of medications that are slightly basic or acidic. In the last 20 years, hydrobromide, mesylate, hydrochloride, fumarate, and acetate have been the most commonly employed counterions for basic chemical entities, while potassium, calcium, and sodium have been the most commonly utilized counterions for weak acidic medicines (Elder et al., 2010). Many of such counterions have been shown to enhance the solubility of water in the aqueous medium. A study conducted by Bastin and colleagues (Bastin et al., 2000) looked at the possibility of salt production for RPR2000765, which has a pH of 5.3 and an inherent neutral base solubility of 10 g/mL. Because of the low water solubility, the drug had low bioavailability in animals. Even though all of the salt formulations tested (hydrobromide, methanesulfonate, hydrochloride, camphor sulfonate, and mesylate) enhanced the solubility of the parent medication, the mesylate salt consistently had a greater solubility of 39 mg/mL at 25°C. Another set of parameters, including hygroscopicity, a clear polymorphism particle size, profile, and flow characteristics, were

considered, and all of such parameters encouraged the creation of a mesylate salt that could be used for future research (Bastin et al., 2000). Accordingly, selecting a proper counterion must not be a one-dimensional exercise in which each aspect is considered in isolation, but rather be an integrated process in which additional important concerns are considered at the same time.

8.3. PHARMACEUTICAL CONSIDERATIONS

8.3.1. Dosage Form Desired

8.3.1.1. A Liquids (Suspensions)

The most prevalent kind of edible liquid dose type is suspensions. Among the most essential issues during medication, formulation synthesis is masking the taste of harsh pharmaceuticals. Various counterions have been successfully used to generate acceptable salt formulations, whether to produce suspensions or to limit solubility such that medications don't dissolve well when applied on the tongue. Erythromycin (neutral base), for instance, is a very well macrolide antibacterial that is soluble in water. Greater solubility, on the other hand, causes rapid disintegration on the tongue, resulting in a sour taste. That distinct feature was discovered to be a significant barrier for pediatric formulations. Later, it was discovered that salt compositions might be used to decrease solubility. The stearic acidic salt was reported to have poor solubility than the other SFs tested, allowing for the creation of a solution that successfully inhibited the harsh taste of the neutral base. It enables the acidic salt version of erythromycin more pharmaceutically acceptable, particularly in children. To lower the solubility of basic or acidic medicine, salts may be created, similarly to erythromycin, to permit the production of a suspension formulation. Calcium salts or anion interchange resonances may be utilized for acidic medicines. Long-chain fatty acid salts (for example, pamoates, and laurates) and cation interchange resonates may be useful for basic medicines (Stahl and Skinner, 2011).

Sweeteners like saccharin or cyclamic acid, for example, maybe utilized to produce salts for basic medications. Basic salts, like triethanolamine, may be used to improve the taste of acidic medications (Stahl and Skinner, 2011). Such cases illustrate that using salt to conceal the taste of sour medications can be a successful strategy.

8.3.1.2. B Solutions

In the creation of parenteral formulations, a drug's solubility in aquatic media is critical. As a result, salt formulations are widely used to generate concentrated parenteral solutions to boost solubility. Solubility tests, which are a key technique for discovering the right candidate, may be used to quickly screen for suitable counterions. Solubility may usually be enhanced by changing the pH of a solution. The solubility of phenytoin sodium is greatly improved by the addition of sodium hydroxide (NaOH), allowing for parenteral delivery at a chosen concentration (Carmichael et al., 1980). Another important element is chemical stability since medications in solution are fewer viable than pharmaceuticals in solid dose formulations. Cephalosporin antiviral, for instance, is unbiased zwitterions that are not particularly stable in solution. Mono-counterion salts were unstable, and while di-counterion salts produced stable solutions, these were acidic with a pH of less than two. Such a pH issue was overcome by making a dihydrochloride salt that was regenerated with two mL of arginine at injection time. It resulted in a medication solution that was stable inside the intended pH range (Stahl and Skinner, 2011). This indicates that salt formulations may be used to create suitable parenteral solutions for a specific therapeutic goal.

8.3.1.3. Creams/Ointments/Gels

Gels, Creams, and ointments are frequent transdermal administration dose formulations. Percutaneous permeation of greatly polar transdermal medication candidates is often inefficient (Marwah et al., 2016). This restricts the usage of several vital medications. Previously, salt production was used to promote transdermal penetration ability. Counterions operate as neutralizing agents by forming a Coulomb force bond with the APIs, allowing passive permeability. The ion matching of salicylates with alkylamines and quaternary ammonium ions, for instance, increased the drug's percutaneous flow. The diethylamine salt of diclofenac was effectively used as a topical gel to higher the penetration, whereas the sodium salt is accessible for permeation (Fini et al., 1999). As a result, a formulation to promote transdermal permeability for desirable systemic side effects may be produced.

8.3.1.4. Aerosols

While inhalation is largely used to deliver drugs locally to the lungs and bronchioles, numerous mechanical and physiochemical aspects must be addressed for successful delivery. The drug's brief residence duration at the site of action is among the most prevalent and significant hurdles to the efficient use of APIs. Salt compositions have been critical in enabling the local administration of medicines with significantly prolonged half-lives. Salmeterol, for instance, is a long-acting beta-adrenergic agonist utilized to treat chronic obstructive pulmonary disease (COPD). Lower solubility was needed to enable a longer duration of action, which was achieved by the synthesis of a xinafoate salt. That slowly dissolves chemical enhanced salmeterol's lengthy half-life. As a result, the xinafoate salt of salmeterol served as a critical composition and a classic illustration of how API characteristics may be adjusted to achieve desired results (Ticehurst and Marziano, 2015).

8.3.2. Ease of Synthesis and Scale-Up

8.3.2.1. Flowability

In general, an API with acceptable flow characteristics is a suitable option for developing commercially effective solid oral dosage forms. The flowability of the medicine may have a considerable impact on the solid dose production processes of mixing, compressing, packing, shipping, and scale-up. APIs with weak flow characteristics can result in undesirable levels of homogeneity, weight fluctuation, and physical irregularity in the end product. The crystalline form of an API is often chosen since it lends itself to flow enhancement strategies (Ahmed et al., 2017). Therefore, an amorphous medication may be synthesized into an appropriate SF that promotes the formation of a crystal lattice, hence improving its solid-state capabilities.

8.3.2.2. Corrosiveness of Counterions

An extremely corrosive medication can significantly complicate the production process. While employing a counterion method to conceal the corrosive group might alleviate some of the difficulty, if the choice is not done properly, it may result in additional issues during the latter stages of drug synthesis. For instance, physically viable salts of substantially stronger counterion acids are required for weak acid medicines with lower dissociation constants (pKa) values (Stephenson et al., 2011). It might result in the formation of the acidic aqueous medium of the salt. Aquatic solutions that are very acidic may damage metal containers, industrial equipment, and other tools. As a result, tableting components like dies, punches, and dying tables are very susceptible to corrosive solids damage due to their continual interaction with tablet mixes at higher and friction and pressure. Corrosion may also occur on the metal surfaces of capsule-filling equipment and the mechanical stresses associated with filling pharmaceuticals. Corrosive salts may render tableting technically challenging and, if employed, may result in the presence of metal residues in tablets after compressing. As a result, such corrosive counterions should either be avoided in salt compositions or suitably diluted with excipients to prevent severe corrosive qualities (Makary, 2014). Additionally, salts of medicinal products having a pH of 2.5 or below in saturated aquatic medium are often corrosive. If the value of pH of a saturated aquatic medium is lower than or equal to 4, corrosion tests must be done. For instance, as Stahl and Skinner (2011) noted, weak basic medicines (pKa = 4.7) were thought to be created either as neutral bases or hydrochloride/methane sulfonate salts. Although, due to its high corrosiveness, the hydrochloride salt was ultimately abandoned. The methane sulfonate was found to be non-corrosive to stainless steel and mildly corrosive to tool steel alloys and gray cast iron. As a result, methane sulfonate had selected as the preferable counterion, with subsequent development (Stahl and Skinner, 2011). Therefore, it is necessary to investigate the special qualities of counterions to appropriately develop noncorrosive medicinal items

8.3.2.3. Compatibility with Excipients

There seem to be several instances in the publications about how to choose salt formulations that don't relate to different types of excipients, which makes it easier to make the drug product chemically. The choice of the counterion must be made depending upon how the excipients communicate with each other.

For instance, the neutral base type of compound CGP6085 was meant to be an antidepressant. Moreover, when lactose was mixed with the tablet excipient, it caused a lot of damage to the active ingredient. Consequently, the free base type was discovered to be a bad idea. Afterwards, the hydrochloride salt type CGP6085 was made, which made the API more stable and prevented it from interacting with lactose (Stahl and Skinner, 2011). When a drug is in SF, it may have a big impact on how long it lasts. Unique counterions may make a drug more stable in the dose form that it's used in (Figure 8.4).





CGP 6085 Free Base

CGP 6085 Salt

Figure 8.4: Salt form and freebase of CGP6085.

Source: https://www.semanticscholar.org/paper/Salts-of-Therapeutic-Agents%3A-Chemical%2C-and-Gupta-Bhatia/335fac4356202d27d11c781652 01aeb186e5936a.

8.3.3. Route of Administration

The route of medicine administration dictates whether the free form (acid/ base) of medicine should be used or if an appropriate salt type should be used. Indeed, for many types of medicine formulations, having a salt state becomes even more critical than having a non-salt state. One of the primary difficulties with injectable dose forms is the drug's low solubility in the very few injectable carriers available. For instance, salt compositions are far very critical for injectable dose states than they are for edible or transdermal dose forms. It is because injectable medications, that are often administered intravenously (IV), need soluble materials to prevent phlebitis or tissue irritation caused by insoluble therapeutic agents (Jamerson et al., 1994). Previously, injectable salt states have been authorized in more numbers than any other type of salt. Paulekuhn et al. (2007) reported in a research article that greater than 70% of injectable dose state forms contained salts, compared to just 50 to 60% of oral dose formats. Growing demand for a highly soluble salt for injectable dose state is one of the primary drivers of salt formulations (Paulekuhn et al., 2007). The three most often utilized anions in oral dose formats are sulfate, maleate, and chloride; the three most frequently utilized anions in injectable pharmaceutical formulations are sulfate, maleate, and chloride. Calcium, potassium, and sodium were the three most frequently utilized cations in parenteral and oral formulations. The lysine counterion has been a good alternative for injectables in current years, accounting for roughly 15% of injectable salts authorized between 2002 and 2006 (Paulekuhn et al., 2007). Consequently, salt production is a critical step in achieving desirable medication properties, like improved solubility for parenteral delivery.

Additionally, various salt versions of similar medicine may be appropriate for various routes of administration. For instance, potassium, diclofenac sodium, and the free acid versions have all been allowed for oral use. Although diclofenac sodium 1% gel (Voltaren Gel®) and diclofenac sodium topical solution one and a 0.5% w/w (Pennsaid®) are also accessible as topical products, its epolamine salt (Flector®) is authorized like a transdermal patch due to its improved skin permeation compared to potassium or sodium salts (McPherson and Cimino, 2013).

8.3.4. Controlled Release Dosage Forms

When APIs are coupled to various counterions, they exhibit distinct dissolving and releasing characteristics; such trait has been used to develop controlled-release medication formulations. Depending upon the intended release properties, one salt formulation can be favored over another in clinical practice. For instance, by employing minimally soluble salts, a completely soluble medicine may be converted into a sustained release formulation. Such reduction in drug solubility can result in the required delay in medication release. Thus, in sustained-release (SR) compositions, choosing an adequate counterion to retard drug release may be beneficial. For instance, imipramine, a tricyclic antidepressant, was first developed as an immediate-release (IR) prescription in the hydrochloride salt state. A controlled release formulation, on the other hand, was preferred to provide persistent therapeutic benefits. Similarly, imipramine pamoate was developed for this purpose, and its solubility was discovered to be much lower than that of the hydrochloride form. Such latency in drug release was appropriate for the Sr composition (Stahl and Skinner, 2011) (Figure 8.5).



Figure 8.5: Salts of imipramine.

Source: https://www.sigmaaldrich.com/PK/en/product/sigma/i0899.

A further illustration of the critical nature of dissolving is the many salt formulations of diclofenac. Fini et al. (1996) investigated the solubility of 30 distinct diclofenac salt formulations. Whereas the rapid release dose format is now available in both a free acid and potassium forms in the United States, the prolonged-release dosage form is only available in the sodium salt state. Hence, various counterions connected to a certain medication might affect the rate of dissolution therefore the dose forms sought in clinical practice.

8.4. PHARMACOKINETICS (PK), PHARMACODY-NAMICS (PD), AND SAFETY CONSIDERATIONS

8.4.1. Toxicological Consideration

Whenever medicine is ingested properly, it can interfere with the lining of the gastrointestinal (GI) tract, resulting in undesirable side effects. That sort of toxicity issue with is APIs critical and may play a significant role in restricting the efficient use of medications. Occasionally, salt methods have been used to mitigate the parent drug's GI toxicity. Numerous instances (Broh-Kahn, 1906; Duesel et al., 1954) indicate similar usage of rapidly metabolized and expelled counterions with low toxicity issues. Therefore, such techniques aided in addressing GI toxicity issues. Salicylates, for instance, are believed to stimulate GI bleeding and accompanying problems, like ulcers. Choline is an essential counterion with low toxicity; choline salicylate was shown to have a reduced frequency of GI damage and was widely supported at greater dosages (Broh-Kahn, 1906). As a result, the GI toxicity of APIs may be successfully minimized by using the proper salt formulations.

8.4.2. Distribution and Clearance

While salt forms are not frequently used, they have been proven to impact the elimination and distribution of a medicinal molecule. Malek et al. (1957) revealed that macromolecular counterions may drastically affect the distribution characteristics of certain antibacterial (Malek et al., 1957). Polyacrylic acids, polysaccharides, sulfonic acids, and polyuric acids were mixed having neomycin and streptomycin. In comparison to streptomycin sulfate salt, such large molecular weight counterion salts of streptomycin demonstrated increased drug transport to lymph nodes and decreased drug existence in plasma. Streptomycin's removal was therefore postponed as a consequence of its selective distribution (Berge et al., 1997). It provides an excellent opportunity for researchers to identify novel macromolecular salt formulations that may be used to tailor the distribution of medicine to attain the ideal therapeutic effects.

8.4.3. Onset and Termination of Therapeutic Effects

Certain medication compositions necessitate a weak start and expiration of therapeutic activity, depending on the therapeutic indication. Various salt formulations have been successfully used to modify the onset and duration of action of medicines. For instance, it was shown that using solitary salt amphetamine in dextroamphetamine formulations wasn't just an ideal option for achieving rapid and sustained psychostimulant actions. Rather than that, Adderall XR® was developed as a mixture of amphetamine's aspartate and sulfate salts, as well as dextroamphetamine's saccharate and sulfate salts. Such distinct salts inside a single medicinal product permitted distinct metabolic rates and onsets of action. This resulted in a more rapid onset of therapeutic impact while sustaining it for an extended period (Gupta et al., 2018). That example demonstrates how salt may be used to alter a drug's onset and duration of action to accomplish its intended impact.

8.4.4. Counteracting Side Effects

Occasionally, counterions are employed in such a way that the counterion reduces the parental medication's adverse impacts. For instance, antihistamine salts of penicillin have been described in the literature, because penicillin may induce an allergic reaction in certain people. The primary goal was to minimize penicillin's allergic reaction with the use of well-documented anti-allergic medicines (JM, 1955). Likewise, benzylpenicillin was co-formulated with benzathine counterion for intramuscular (IM) injection. Benzathine is a famous local anesthetic that relaxes the injection site in an IM injection. Such co-formulation alleviates the discomfort associated with a quite heavy IM depot dosage of benzylpenicillin that is essential for the treatment of some illnesses like syphilis (Engel et al., 1990). A more well instance of counterions being utilized to limit adverse impacts is Dramamine® (diphenhydramine + 8-chloro-theophylline), in which the 8-chloro-theophylline works as a booster to counteract the sleepiness induced by diphenhydramine (David et al., 2012; Bander et al., 2017).

8.4.5. Drug Interactions

Whenever medicine is co-manufactured or co-administered with other pharmaceuticals, the existence of free acidic/basic formulation or a specific counterion might have significant clinical pharmacological interactions. When used with proton pump inhibitors (PPIs), prasugrel is a good existence of a drug interaction (Seiler et al., 2011). As contrasted to the free base state, prasugrel is accessible like a hydrochloride salt, which is being reported to enable greater uptake at increased stomach pH. Furthermore, it has been discovered that throughout medication manufacture, the base-acid interaction may transform the salt state to the free base state, influencing PK. This is exacerbated considerably by the utilization of PPIs in conjunction with prasugrel since co-administration might change stomach pH and the salt-to-base ratio. As a result, bioequivalence investigations using PPIs or not become therapeutically relevant. Whenever prasugrel in various salt/ base ratios was co-administered having lansoprazole, the degree of uptake was determined to be equal in all formulations; although, the absorption rate was shown to be varied (Seiler et al., 2011). It was a noteworthy clinical result because a higher salt to base transformation postponed prasugrel's peak platelet aggregation, which is an essential therapeutic objective after myocardial infarction. As a result, salt formulations and medication combinations may have significant clinical effects (Seiler et al., 2011).

8.5. ECONOMIC CONSIDERATIONS

Several generic drug companies have attempted to enter the market with various salt formulations of authorized APIs over the decades, since before the original copyright had ended. Improved salt formulas, on the other hand, have aided original copyright holders in extending their intellectual rights or granting marketing authorization to a generic producer. The simplest manufacturing process, very viable analogs, modern paths of administration, or an opposite therapeutic utilize are some of the advantages offered by creative salt formulations that can warrant patent protection (Song and Han, 2016).

A familiar instance is Dr. Reddy's Laboratories' appeal for marketing authorization of amlodipine maleate since the patent on amlodipine besylate expired. In favor of the original patent, that argument was dismissed. Certain producers, on the other hand, were effective in changing specific dose parameters because they proved distinct benefits. *Diclofenac epolamine* (Flector®) is a well-known instance of a transdermal patch that was authorized and patented whereas its potassium and sodium salts were already accessible as topical gels, generic tablets, solutions, and capsules. The conventional composition received its first patent on 4 March 1997 (Akazawa, 1997). Flector® has a new patent from the Institut Biochimique SA (IBSA), which was authorized by the FDA on January 31, 2007, and is applicable till April 13, 2019. The prolonged patent and marketing exclusivity was warranted due to the new composition. It shows how patenting new salt formulations may provide certain items market exclusivity and assist corporations to safeguard their intellectual property.

For simplicity, all elements impacting the salt chosen procedure are described in the diagram Figure 8.6.





Source: https://www.mdpi.com/1420-3049/23/7/1719/htm.

8.6. SCREENING, PREPARATION, AND CHARACTERIZATION OF SALTS

Numerous works discuss salt testing, manufacturing, and characterization (Black et al., 2007; Thorson et al., 2011). The objective of this analysis does not provide an exhaustive overview of the methods concerned, however rather provide a synopsis of the choice, testing, production, and

characterization of salts. The testing of salts begins with the identification of probable counterions for the salt's formation (Wiedmann and Naqwi, 2016). The salts of parent compounds (PC) are discovered by the testing of a great number of salt forms (SFs) under a range of crystallization settings. Historically, comprehensive screens have been undertaken under a variety of circumstances to discover salts with the optimum characteristics for formulation development (Black et al., 2007). To facilitate salt production, the medication should be entirely ionized in a solitary state ionization, as partial ionization might result in the precipitation of the unionized form. Even though indicated before in the pKa portion, the optimum pKa gap must be sustained in the solvent system utilized for crystallization; the difficulty with this criterion is that non-aqueous or combined solvent systems are frequently employed for crystallization, affecting pKa. New advancements, including a microfluidic system, have the potential to bypass the solvent incompatibility constraint. In all, 48 wells make up the microfluidic platform, with every well containing roughly 87.5 nL of fluid volume. Because of the decrease in volume, salt testing may be performed on specimens as little as 1 mg. There are four ways for preparing the API salt: heat, evaporation, slurry conversion and anti-solvent, all of which are described here (Wiedmann and Naqwi, 2016). Crystallization is affected by several factors, including concentration, pH, ionic strength and the additive kind, regardless of the technique applied. To determine if the salt is amorphous or crystalline, X-ray powder diffraction is used to examine the specimen under consideration. Additional spectroscopic techniques such as Raman, infrared (IR), and nuclear magnetic resonance (NMR) spectroscopy can be used to gather information regarding the interaction between the parent molecule and the counterion. DSC and other thermal procedures are utilized to identify the melting temperature and enthalpy of fusion of a substance. It is possible to anticipate the stability and solubility of salts based on both of these qualities (Wiedmann and Naqwi, 2016). Because of the clarity of the endotherm, it is possible to determine the purity and crystalline nature of the specimen. Additionally, the type of the endotherm may provide information on the presence of solvates and hydrates inside the crystalline lattice. Thorson et al. (2011) currently published a paper describing a semiautomated approach for screening cationic API salts at higher throughput utilizing cationic API salts. Using nanoliters of the analyte solution for crystallization, the researchers were able to produce single crystals of adequate size for characterization by a single-crystal X-ray structural characterization (Thorson et al., 2011).

8.7. SUMMARY

An APIs salt form is a critical component of the formulation development procedure. Historically, one of the primary reasons for using salt formulations has been to increase solubility. That article discussed the fact that a distinctive salt state may have consequences that extend beyond solubility. The optimal salt formulation may enhance the APIs solid-state characteristics and alleviate the burden of time-consuming and costly composition creation. The counterions in the salts utilized may enhance the drug's usability in a variety of dose formulations by increasing the composition qualities. The correct salt formulation of the API is critical for achieving the intended result and may also have a significant economic impact.

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The Study of lons and Salts in Chemistry

Positive and negative ions are bound together by ionic bonding in most of the compounds that make up the Earth's crust. An ionic compound is one that contains both negative and positive ions and is electrically neutral. W.H. Bragg and W.L. Bragg discovered the crystalline structure of sodium chloride salt in 1913. This revealed that each atom had six equidistant closest neighbors, indicating that the components were not organized in molecules or limited aggregates, but rather as a networked structure with the long-range crystalline organization. More inorganic compounds were discovered that share structural similarities. These compounds were quickly identified as containing ions rather than neutral atoms, but verification of this theory did not come until the late 1920s, when X-ray tests (which determine the density of electrons) were carried out.

Max Born, Alfred Landé, Fritz Haber, Erwin Madelung, Kazimierz Fajans, and Paul Peter Ewald were known major contributors to the creation of a theoretical explanation of ionic crystal formations. Max Born projected crystallization energies based on the idea of ionic components, which matched thermochemical data well, confirming the hypothesis. Precipitation, evaporation, or freezing can form ionic compounds (including salts) from their constituent ions. Reactive metals, such as alkali metals can generate an ionic product by reacting directly with strongly electronegative halogen gasses. They can also be made as a result of a high-temperature solid-solid reaction.

This book contains detailed information about ions, ionic compounds, different types of salts, and their applications. There are eight chapters in the book. The book is mainly divided into two parts. The first part consists of the initial four chapters, which deal with the properties, classifications, and applications of ions and ionic compounds. The second part introduces the readers with the fundamentals of different types of salts and their applications.

Chapter 1 introduces the readers with the fundamentals of ions and ionic compounds with emphasis on ionic bonding and classifications of ions. Chapter 2 deals with the salient features of ions and ionic compounds. Chapter 3 contains information regarding the basics of ion extraction and ion mobility. Chapter 4 introduces the readers with novel concepts of ionic liquids and their applications.

Chapter 5 explains the key concepts of salt chemistry and aqueous solutions. Chapter 6 illustrates the role of salts in public health and food sciences. Chapter 7 contains information about the saline environment and the use of saline water and salts in agriculture. Finally, Chapter 8 describes the fundamental concepts of salts and their uses in pharmaceutical industries. This book is primarily written for chemistry students who wish to learn more about the connections between atomic structure and bonding, as well as the macroscopic features of ionic compounds and salts. Similarly, the book aims to help teachers and educators to substantiate their lessons through a simple and informative manner of explaining the chemistry of ions and salts.



Dr. Rose obtained her PhD in Chemical Engineering from the University of the Philippines-Diliman in 2013, while her Masters in Chemical Engineering and BS Chemical Engineering degree was obtained from Adamson University. She is also a Professor in the Graduate School Department under the Master of Engineering Program at Adamson University since 2006. In 2017, she obtained her Post Doctorate Degree in Green Power: Hydrogen Generation and Fuel Cell Development from the University of California Merced, USA (in collaboration with the Energy Storage and Conversion Materials Laboratory of the University of the Philippines, Diliman). She is a visiting scientist to several universities abroad such as the University of California Merced in USA, Kindai University in Japan, National Taiwan University and Chia Nan University of Pharmacy and Science in Taiwan. She has published more than 20 research papers in water treatment and remediation, green technology, fuel cells, electrodialysis, nanomaterials, high voltage spatial electricity, batteries in peer-reviewed journals, and have more than 15 textbooks published in chemical engineering and processes. As an educator, she is very active in publishing her research to local peer reviewed journals. An advocate of Climate Action, a Climate Reality Leader Corp Member and a budding Sustainability and Circularity talent, Dr. Mendoza is also presently actively engaged in several local and international Green Federation as Board Member and Officer such as the Green Party of the Philippines, and Treasurer of the Asian Pacific Federation of Green Women's Network. She is also one of the Board of Directors of the Philippine Society of Engineering Educators, Mark Energy Revolution Corporation and one of the pioneering members of the Philippine Institute of Chemical Engineers, CaMaNaVa Chapter, and an Associate Member of the National Research Council of the Philippines (NRCP).



