Basic Chemistry for Geological Sciences

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What will we learn?

- Atoms and atomic structure
- Chemical bonds (covalent, ionic, metallic, Van der Waals)
- Hydrogen bond (which is not a chemical bond)
- How is water a special molecule (it is dipolar)
- What are isotopes and why do we study them in geology?

Why chemistry in a geology course?

- Rocks are made of minerals
- Minerals are made of atoms, that stay together because of different kinds of chemical bonds
- Different kinds of chemical bonds determine different behaviors of rocks and minerals in nature
  - Why does salt dissolve in water and quartz does not?
- Isotopes are important in geology to both track variations of certain properties in time (stable isotopes) and tell numerical time (unstable, or radioactive isotopes)

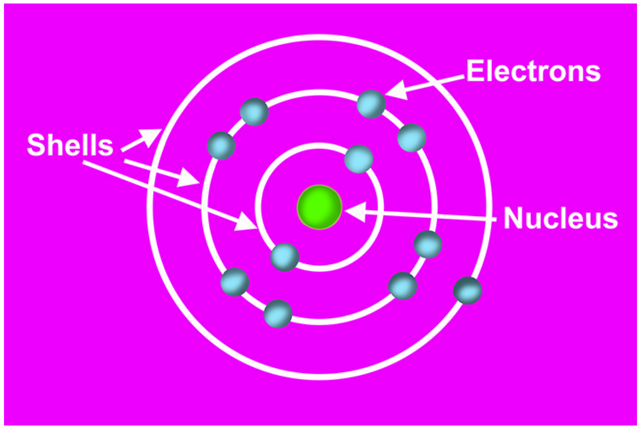
Atoms

- Atoms are the basic building blocks for all matter
- Atoms include subatomic particles called protons, neutrons, electrons

Subatomic Particle	Charge	Mass
Protons	+ (positive)	yes
Neutrons	none (neutral)	yes
Electrons	- (negative)	no* *(1/2056 smaller than protons and neutrons)

- Protons and neutrons reside at the center of an atom, its **nucleus**

- Electrons orbit around the nucleus along a spherical surface (a **shell**)
  - Notice that:
    - the shell is just a space where electrons orbit, not a solid structure
    - a spherical orbit is *not the same as a circular orbit*, like that of Earth around the Sun



- There are different kinds of atoms (elements)
- There are 92 different naturally occurring elements
- The number of protons in an atom is defined as its **atomic number** (“N”)
- N determines what that element is
  - for instance:
    - If N = 1, that is an atom of hydrogen (H)
    - If N = 8, that is an atom of oxygen (O)
    - If N = 92, that is an atom of uranium (U)

What are all those symbols?

center:

Symbol of element

in this case, O stands for oxygen

Always used

upper left:

Atomic Mass

(sum of protons and neutrons)

used only when dealing with isotopes

upper right:

Oxidation Number

(charge of atom if outer shell is full)

used only for ions or when dealing with bonds

$$^{16}_{8}O_2^{-2}$$

bottom left:

Atomic Number

(number of protons)

rarely used

bottom right:

Number of atoms in a molecule

commonly used in chemical formulas

Are atoms always stable?

- In order for an atom to be stable, two conditions are required:
  - There has to be no charge
    - We must have the same number of protons and electrons
  - The (outermost) shell, where the electrons orbit must be full
    - If a shell does not have the exact number of electrons required to fill it, the atom cannot stand by itself

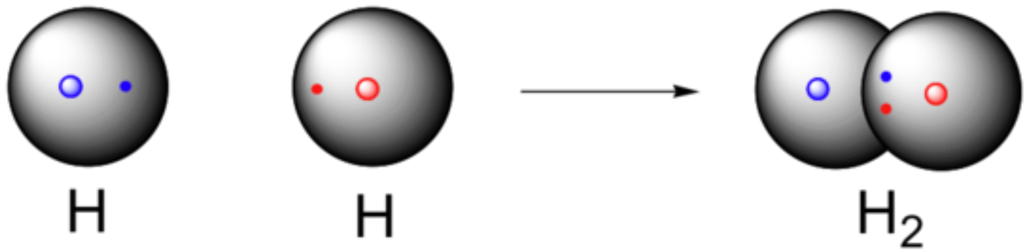
… not always!

- Usually, atoms have the same number of protons and electrons, but ..
- Electrons have to fill shells, and that is not often possible
- In these cases, atoms must bond together, and form **molecules**

H cannot stand by itself …

- Let’s start from the smallest possible atom: H

- H has 1 proton (+), and 1 electron (-), so there is no charge
- But, that single electron is orbiting a shell that has space for two electrons
  - I cannot add another electron, otherwise there would be an electrical charge
  - Solution: two H atoms bond together to form a H_2 molecule



In this image, the two H atoms on the left, each with a proton (big dot) and an electron (small dot) bond together by sharing their electrons to form a molecule (on the right)

The molecule has no charge (2 protons and 2 electrons)
Each atom “sees” 2 electrons on its outer shell

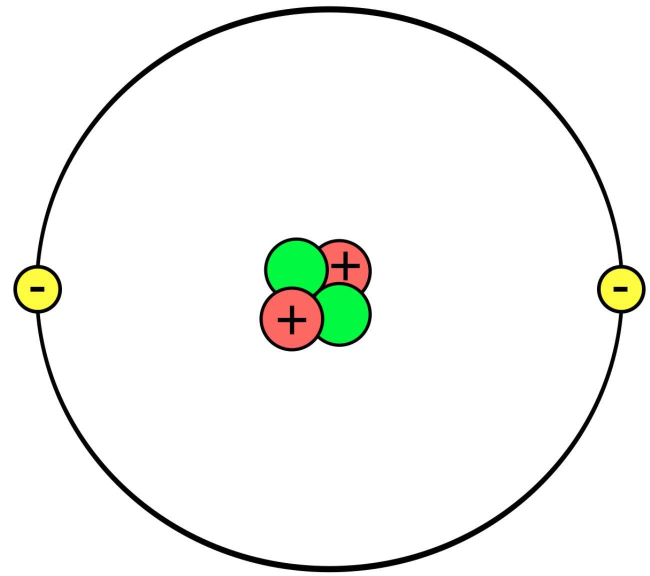
Both requirements are satisfied

A bond where electrons are put in common, or shared, is called a **covalent bond**

The number of atoms used in a molecule is indicated by a subscript on the right

… but He can stand by itself

- The next step is the atom of Helium (He), where N=2
- The single atom of He has 2 protons and 2 electrons (no charge)
- The 2 electrons are filling up the outer shell
- Both requirements are satisfied
  - the atom of He is happy by itself
  - it does not need to bond with other atoms
  - it is part of a group called “noble gases”, that do not bond



In this image, two protons (red) and two neutrons (green) are in the nucleus, while two electrons orbit around them.

There is no charge, and the shell is full: the atom does not need to bond to satisfy requirements

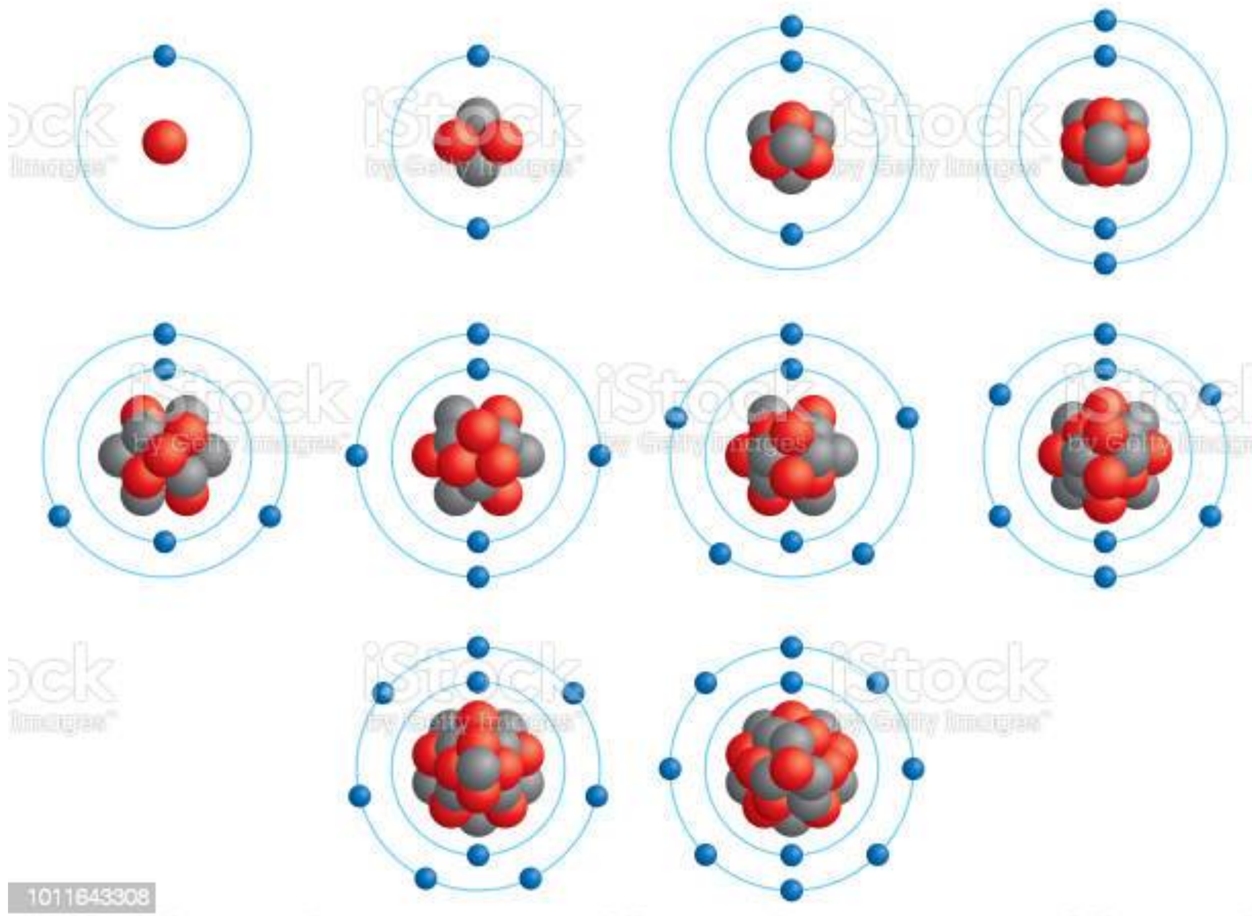
… and beyond He?

- With increasing number of protons, there will be more electrons also
- The outer shell seen so far for H and He can only contain two electrons, so more shells are necessary
- A second outer shell will have space for 8 electrons, and so will a third and a fourth shell
- Past that point, things get complicated and beyond what we need to understand how minerals form
  - These basic notes are already very simplified

Atomic structure
for atoms with N from 1 to 10

(protons in red, neutrons in gray, electrons in blue: neutrons have NO EFFECT on bonding)

notice that the only two atoms with a full outer shell are N=2 Helium (He), and N=10 Neon (Ne)



Periodic Table of the Elements

- All atoms are displayed, in order of increasing atomic number, in the Mendeleev Periodic Table of the Elements
- Notice (next slide) how the first row of the Table has two atoms, while the second and the third have eight atoms
- That matches the number of electrons in the outer shell of those atoms
- There are more than 92 elements in the Table because some of them can be generated in the lab, albeit they have a very short, ephemeral life

Periodic Table of the Elements

Atomic Number → 1; Symbol ← H; Name → Hydrogen; Atomic Weight ← 1.008; Electrons per shell → 1

State of matter (color of name)
GAS LIQUID SOLID UNKNOWN

Subcategory in the metal-metalloid-nonmetal trend (color of background)
- Alkali metals
- Alkaline earth metals
- Transition metals
- Lanthanides
- Actinides
- Post-transition metals
- Metalloids
- Reactive nonmetals
- Noble gases
- Unknown chemical properties

1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIIIB	9 VIIIB	10 VIIIB	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1 H Hydrogen 1.008 1																	2 He Helium 4.0026 2
3 Li Lithium 6.94 2-1	4 Be Beryllium 9.0122 2-2											5 B Boron 10.81 2-3	6 C Carbon 12.011 2-4	7 N Nitrogen 14.007 2-5	8 O Oxygen 15.999 2-6	9 F Fluorine 18.998 2-7	10 Ne Neon 20.180 2-8
11 Na Sodium 22.98976928 2-8-1	12 Mg Magnesium 24.305 2-8-2											13 Al Aluminium 26.982 2-8-3	14 Si Silicon 28.085 2-8-4	15 P Phosphorus 30.974 2-8-5	16 S Sulfur 32.06 2-8-6	17 Cl Chlorine 35.45 2-8-7	18 Ar Argon 39.948 2-8-8
19 K Potassium 39.0983 2-8-8-1	20 Ca Calcium 40.078 2-8-8-2	21 Sc Scandium 44.955908 2-8-9-2	22 Ti Titanium 47.867 2-8-10-2	23 V Vanadium 50.9415 2-8-11-2	24 Cr Chromium 51.9961 2-8-13-1	25 Mn Manganese 54.938044 2-8-13-2	26 Fe Iron 55.845 2-8-14-2	27 Co Cobalt 58.933 2-8-15-2	28 Ni Nickel 58.693 2-8-16-2	29 Cu Copper 63.546 2-8-18-1	30 Zn Zinc 65.38 2-8-18-2	31 Ga Gallium 69.723 2-8-18-3	32 Ge Germanium 72.630 2-8-18-4	33 As Arsenic 74.922 2-8-18-5	34 Se Selenium 78.971 2-8-18-6	35 Br Bromine 79.904 2-8-18-7	36 Kr Krypton 83.798 2-8-18-8
37 Rb Rubidium 85.4678 2-8-18-8-1	38 Sr Strontium 87.62 2-8-18-8-2	39 Y Yttrium 88.90584 2-8-18-9-2	40 Zr Zirconium 91.224 2-8-18-10-2	41 Nb Niobium 92.90637 2-8-18-12-1	42 Mo Molybdenum 95.95 2-8-18-13-1	43 Tc Technetium (98) 2-8-18-13-2	44 Ru Ruthenium 101.07 2-8-18-15-1	45 Rh Rhodium 102.91 2-8-18-16-1	46 Pd Palladium 106.42 2-8-18-18	47 Ag Silver 107.87 2-8-18-18-1	48 Cd Cadmium 112.41 2-8-18-18-2	49 In Indium 114.82 2-8-18-18-3	50 Sn Tin 118.71 2-8-18-18-4	51 Sb Antimony 121.76 2-8-18-18-5	52 Te Tellurium 127.60 2-8-18-18-6	53 I Iodine 126.90 2-8-18-18-7	54 Xe Xenon 131.29 2-8-18-18-8
55 Cs Caesium 132.90545196 2-8-18-18-8-1	56 Ba Barium 137.327 2-8-18-18-8-2	57-71 Lanthanides	72 Hf Hafnium 178.49 2-8-18-32-10-2	73 Ta Tantalum 180.94788 2-8-18-32-11-2	74 W Tungsten 183.84 2-8-18-32-12-2	75 Re Rhenium 186.21 2-8-18-32-13-2	76 Os Osmium 190.23 2-8-18-32-14-2	77 Ir Iridium 192.22 2-8-18-32-15-2	78 Pt Platinum 195.08 2-8-18-32-17-1	79 Au Gold 196.97 2-8-18-32-18-1	80 Hg Mercury 200.59 2-8-18-32-18-2	81 Tl Thallium 204.38 2-8-18-32-18-3	82 Pb Lead 207.2 2-8-18-32-18-4	83 Bi Bismuth 208.98 2-8-18-32-18-5	84 Po Polonium (209) 2-8-18-32-18-6	85 At Astatine (210) 2-8-18-32-18-7	86 Rn Radon (222) 2-8-18-32-18-8
87 Fr Francium (223) 2-8-18-32-18-8-1	88 Ra Radium (226) 2-8-18-32-18-8-2	89-103 Actinides	104 Rf Rutherfordium (267) 2-8-18-32-32-10-2	105 Db Dubnium (268) 2-8-18-32-32-11-2	106 Sg Seaborgium (269) 2-8-18-32-32-12-2	107 Bh Bohrium (270) 2-8-18-32-32-13-2	108 Hs Hassium (277) 2-8-18-32-32-14-2	109 Mt Meitnerium (278) 2-8-18-32-32-15-2	110 Ds Darmstadtium (281) 2-8-18-32-32-17-1	111 Rg Roentgenium (282) 2-8-18-32-32-17-2	112 Cn Copernicium (285) 2-8-18-32-32-18-2	113 Nh Nihonium (286) 2-8-18-32-32-18-3	114 Fl Flerovium (289) 2-8-18-32-32-18-4	115 Mc Moscovium (290) 2-8-18-32-32-18-5	116 Lv Livermorium (293) 2-8-18-32-32-18-6	117 Ts Tennessine (294) 2-8-18-32-32-18-7	118 Og Oganesson (294) 2-8-18-32-32-18-8
		57 La Lanthanum 138.91 2-8-18-18-9-2	58 Ce Cerium 140.12 2-8-18-19-9-2	59 Pr Praseodymium 140.91 2-8-18-21-8-2	60 Nd Neodymium 144.24 2-8-18-22-8-2	61 Pm Promethium (145) 2-8-18-23-8-2	62 Sm Samarium 150.36 2-8-18-24-8-2	63 Eu Europium 151.96 2-8-18-25-8-2	64 Gd Gadolinium 157.25 2-8-18-25-9-2	65 Tb Terbium 158.93 2-8-18-27-8-2	66 Dy Dysprosium 162.50 2-8-18-28-8-2	67 Ho Holmiun 164.93 2-8-18-29-8-2	68 Er Erbium 167.26 2-8-18-30-8-2	69 Tm Thulium 168.93 2-8-18-31-8-2	70 Yb Ytterbium 173.05 2-8-18-32-8-2	71 Lu Lutetium 174.97 2-8-18-32-9-2	
		89 Ac Actinium (227) 2-8-18-32-18-9-2	90 Th Thorium 232.04 2-8-18-32-18-10-2	91 Pa Protactinium 231.04 2-8-18-32-20-9-2	92 U Uranium 238.03 2-8-18-32-21-9-2	93 Np Neptunium (237) 2-8-18-32-22-9-2	94 Pu Plutonium (244) 2-8-18-32-24-8-2	95 Am Americium (243) 2-8-18-32-25-8-2	96 Cm Curium (247) 2-8-18-32-25-9-2	97 Bk Berkelium (247) 2-8-18-32-27-8-2	98 Cf Californium (251) 2-8-18-32-28-8-2	99 Es Einsteinium (252) 2-8-18-32-29-8-2	100 Fm Fermium (257) 2-8-18-32-30-8-2	101 Md Mendelevium (258) 2-8-18-32-31-8-2	102 No Nobelium (259) 2-8-18-32-32-8-2	103 Lr Lawrencium (266) 2-8-18-32-32-8-3	

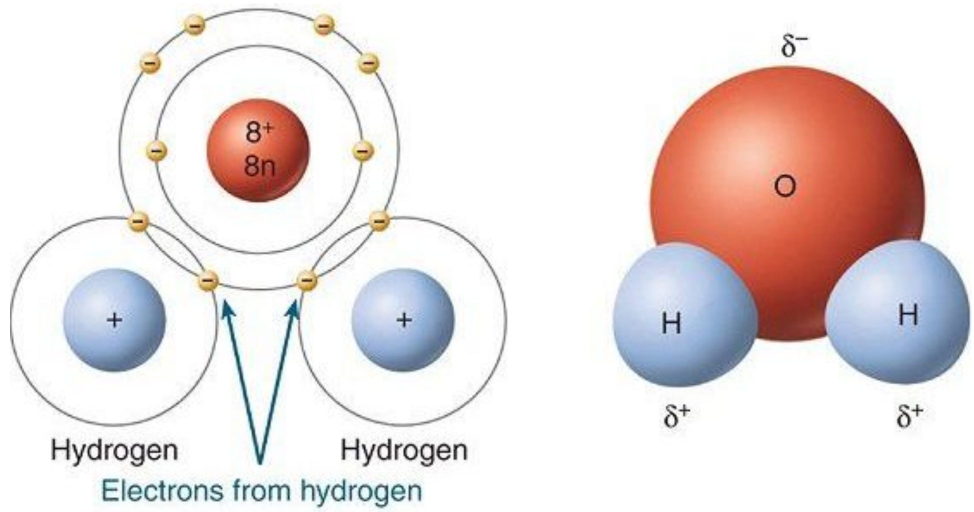
The **Water** molecule (H_2O)

- Before looking into other chemical bonds, we need to study a special molecule: water

- Water is H_2O, two H atoms and one O

- H has 1 proton and 1 electron
- O has 8 protons and 8 electrons

- So how does water exist?



(a) Electron shells in a water molecule

(b) Distribution of partial charges in a water

- O has 8 protons and 8 electrons, while H has 1 proton and 1 electron
- Of the 8 O electrons, 2 are in the inner shell, 6 in the outer shell
- The outer shell has space for 8 electrons, so two are missing to fill it out
- We cannot simply add two electrons, or O would have a charge
- So two atoms of H bond with one O, each providing their single electron in a covalent bond
- In water, H always bond with O by staying on the same side, and not opposite sides of the molecule
- This causes electrons to spend more time on O side, making it more “negative”, and leave the H side “uncovered”, making it more “positive”.

- So we can say that H_2O has a partial charge, negative on the O side (∂-), and positive on the H side (∂+), like a magnet has a positive and a negative side

- Hence, the H_2O molecule is defined as dipolar (two poles)

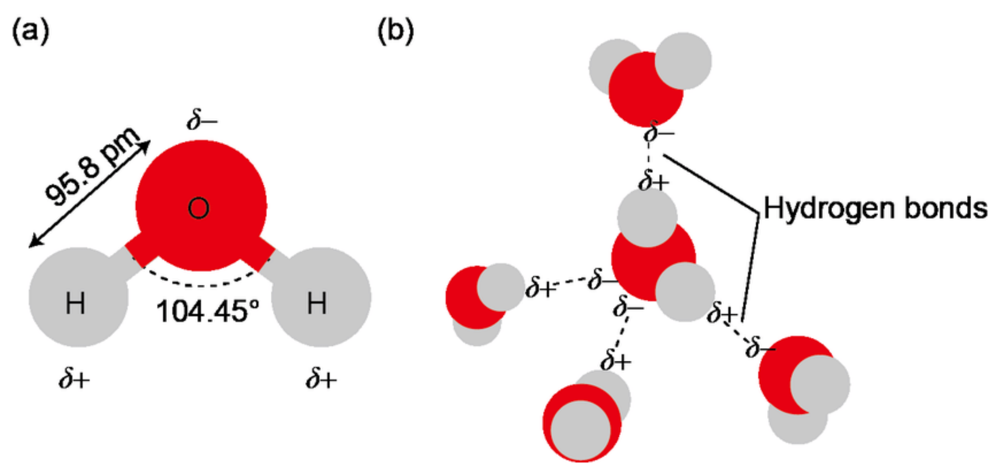
- Hence, that charge can attract or repel any other atom or molecule with a charge

So that is why water is a liquid at room temperature!

The positive side of a water molecule attracts the negative side of another water molecule: water molecules stick to each other!
(non polar molecules that are similar to water, like CO_2, are gases and not liquids at room temperature because they do not stick to each other)

That "sticking" is what we call a hydrogen bond
(notice that the hydrogen bond connects two molecules, so it is NOT an atomic bond)

The hydrogen bond is relatively weak: you can easily break it by boiling water: the energy at 100°C is high enough to break up the bond



back to chemical bonds!

- We have seen (slide 9) the **covalent bond**, a bond where electrons are shared between atoms

- We will now look at the **ionic bond**, a bond where electrons are physically moved from one atom to another, creating ions

The Ionic Bond

- Let's start from a very common compound, table salt

- Table Salt is $NaCl$

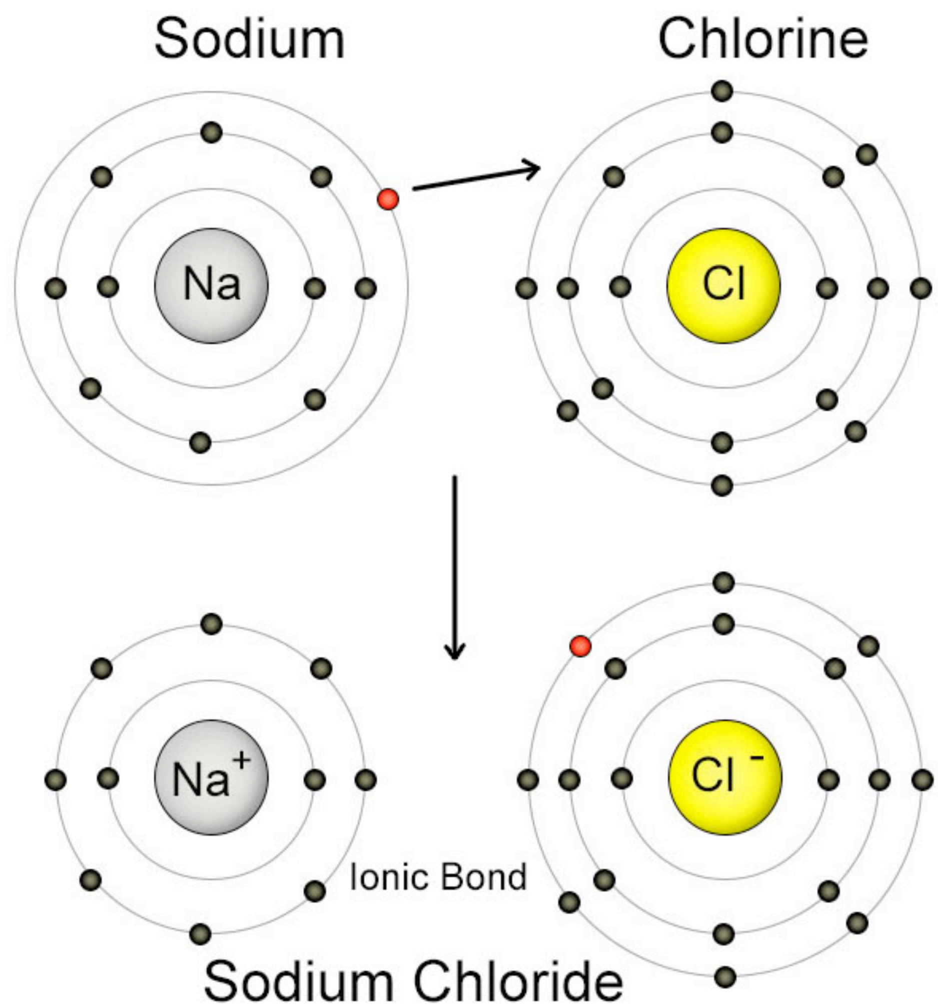
- The atomic numbers of Na (sodium) and Cl (chlorine) are, respectively, 11 and 17 (see the periodic table on slide 14)

- That means that (check it out!) sodium has a lonely electron on its outer third shell, while chlorine has seven, and only misses one to a have a full shell

- What happens is that the lonely Na electrons moves onto the Cl outer shell, so that both atoms have a full outer shell

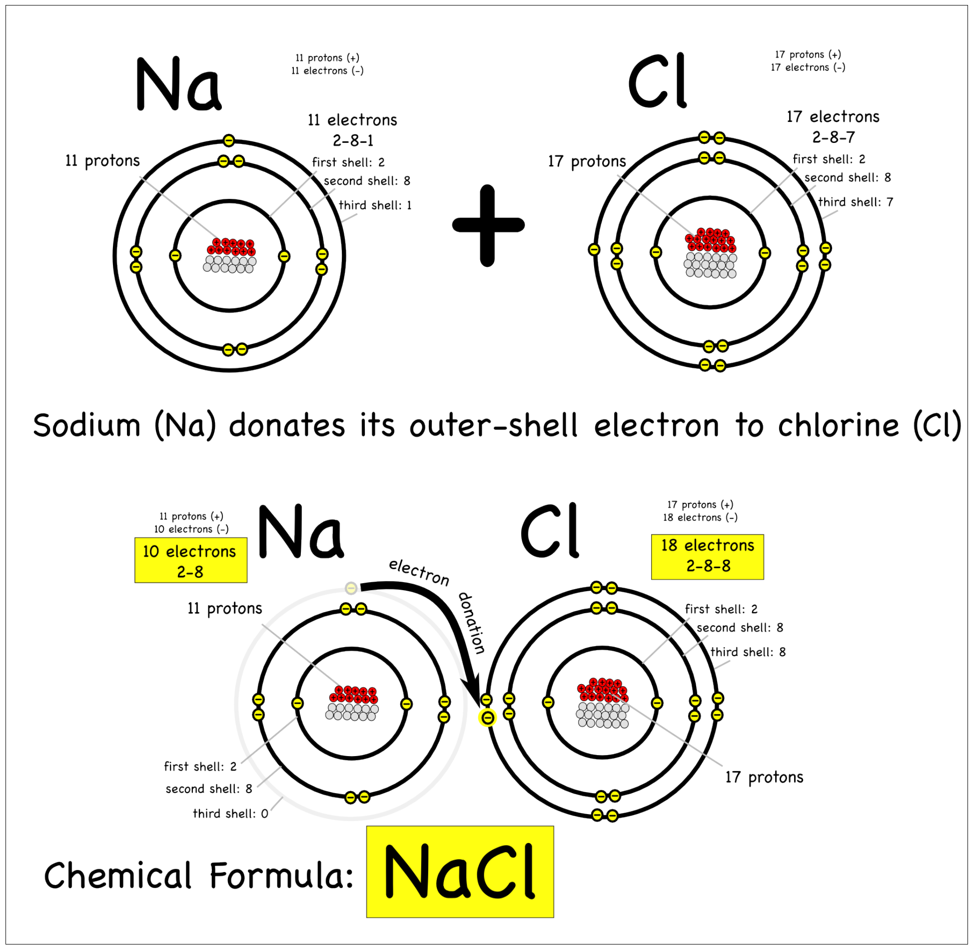
- But, then the atoms would have a charge, and cannot exist as such alone!

- That is true, so in the moment these ions are exchanged, the two atoms, now called ions, become strongly bonded to each other



A chemical bond where electrons are exchanged is called

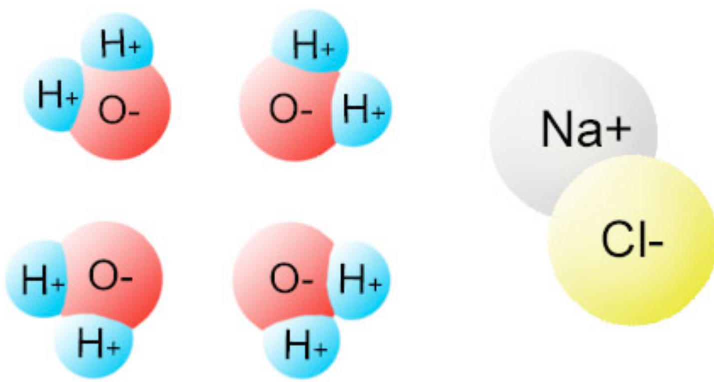
Ionic Bond



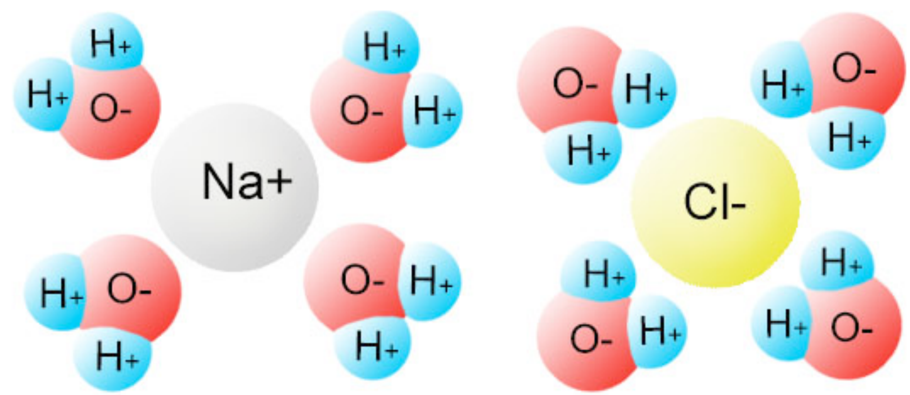
So, why does salt dissolve in water?

(and other minerals do not!)

- Water breaks the ionic bond in salt and neutralizes the charges thanks to its partial charges
- It takes 4 water molecules to neutralize one charge, so 8 water molecules to dissolve 1 molecule of salt
- The negative sides of 4 water molecules surround one Na ion, and the positive sided of 4 more water molecules surround one Cl ion
- If there are not 8 water molecules, salt would not dissolve



Four water and one table salt molecules



Two ions surrounded (neutralized) by eight water molecules

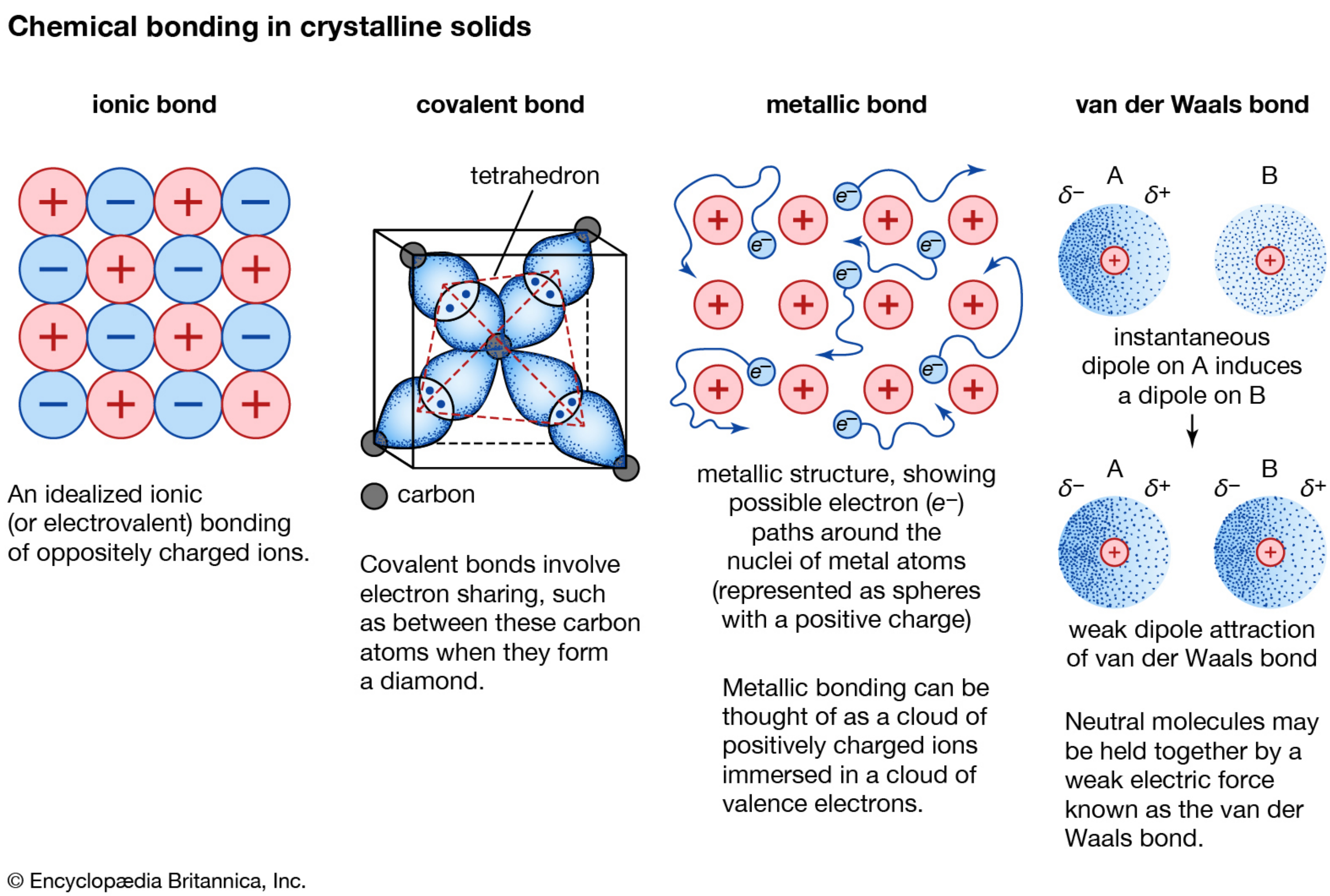
More than one bond can exist in the same molecule

- Some minerals, such as $CaCO_3$ (calcite) are kept together by both covalent and chemical bonds
- In water, $CaCO_3$ splits into Ca^{2+} and CO_3^{2-}.
  - Ca^{2+} is attached ionically to CO_3^{2-} and it would separate from it in water
  - In the CO_3^{2-} ion, C and O are attached through covalent bonds, that would not break up in water

Metallic and van Der Waals bonds

- In **metallic bonds**, electrons are not tied to shells, but are free to roam
- In **Van Der Waals bonds**, weak electrical forces keep atoms together

summary


Chemical bonding in crystalline solids
ionic bond
covalent bond
metallic bond
van der Waals bond
An idealized ionic (or electrovalent) bonding of oppositely charged ions.
tetrahedron
carbon
Covalent bonds involve electron sharing, such as between these carbon atoms when they form a diamond.
metallic structure, showing possible electron (e−) paths around the nuclei of metal atoms (represented as spheres with a positive charge)
Metallic bonding can be thought of as a cloud of positively charged ions immersed in a cloud of valence electrons.
A
B
δ−
δ+
instantaneous dipole on A induces a dipole on B
weak dipole attraction of van der Waals bond
Neutral molecules may be held together by a weak electric force known as the van der Waals bond.
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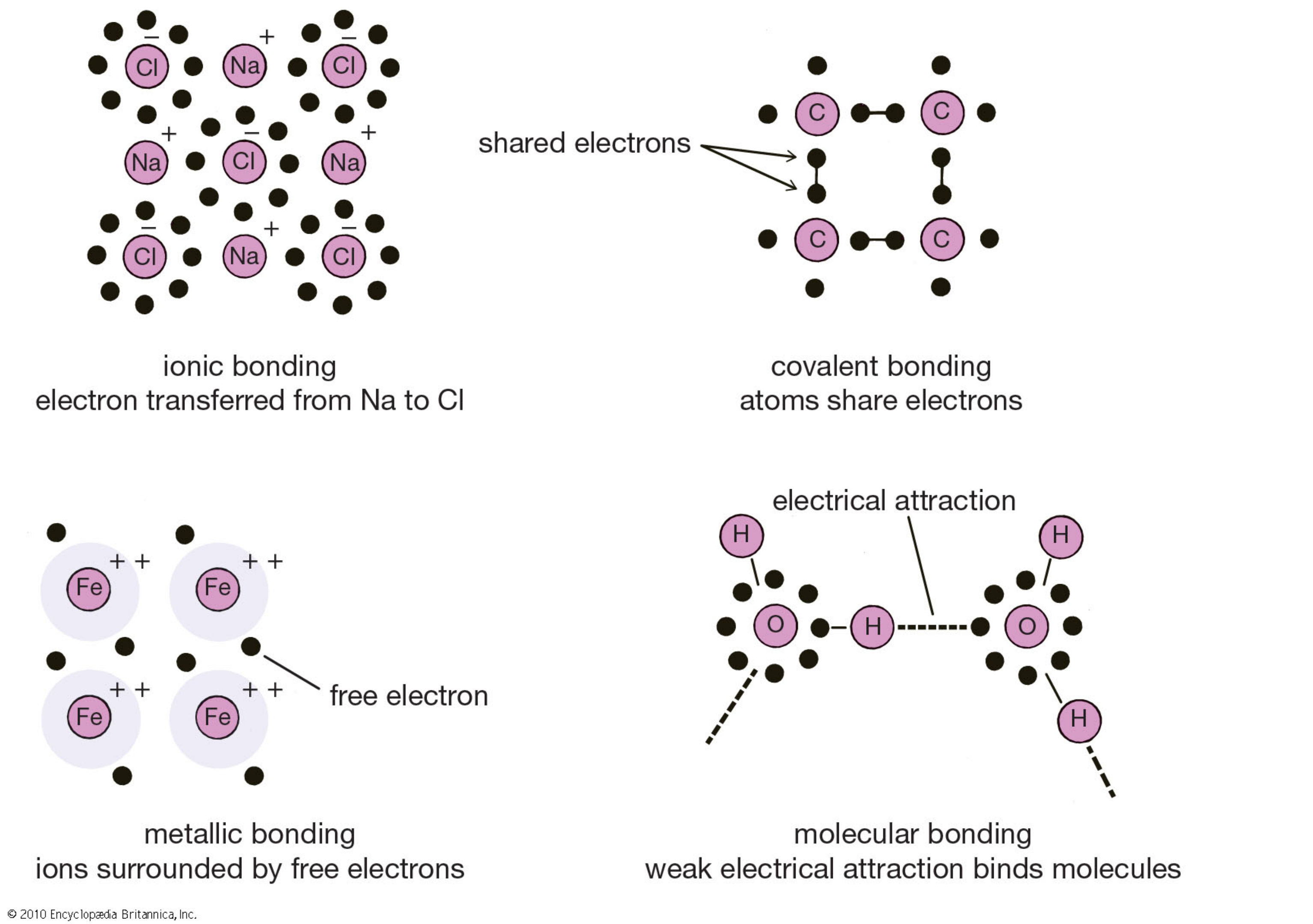
summary


Cl
Na
Cl
Na
Cl
Na
Cl
Na
Cl
ionic bonding
electron transferred from Na to Cl
shared electrons
C
C
C
C
covalent bonding
atoms share electrons
Fe
Fe
Fe
Fe
free electron
metallic bonding
ions surrounded by free electrons
electrical attraction
H
O
H
O
H
H
molecular bonding
weak electrical attraction binds molecules
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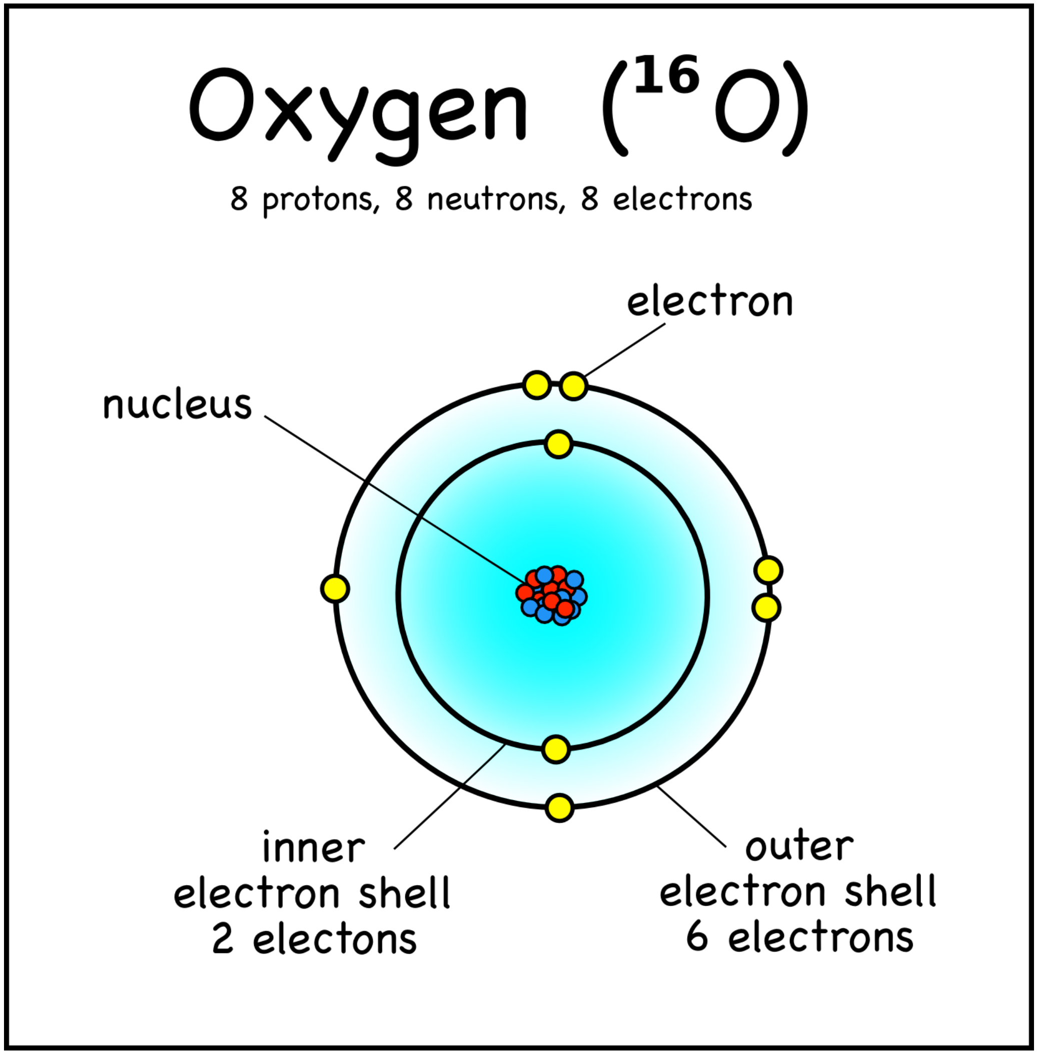
Oxidation Number, or Valence

- The Oxidation Number of an atom represents how many electrons would be needed to have a complete, stable electronic structure
- It determines the kind of chemical bond
- It determines who is bonding with who
- In a mineral, the sum of oxidation number must be zero!

Oxygen (-2):
a negative oxidation number



The outer shell of an atom has space for 8 electrons.

Oxygen only has 6 electrons in the outer shell.

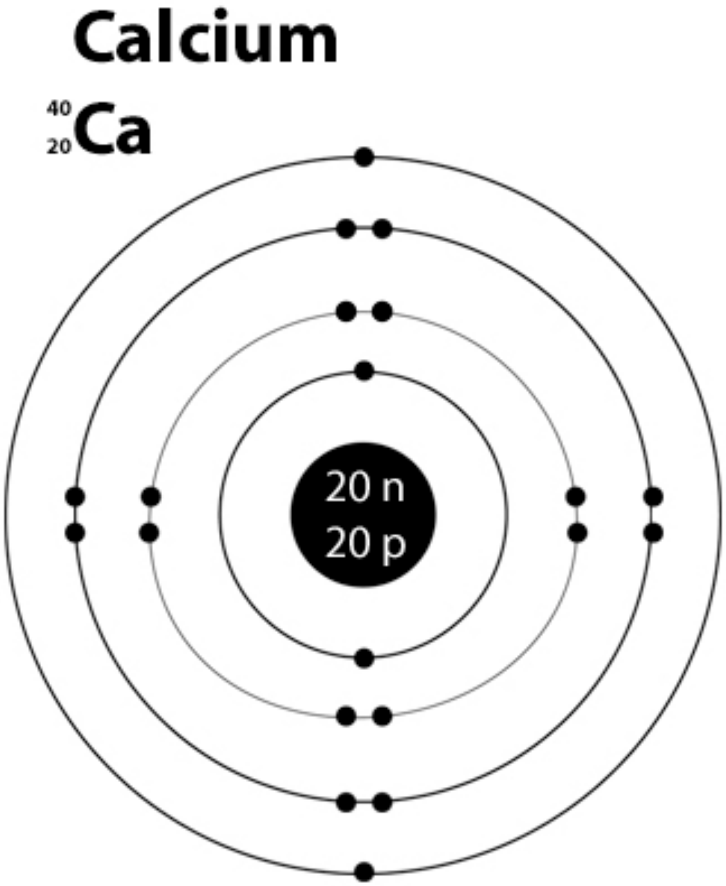
With two more electrons it would reach the stage of "full shell".

But, if we have two extra electrons, the atom would have a charge, and that is not possible, unless it bonds with one or more other atoms.

So, Oxygen would only bond with atoms that would provide it with two extra electrons.

That would imply that Oxygen is looking for two negative charges (-2), and that is how its Oxidation Number is calculated

Calcium (+2): a positive oxidation number



http://www.micromountain.com/sci_diagrams/at_struct/at_struct_pages/calcium_lab_eng.htm

- Calcium only has 2 electrons in the outer shell.
- By losing those two more electrons it would reach the stage of “full shell”.
- But, if we lose two electrons, the atom would have a charge, and that is not possible, unless it bonds with one or more other atoms.
- So Calcium would only bond with atoms that would take from it those two extra electrons.
- That would imply that calcium is looking to give out two negative charges, leaving two positive charges (+2) uncovered, and that is how its Oxidation Number is calculated

The 8 most common elements in Earth's crust

ELEMENT	SYMBOL	VALENCE, or OXIDATION NUMBER	% BY WEIGHT	% BY VOLUME	% OF ATOMS
Oxygen	O	-2	46.6	93.8	60.5
Silicon	Si	+4	27.7	0.9	20.5
Aluminum	Al	+3	8.1	0.8	6.2
Iron	Fe	+2 (+3)	5.0	0.5	1.9
Calcium	Ca	+2	3.6	1.0	1.9
Sodium	Na	+1	2.8	1.2	2.5
Potassium	K	+1	2.6	1.5	1.8
Magnesium	Mg	+1	2.1	0.3	1.4
all others			1.5		3.3

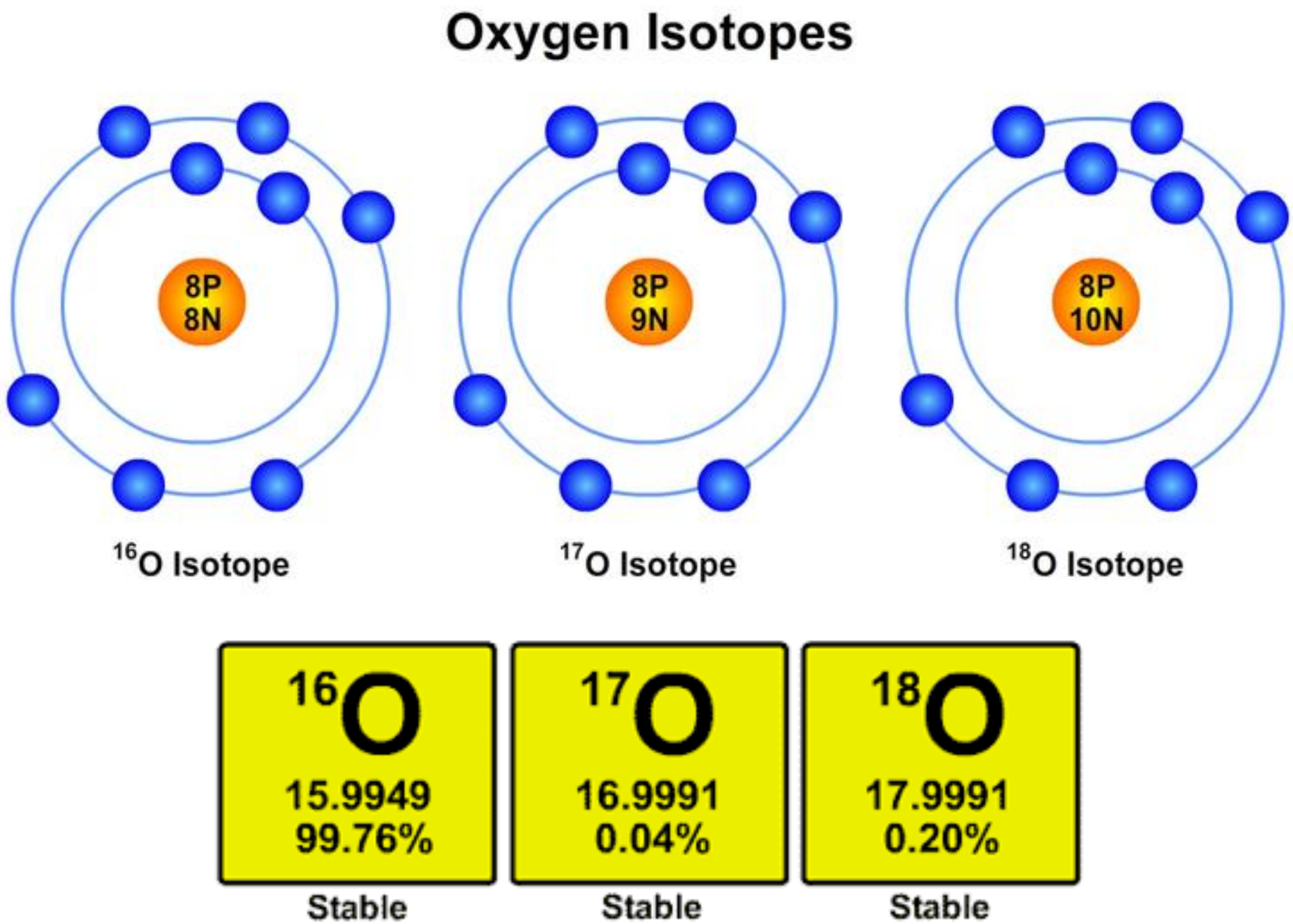
Protons and electrons determine the chemical bond but what about **neutrons**?

- Neutrons have no charge, so they do not affect who bonds with who
- A neutron can theoretically be seen as the sum of a proton and an electron
- Neutrons though do have a mass, like a proton
- So having more or less neutrons would make the atoms heavier or lighter

Atomic Number vs. Atomic Mass

- Most atoms exist in forms with different amounts of neutrons
  - That is, one element has a specific number of protons (the **atomic number**) but that element can exist with different number of neutrons
    - Example: oxygen always has 8 protons and 8 electrons, but can exist with 8, 9, or 10 neutrons
  - The sum of protons and neutrons is the **atomic mass**
  - In the previous case, the atomic mass of oxygen is, respectively, 16, 17, and 18

- These three variety of oxygen are called **isotopes**, and written as ^{16}O, ^{17}O and ^{18}O
- The only difference between them is that ^{16}O is the lightest and ^{18}O is the heaviest
  - The difference is physical (weight)
  - There is no chemical difference
    - Water can be $H_2{}^{16}O$ or $H_2{}^{18}O$



Most O is ^{16}O (99.76%)

Isotopes

- So, isotopes are atoms with the same atomic number (same number of protons), but different atomic mass (caused by different number of neutrons)

- Isotope means “same place” because isotopes occupy the same spot in the periodic table of elements

Isotopes can be stable or radioactive

- Some isotopes are stable, like the three O isotopes we have seen
- Some isotopes instead are unstable, or radioactive
  - Radioactive isotopes decay over time, that is the are reduced by losing energy and subatomic particles to the environment

Why do we study isotopes?
We are not chemists, or physicists

- **Stable isotopes** are used to track variations of certain properties, mostly (but not only) tied to climate change

- **Radioactive isotopes** are used as clock to tell numerical time (the age of a rock)

Use of O isotopes in studying ancient climate: **greenhouse time** (no permanent ice at sea level)

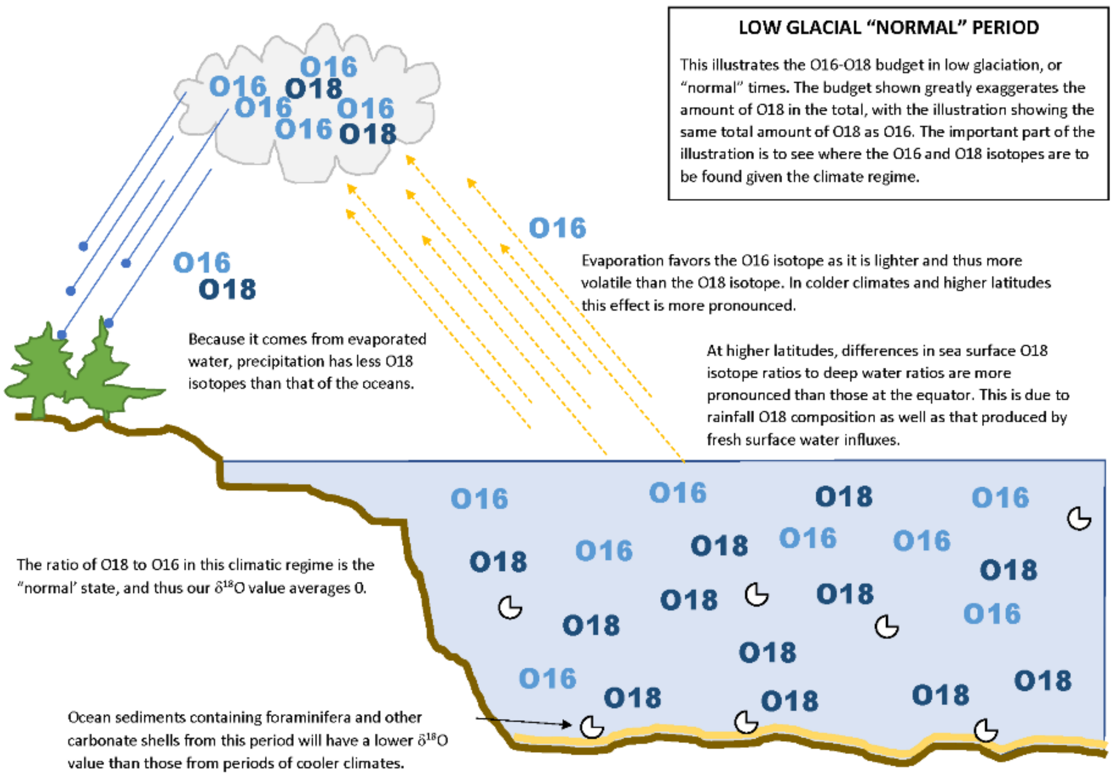


Figure 1. Oxygen isotope balance during a low glacial "normal" period.

Use of O isotopes in studying ancient climate:

icehouse time (permanent ice at sea level)*

*like today

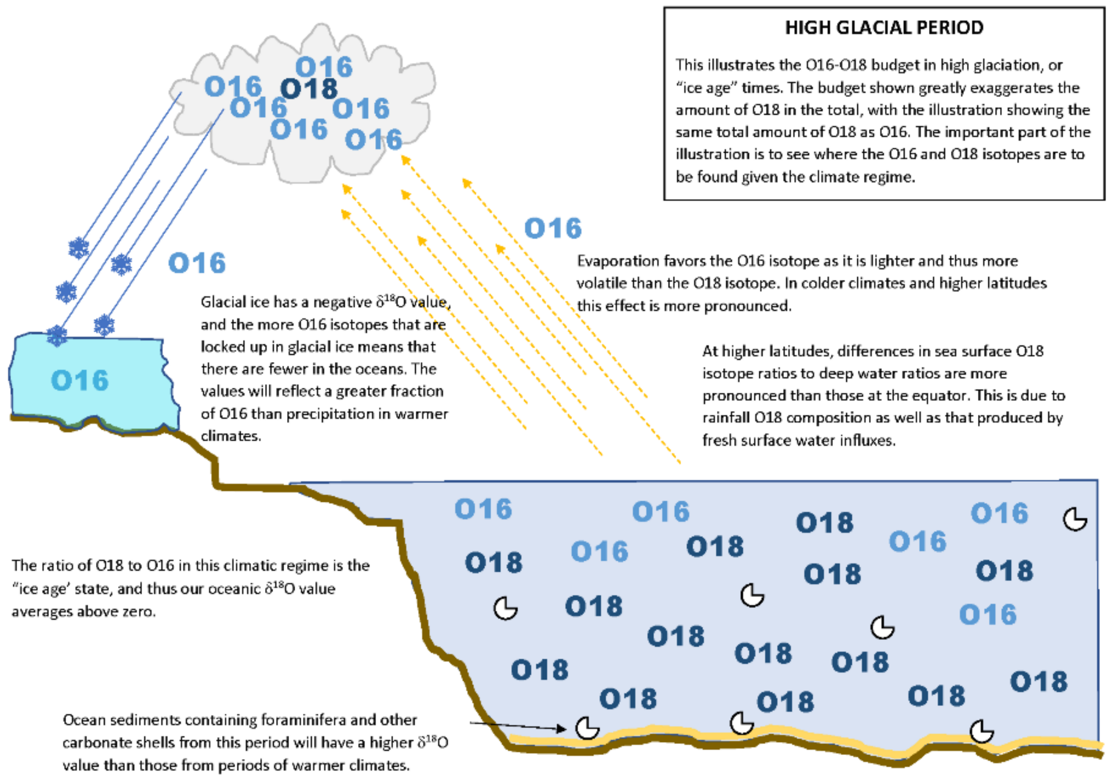
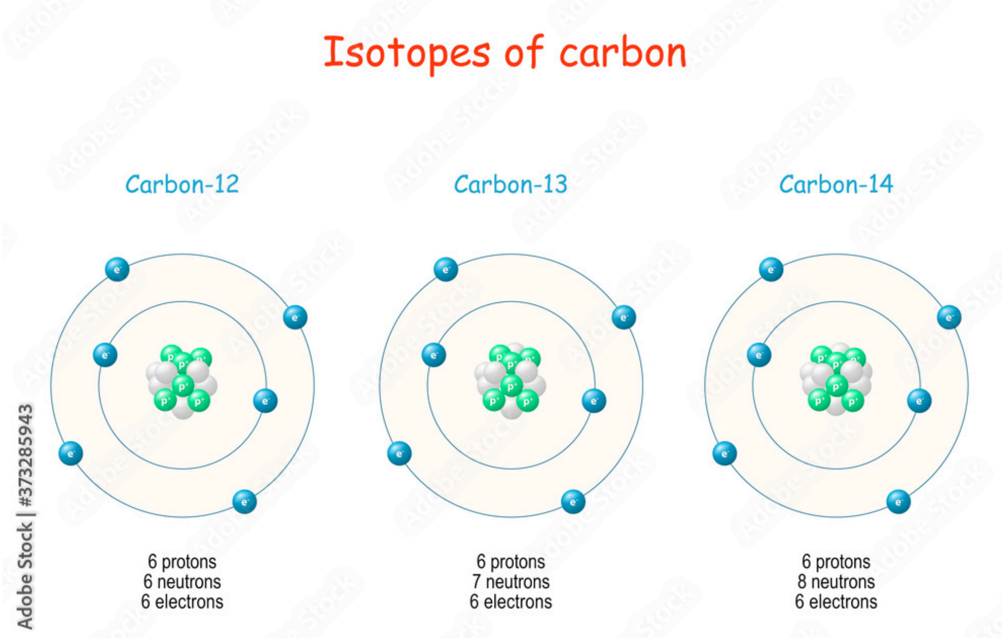


Figure 2. Oxygen isotope balance during a high glacial period.

Carbon (C) too has important isotopes we need to know about

- ^{12}C and ^{13}C are stable and used to study, among other things, past climate change and sequestration of organic matter

- ^{14}C is radioactive and is used to tell the age of very recent (less than 50,000 years old) organic matter



Radioactive Isotopes

- Radioactive isotopes, like uranium (U) are used to establish the age of certain rocks
- While we will study them later on (Geological Dating), this is possible because we know that radioactive isotopes (called parent isotopes) decay at a known pace into stable isotopes (daughter isotopes)
- We look for parent and daughter isotopes in these rocks
  - We know how long it takes for them to change from P to D
  - We count how many of them we still have
  - We establish the age of the rock

An example: ^{238}U turns into ^{206}Pb

- U (uranium) has atomic number 92
  - If 238 is its atomic mass, 238 - 92 is its number of neutrons. That is 146
- Pb (lead) has atomic number 82
  - If 206 is its atomic mass, 206 - 82 is its number of neutrons. That is 124

- So when U turns into Pb:
  - it loses 10 protons (92 - 82)
  - it loses 22 neutrons (146 – 124)
    - these particles are the radiation component
  - it loses energy as heat
    - the heat is what powers plate tectonics

  - For a total of 10 + 22 particles = 32
  - 238 - 206 = 32