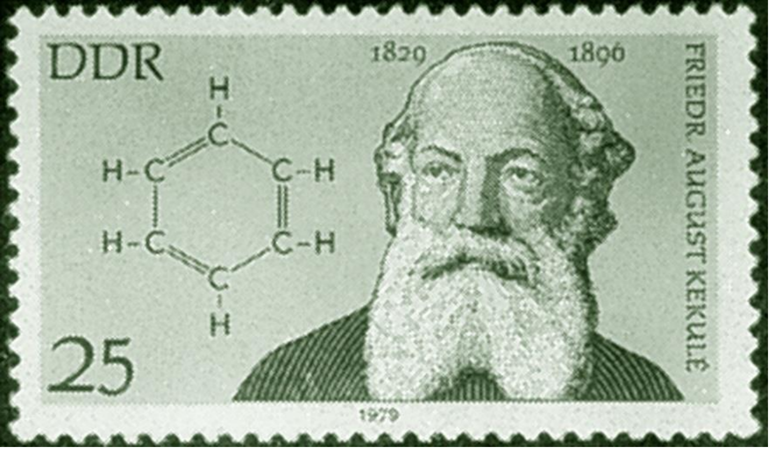
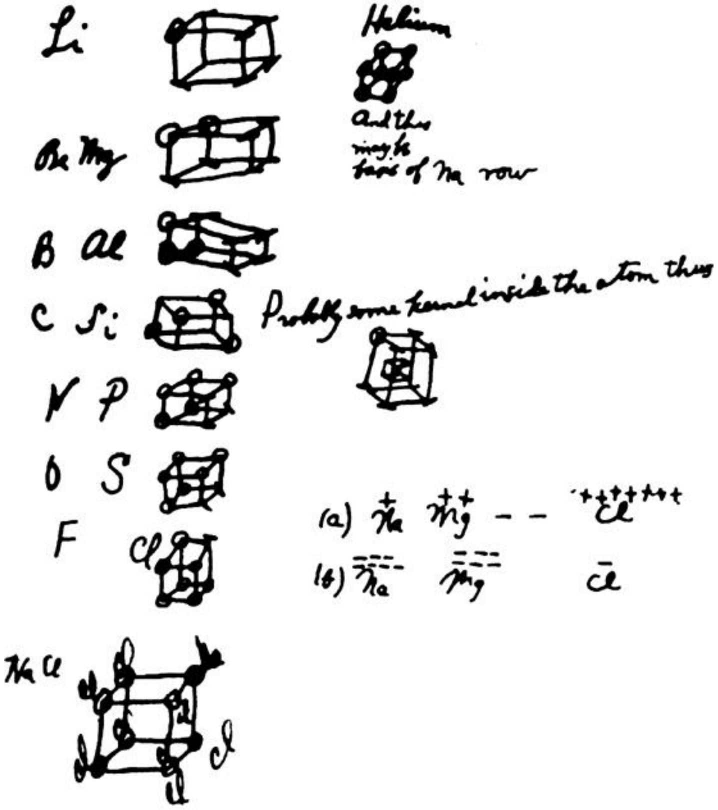


Chemical Bonding I: Basic Concepts



Bonding Theories

- Explain how and why atoms attach together to form molecules
- Explain why some combinations of atoms are stable and others are not
  - Why is water H_2O, not HO or H_3O?
- Can be used to predict the shapes of molecules
- Can be used to predict the chemical and physical properties of compounds

Lewis Model

- One of the simplest bonding theories is called **Lewis theory**.
- Lewis theory emphasizes valence electrons to explain bonding.
- Using Lewis theory, we can draw models, called **Lewis structures**.
    - Also known as electron dot structures
- Lewis structures allow us to predict many properties of molecules.
    - Molecular stability, shape, size, and polarity

Why Do Atoms Bond?

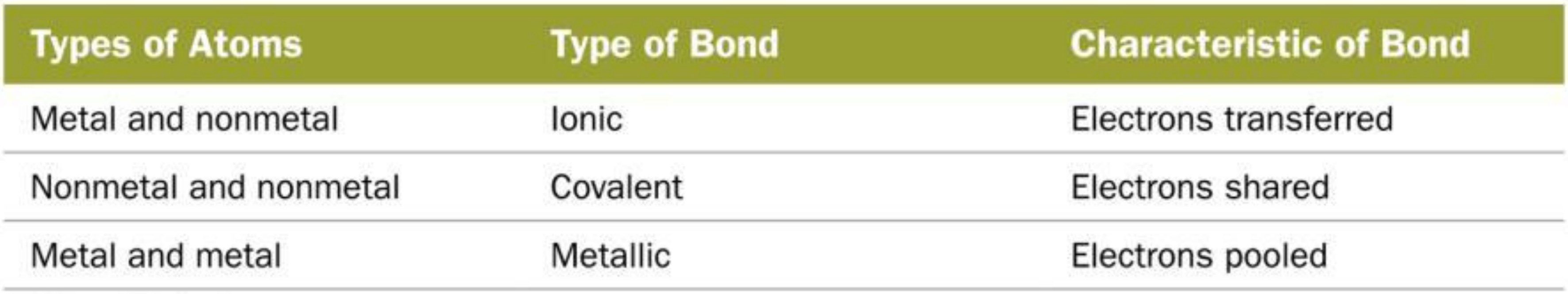
- Chemical bonds form because they lower the potential energy between the charged particles that compose atoms.

- A chemical bond forms when the potential energy of the bonded atoms is less than the potential energy of the separate atoms.

- To calculate this potential energy, you need to consider the following interactions:
  - Nucleus-to-nucleus repulsions
  - Electron-to-electron repulsions
  - Nucleus-to-electron attractions

Types of Bonds

- We can classify bonds based on the



Types of Atoms	Type of Bond	Characteristic of Bond
Metal and nonmetal	Ionic	Electrons transferred
Nonmetal and nonmetal	Covalent	Electrons shared
Metal and metal	Metallic	Electrons pooled

Ionic Bonds

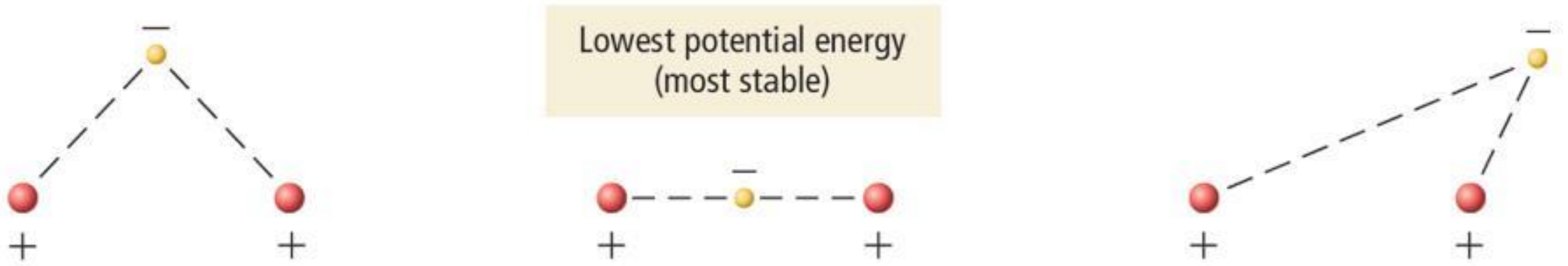
- When a metal atom loses electrons it becomes a **cation**.
  - Metals have low ionization energy, making it *relatively* easy to remove electrons from them.

- When a nonmetal atom gains electrons it becomes an **anion**.
  - Nonmetals have high electron affinities, making it advantageous to add electrons to these atoms.

- The oppositely charged ions are then attracted to each other, resulting in an **ionic bond**.

Covalent Bonds

- Nonmetal atoms have relatively high ionization energies, so it is difficult to remove electrons from them.
- When nonmetals bond together, it is better in terms of potential energy for the atoms to share valence electrons.
  - Potential energy is lowest when the electrons are between the nuclei.
- Shared electrons hold the atoms together by attracting nuclei of both atoms.



Metallic Bonds

- The *relatively* low ionization energy of metals allows them to lose electrons easily.

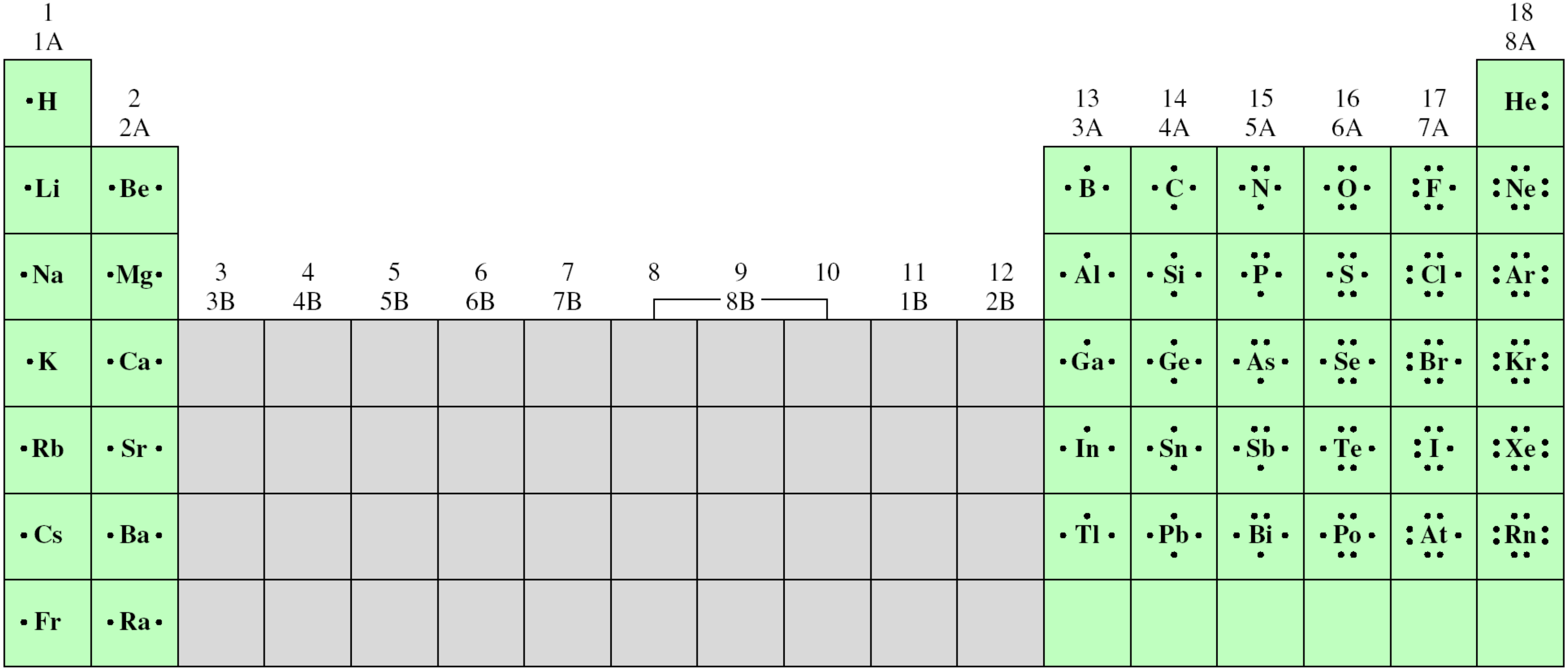
- The simplest theory of metallic bonding involves the metal atoms releasing their valence electrons to be shared as a pool by all the atoms/ions in the metal.
  - An organization of metal cation islands in a sea of electrons
  - Electrons delocalized throughout the metal structure

- Bonding results from attraction of cation for the delocalized electrons.

Valence electrons are the outer shell electrons of an atom. The valence electrons are the electrons that particpate in chemical bonding.

Group	e^- configuration	# of valence e^-
1A	ns^1	1
2A	ns^2	2
3A	ns^2np^1	3
4A	ns^2np^2	4
5A	ns^2np^3	5
6A	ns^2np^4	6
7A	ns^2np^5	7

Lewis Dot Symbols for the Representative Elements & Noble Gases



1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8	9 8B	10	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
$\cdot\mathrm{H}$																	$\mathrm{He}:$
$\cdot\mathrm{Li}$	$\cdot\mathrm{Be}\cdot$											$\cdot\overset{\cdot}{\mathrm{B}}\cdot$	$\cdot\overset{\cdot}{\underset{\cdot}{\mathrm{C}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot}{\mathrm{N}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{O}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{F}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Ne}}}:$
$\cdot\mathrm{Na}$	$\cdot\mathrm{Mg}\cdot$											$\cdot\overset{\cdot}{\mathrm{Al}}\cdot$	$\cdot\overset{\cdot}{\underset{\cdot}{\mathrm{Si}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot}{\mathrm{P}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{S}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Cl}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Ar}}}:$
$\cdot\mathrm{K}$	$\cdot\mathrm{Ca}\cdot$											$\cdot\overset{\cdot}{\mathrm{Ga}}\cdot$	$\cdot\overset{\cdot}{\underset{\cdot}{\mathrm{Ge}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot}{\mathrm{As}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Se}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Br}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Kr}}}:$
$\cdot\mathrm{Rb}$	$\cdot\mathrm{Sr}\cdot$											$\cdot\overset{\cdot}{\mathrm{In}}\cdot$	$\cdot\overset{\cdot}{\underset{\cdot}{\mathrm{Sn}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot}{\mathrm{Sb}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Te}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{I}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Xe}}}:$
$\cdot\mathrm{Cs}$	$\cdot\mathrm{Ba}\cdot$											$\cdot\overset{\cdot}{\mathrm{Tl}}\cdot$	$\cdot\overset{\cdot}{\underset{\cdot}{\mathrm{Pb}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot}{\mathrm{Bi}}}\cdot$	$\cdot\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Po}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{At}}}\cdot$	$:\overset{\cdot\cdot}{\underset{\cdot\cdot}{\mathrm{Rn}}}:$
$\cdot\mathrm{Fr}$	$\cdot\mathrm{Ra}\cdot$																

The Ionic Bond

Ionic bond: *the electrostatic force that holds ions together in an ionic compound.*

$$\cdot\text{Li} \;+\; :\ddot{\underset{\cdot\cdot}{\text{F}}}\cdot \longrightarrow \text{Li}^{+}:\ddot{\underset{\cdot\cdot}{\text{F}}}:^{-}$$

$1s^22s^1$ $1s^22s^22p^5$ [He] $1s^22s^22p^6$ [Ne]

$$\cdot\text{Li} \longrightarrow \text{Li}^{+} + e^{-}$$

$$e^{-} + :\ddot{\underset{\cdot\cdot}{\text{F}}}\cdot \longrightarrow :\ddot{\underset{\cdot\cdot}{\text{F}}}:^{-}$$

$$\text{Li}^{+} + :\ddot{\underset{\cdot\cdot}{\text{F}}}:^{-} \longrightarrow \text{Li}^{+}:\ddot{\underset{\cdot\cdot}{\text{F}}}:^{-}$$

Quantitative: định lượng
(có number)

Qualitative: định tính
(này cao hơn kia, nay lạnh quá)

Electrostatic (Lattice) Energy

Lattice energy (U) is the energy required to completely separate one mole of a solid ionic compound into gaseous ions.

$$E = k\frac{Q_+ Q_-}{r}$$

E is the potential energy

Q_+ is the charge on the cation

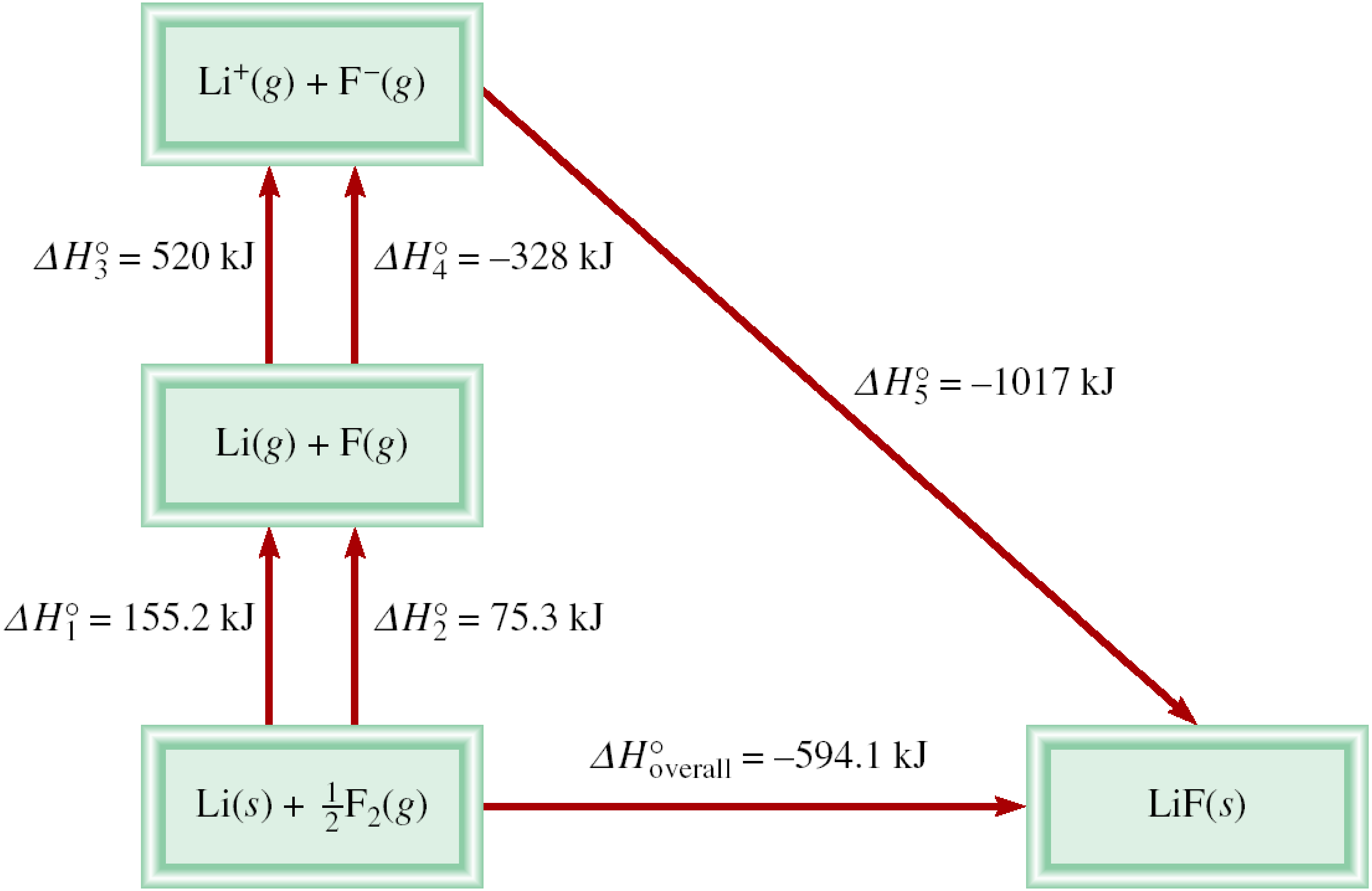
Q_- is the charge on the anion

r is the distance between the ions

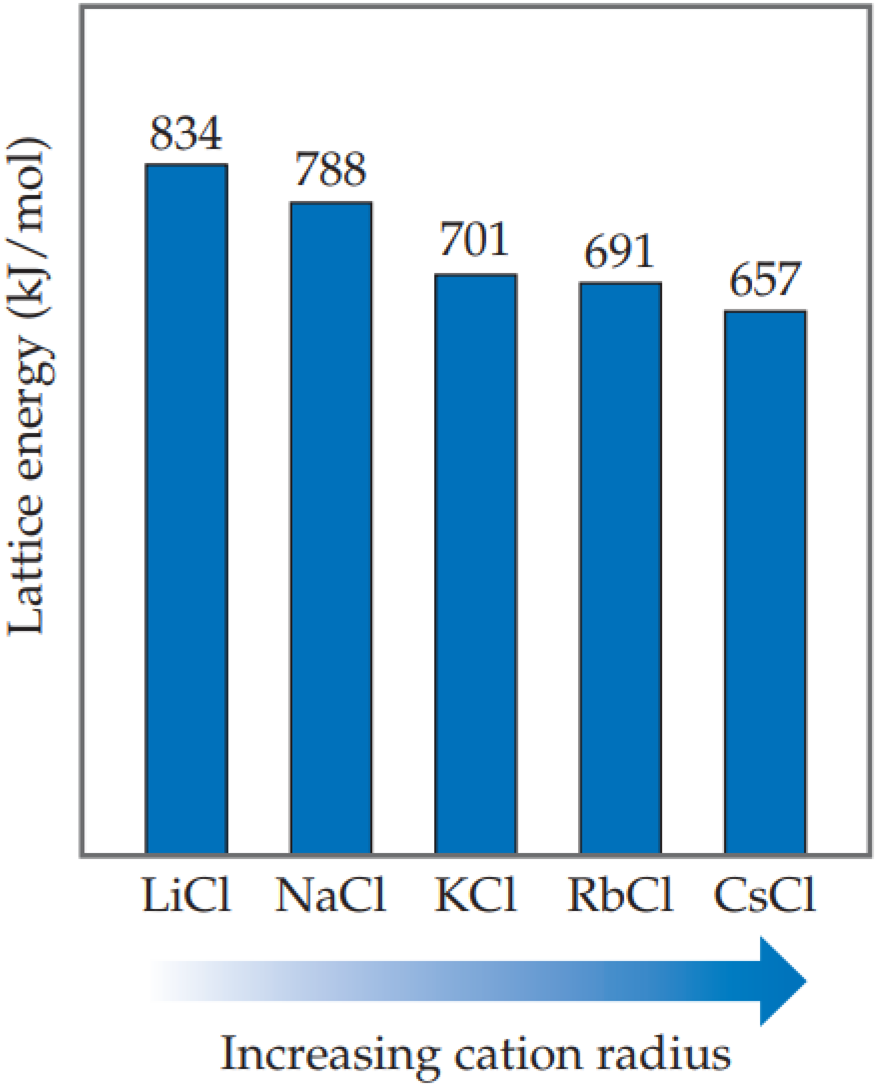
Compound	Lattice Energy (kJ/mol)	
MgF_2	2957	Q: +2,-1
MgO	3938	Q: +2,-2
LiF	1036	$r\ F^- < r\ Cl^-$
LiCl	853	

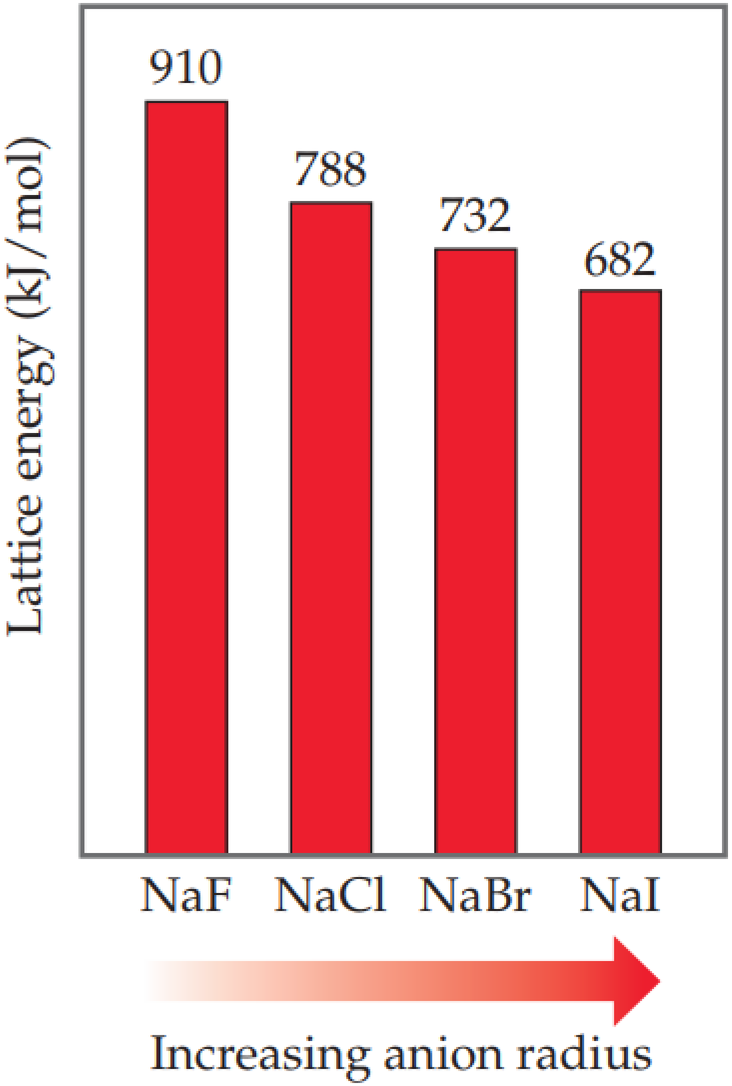
Lattice energy increases as ***Q increases*** and/or as ***r decreases***.

Born-Haber Cycle for Determining Lattice Energy



$$\Delta H^o_{overall} = \Delta H^o_1 + \Delta H^o_2 + \Delta H^o_3 + \Delta H^o_4 + \Delta H^o_5$$


Lattice energy (kJ/mol)
834
788
701
691
657
LiCl
NaCl
KCl
RbCl
CsCl
Increasing cation radius


Lattice energy (kJ/mol)
910
788
732
682
NaF
NaCl
NaBr
NaI
Increasing anion radius

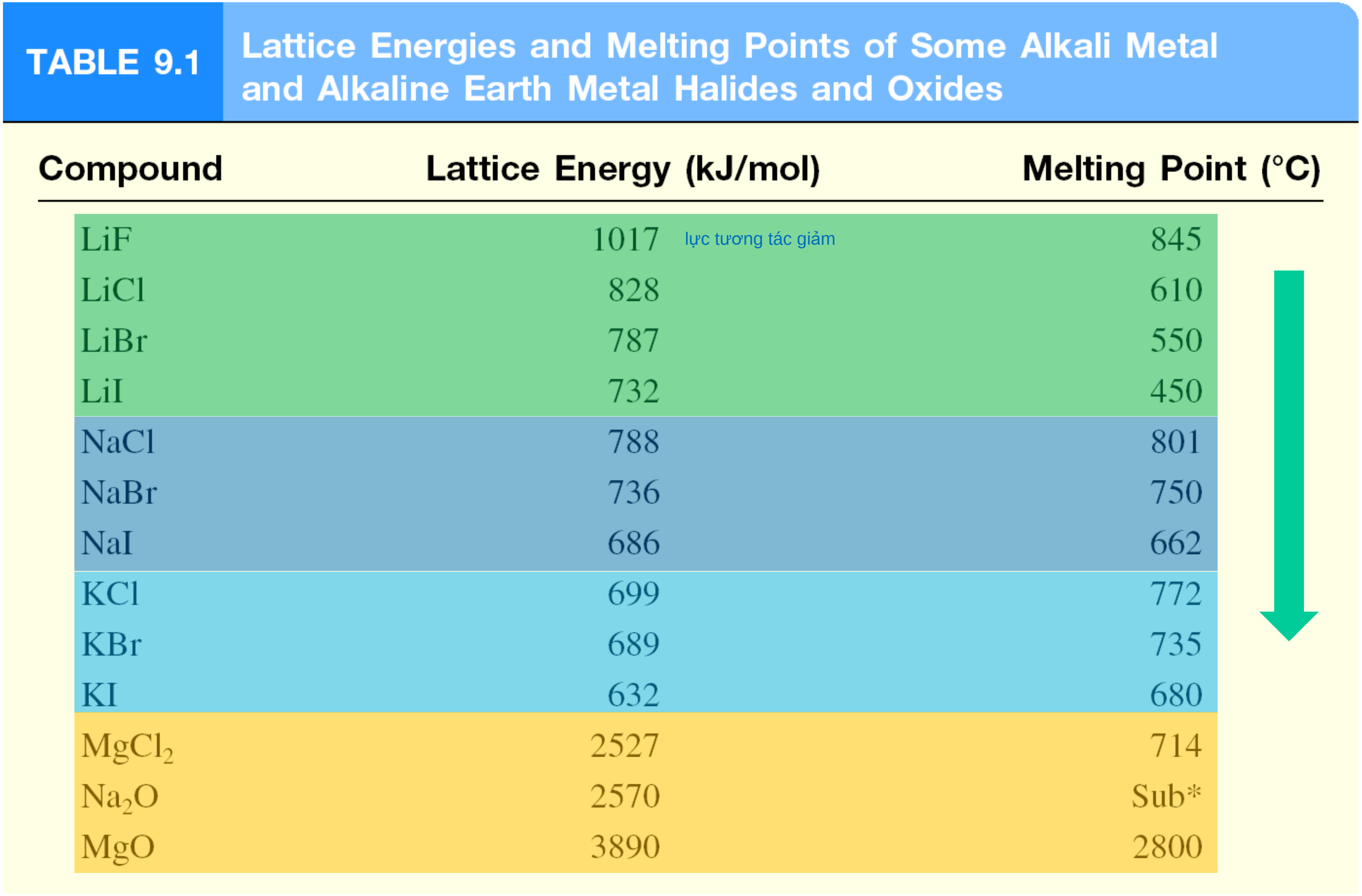


TABLE 9.1 Lattice Energies and Melting Points of Some Alkali Metal and Alkaline Earth Metal Halides and Oxides

Compound	Lattice Energy (kJ/mol)	Melting Point (°C)
LiF	1017	845
LiCl	828	610
LiBr	787	550
LiI	732	450
NaCl	788	801
NaBr	736	750
NaI	686	662
KCl	699	772
KBr	689	735
KI	632	680
$MgCl_2$	2527	714
Na_2O	2570	Sub*
MgO	3890	2800

lực tương tác giảm

*Na_2O sublimes at 1275°C.

Chemistry In Action:

Sodium Chloride: A Common and Important Compound

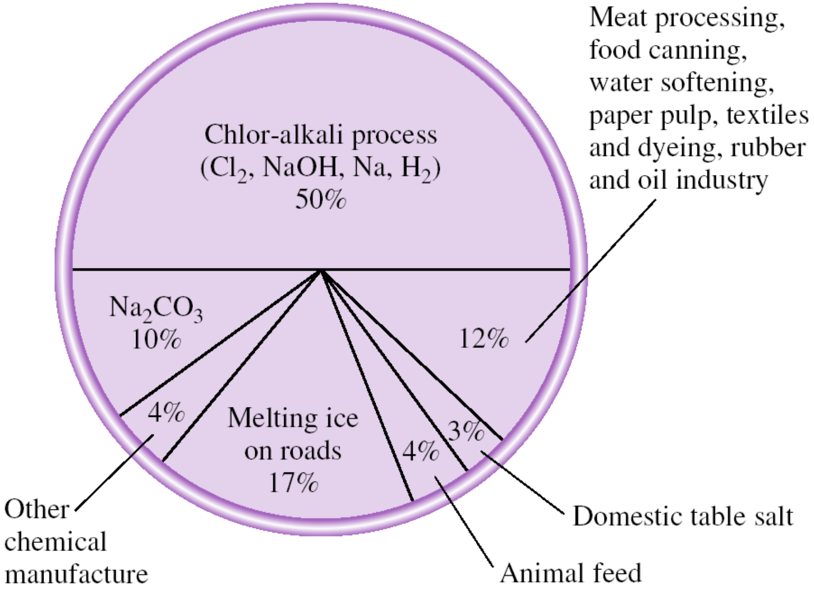
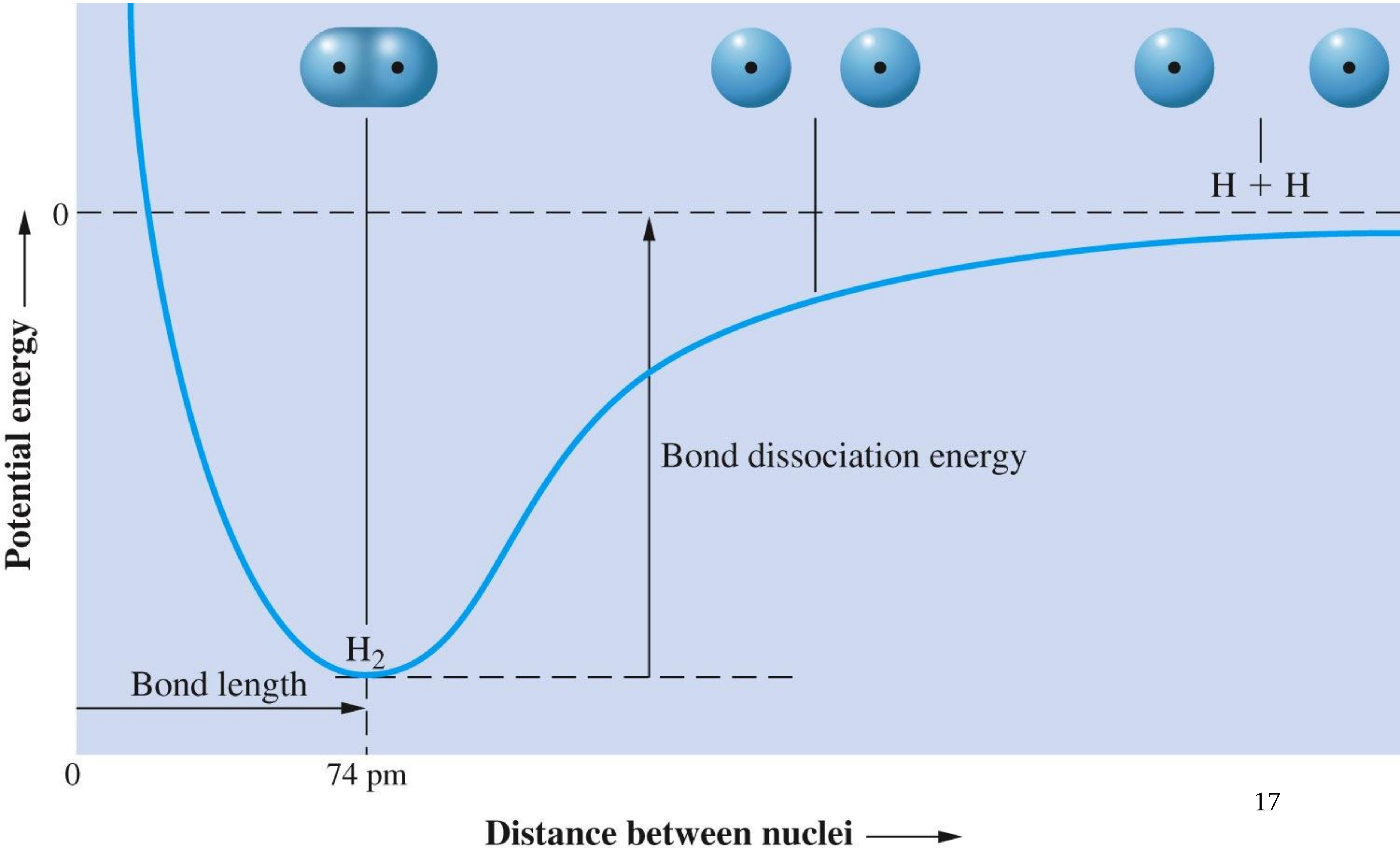


table salt

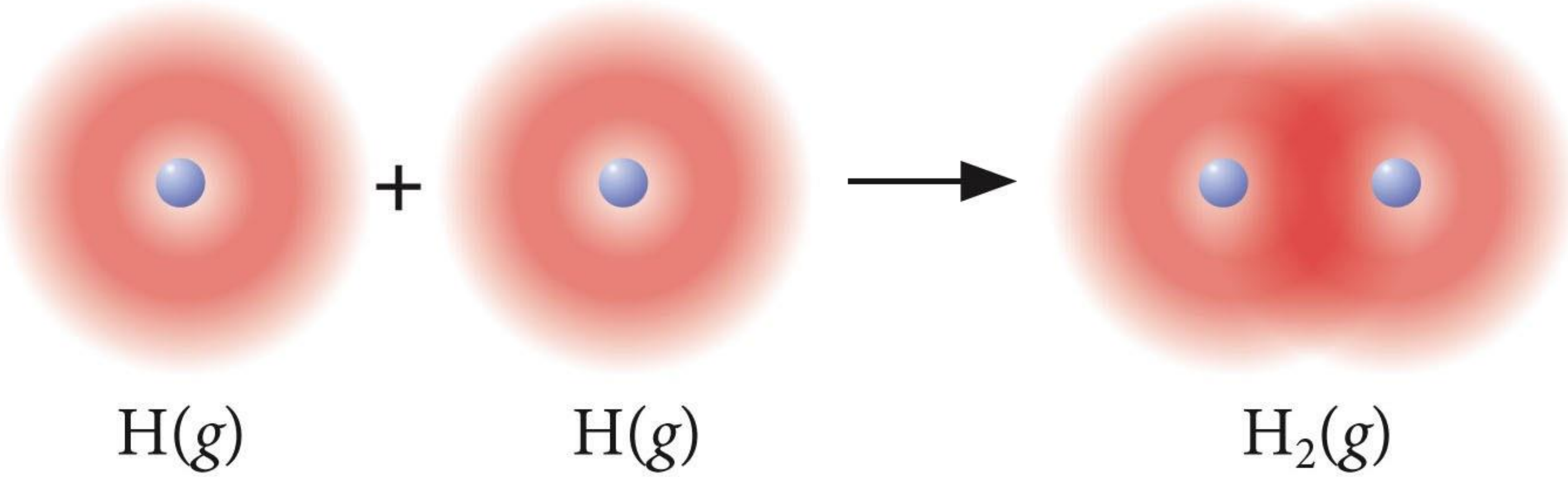
Mining Salt

Solar Evaporation for Salt

A ***covalent bond*** is a chemical bond in which two or more electrons are shared by two atoms.

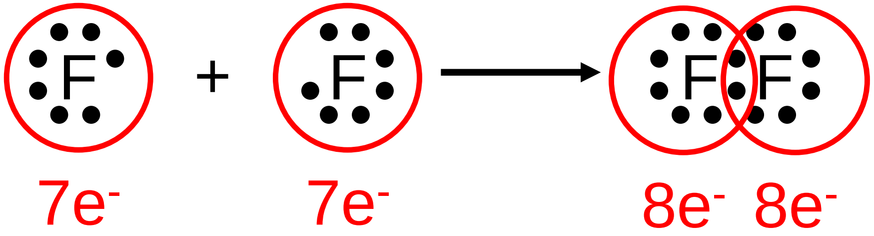


As the hydrogen atoms move closer together, the electron of each atom is attracted to both its own nucleus and the nucleus of the second atom. The electron probability distribution illustrates this relationship.

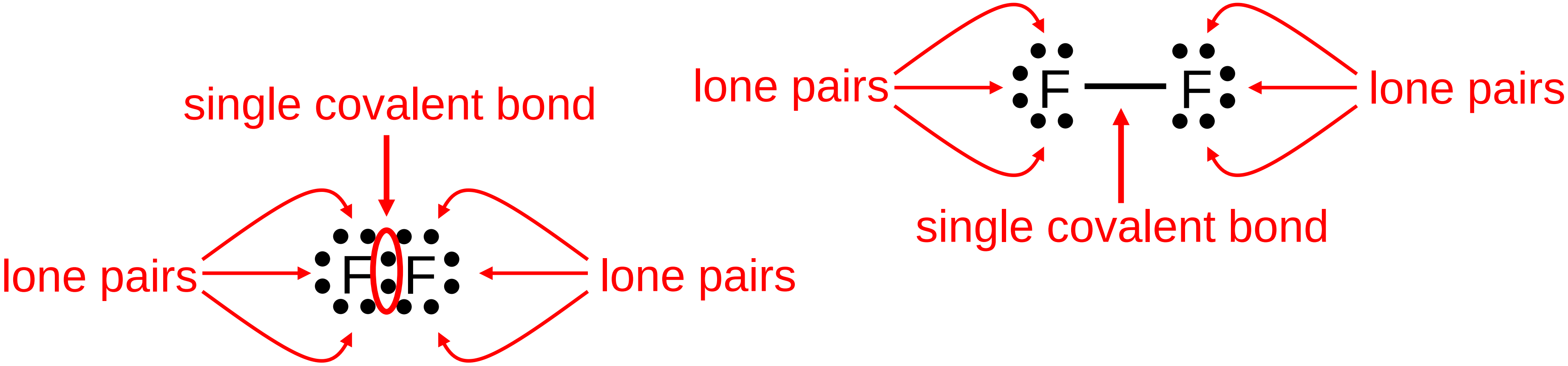


A ***covalent bond*** is a chemical bond in which two or more electrons are shared by two atoms.

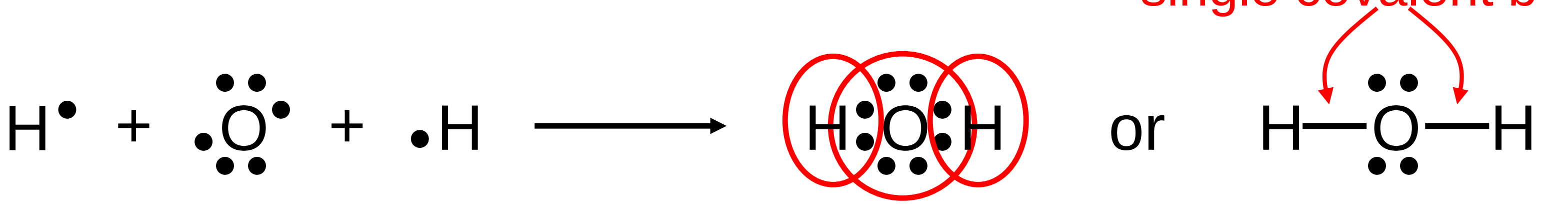
Why should two atoms share electrons?



Lewis structure of F_2



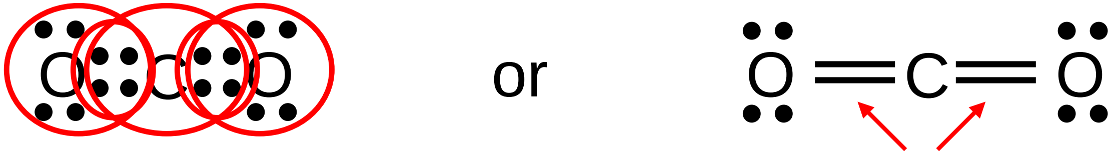
Lewis structure of water



single covalent bonds

$2e^-$ $8e^-$ $2e^-$

Double bond – two atoms share two pairs of electrons

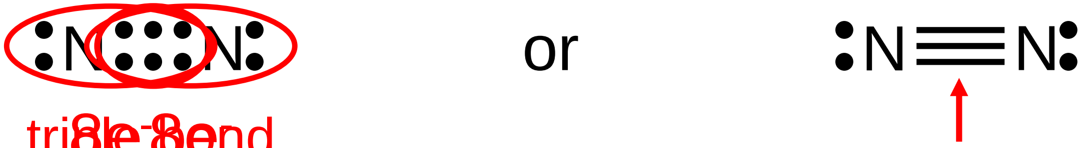


$8e^-$ $8e^-$ $8e^-$

double bonds

double bonds

Triple bond – two atoms share three pairs of electrons

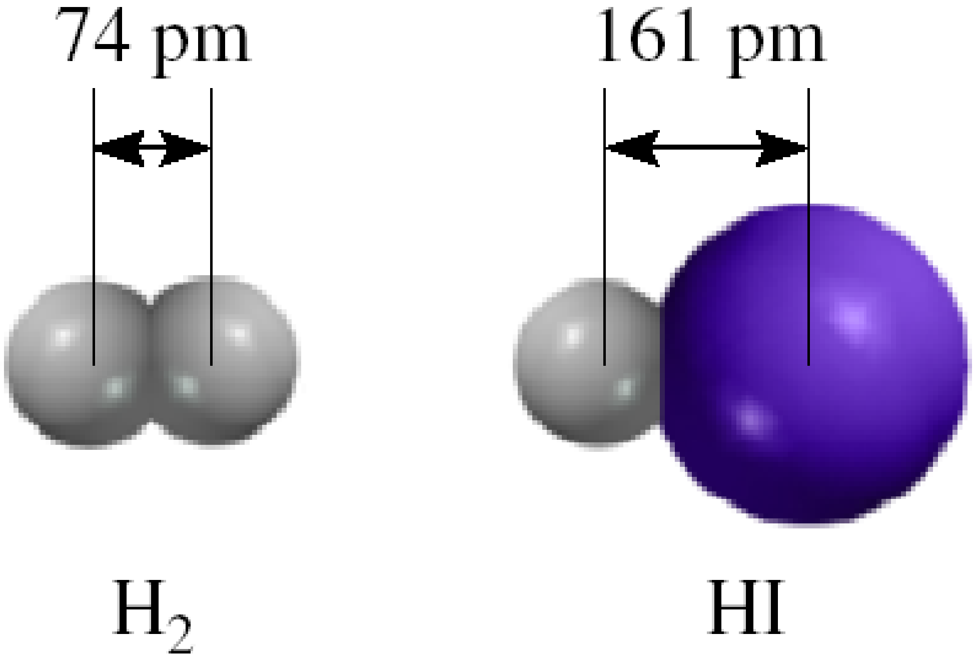


$8e^-$ $8e^-$

triple bond

triple bond

Lengths of Covalent Bonds



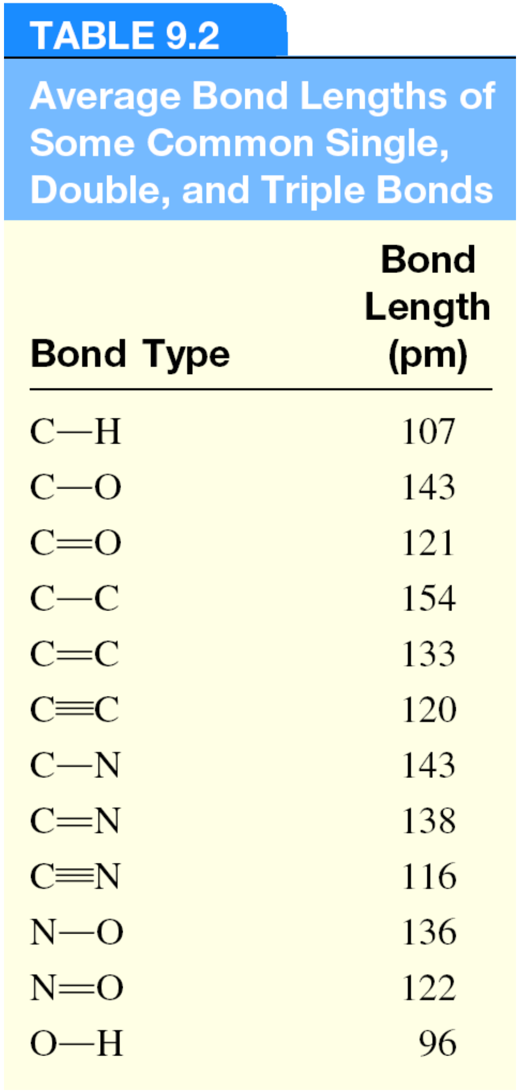


TABLE 9.2

Average Bond Lengths of Some Common Single, Double, and Triple Bonds

Bond Type	Bond Length (pm)
C—H	107
C—O	143
C=O	121
C—C	154
C=C	133
C≡C	120
C—N	143
C=N	138
C≡N	116
N—O	136
N=O	122
O—H	96

Bond Lengths

Triple bond < Double Bond < Single Bond

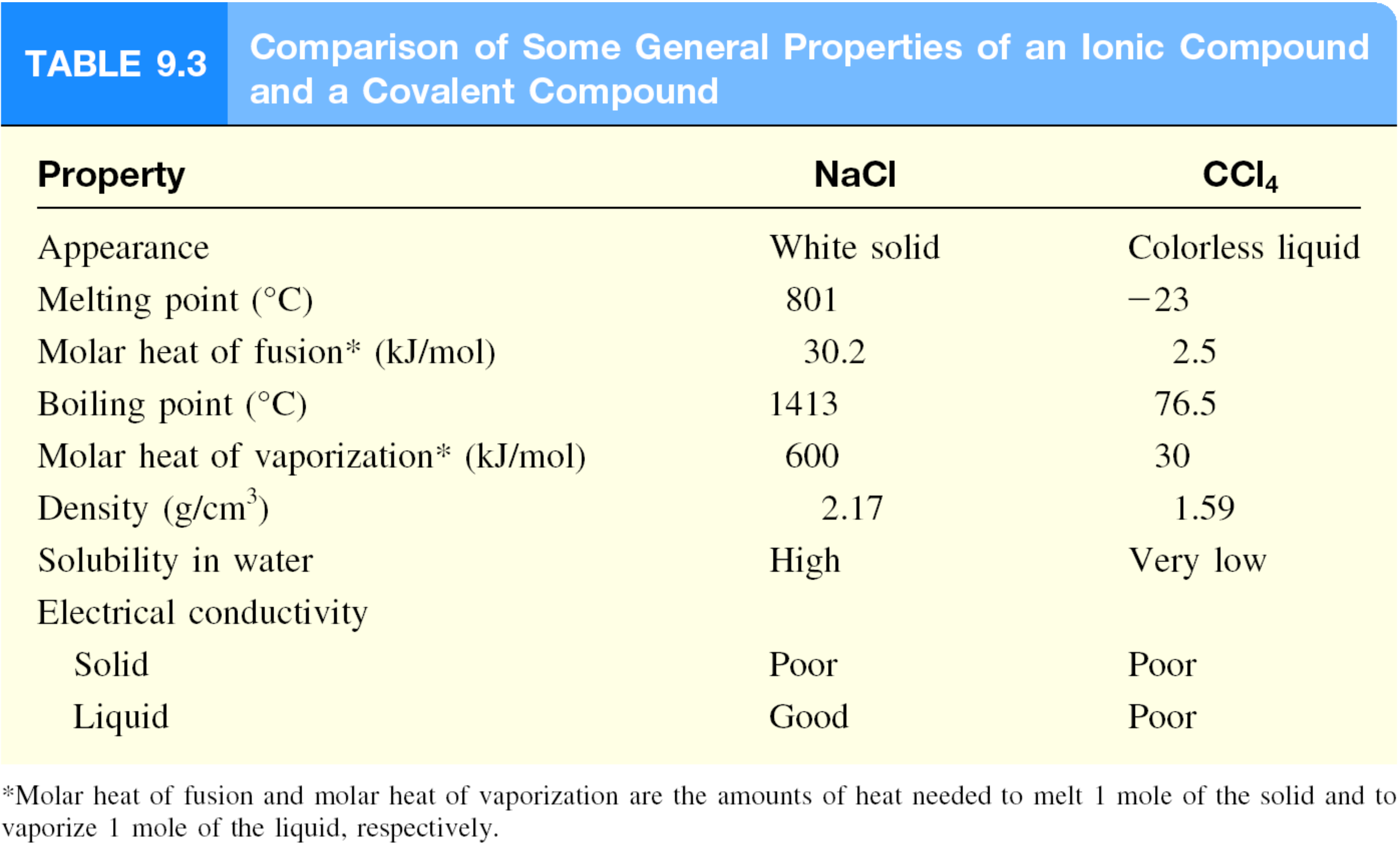
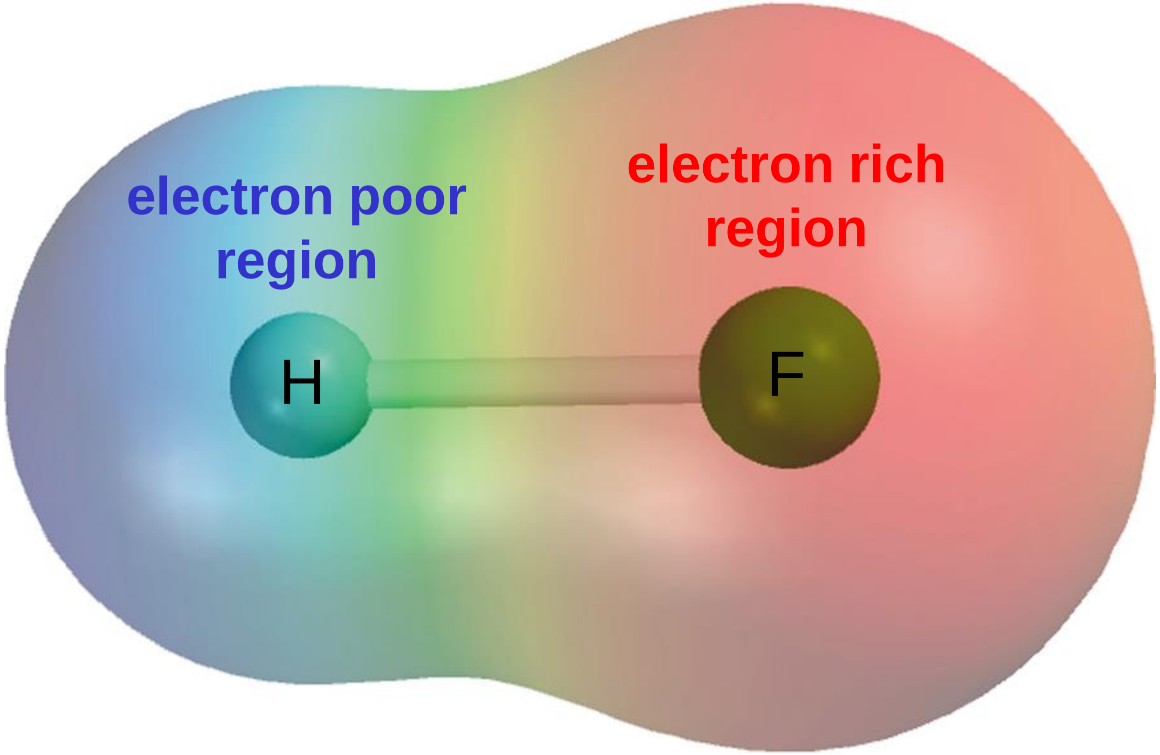


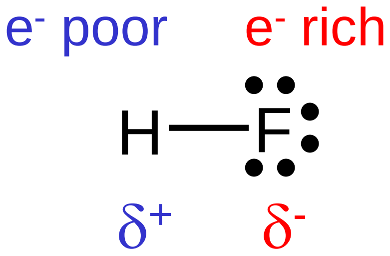
TABLE 9.3 **Comparison of Some General Properties of an Ionic Compound and a Covalent Compound**

Property	NaCl	CCl_4
Appearance	White solid	Colorless liquid
Melting point (°C)	801	−23
Molar heat of fusion* (kJ/mol)	30.2	2.5
Boiling point (°C)	1413	76.5
Molar heat of vaporization* (kJ/mol)	600	30
Density (g/cm^3)	2.17	1.59
Solubility in water	High	Very low
Electrical conductivity		
Solid	Poor	Poor
Liquid	Good	Poor

*Molar heat of fusion and molar heat of vaporization are the amounts of heat needed to melt 1 mole of the solid and to vaporize 1 mole of the liquid, respectively.

Polar covalent bond or ***polar bond*** is a covalent bond with greater electron density around one of the two atoms





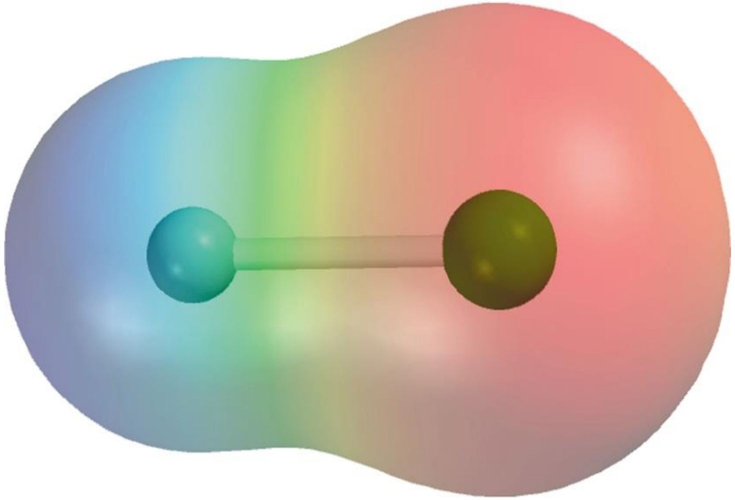
Electronegativity is the ability of an atom to attract toward itself the electrons in a chemical bond.

độ âm điện

Electron Affinity - measurable, Cl is highest

$$X_{(g)} + e^- \longrightarrow X^-_{(g)}$$

Electronegativity - relative, F is highest



Electronegativity: Linus Pauling Scale (1932)

$$\chi_A - \chi_B = (\mathrm{eV})^{-1/2}\sqrt{\mathrm{E_d(AB)} - [\mathrm{E_d(AA)} + \mathrm{E_d(BB)}]/2}$$

$\chi_A - \chi_B$: electronegativity difference between to elements

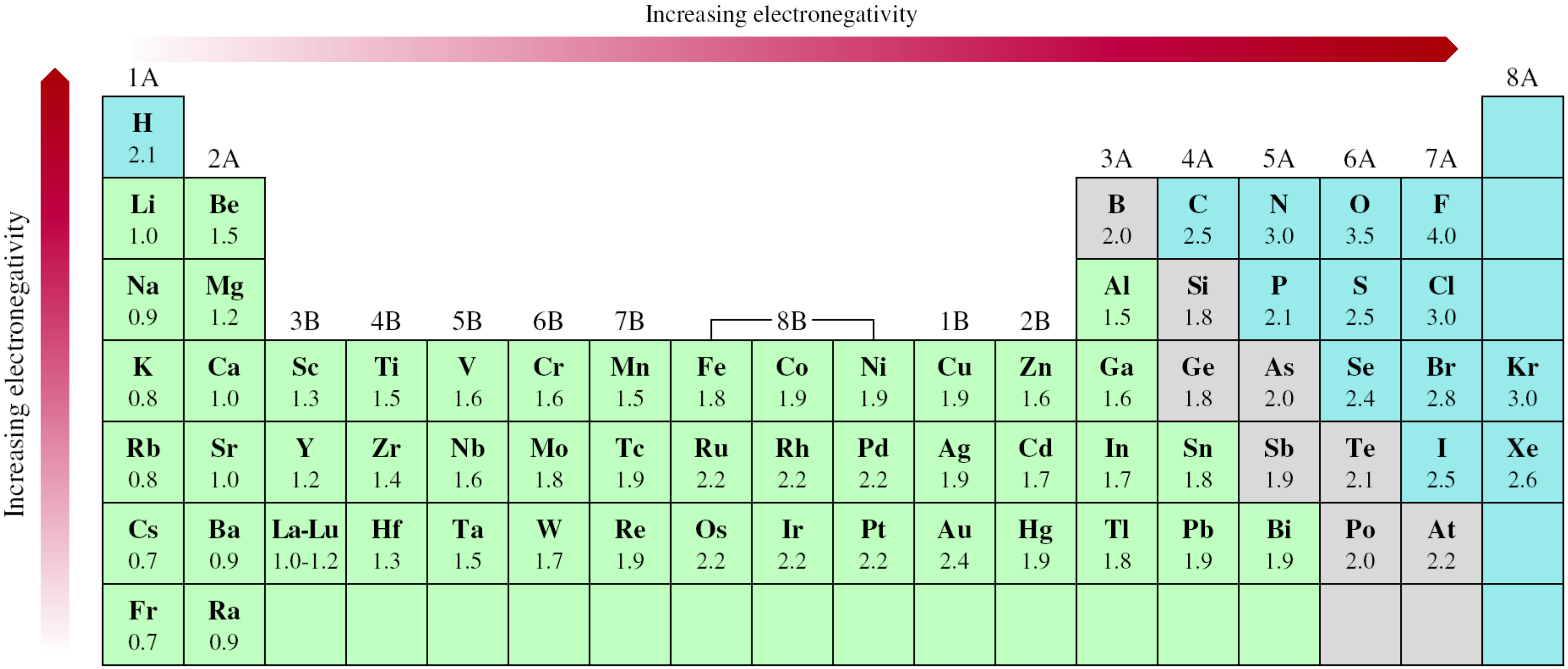
E_d: dissociation energy, electronvolts

$\chi_F - \chi_H$ between hydrogen and bromine is 0.73 (dissociation energies: H–Br, 3.79 eV; H–H, 4.52 eV; Br–Br 2.00 eV)

H as an arbitrary reference point, as it forms covalent bonds with a large variety of elements: its electronegativity was set at 2.1.

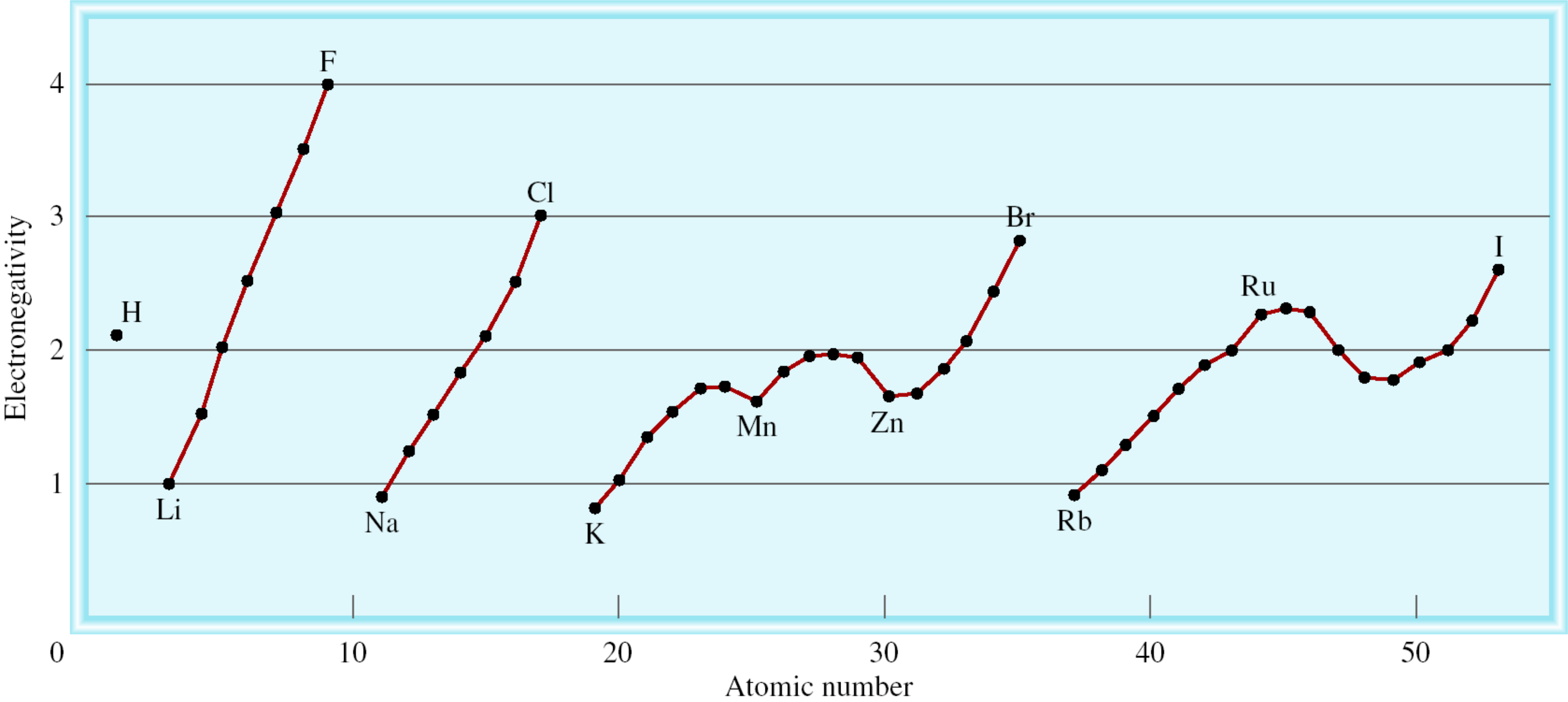
$$\chi_{\mathrm{Br}} - 2.1 = 0.73, \chi_{\mathrm{Br}} = 2.83$$

The Electronegativities of Common Elements

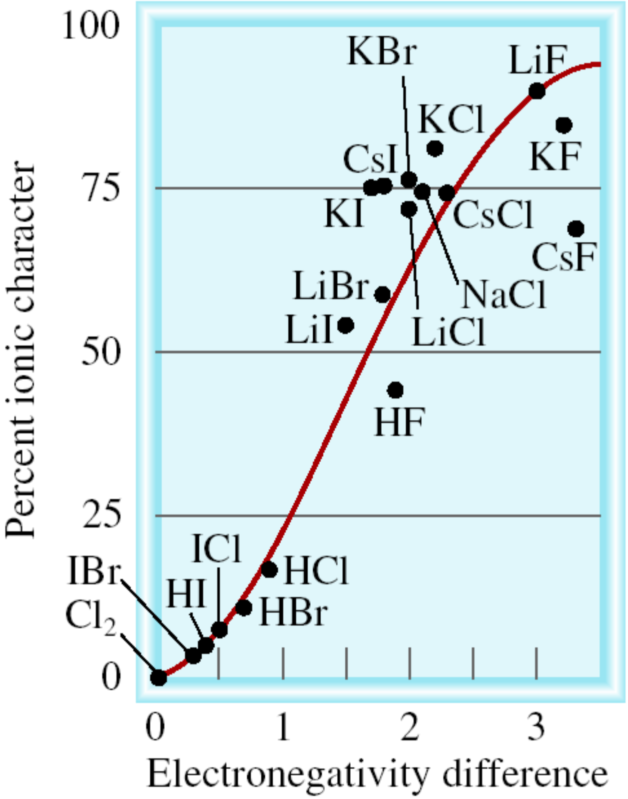


1A	2A	3B	4B	5B	6B	7B	8B			1B	2B	3A	4A	5A	6A	7A	8A
H 2.1																	
Li 1.0	**Be** 1.5											**B** 2.0	**C** 2.5	**N** 3.0	**O** 3.5	**F** 4.0	
Na 0.9	**Mg** 1.2											**Al** 1.5	**Si** 1.8	**P** 2.1	**S** 2.5	**Cl** 3.0	
K 0.8	**Ca** 1.0	**Sc** 1.3	**Ti** 1.5	**V** 1.6	**Cr** 1.6	**Mn** 1.5	**Fe** 1.8	**Co** 1.9	**Ni** 1.9	**Cu** 1.9	**Zn** 1.6	**Ga** 1.6	**Ge** 1.8	**As** 2.0	**Se** 2.4	**Br** 2.8	**Kr** 3.0
Rb 0.8	**Sr** 1.0	**Y** 1.2	**Zr** 1.4	**Nb** 1.6	**Mo** 1.8	**Tc** 1.9	**Ru** 2.2	**Rh** 2.2	**Pd** 2.2	**Ag** 1.9	**Cd** 1.7	**In** 1.7	**Sn** 1.8	**Sb** 1.9	**Te** 2.1	**I** 2.5	**Xe** 2.6
Cs 0.7	**Ba** 0.9	**La-Lu** 1.0-1.2	**Hf** 1.3	**Ta** 1.5	**W** 1.7	**Re** 1.9	**Os** 2.2	**Ir** 2.2	**Pt** 2.2	**Au** 2.4	**Hg** 1.9	**Tl** 1.8	**Pb** 1.9	**Bi** 1.9	**Po** 2.0	**At** 2.2	
Fr 0.7	**Ra** 0.9																

Variation of Electronegativity with Atomic Number



Classification of bonds by difference in electronegativity



Difference	Bond Type
0	Covalent
≥ 2	Ionic
0 < and <2	Polar Covalent

Increasing difference in electronegativity →

Covalent → Polar Covalent → Ionic

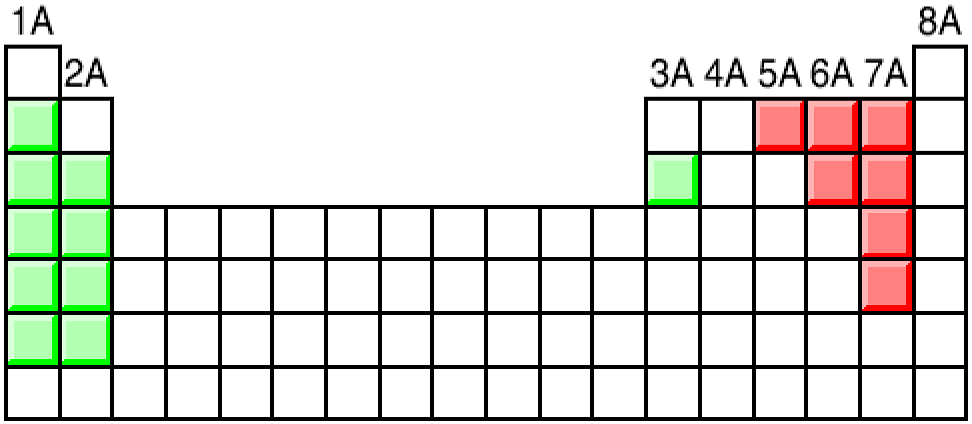
share e^-

partial transfer of e^-

transfer e^-

Classify the following bonds as ionic, polar covalent, or covalent: The bond in CsCl; the bond in H_2S; and the NN bond in H_2NNH_2.

Cs – 0.7	Cl – 3.0	3.0 – 0.7 = 2.3	Ionic
H – 2.1	S – 2.5	2.5 – 2.1 = 0.4	Polar Covalent
N – 3.0	N – 3.0	3.0 – 3.0 = 0	Covalent



Writing Lewis Structures

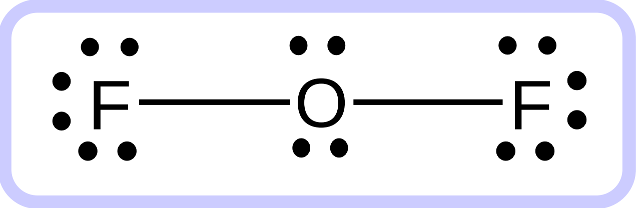
1. Write the correct skeletal structure for the molecule.
    - Hydrogen atoms are always terminal.
    - The more electronegative atoms are placed in terminal positions.
2. Calculate the total number of electrons for the Lewis structure by summing the valence electrons of each atom in the molecule.
3. Distribute the electrons among the atoms, giving octets (or duets in the case of hydrogen) to as many atoms as possible.
4. If any atoms lack an octet, form double or triple bonds as necessary to give them octets.

Write the electron dot formulas for the following:

- a. OF_2
- b. NF_3
- c. NH_2OH, hydroxylamine

Count the valence electrons in OF_2**:**

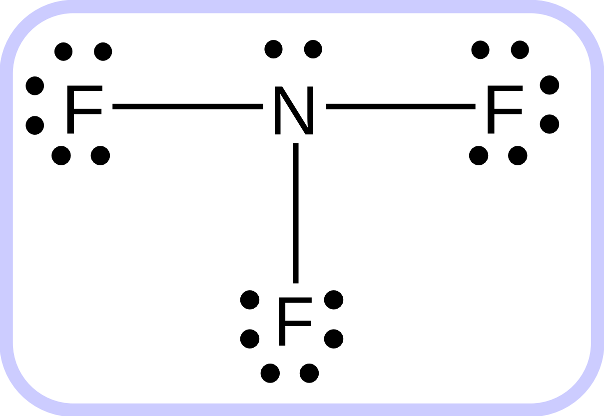
O	1(6)
F	2(7)
	20 valence electrons



O is the central atom (it is less electronegative). Now, we distribute the remaining 16 electrons, beginning with the outer atoms. The last four electrons go on O.

Count the valence electrons in NF_3:

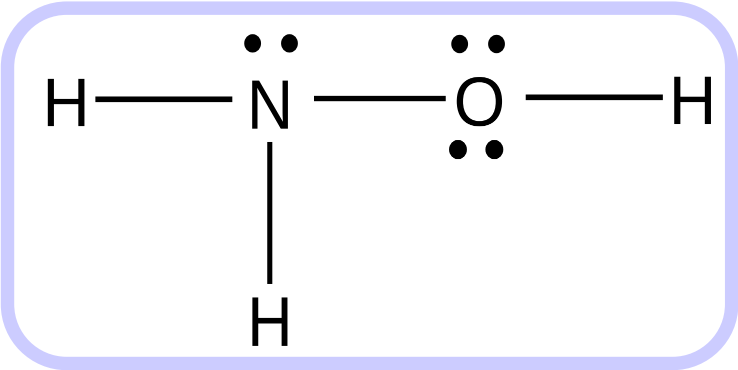
N	1(5)
F	<u>3(7)</u>
	26 valence electrons



N is the central atom (it is less electronegative). Now, we distribute the remaining 20 electrons, beginning with the outer atoms. The last two electrons go on N.

Count the electrons in NH_2OH:

N	1(5)
H	3(1)
O	1(6)
	14 valence electrons



N is the central atom. Now, we distribute the remaining six electrons, beginning with the outer atoms. The last two electrons go on N.

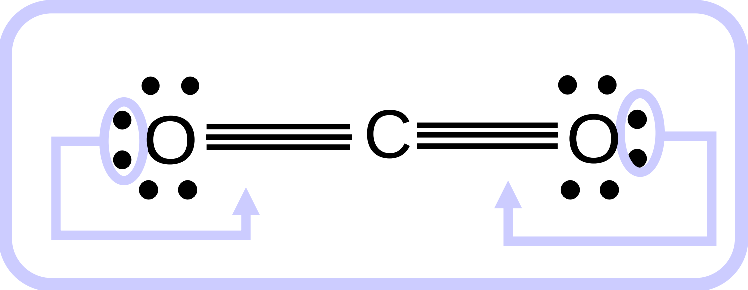
Write electron-dot formulas for the following:

a. CO_2

b. HCN

Count the electrons in CO_2:

C	1(4)
O	<u>2(6)</u>
	16 valence electrons

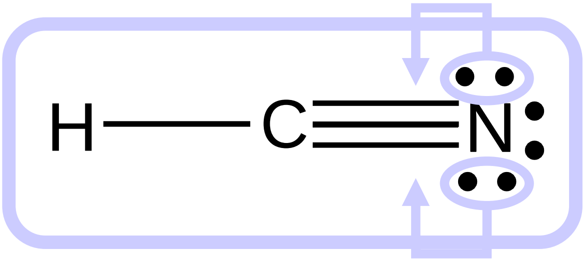


C is the central atom. Now, we distribute the remaining 12 electrons, beginning with the outer atoms.

Carbon does not have an octet, so two of the lone pairs shift to become a bonding pair, forming double bonds.

Count the electrons in HCN:

H	1(1)
C	1(4)
N	1(5)
	10 valence electrons



C is the central atom. The remaining electrons go on N.

Carbon does not have an octet, so two of the lone pairs shift to become a bonding pair, forming a triple bond.

Phosphorus pentachloride exists in solid state as the ionic compound $[PCl_4]^+[PCl_6]^-$; it exists in the gas phase as the PCl_5 molecule. Write the Lewis formula of the PCl_4^+ ion.

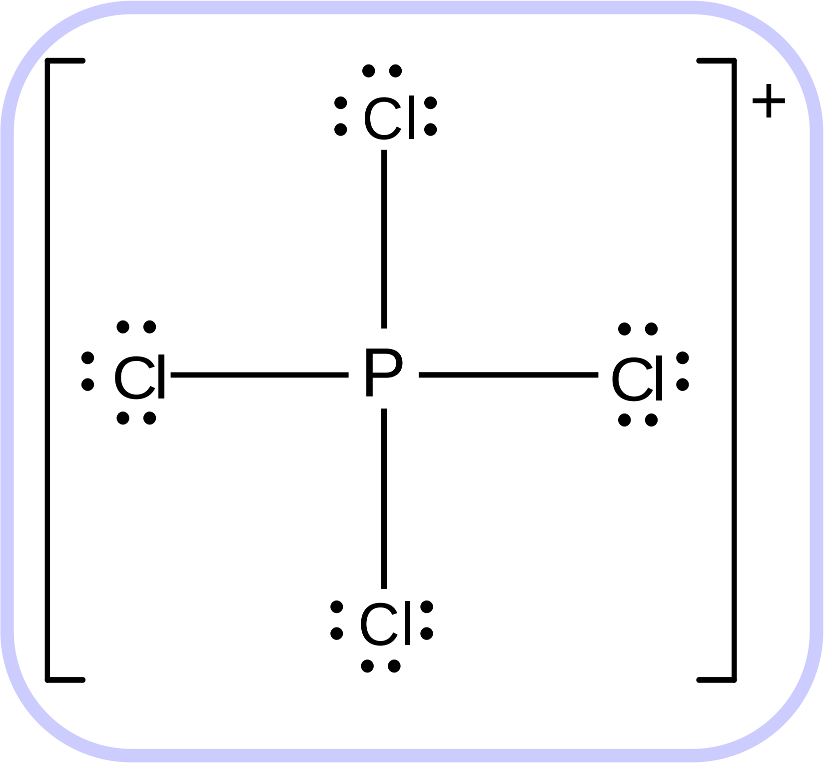
Count the valence electrons in PCl_4^+:

P 1(5)

Cl 4(7)

$\underline{-1}$

32 valence electrons



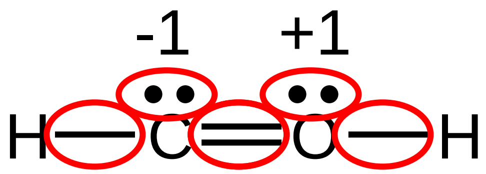
P is the central atom. The remaining 24 nonbonding electrons are placed on Cl atoms. Add square brackets with the charge around the ion.

Two possible skeletal structures of formaldehyde (CH_2O)

An atom's ***formal charge*** is the difference between the number of valence electrons in an isolated atom and the number of electrons assigned to that atom in a Lewis structure.

$$\text{formal charge on an atom in a Lewis structure} = \text{total number of valence electrons in the free atom} - \text{total number of nonbonding electrons} - \frac{1}{2}\left(\text{total number of bonding electrons}\right)$$

The sum of the formal charges of the atoms in a molecule or ion must equal the charge on the molecule or ion.



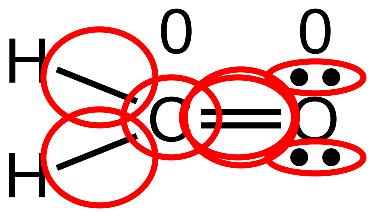
C – 4 e^-
O – 6 e^-
2H – 2x1 e^-
12 e^-

2 single bonds (2x2) = 4
1 double bond = 4
2 lone pairs (2x2) = 4
Total = 12

$$\text{formal charge on an atom in a Lewis structure} = \text{total number of valence electrons in the free atom} - \text{total number of nonbonding electrons} - \frac{1}{2}\left(\text{total number of bonding electrons}\right)$$

formal charge on C = 4 -2 -½ x 6 = -1

formal charge on O = 6 -2 -½ x 6 = +1



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12 e^-

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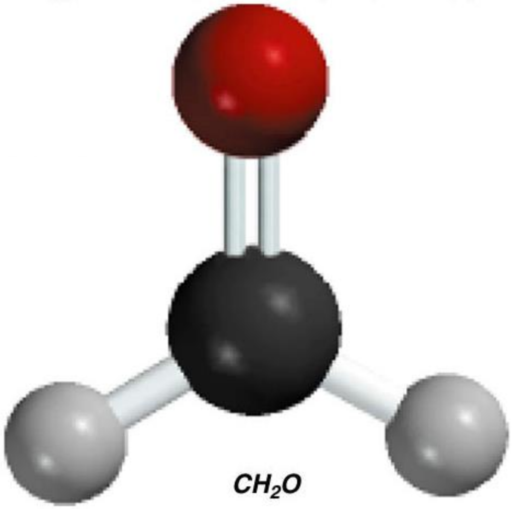
$$\text{formal charge on an atom in a Lewis structure} = \text{total number of valence electrons in the free atom} - \text{total number of nonbonding electrons} - \frac{1}{2}\left(\text{total number of bonding electrons}\right)$$

formal charge on C $= 4 - 0 - ½ \times 8 = 0$

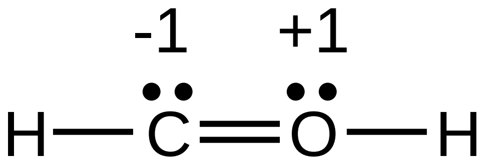
formal charge on O $= 6 - 4 - ½ \times 4 = 0$

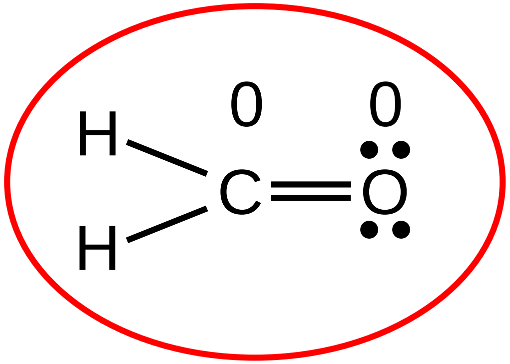


Formal Charge and Lewis Structures

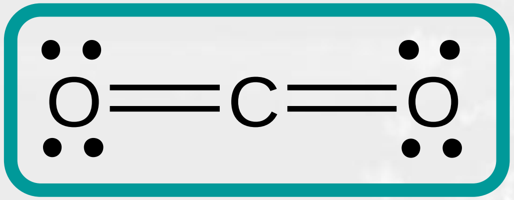
1. For neutral molecules, a Lewis structure in which there are no formal charges is preferable to one in which formal charges are present.
2. Lewis structures with large formal charges are less plausible than those with small formal charges.
3. Among Lewis structures having similar distributions of formal charges, the most plausible structure is the one in which negative formal charges are placed on the more electronegative atoms.

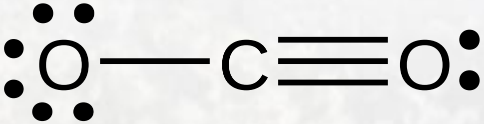
Which is the most likely Lewis structure for CH_2O?





Compare the formal charges for the following electron-dot formulas of CO_2.





Formal charge = group number – (number of bond pairs) – (number of nonbonding electrons)

For the left structure:

C: $4 - 4 - 0 = 0$

O: $6 - 2 - 4 = 0$

For the right structure:

C: $4 - 4 - 0 = 0$

O: $6 - 1 - 6 = -1$

O: $6 - 3 - 2 = +1$

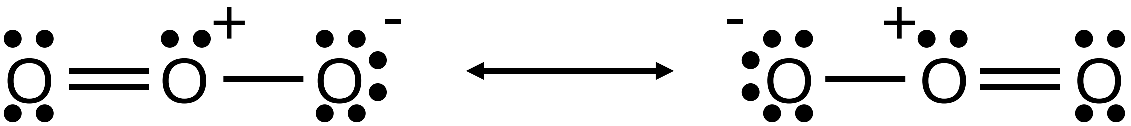
The left structure is better.

Resonance structure

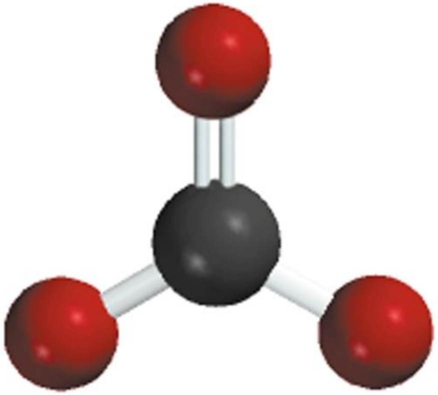
Delocalized bonding is a type of bonding in which a bonding pair of electrons is spread over a number of atoms rather than being localized between two atoms.

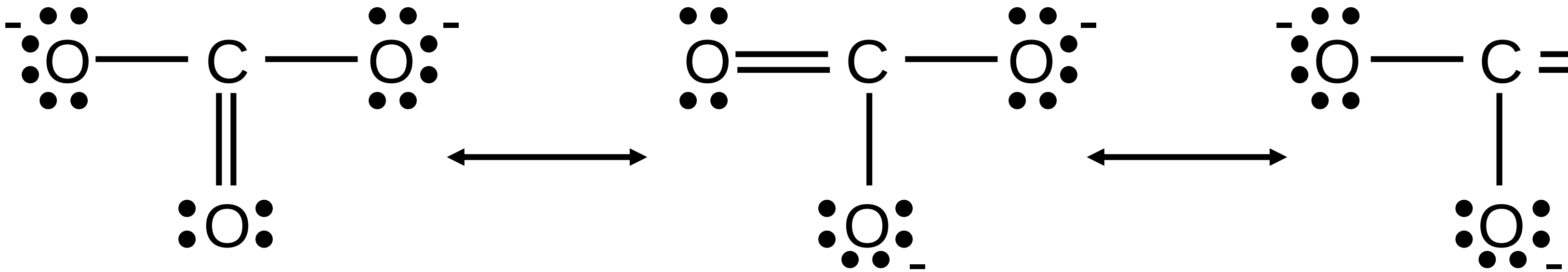
A single electron-dot diagram cannot properly describe delocalized bonding. Using the resonance description, the electron structure of a molecule or ion having delocalized bonding is given by writing all possible electron-dot formulas. They are connected with a double-headed arrow.

A ***resonance structure*** is one of two or more Lewis structures for a single molecule that cannot be represented accurately by only one Lewis structure.



What are the resonance structures of the carbonate (CO_3^{2-}) ion?





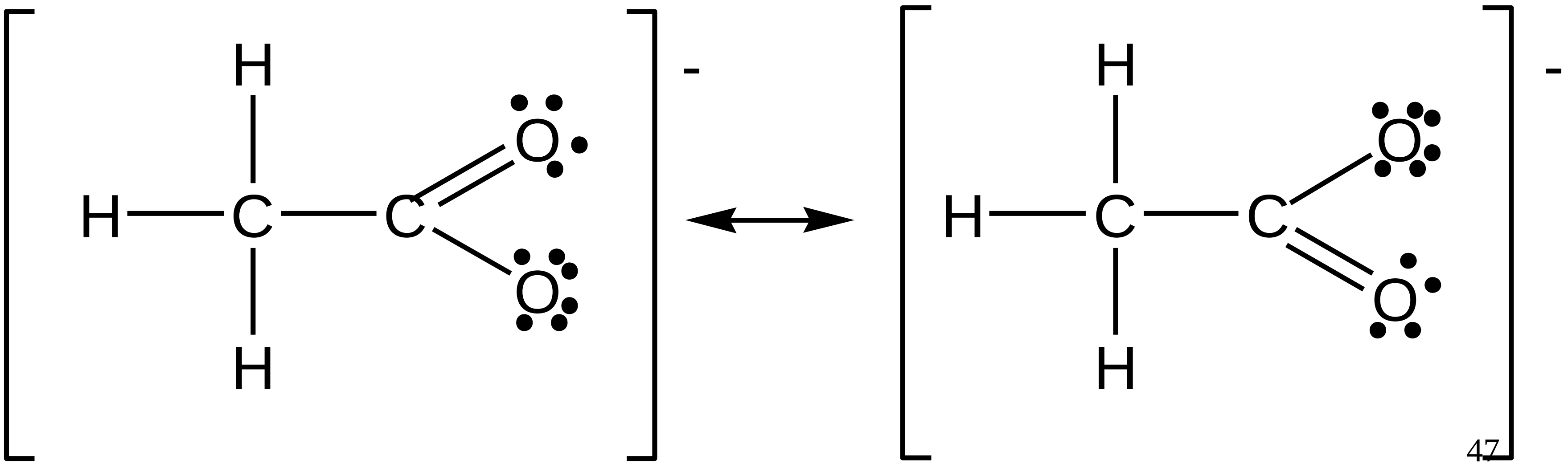
CH_3COO^-

Valence electrons: 2(4) + 3(1) + 2(6) + 1 = 24

C is the central atom.

A double bond is needed between C—O.

There are two equivalent places for it, so two resonance structures are required.

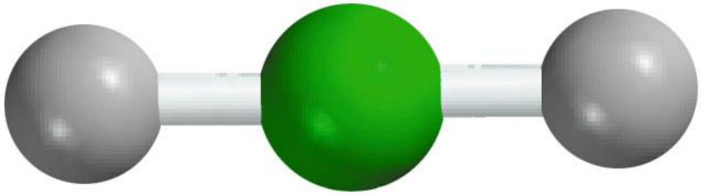


Exceptions to the Octet Rule

The Incomplete Octet

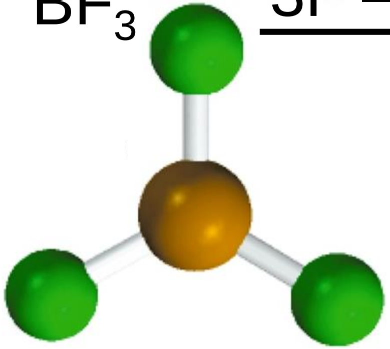
BeH_2

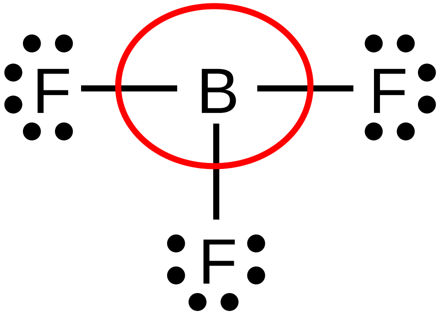
Be – $2e^-$
2H – $2x1e^-$
$4e^-$



BF_3

B – $3e^-$
3F – $3x7e^-$
$24e^-$





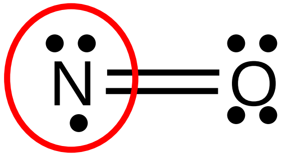
3 single bonds (3x2) = 6
9 lone pairs (9x2) = 18
Total = 24

Exceptions to the Octet Rule

Odd-Electron Molecules

NO

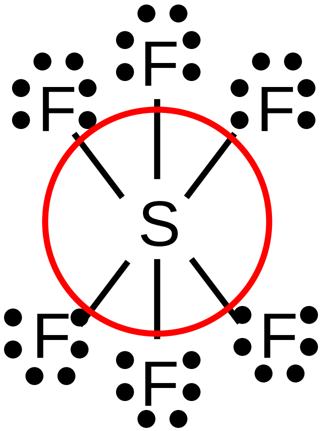
N – 5e$^-$
O – 6e$^-$
11e$^-$



The Expanded Octet (central atom with principal quantum number n > 2)

SF_6

S – 6e$^-$
6F – 42e$^-$
48e$^-$

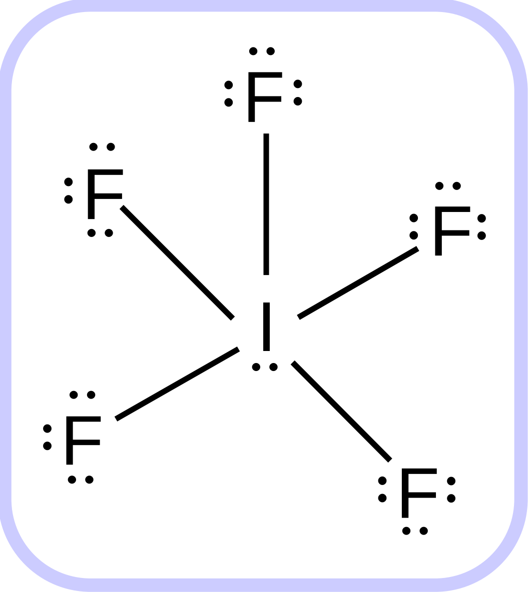


6 single bonds (6x2) = 12
18 lone pairs (18x2) = 36
Total = 48

Exceptions to the Octet Rule

Count the valence electrons in IF_5:

I	1(7)
F	5(7)
	42 valence electrons



I is the central atom. Thirty-two electrons remain; they first complete F octets. The remaining electrons go on I.

The enthalpy change required to break a particular bond in one mole of gaseous molecules is the ***bond enthalpy***.

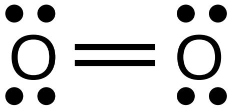
Bond Enthalpy

$H_{2\,(g)} \longrightarrow H_{(g)} + H_{(g)}$ $\Delta H^0 = 436.4$ kJ

$Cl_{2\,(g)} \longrightarrow Cl_{(g)} + Cl_{(g)}$ $\Delta H^0 = 242.7$ kJ

$HCl_{(g)} \longrightarrow H_{(g)} + Cl_{(g)}$ $\Delta H^0 = 431.9$ kJ

$O_{2\,(g)} \longrightarrow O_{(g)} + O_{(g)}$ $\Delta H^0 = 498.7$ kJ



$N_{2\,(g)} \longrightarrow N_{(g)} + N_{(g)}$ $\Delta H^0 = 941.4$ kJ

Bond Enthalpies

Single bond < Double bond < Triple bond

Average ***bond enthapy*** in polyatomic molecules

$$H_2O_{(g)} \longrightarrow H_{(g)} + OH_{(g)} \quad \Delta H^0 = 502 \text{ kJ}$$

$$OH_{(g)} \longrightarrow H_{(g)} + O_{(g)} \quad \Delta H^0 = 427 \text{ kJ}$$

$$\text{Average OH bond enthalpy} = \frac{502 + 427}{2} = 464 \text{ kJ}$$

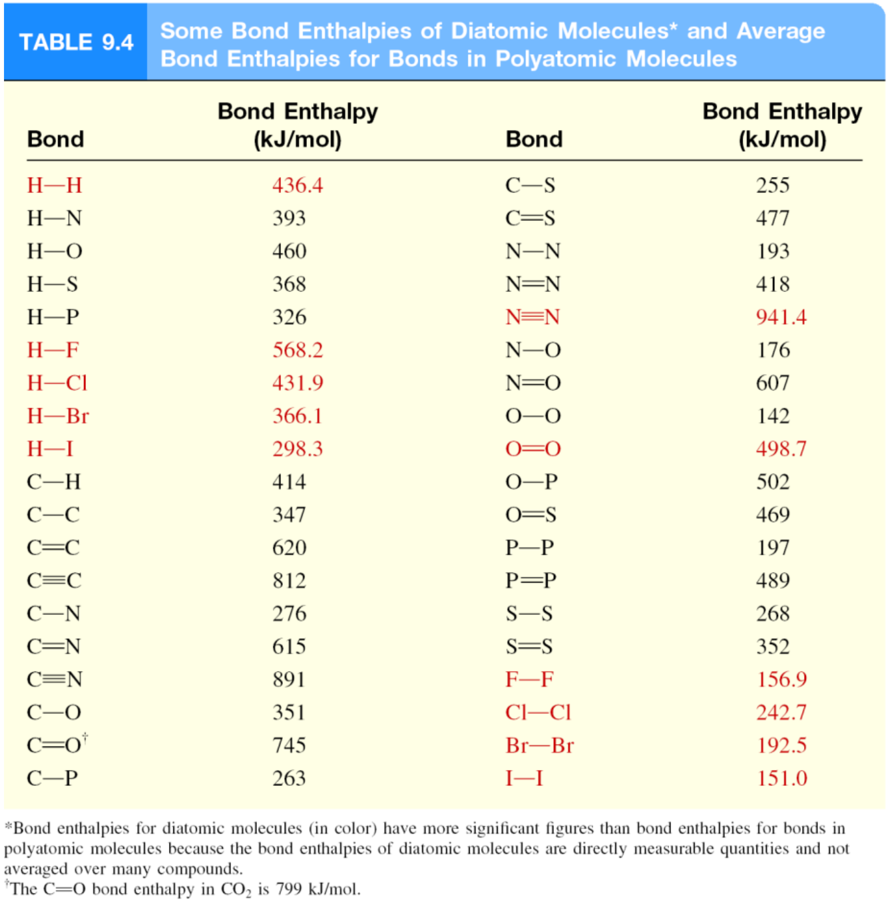


TABLE 9.4 Some Bond Enthalpies of Diatomic Molecules* and Average Bond Enthalpies for Bonds in Polyatomic Molecules

Bond	Bond Enthalpy (kJ/mol)	Bond	Bond Enthalpy (kJ/mol)
H—H	436.4	C—S	255
H—N	393	C═S	477
H—O	460	N—N	193
H—S	368	N═N	418
H—P	326	N≡N	941.4
H—F	568.2	N—O	176
H—Cl	431.9	N═O	607
H—Br	366.1	O—O	142
H—I	298.3	O═O	498.7
C—H	414	O—P	502
C—C	347	O═S	469
C═C	620	P—P	197
C≡C	812	P═P	489
C—N	276	S—S	268
C═N	615	S═S	352
C≡N	891	F—F	156.9
C—O	351	Cl—Cl	242.7
C═O[†]	745	Br—Br	192.5
C—P	263	I—I	151.0

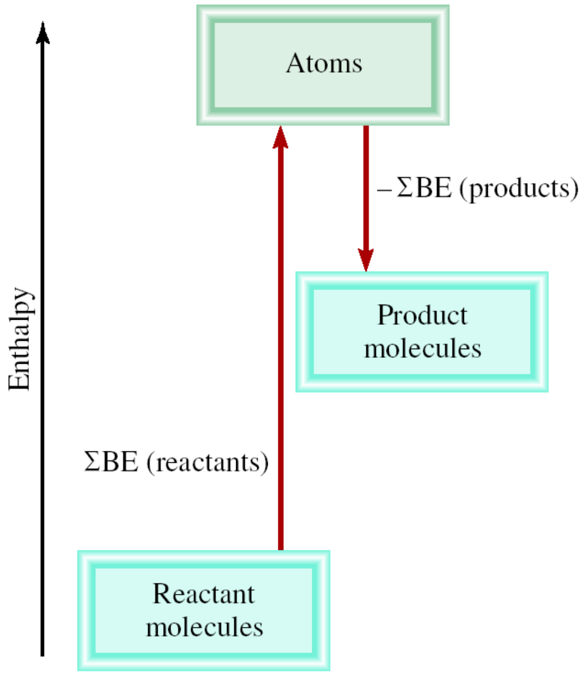
*Bond enthalpies for diatomic molecules (in color) have more significant figures than bond enthalpies for bonds in polyatomic molecules because the bond enthalpies of diatomic molecules are directly measurable quantities and not averaged over many compounds.

[†] The C═O bond enthalpy in CO_2 is 799 kJ/mol.

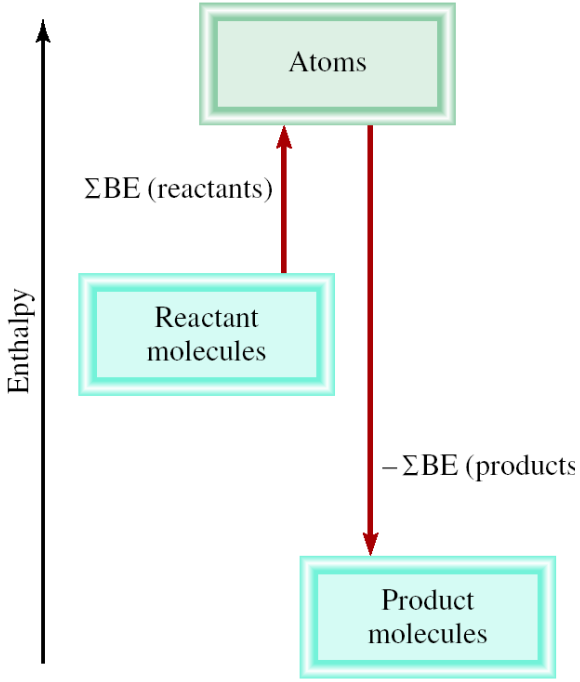
Bond Enthalpies (BE) and Enthalpy changes in reactions

Imagine reaction proceeding by breaking all bonds in the reactants and then using the gaseous atoms to form all the bonds in the products.

$$\Delta H^0 = \text{total energy input} - \text{total energy released}$$
$$= \Sigma\text{BE(reactants)} - \Sigma\text{BE(products)}$$

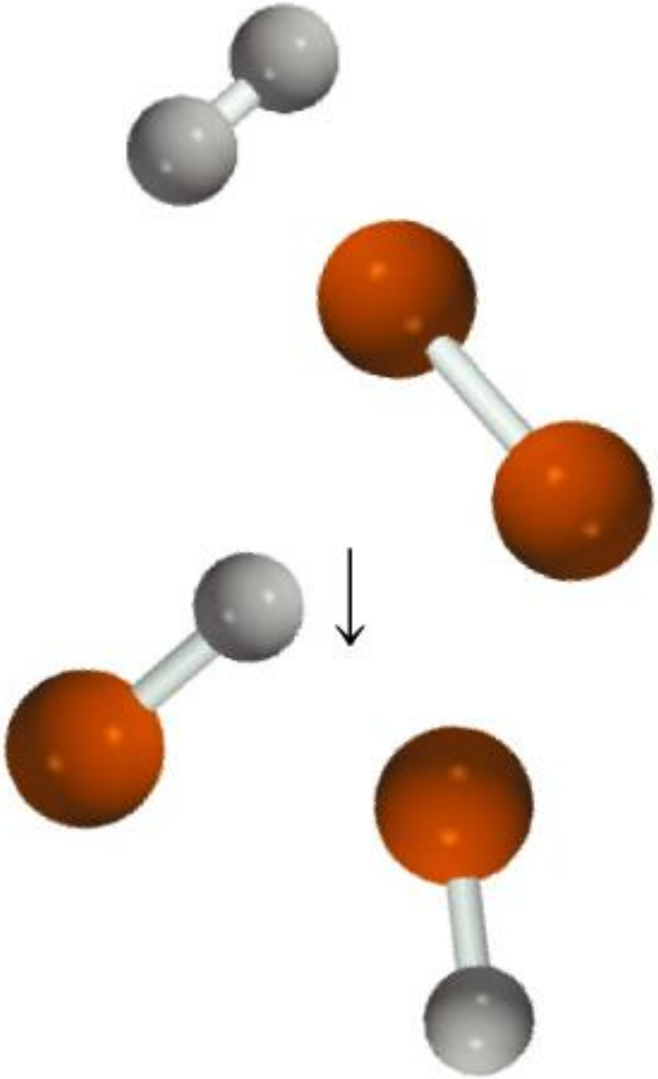


endothermic

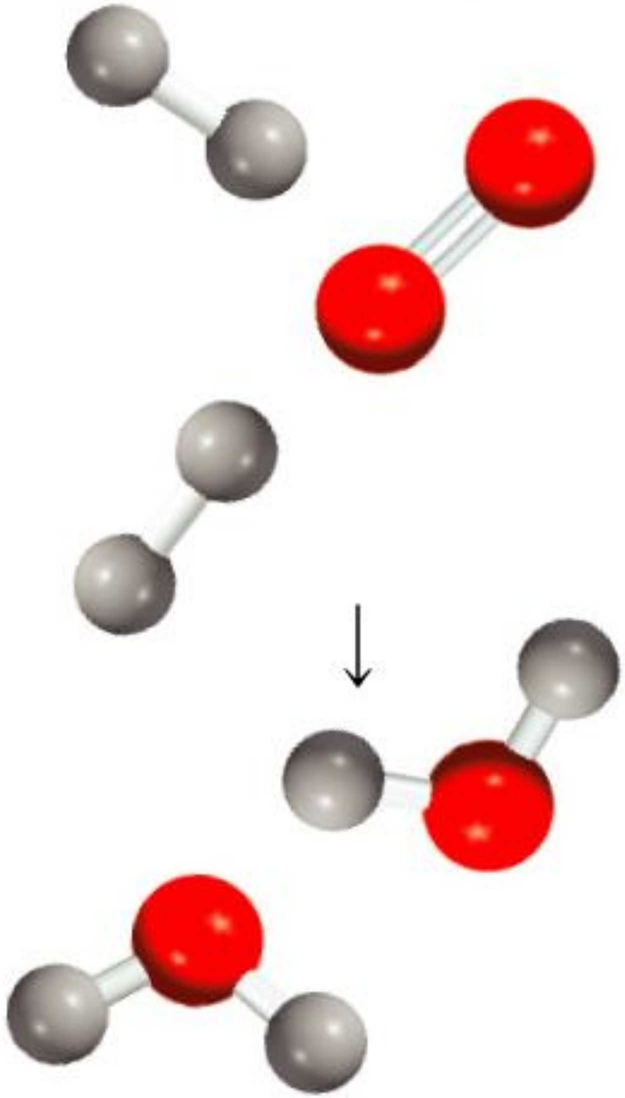


exothermic

$H_2\ (g) + Cl_2\ (g) \longrightarrow 2HCl\ (g)$



$2H_2\ (g) + O_2\ (g) \longrightarrow 2H_2O\ (g)$



Use bond enthalpies to calculate the enthalpy change for:

$$H_{2\ (g)} + F_{2\ (g)} \longrightarrow 2HF_{\ (g)}$$

$$\Delta H^0 = \Sigma BE(\text{reactants}) - \Sigma BE(\text{products})$$

Type of bonds broken	Number of bonds broken	Bond enthalpy (kJ/mol)	Enthalpy change (kJ/mol)
H—H	1	436.4	436.4
F—F	1	156.9	156.9

Type of bonds formed	Number of bonds formed	Bond enthalpy (kJ/mol)	Enthalpy change (kJ/mol)
H—F	2	568.2	1136.4

$$\Delta H^0 = 436.4 + 156.9 - 2 \times 568.2 = -543.1 \text{ kJ/mol}$$