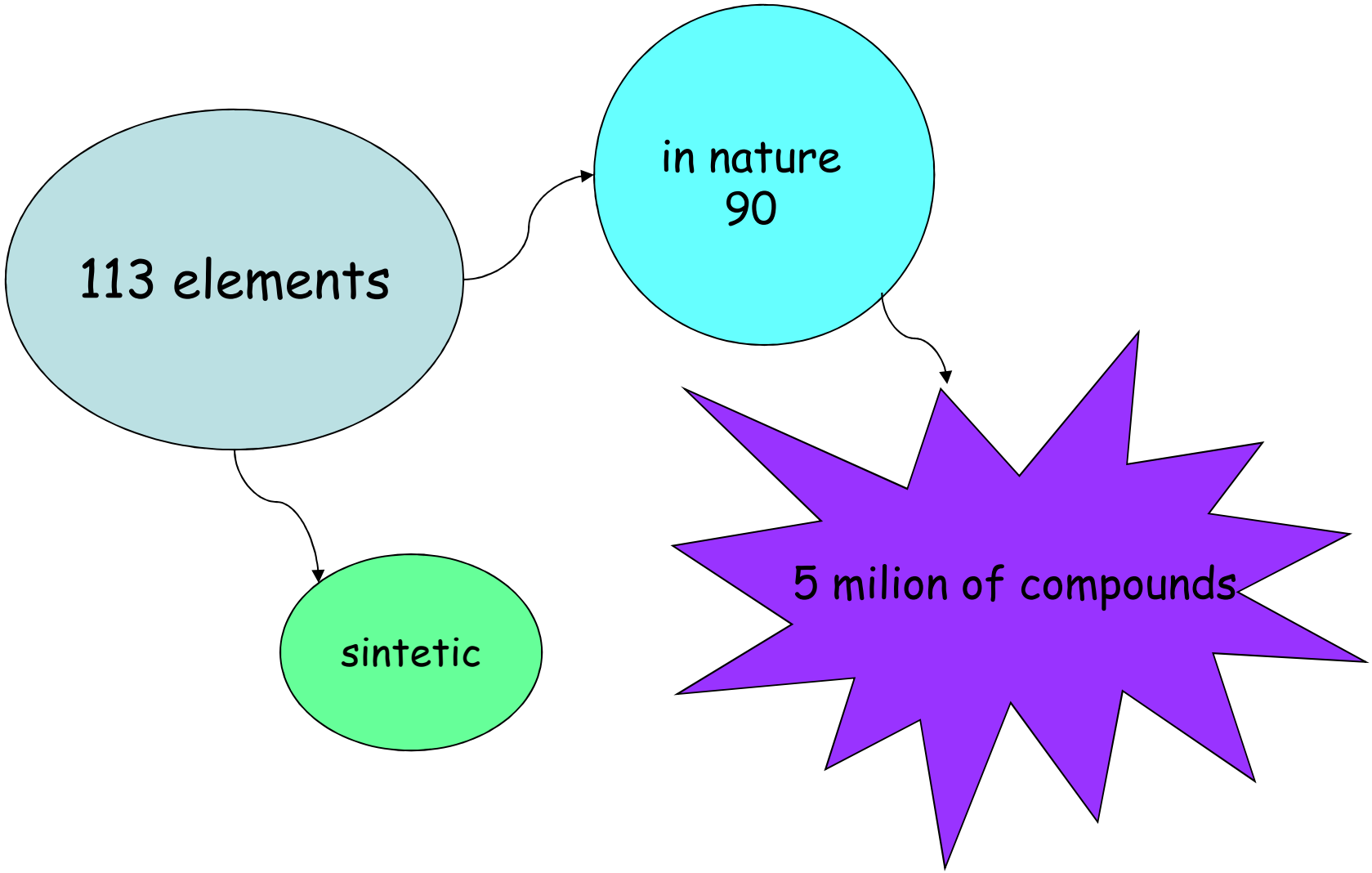
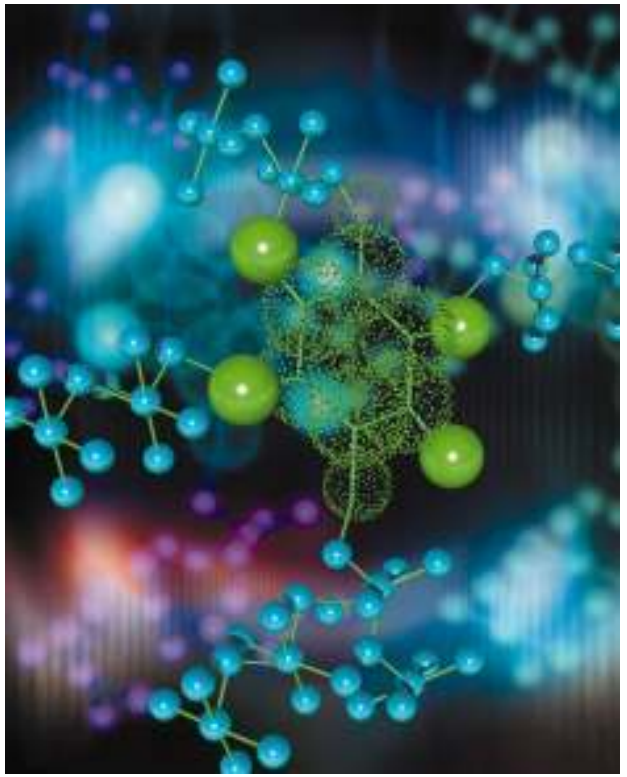

Chemical bonds


113 elements
in nature
90
sintetic
5 milion of compounds

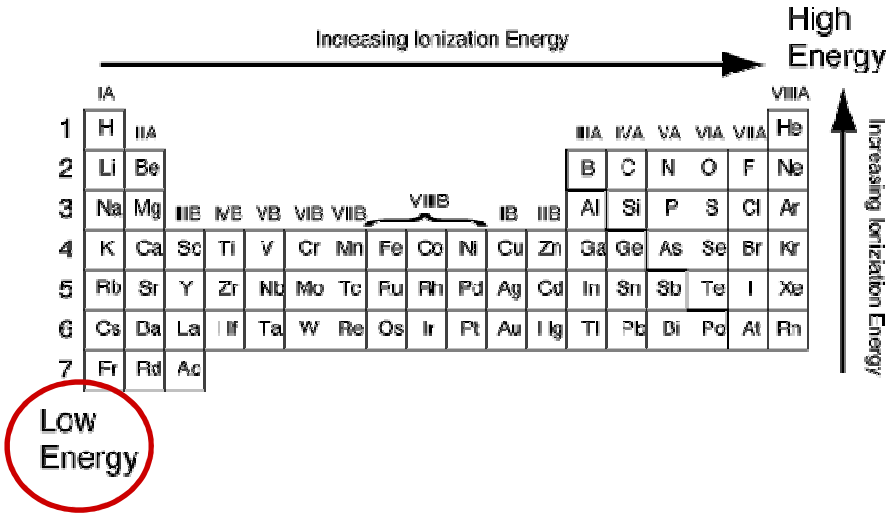
# Chemical bonds

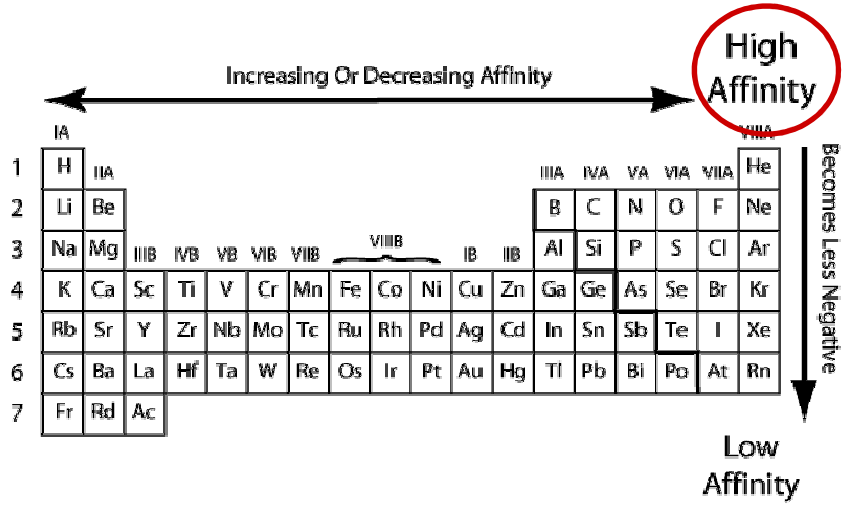
- The atoms are joined because so attached they form more stable energy system
- Atoms realize their bonds through outer or valence electrons
- IONIC, COVALENT and METALLIC BOND



# IONIC BOND

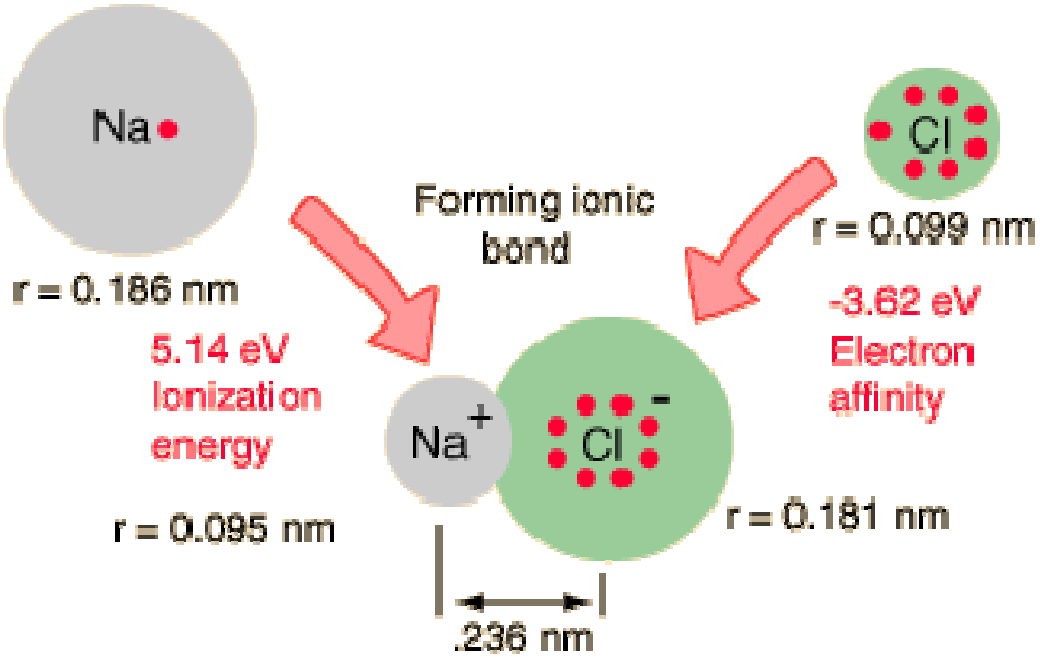
- Connecting the metals atoms having low ionization energy with a nonmetal atoms that have high electron affinity
- Metals in 1st and 2nd group and nonmetals in 17th and 16th group



# IONIC BOND

Formation of NaCl from sodium and chlorine in three phases:




Electric potential energy

$$\frac{-Ke^2}{r} = \frac{-1.44 \text{ eV nm}}{0.236 \text{ nm}} = -6.1 \text{ eV}$$

Change of energy:

5.14 eV ionization energy
-3.62 eV electron affinity
-6.10 eV Coulomb's force

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-4.58 eV

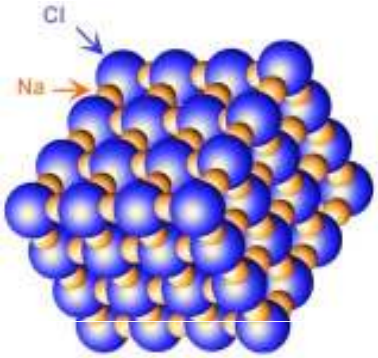
Ionic pair $Na^+$ and $Cl^-$ that were attracted is for 4:58 eV poorer than Na and Cl atoms, that is more stable

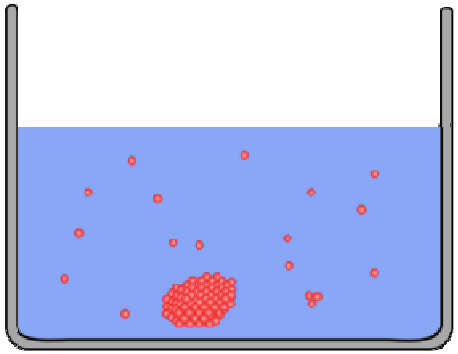
# IONIC BOND

- Released potential energy is an important factor in the creation of ionic compound because it compensate ionization energy and represents the ENERGY OF THE CRYSTAL LATTICE
- Lattice energy is the quantity of energy released at the formation of one mole of single crystal of infinitely distant ions in the gas phase.
- E of lattice depends on the radius: radius smaller → E of lattice larger
- E of lattice depends on the charge of ion: charge larger → E of lattice larger

# IONIC BOND

- connection between ions is of electrical nature
- not directed in space because electric field acts around the entire ion
- all ionic compounds are crystalline nature, packed compact structure, high melting point and boiling point
- easily soluble in water
- aqueous solutions and melts conduct electricity due to the existence of free ions



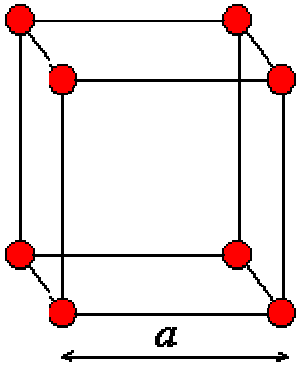



# Crystals

- crystal has a form
- angles between the planes of the crystal are constant
- parts created cleaving crystals have flat surfaces of constant angles
- the smallest unit of the crystal is unit cell

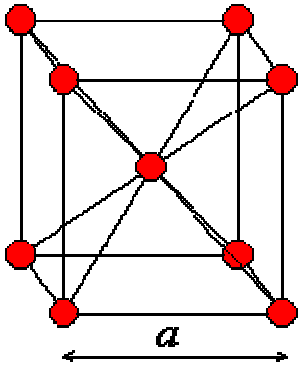
# Crystals

- The most common is CUBIC STRUCTURE



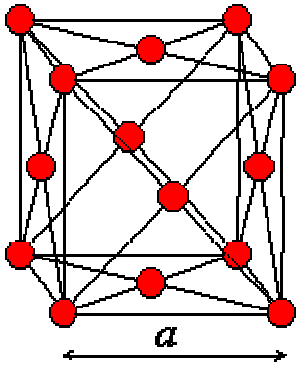

**Simple cubic lattice**

i.e. ice, $I_2$, camphor, diamond...




**Body-centered cubic lattice**

i.e. Fe

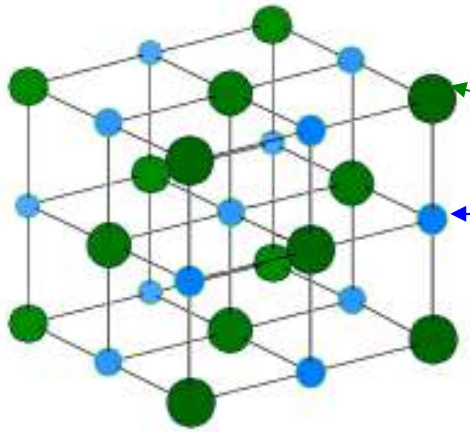


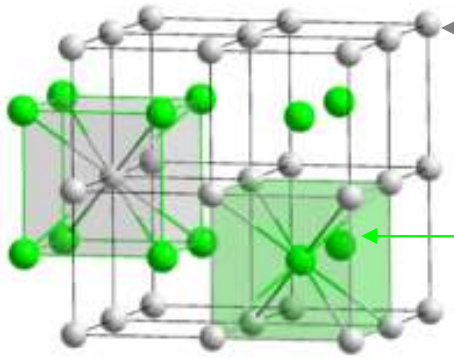

**Face-centered cubic lattice**

i.e. Cu, Ag...

# Ionic crystals

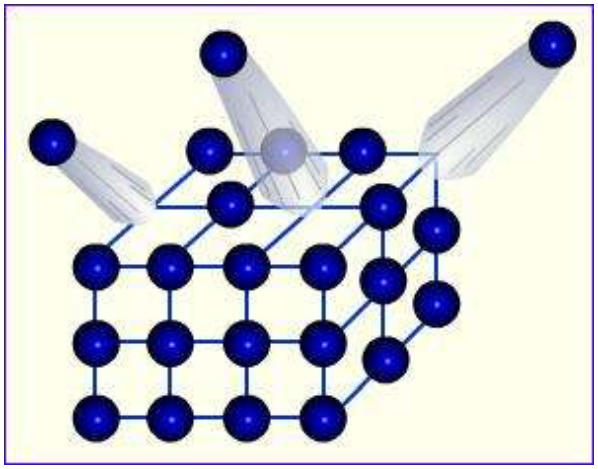
- each cation is surrounded by a number of anions and vice versa
- they are gathered by attractive force which are stronger with higher charge and smaller ion
- lattice structure depends on the size of cations and anions, their charge and stoichiometry

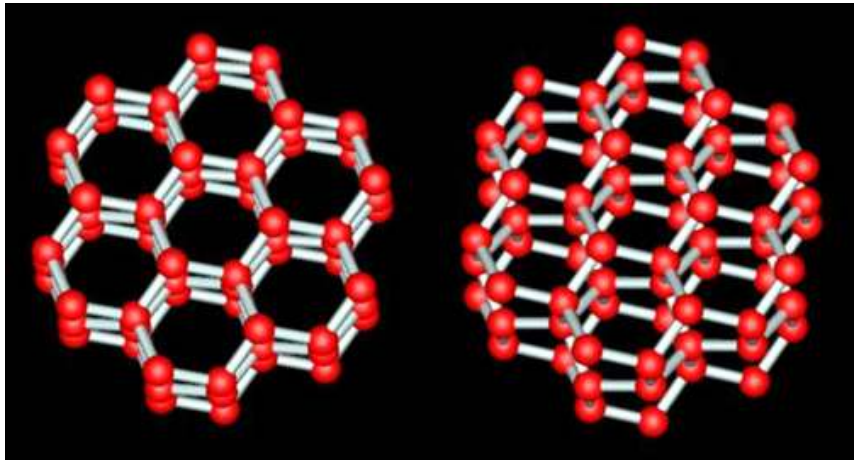


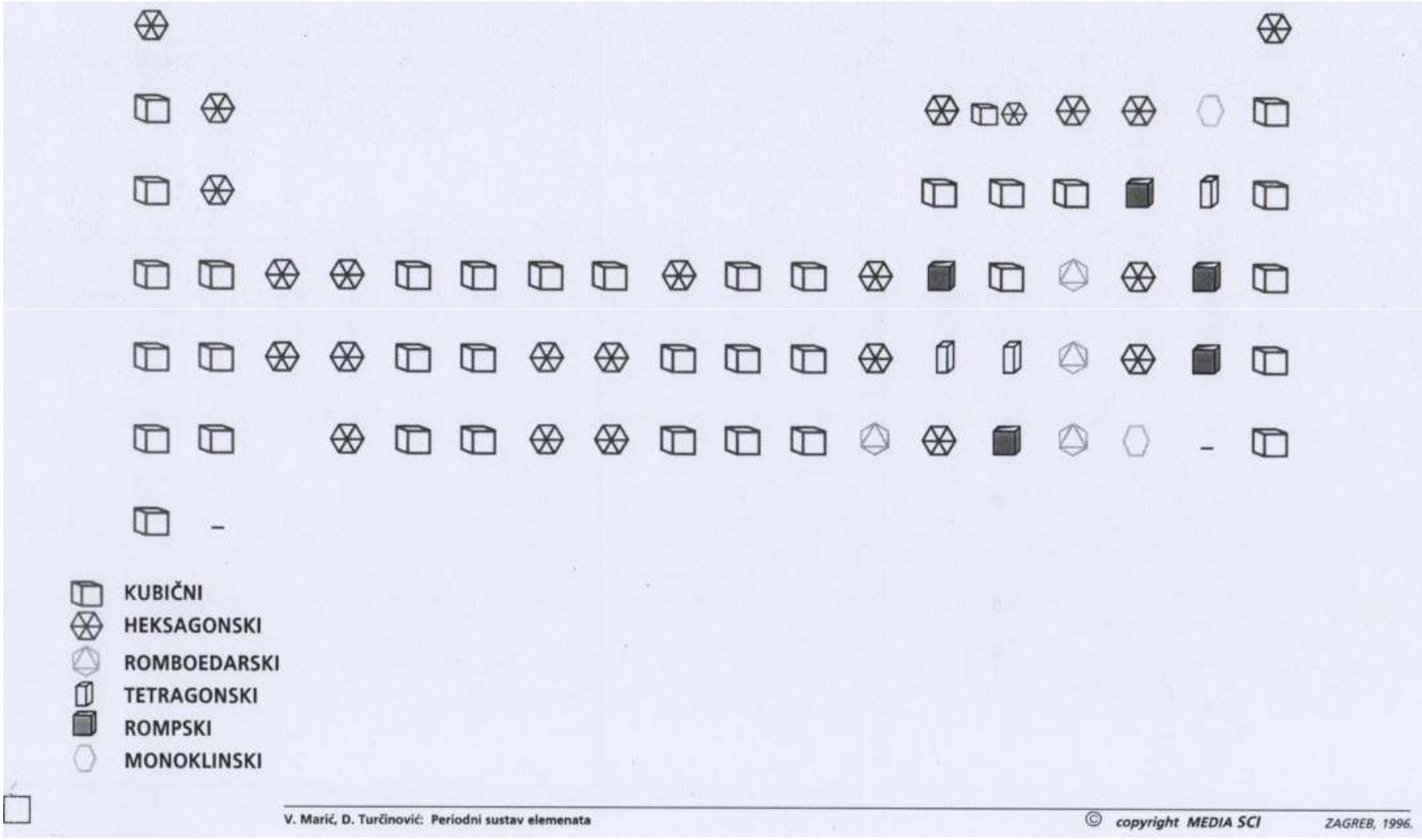
# Molecular crystals

- structural units are molecules
- gathered by weak attractive van der Waals forces
- sublimate
- have lower melting and boiling points of ionic crystals
- i.e. ice, iodide, camphor





# Crystal system of elements in the solid state



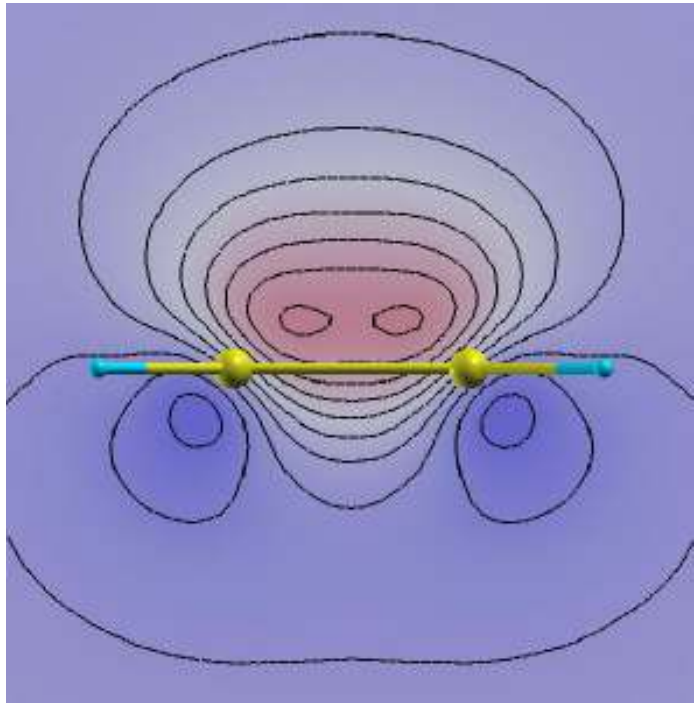
# COVALENT BOND

- Lewis theory: creating of a common electronic pairs between two atoms. Common el. pair lies between the two nuclei.
- Simple theory, but it does not explain the shape nor the magnetic properties of molecules

H••H → H:H → H—H

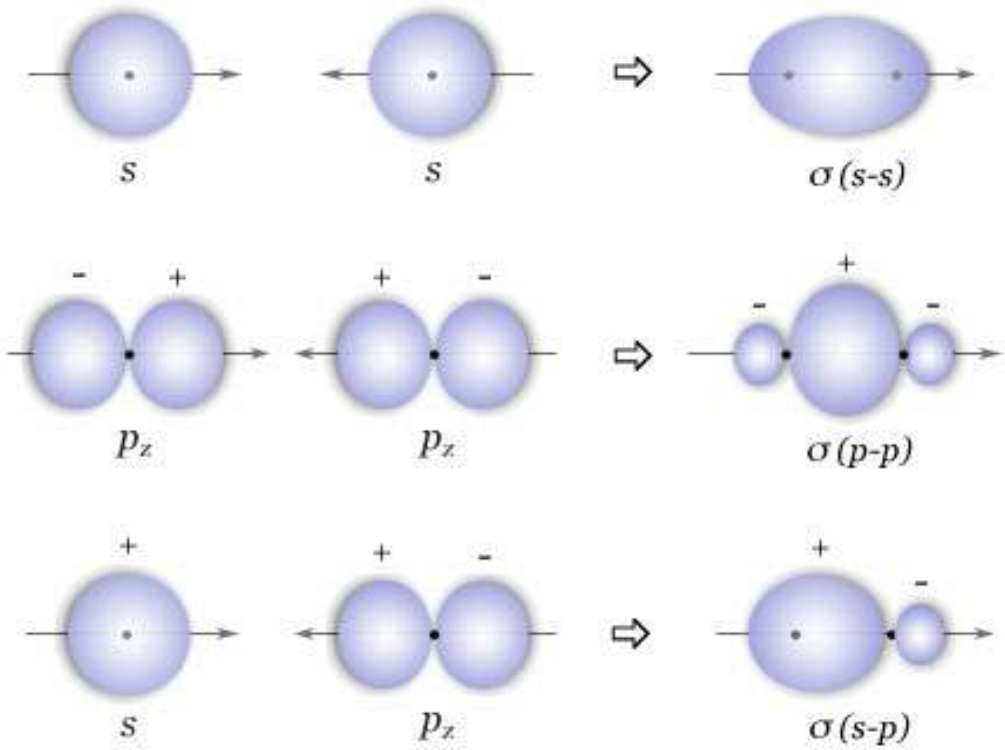
# COVALENT BOND

- Quantum-mechanics theory: valence orbitals of two atoms with one electron of opposite spin overlap. The strength of the bond depends on the bond type and amount of overlapping.
- σ – sigma bond
- π – pi bond



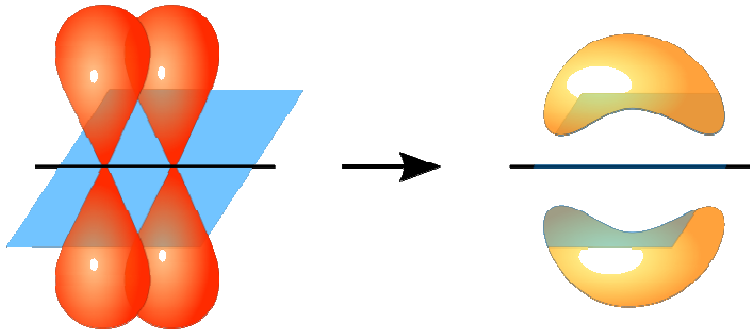
# σ - bond

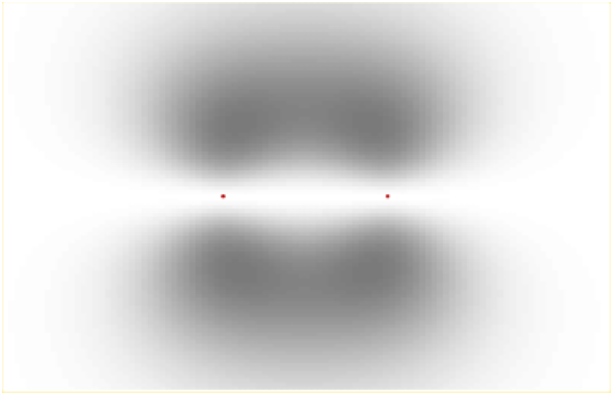
- primary
- maximum electron density between the nuclei
- symetric

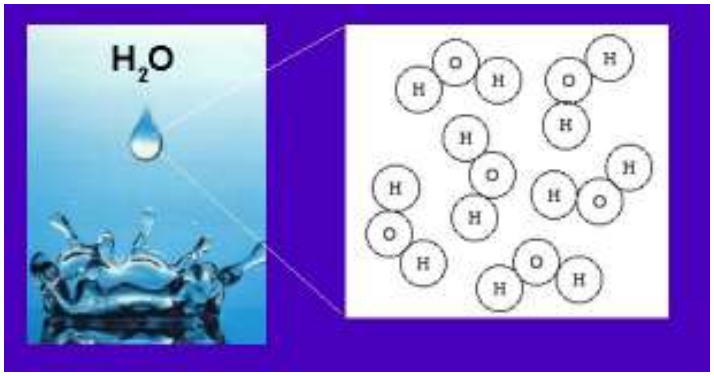


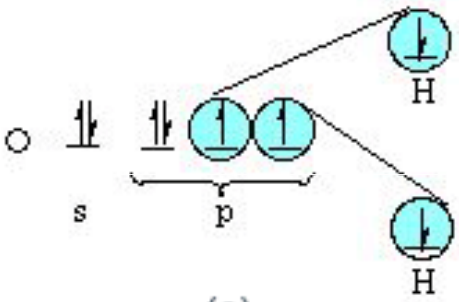
# π - bond

- secondary e.g. occurs after the occurrence of σ-bond which closer nuclei
- weaker than σ-bond because el. density is maximum above and below the plane of nuclei
- perpendicular to the σ-bond
- in chem. reaction breaks before σ-bond. The next bond that emerges is again π-bond perpendicular to the σ-bond and the previous π-bond. There are two electron clouds, above and below the axisis
- non-symmetric, shaped bananas

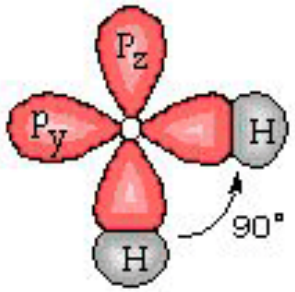




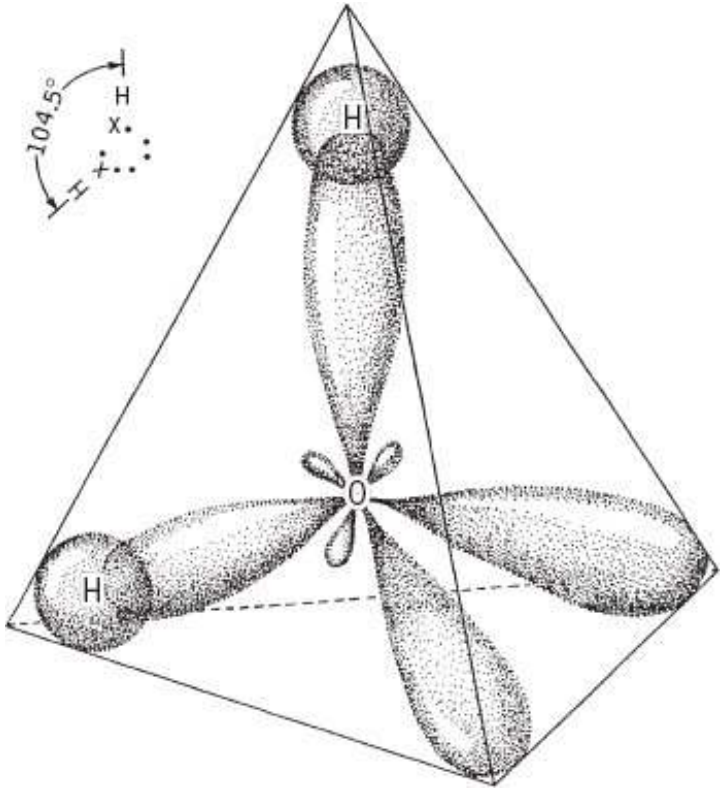



(a)



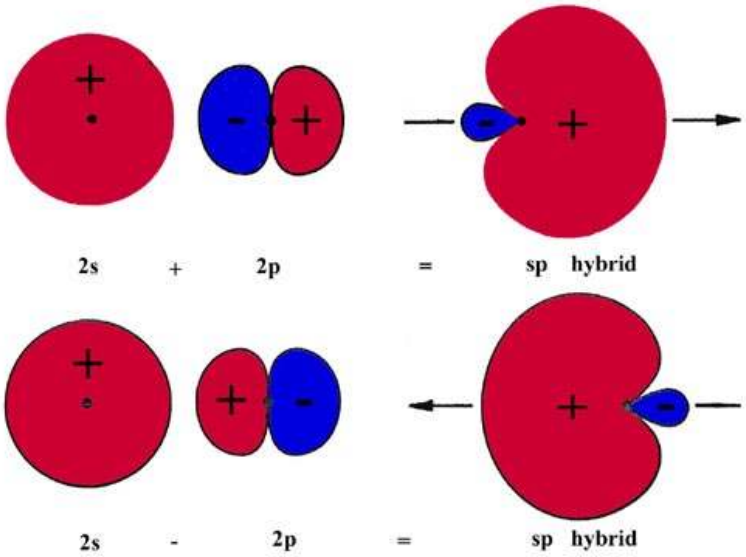

(b)



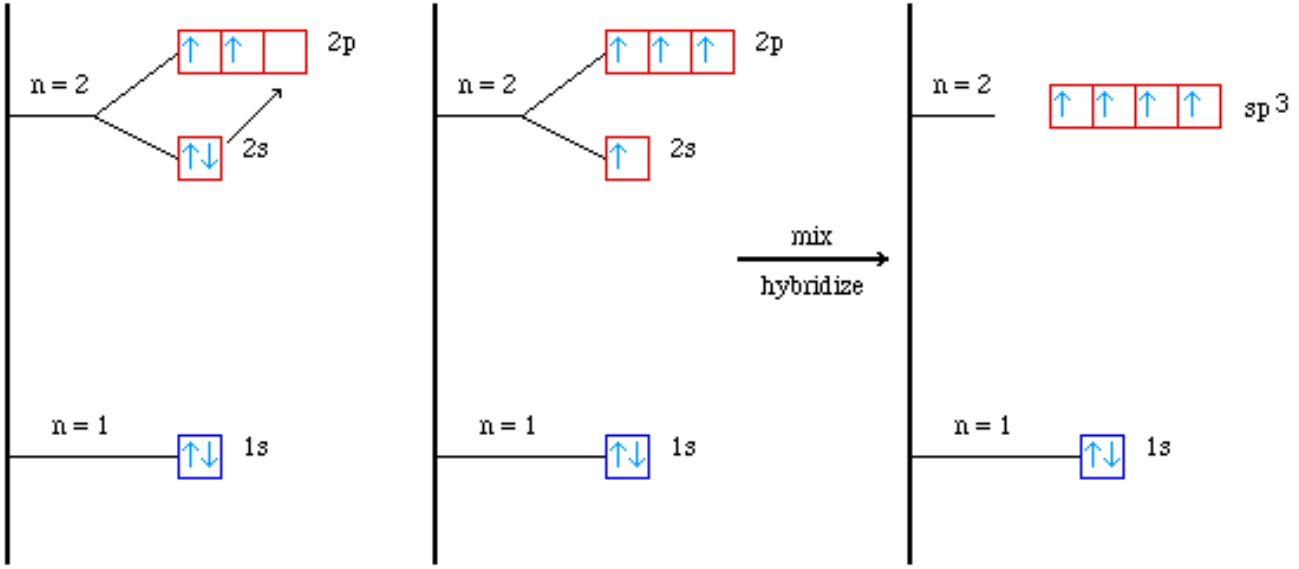
# Hybrid orbitals

- theory and form of many molecules can be explained by the theory of hybrid atomic orbitals.
- occur in the same atom by mixing atomic orbitals of similar energy. This occurs at the formation of chemical bond because hybrid orbitals are not detected in the isolated atom.
- hybridization is present in larger atoms
- mixing of one 2s and one 2p → two sp
- mixing of one 2s and two 2p → three $sp^2$
- mixing of one 2s and three 2p → four $sp^3$

# Hybrids



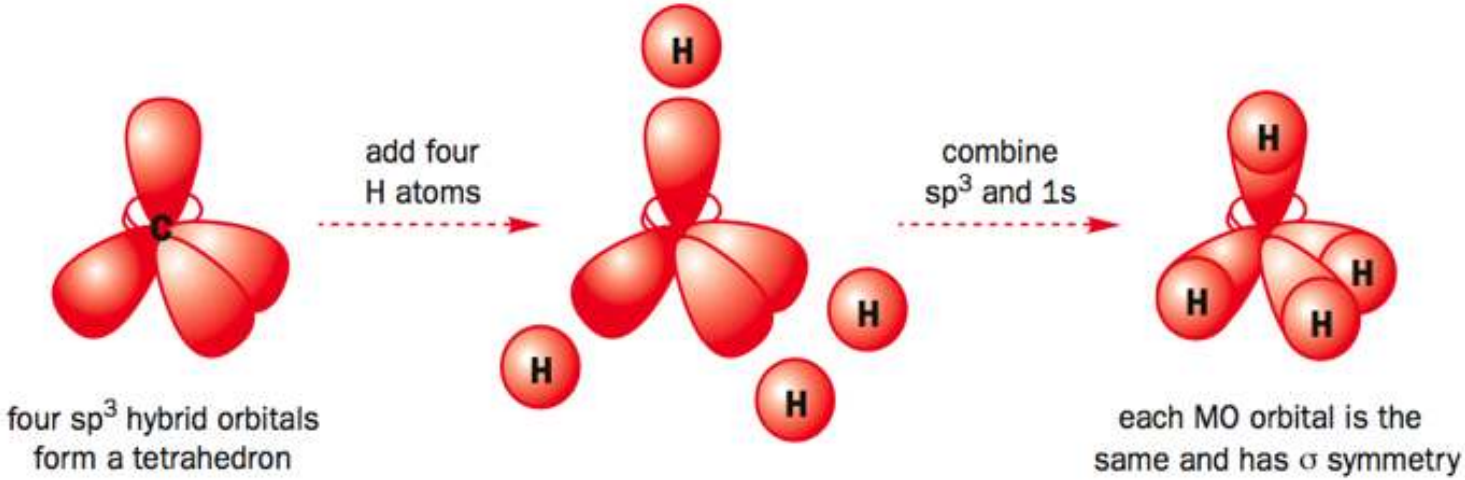

| | | | |
|---|---|---|---|
| 1 *s* orbital & 1 *p* orbital | sp hybrid (2 orbitals) | 2 | linear |
| 1 *s* orbital & 2 *p* orbitals | $sp^2$ hybrid (3 orbitals) | 3 | trigonal planar |
| 1 *s* orbital & 3 *p* orbitals | $sp^3$ hybrid (4 orbitals) | 4 | tetrahedral |
| 1 *s* orbital & 3 *p* orbitals & 1 *d* orbital | $dsp^3$ hybrid (5 orbitals) | 5 | trigonal bipyramidal |
| 1 *s* orbital & 3 *p* orbitals & 2 *d* orbitals | $d^2sp^3$ hybrid (6 orbitals) | 6 | octahedral |




Energy level diagram for carbon

promotion of a 2s electron

four hybrid $sp^3$ orbitals are formed

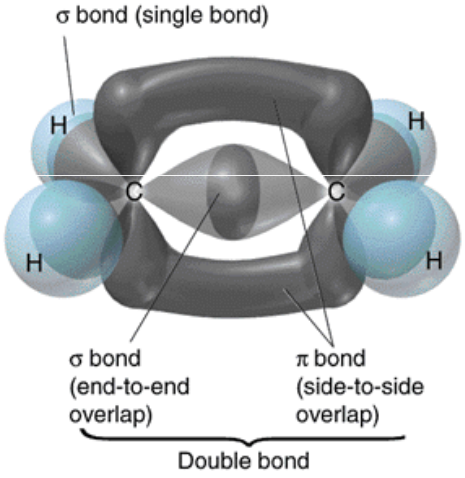


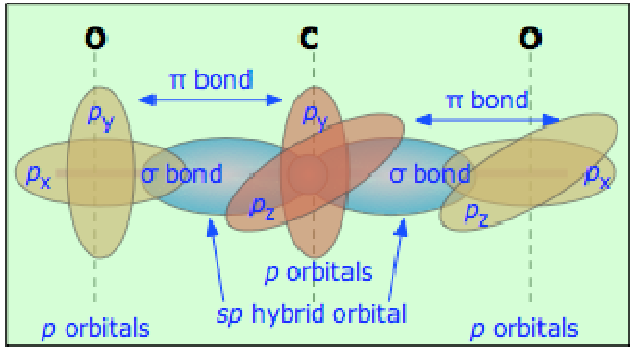

four $sp^3$ hybrid orbitals form a tetrahedron

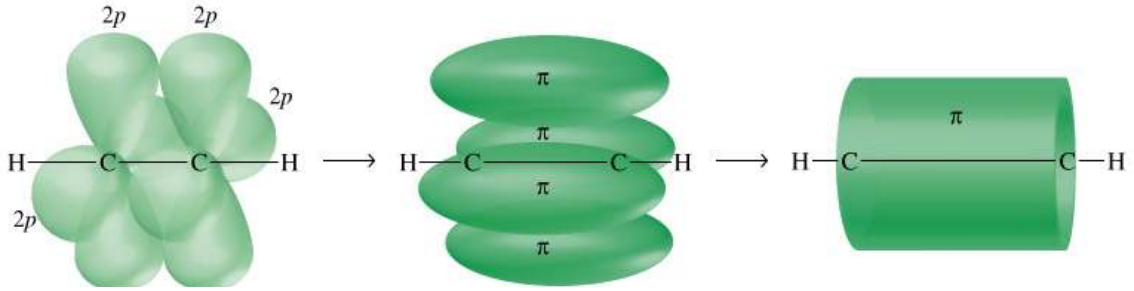
each MO orbital is the same and has σ symmetry

# Hybrid orbitals

- all organic compounds are produced by overlapping of hybrid orbitals

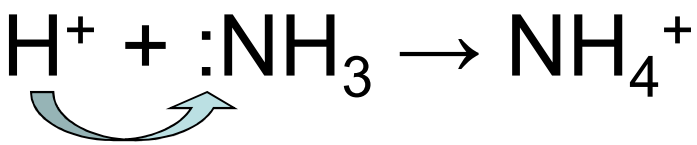


# COVALENT BOND

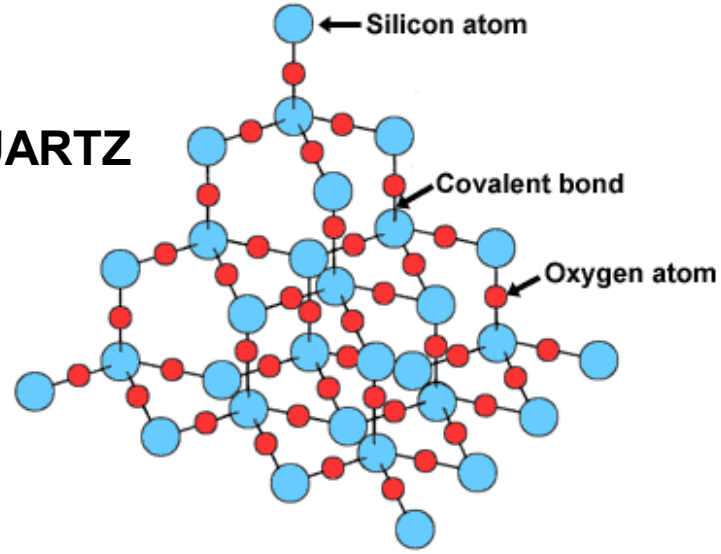
- covalent bond can also occur so that both electrons are given from a single atom



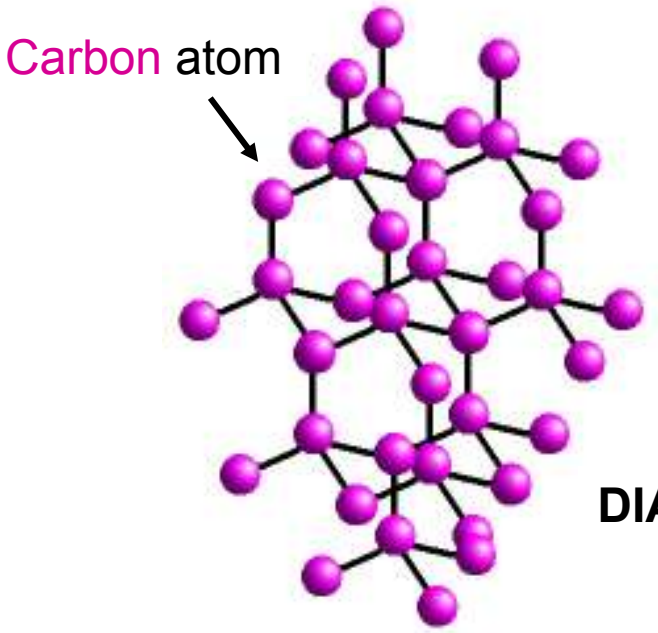

- Symetry of molecule depends on repulsing of orbitals with shared electrons and orbitals with undivided electron pair

# Properties of covalent compounds

- build molecules that have the shape and structure
- covalent bond is a directed and rigid
- between molecules there are weak attractive forces so covalent substances are gases or liquids. If they are solids, they have low melting and boiling point, and can easily sublimate (exceptions diamond and quartz - atomic lattice)
- poorly soluble in water




**QUARTZ**




**DIAMOND**

# Polarity of covalent bond

- two identical atoms covalently bound equally share an electron pair.

  H — H  or  Cl — Cl

  electron density is equal around each atom

- different atoms share an electron pair.

  H — Cl  ili  H — O — H

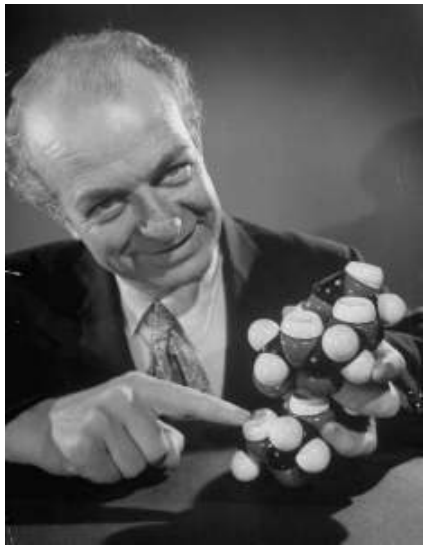
- then one atom attracts more common el. pair. This part of the molecule has a higher el. density, i.e. has a partial negative charge.

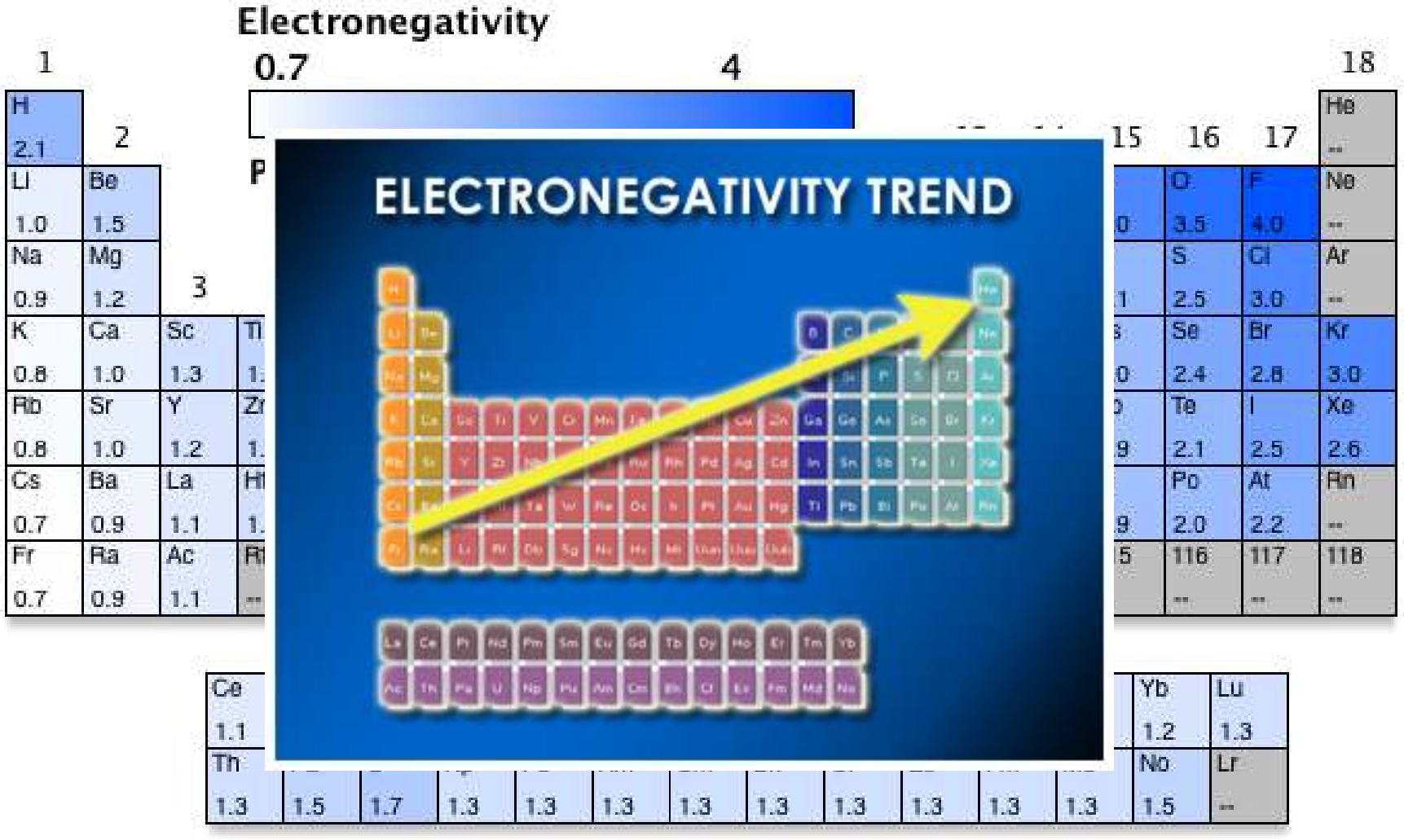
  $^{\delta+}$H — Cl$^{\delta-}$

  covalent bond has a partial ionic character

# Electronegativity

- the tendency of an atom or a functional group to attract electrons (or electron density) towards itself.
- L. Pauling experimentally determined coefficients of relative electronegativity of atoms
- that is how oxidation numbers of covalently bound atoms are determined



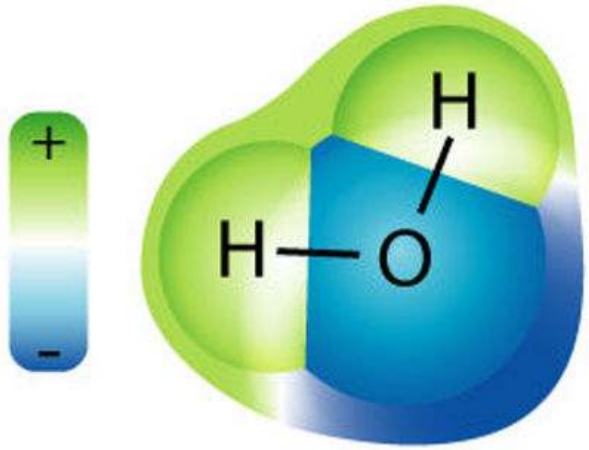


# Molecular dipole

- partial ionic character of covalent bonds can cause molecular polarity or molecular dipole

- measure for the molecular polarity is of MOLECULAR DIPOLE MOMENT, which is determined experimentally

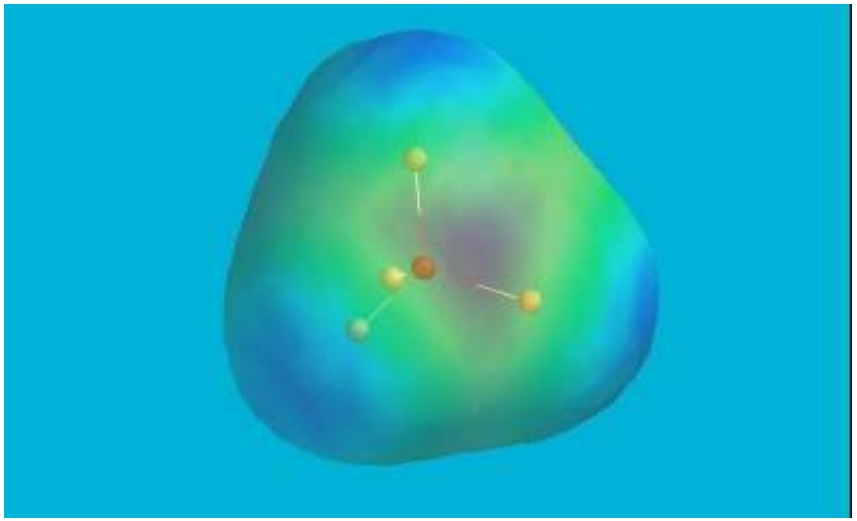
- molecule of water is the most important molecular dipole




- water molecular dipole is the basis of ionic compounds dissolving

# Dipole vs non-dipole

- all covalent bonds in molecule may have a partial ionic character and molecule may not be dipole ($CH_4$, $CCl_4$, $C_6H_6$..)

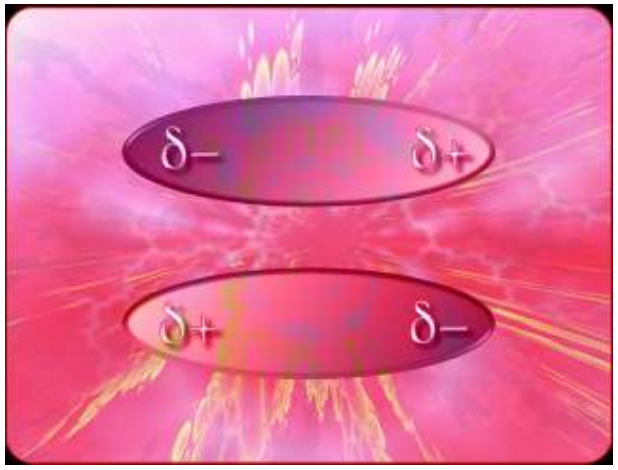


• consequence of molecular dipole are attractive forces between them, called intermolecular attractive forces

# Intermolecular attractive forces

1. Van der Waals attractive forces

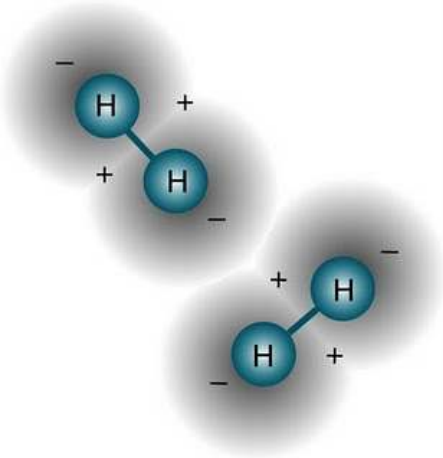
- molecular dipoles are mutually attracted to each other with opposite charges
- these compounds melt and volatilize more difficult
- it is dipole-dipole attraction
- molecular dipole can attract other molecular dipole and ions (ionic-dipole attraction)



# Intermolecular attractive forces

## 2. London attraction forces

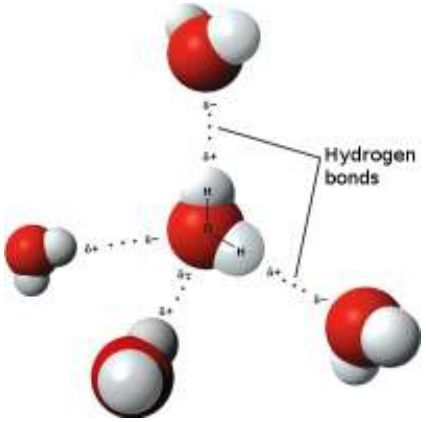
- occur in molecules which are not dipoles, and in conditions of high pressure and low temperatures may become dipoles due to the current asymmetry of electron density

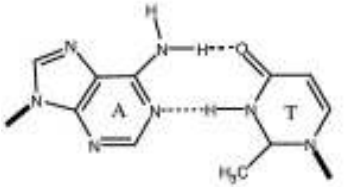


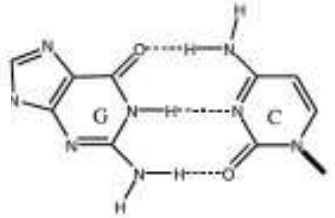
# Intermolecular attractive forces

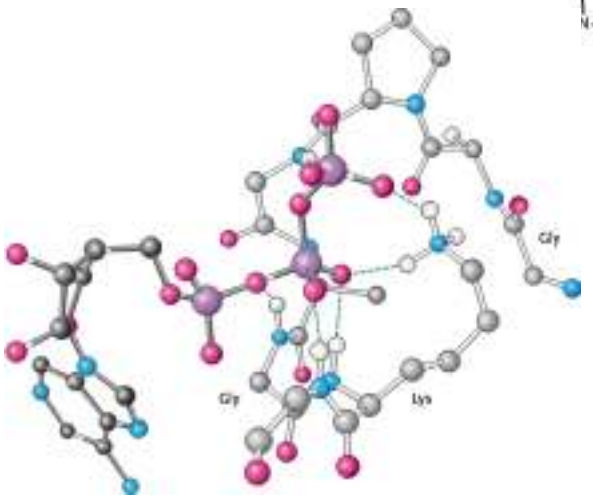
## 3. Hydrogen bonding

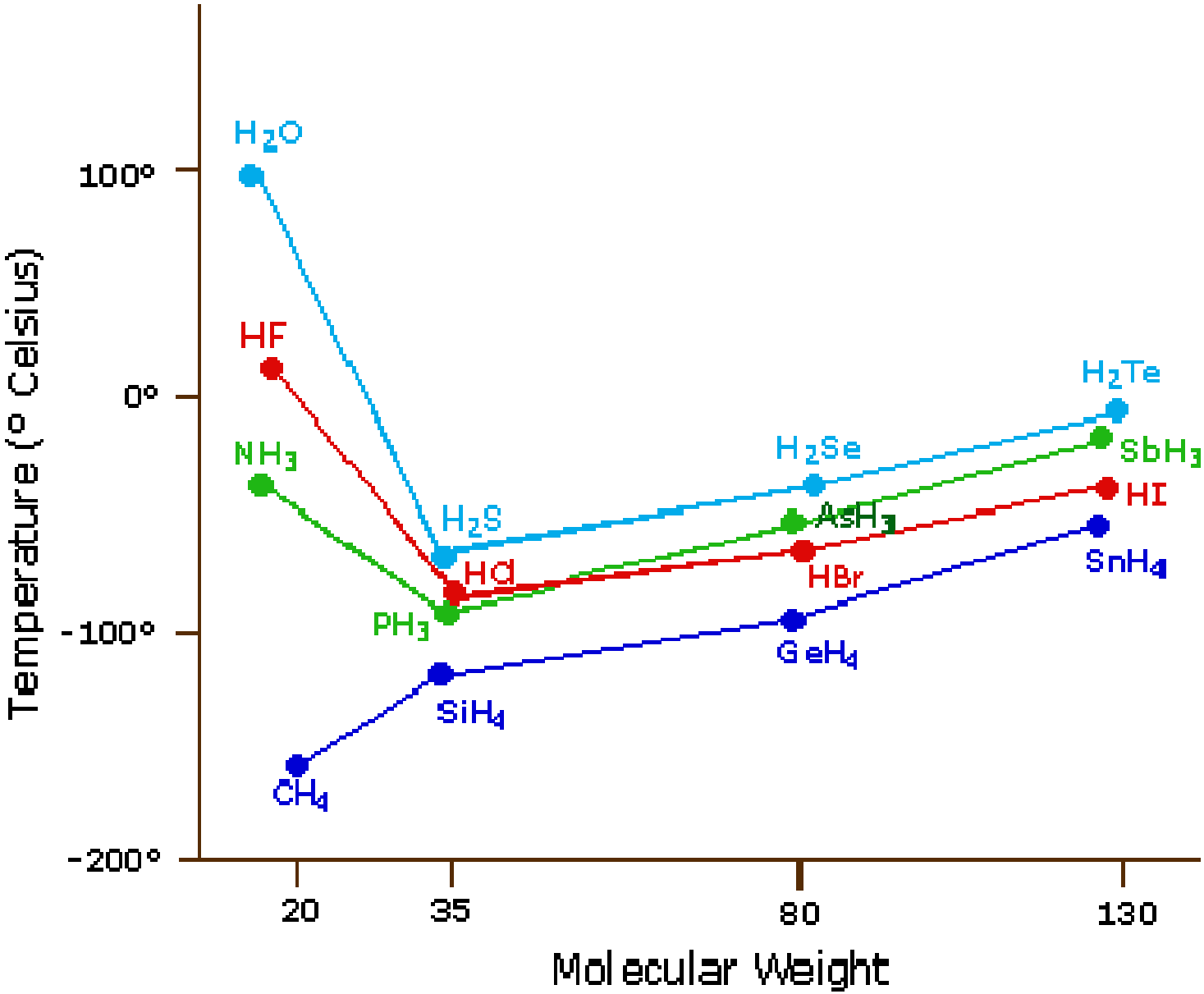
- occurs between the molecules in which the hydrogen is covalently bonded to a very small and highly electronegative atom such as F, O, or N
- electrostatic attraction, but is separately studied because this bond is stronger than the van der Waals
- moleculs are associated
- higher melting point and the boiling point of the analog compounds that have no hydrogen bond
- strength: 1/10 σ-bond, length: 2x σ-bond



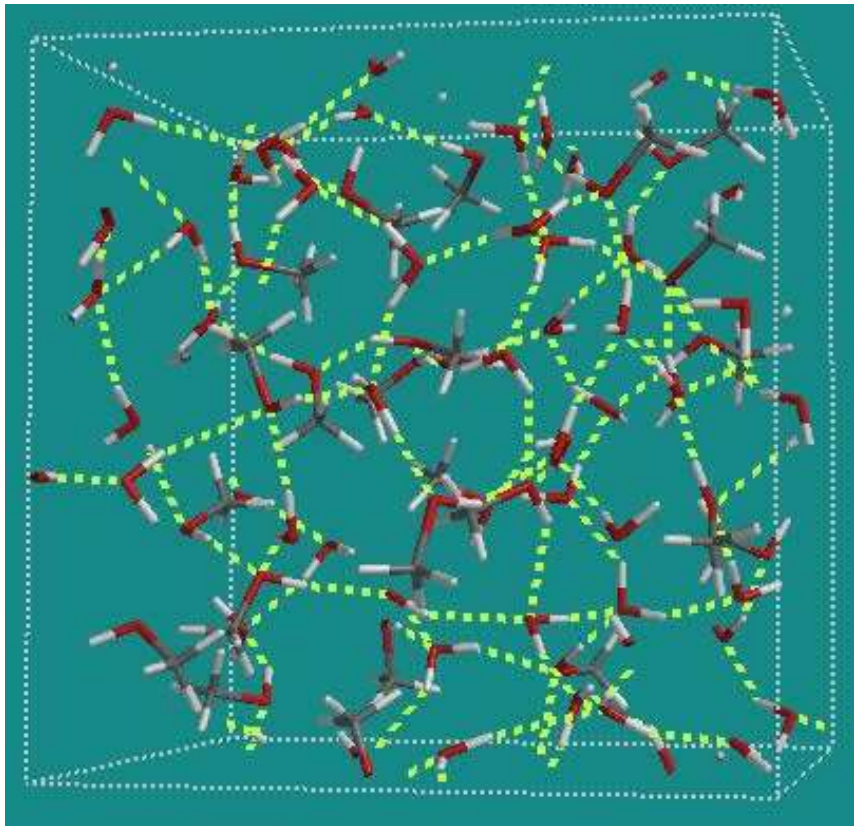




Temperature (° Celsius)
100°
0°
-100°
-200°
$H_2O$
HF
$NH_3$
$H_2S$
HCl
$PH_3$
$CH_4$
$SiH_4$
$H_2Se$
$AsH_3$
HBr
$GeH_4$
$H_2Te$
$SbH_3$
HI
$SnH_4$
20
35
80
130
Molecular Weight

# Similar is soluble in a similar

Solubility of methanol in water:

- H bonds in water and methanol are similar in type and strength and can be replaced. Therefore, the methanol is soluble in water, namely water and methanol are mixed



# Importance of hydrogen bonding for water

- ice floats on water – hydrogen bonds are rigid, they break with warming and molecule can be arranged densely. Above +4ºC number of hydrogen bonds decreases, as well as density
- high boiling and melting point comparing to analog compounds. If there were not this bond, boiling point of water would be app. -80ºC
- we could say that hydrogen bond allows life on Earth