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Thermodynamics

Understanding what drives chemical and physical changes

Intermolecular forces and solubility

Solubility

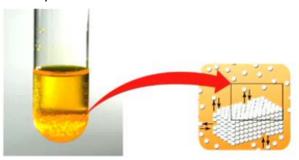
- > Definition: Maximum amount of solute (minor component) that dissolve in a given amount of solvent (major component) at specific temperature
- ➤ Molecular structure is important
- Polar solvent/ polar solute or nonpolar solvent/ nonpolar solute favored
- Polar dissolves in polar and nonpolar dissolves in nonpolar(like dissolves like)
- e.g. Hexane is better solvent for grease than methanol

Intermolecular interactions drive solubility

Increasing Strength of attraction Hydrogen bonding

Dispersion Dipole-dipole

- > Solute-solvent interactions must be stronger than solute-solute interactions for substance to dissolve
- This is because the solvent has to overcome the forces and interactions it starts with (the ones that is holding the solid together)
- They have to turn into interactions between the solvent now



Polarity and solubility (dw about it for now)

- Polar solute dissolves in polar solvent, e.g. water, because its molecules are attracted to the polar water molecules
- lowering of energy (enthalpy)
- Enthalpy is the energy in the bonds
- Nonpolar solute dissolves in a nonpolar solvent because the dispersion forces are of comparable strength
- There is no change in enthalpy but molecules being mixed up (dissolved) is more probable.
- Entropy (increased probability) is the driving force!
- Entropy is basically the disorder

Thermodynamics

- > Definition: energy can be harnessed to provide heat and work
- To see if a reaction occurs spontaneously or non-spontaneously and if it does, does it release or give away heat and does it do work or get work done on it

Release of energy can:

- Heat surroundings
- Produce mechanical work when fuel burns in an engine
- > Produces electrical work from a chemical reaction- pumps electrons through circuit
- Produce chemical work during biological processes

Thermodynamics

Quantitative study of transformations of energy

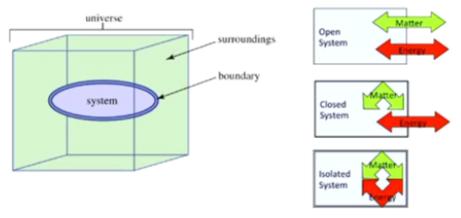
Chemical thermodynamics

- ➤ Definition: the ability to predict both the direction and the extent of **spontaneous** chemical and physical change under particular conditions.
- What will happen under given conditions:
- So whether it move from reactants to products
- And how far it moves along that path

Thermochemistry

- > Definition: the study of energy changes involved with chemical reactions. Virtually all chemical reactions absorb or release energy
- In order to understand this, we need to focus on a limited, well-defined part of universe, called the **system**. Everything else Is called **surroundings**.
- The properties of a system at any one time is its 'state'

The System + Surroundings = Universe.



E.g.

- > Cup of coffee with no lid on it is an open system
- · Coffee is evaporating
- Losing energy
- > Cup of coffee with a lid on it is an closed system
- Coffee is not evaporating
- But still losing energy
- Coffee placed in a very very insulated cup that is sealed
- Neither matter no energy translates between system and sounding

Chemical reactions involve energy transfer

- Work and heat are the two fundamental ways in which energy is transferred to or from a system
- The **system** is usually the chemical reactants and products. The system is our frame of reference and what we can experimentally measure.
- > Energy is transferred to <u>or</u> from a system from <u>or</u> to the **surroundings**

Heat and work are the only ways that a chemical system can exchange energy with its surroundings:

1) The capacity to do work (w). e.g. lifting an object

> Definition: got to move something against the force

 $work = force \times distance$

2) The capacity to transfer heat (g)

Heat

- > Definition: the process of transfer of thermal energy between two bodies or system at different temperatures.
- · We consider that heat cannot do work

What drives chemical change?

Evidence of chemical change

- Exothermic reaction (heat released)
- > Endothermic reaction (heat absorbed)
- Chemical change (new substances)
- Useful for work (gas generated)
- > Combustion of fat releases energy in form of heat (energy flows from system to surroundings). The release of heat is an **exothermic process**

 $Fat + O_2 \cdots > CO_2 + H_2O + energy$

> Other reactions cause energy to flow from surroundings to system: endothermic process

$$N_2 + O_2 + energy \cdots > 2NO_2$$

Note: Energy is no created or destroyed, just transferred from one place to another

The First law of Thermodynamics

> Definition: Energy cannot be created or destroyed, it can only be converted from one form to another

Potential energy

Definition: Difference between reactants and products (stored energy)

The combustion of methane:

$$CH_4(g) + 2O_2(g) \cdots > CO_2(g) + 2H_2O$$

- The energy that is transferred comes from the systems internal energy, U
- > The internal **energy, U** is the sum of all the energies for an individual particle- e.g. potential, kinetic
- > We are only interested in the change in internal energy

Internal energy, U

U is the sum of all the energies (potential and kinetic energy)- for all particles in the system

Kinetic energy:

- > Definition: thermochemistry involves the movement of atoms, molecules or ions (including vibration, translation and rotation)
- E(kinetic)= $\frac{1}{2}mu^2$

Potential energy (depends on the position)

- > Definition: potential energy at the molecular level due to the electronic states of the atoms, molecules or ions and their relative positions to each other.
- Depends on the position and the bonding

The symbol Δ is used to express the change in a variable

The change in internal energy during reactions

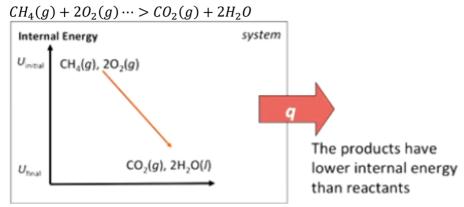
$$\Delta U = U_{final} - U_{initial}$$

(the absolute value of U is impossible to determine)

- \triangleright If the value of ΔU is positive: the system gains energy
- The products have more internal energy than the reactants

- \triangleright If the value of ΔU is negative: the system loses energy
- The reactant have more internal energy than the products
- All energy must be released or gained from the surroundings so: $\Delta U_{system} = -\Delta U_{surroundings}$

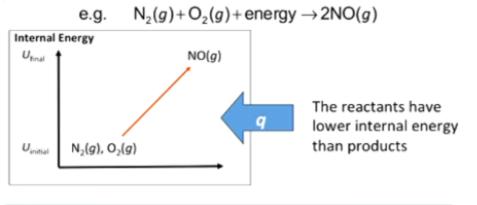
The combustion of methane:



In the combustion of methane the system has lower energy at the end of the reaction-energy has been transferred to the surroundings. **Exothermic reaction**

The First Law of Thermodynamics

Reactions also may cause energy to flow from surroundings to system: endothermic.



In chemical reactions energy is exchanged with the surrounding as either heat(q) or work (w)

ightharpoonup With respect to chemical reactions: the first law can be expressed in: terms of w and q $\Delta U=q+w$

q= heat added to system (q<0 means heat removed)

w= work done on system (w<0 means work by system and is w>0 means the surrounding are doing work on the system)

Important convention

- > Positive work or heat implies that energy of system increases
- ➤ Negative work or heat implies that energy of system decreases