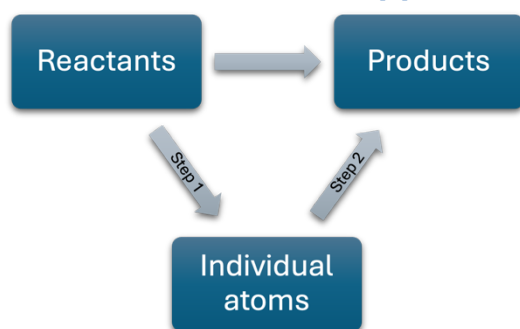


Energy cycles in reactions

A first energetic approach to chemical reactions

1. "LEGO® approach" of a chemical reaction



From an energetical point of view, a chemical reaction can be described as a 2-steps process:

The first step involves an energy input, to break the bonds between atoms of the reactants, thus forming individual atoms. Enthalpy change involved in step 1 is positive.

The second step consists in the creation of new bonds, thus forming the products. It produces energy, which is lost to the environment as heat. Enthalpy change involved in step 2 is negative.

2. Bonding enthalpy

Enthalpy change involved in breaking or forming of covalent bonds is usually called "bonding enthalpy".

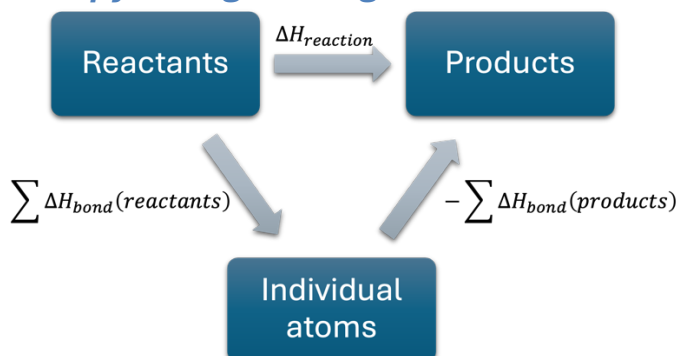
Usually given in $\text{kJ}\cdot\text{mol}^{-1}$, it is defined as the enthalpy needed to break 1 mole of bonds.

Note: Bonding enthalpy as it is defined is positive. When a covalent bond is formed, the change in enthalpy involved has the same value, but is negative.

Bond	Bond Enthalpy ($\text{kJ}\cdot\text{mol}^{-1}$)
C-C	+347
C-H	+413
O=O	+498
O-H	+464
C=O (in CO_2)	+805
C-O	+358
H-H	+436
C=C	+612

Note for later: The bonding enthalpy of a C=C double bond is not equal to the bonding enthalpy of a C-C single bond. This leads to the idea that 1 double bond has to be different of the addition of 2 single bonds.

3. Hess's law: Enthalpy change during a chemical reaction



Hess's law:

$$\Delta H_{\text{reaction}} = \sum \Delta H_{\text{bond}}(\text{reactants}) - \sum \Delta H_{\text{bond}}(\text{products})$$

- If $\Delta H_{\text{reaction}}$ is positive, there is an overall energy output. The reaction is said to be exothermic. The products being lower in energy than the reactants, they are more stable.
- If $\Delta H_{\text{reaction}}$ is negative, there is an overall energy input. The reaction is said to be endothermic. The products being higher in energy than the reactants, they are less stable.
- Sometimes, enthalpy changes in steps 1 and 2 compensate. No overall change in enthalpy occurs. The reaction is then said to be athermic.

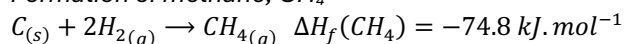
HL: Formation and combustion of a compound

1. Enthalpy of formation of a compound

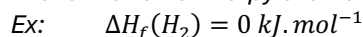
A compound is obtained through the chemical reaction between its elements in a pure stable state.

The change in enthalpy involved in this chemical reaction is the enthalpy of formation, ΔH_f . Its value is usually available in tables.

Ex: Formation of methane, CH_4



Note: The formation enthalpy of an element in its pure stable state is equal to 0.

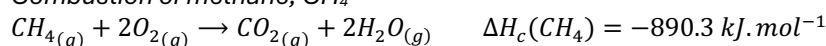


2. Enthalpy of combustion of a chemical

A combustion reaction is a reaction between a chemical and oxygen gas, O_2 .

The change in enthalpy involved in this chemical reaction is the enthalpy of combustion, ΔH_c . Its value is usually available in tables.

Ex: Combustion of methane, CH_4

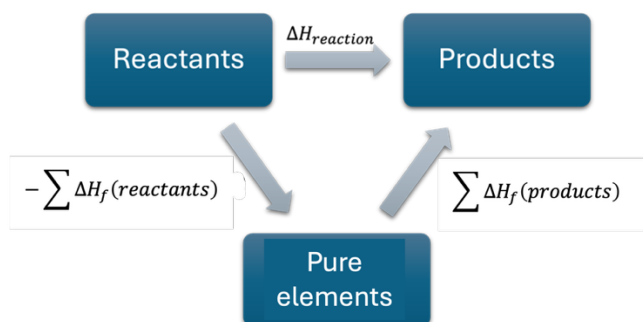


3. Enthalpy of a reaction and enthalpies of formation

From an energetical point of view, a chemical reaction can be described as a 2-steps process:

The first step involves an energy input, to turn the reactants into the pure elements they are issued from.

The second step consists in the formation of the products from the pure elements from step 1. It produces energy, which is lost to the environment as heat.



$$\Delta H_{\text{reaction}} = \sum \Delta H_f(\text{products}) - \sum \Delta H_{\text{bond}}(\text{reactants})$$

Ex: Combustion of methane

$$\Delta H_c(CH_4) = -\Delta H_f(CH_4) - 2\Delta H_f(O_2) + \Delta H_f(CO_2) + 2\Delta H_f(H_2O)$$

$$\Delta H_c(CH_4) = -(-74.8) - 2 \times (0) + (-393.5) + 2 \times (-285.8) = -890.3 \text{ kJ} \cdot \text{mol}^{-1}$$

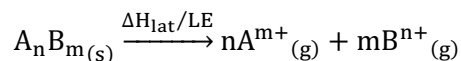
Note: The same can be done with the enthalpies of combustion

$$\Delta H_{\text{reaction}} = \sum \Delta H_c(\text{reactants}) - \sum \Delta H_c(\text{products})$$

HL: Energy in ionic compounds

1. What holds an ionic lattice together?

An ionic compound is a lattice of cations and anions, held together by electrostatic interactions. Using an analogy to the bonding enthalpy, a lattice enthalpy ΔH_{lat} (or LE) can be defined: measured in $\text{J}\cdot\text{mol}^{-1}$, it is the energy needed to separate the lattice into individual non-interacting ions.



2. From atoms to ions

Metal atoms (elements of columns 1 to 13 of the periodic table) are susceptible of losing electrons to form cations.

Ionization energy IE, measured in $\text{kJ}\cdot\text{mol}^{-1}$, is the enthalpy change involved in pulling an electron away from these atoms

Note: Pulling a second electron doesn't involve the same energy than pulling the first electron of an atom. Therefore, we distinguish first ionization energy and second ionization energy.

Non-metal atoms (elements of columns 14 to 17 of the periodic table) are susceptible of gaining electrons to form anions.

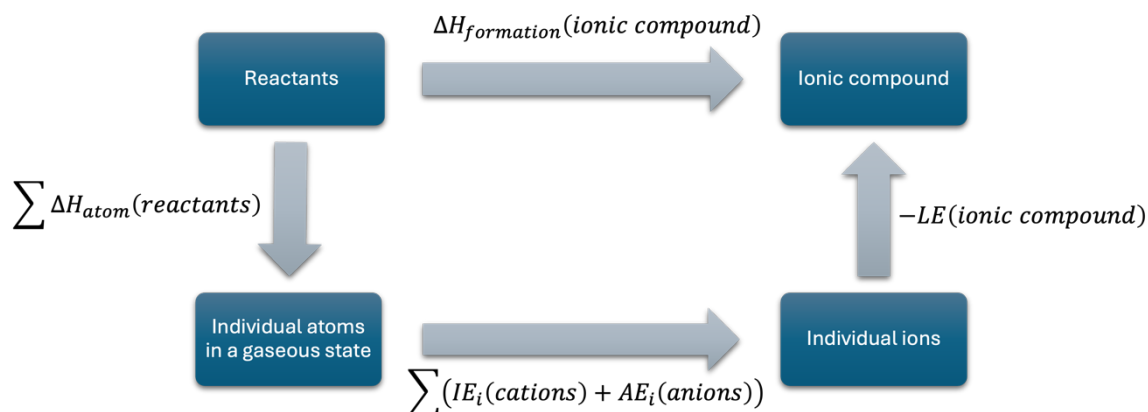
Electron affinity EA, measured in $\text{kJ}\cdot\text{mol}^{-1}$, is the enthalpy change involved in adding an electron to these atoms.

Note: Ionizing a metal atom, turning it into a cation, involves an energy input to go against the natural pull of the nucleus on the electrons $\Rightarrow \text{IE} > 0$.

Ionizing a non-metal atom, turning it into an anion, benefits from the natural pull of the positively charged nucleus on the negatively charged electron. This leads to an energy output $\Rightarrow \text{EA} < 0$.

3. Born-Haber cycle

Forming an ionic compound from the initial elements can be modelised by a Born-Haber cycle:



Step 1: Atomization of the elements: They are turned into individual non-interacting atoms (thus in gaseous form). This involves bonding enthalpy and/or change of state enthalpy

Step 2: Ionization of the atoms. This involves Ionization Energy and Electron Affinity.

Step 3: Interaction between the ions to form the lattice. This involves Lattice Enthalpy.

Note: Lattice enthalpy is a value that cannot be measured experimentally, unlike the other data involved (including the enthalpy of formation of the ionic compound).

The main purpose of using a Born-Haber cycle is therefore to determine the lattice enthalpy of an ionic compound.