

Les molécules

TP 4

Objectifs

- ★ Containers manipulation
- ★ Iterator manipulation

Practical preparation

- A set of unit tests is provided in the folder `tests`, you can compile them with `make testcase`. The tests are using the library `doctest`, to learn more you can go on the project website <https://github.com/doctest/doctest>.
- The practical must be put on moodle at the end of the practical. It could be updated until the day before the next practical.

Concept

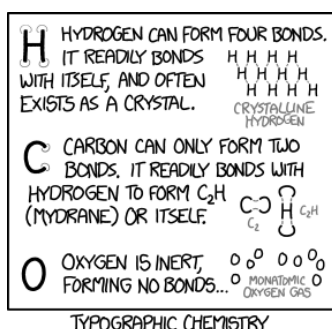


Figure 1: These are all sans-serif compounds. Serif compounds are dramatically different and usually much more reactive.xkcd

1 Normalisation of a molecule form

A chemical molecule is an assembly of individual elements (atom). Each molecule can be written in exploded form: H-O-H , O-Nb-O-Nb-O or in normal form: H_2O , Nb_2O_3 . The exploded form is therefore a sequence of atoms separated by dashes. In normal form, the atoms are grouped by name and arranged in alphabetical order. The aim of the exercise is to write a function to transform an exploded form into a normal form. normal form.: H_2O , Nb_2O_3

1. Write a class `Molecule` that has an attribute containing all its atoms in exploded form.
2. Write the constructor that creates, from a character string representing a molecule in exploded form, a vector of `std::string` representing the same exploded form. For example, the function will give the vector `[O;Nb;O;Nb;O]` from the molecule O-Nb-O-Nb-O . Test this construction with the molecules in the file `"molecules.txt"`.

3. Write a method `std::string normalise() const` which creates, from the atom vector, the molecule's normal shape. This function must :

- sort atoms by name
- count the occurrences of each atom in the molecule

`res_normalisation.txt`.

4. Test this function with the molecules in the file `"molecules.txt"`. Display the result of the normalized form of each of the molecules in a file `res_normalisation.txt`.

2 Chemical reaction normalisation

We now wish to standardize the writing of chemical reactions given in exploded form. For example, the reaction $\text{Na-O-Na} + \text{H-O-H} \rightarrow \text{Na-O-H} + \text{Na-H-O}$ will be normalized to :



1. Write the class `Reaction` which has two attributes corresponding to the set of atoms on the left and the set of atoms on the right of the reaction.
2. Write the constructor creating, from a character string representing an equation in exploded form, two vectors "left" and "right" and "right" vectors containing, respectively, the list of molecules to the left and right of the arrow.
3. Write a method `std::string normalise() const` transforming a reaction given in exploded form into a normalized reaction. Test your function on the file `"reactions.txt"`. Display the result of the normalized form of each molecule in a file `res_reactions.txt`.

Bonus

Overload the outgoing flow operator (`operator<<`) for the two preceding classes.