Chemical reactions & the reasoning system in chemistry.

① Empirical observations of reactivity (upto the end of 18th century)

$B_1 \sim B'_1$

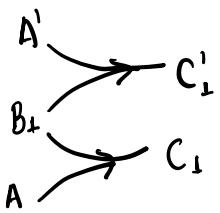
$A + B_1 \to C_1$ ⋮ $A + B_n \to C_n$

$A' + B'_1 \to C'_1$ ⋮ $A' + B_n \to C'_n$

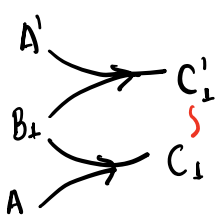
Two chemical substances A & A' are similar if

Hilb.

They react with the same substances:



If they react with the same substances to produce similar substances C_1 & C'_1



$A \sim A'$ if they react with similar substances to produce similar substances C_+ & C'_+

$$A' \in [A] \iff B'_i \in [B_i] \;\&\; C'_i \in [C_i] \;\forall i \leq n.$$

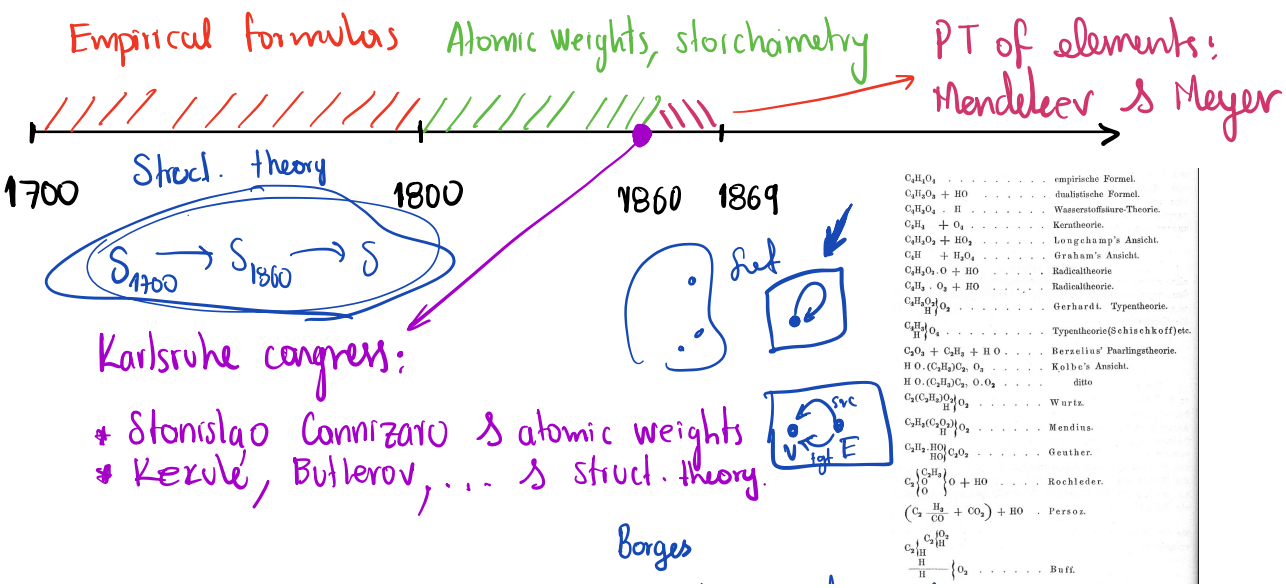
you: What?

Chemists: oh, yeah! Will produce and characterize substances using this similarity principle!

Will call it "Marcha analítica". A generalized form of Voreula.

Several attempts to formalize this similarity & affinity principles (mainly from physics) failed.

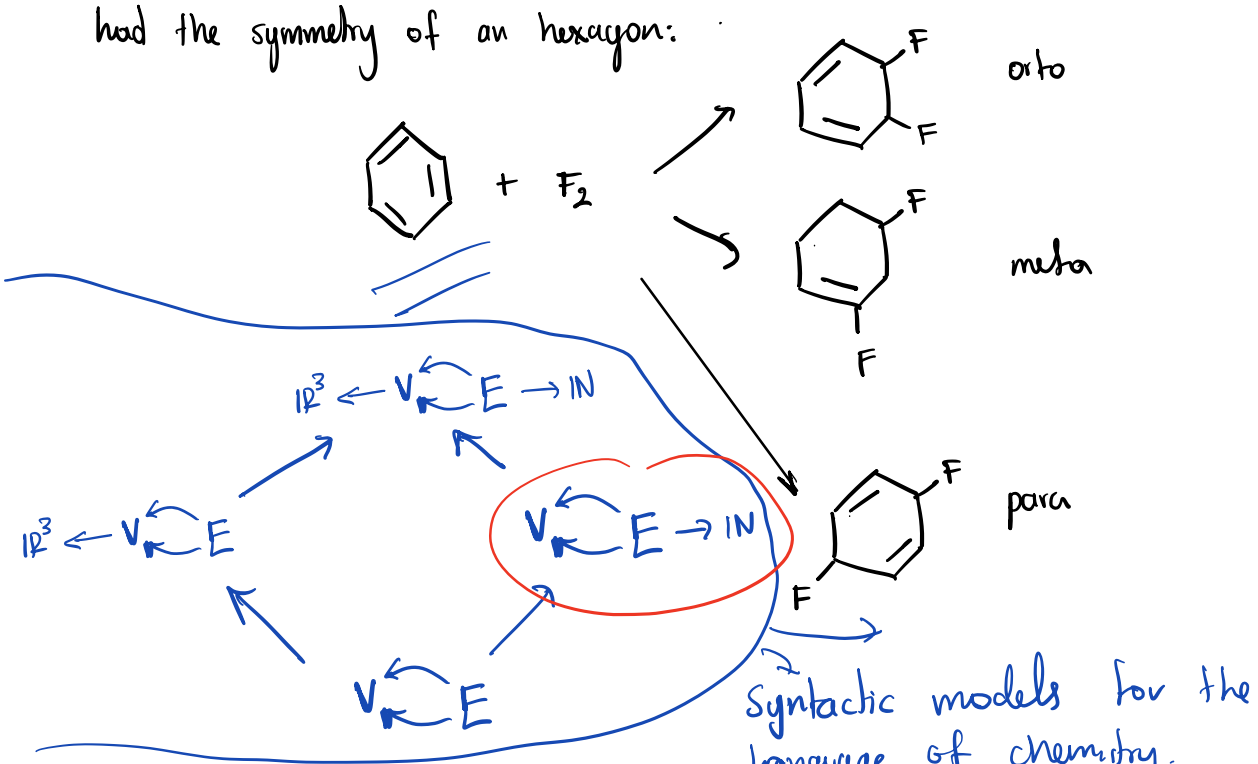
② Empirical formulas, stoichiometry & first glance at the structure of matter



La biblioteca de Babel.

~ 1864: Atoms occupy a fixed position in molecules & are respons. for properties.

③ Trying to explain the number of products obtained by substitution reactions of benzene, Kekulé realized that such reactivity pattern had the symmetry of an hexagon:

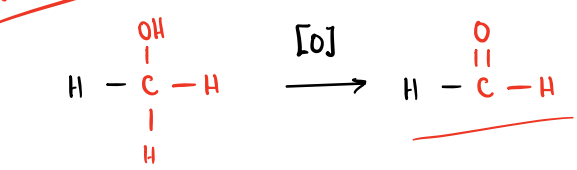


Syntactic models for the language of chemistry.

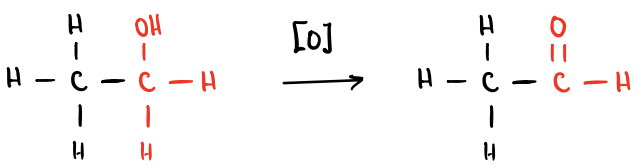
* substances are chemically similar if they undergo similar reactions.

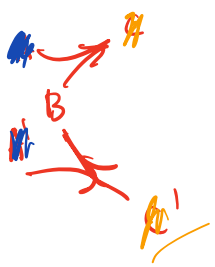
alcohols

$A \in [A']$ because they share their functionalities.



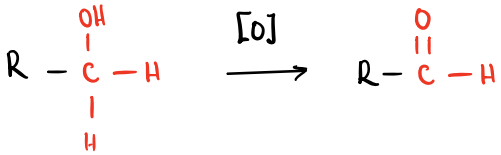
bond order.





Certain arrays of atoms determine the similarity & affinity relation

* Reaction occur because of the presence of functional groups



Primary alcohol Aldehyde.

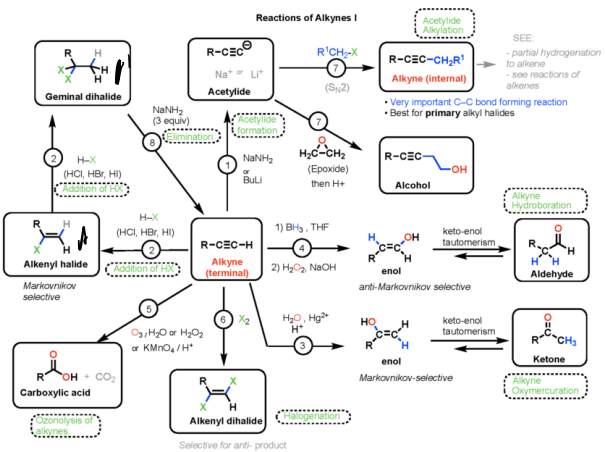
Primary alcohols are substances that react in a similar fashion because they share functional groups.

$A' \in [A] \iff B_i \in [B_i]$ & $C_i \in [C_i] \; \forall i \leq n$.

- Ethanol oxidates into Aldehydes

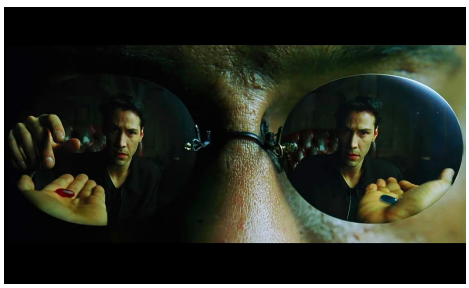
Ethanol $\in$ [methanol] = Alcohols $\iff$ ⋮

Chemistry is therefore a grammar of molecular structures & the rules of this grammar are given by an affinity relation (algebra of functional groups).



Although chemists have used these informal ideas, a formal model of this system is still missing.

④ Red pill or blue pill ?



(4.1) The set-point topology solution: Substances, functional groups & Galois connections.

$$\varphi : 2^{S} \longrightarrow 2^{FG} \qquad \psi : 2^{FG} \longrightarrow 2^{S}$$

$$cl := \psi \circ \varphi : 2^{S} \longrightarrow 2^{S}$$

Data needed:

- S
- FG
- which functional groups belong to which substances:

$$R \subseteq S \times FG$$

φ & ψ via polarities:

$$\varphi : 2^{S} \longrightarrow 2^{FG} \qquad \psi : 2^{FG} \longrightarrow 2^{S}$$

$$A \longmapsto \varphi(A) = \{f \in FG : \forall a \in A, aRf\} \qquad B \longmapsto \psi(B) = \{a \in A : \forall f \in B, aRf\}$$

$$cl := \psi \circ \varphi : 2^S \longrightarrow 2^S$$

Takes a set of substances and gives back a class of similar substances.

Example: If $A \in 2^S$ with $A = \{\text{Ethanol}, \text{Methanol}\}$, then

$cl(A) =$ Alcohols.

ψ & φ form a Galois connection & their composition yields two operators that determine, simultaneously, the similarity classes on S & FG.

$$cl := \psi \circ \varphi : 2^S \longrightarrow S^S \qquad \text{Int} : \psi \circ \varphi : 2^{FG} \longrightarrow 2^{FG}$$

Closure operator — Interior operator

(4.2) Molecules are not points, but what are they? The syntax of chemistry.

What can be represented?

* strings (substance prediction via machine learning)
* Graphs (V, E)
* Copresheaves $F : C \longrightarrow Set$

Syntax of chemistry

M.S.

$V = \{C_1, \ldots, C_6, H_1, \ldots, H_6\}$

$E = \{e_1, \ldots, e_5\}$

$E \xrightarrow{f} \mathbb{N}$

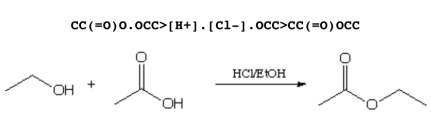
$e_1 \longmapsto f(e_1) = 1$

$e_2 \longmapsto 2$

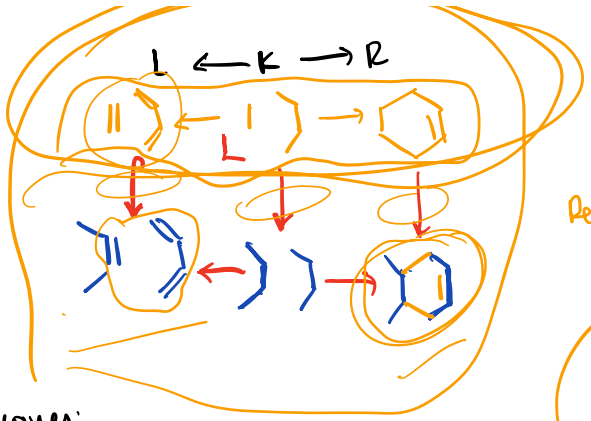
$e_3 \longmapsto 1$

(4.3) chemical reactions and molecular rewritting:

* Strings



* Graphs

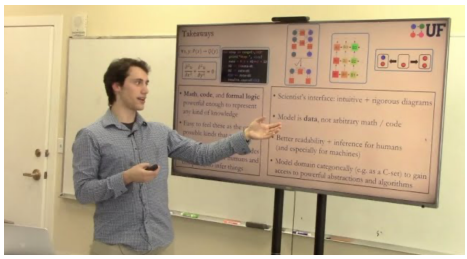


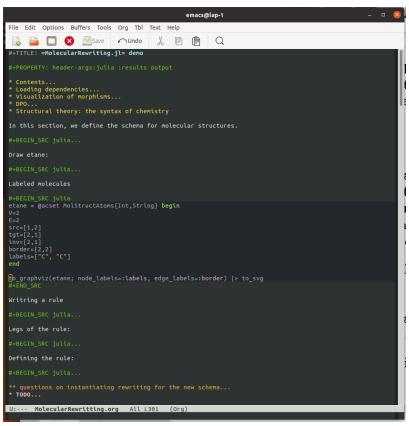
- Copresheaves:

  Data:

  - Substances: $S \subsetneq \{ F: C \to Set \}$
  - Reactions: There is a reaction from $A \subseteq S$ to $B \subseteq S$ if there is a rule $L \leftarrow K \rightarrow R$ that can be applied to A to produce B.
  - Synthetic path: reaction composition / rule composition

(44) Florida: Sun, gators & ACset rewritting.


Takeaways
• Math, code, and formal logic
• Scientist's interface: intuitive + rigorous diagrams
• Model is data, not arbitrary math / code
• Better readability + inference for humans (and especially for machines)
• Model domain categorically (e.g. as a C-set) to gain access to powerful abstractions and algorithms


emacs@iap-1
File Edit Options Buffers Tools Org Tbl Text Help
#+TITLE: =MolecularRewritting.jl= demo
#+PROPERTY: header-args:julia :results output
* Contents...
* Loading dependencies...
* Visualization of morphisms...
* SPO...
* Structural theory: the syntax of chemistry
In this section, we define the schema for molecular structures.
#+BEGIN_SRC julia...
Draw etane:
#+BEGIN_SRC julia...
Labeled molecules
#+BEGIN_SRC julia
etane = @acset MolStructAtoms{Int,String} begin
V=2
E=2
src=[1,2]
tgt=[2,1]
tbv=[2,1]
border=[2,2]
labels=["C", "C"]
end
to_graphviz(etane; node_labels=:labels, edge_labels=:border) |> to_svg
#+END_SRC
Writring a rule
#+BEGIN_SRC julia...
Legs of the rule:
#+BEGIN_SRC julia...
Defining the rule:
#+BEGIN_SRC julia...
** questions on instantiating rewriting for the new schema...
* TODO...
U:--- MolecularRewritting.org All L301 (Org)