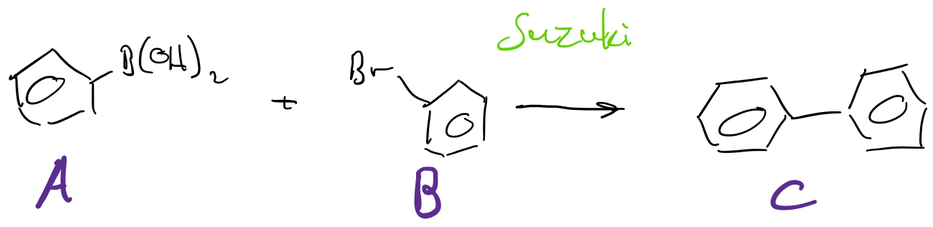
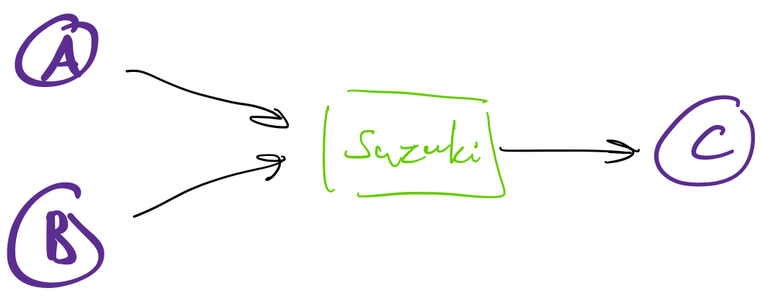
20210610 Reaction templates

Thursday, June 10, 2021 12:19 PM

→ "scale" vs "mols"





* 1. scale(A) = 1 mmol ⇒ StepScore: mols(A), mols(B)

2. RxnTemplate(A,B) ⇒ mols(A), mols(B) → StepScore

↳ scale ⇒ update { A → mols(A); B → mols(B)

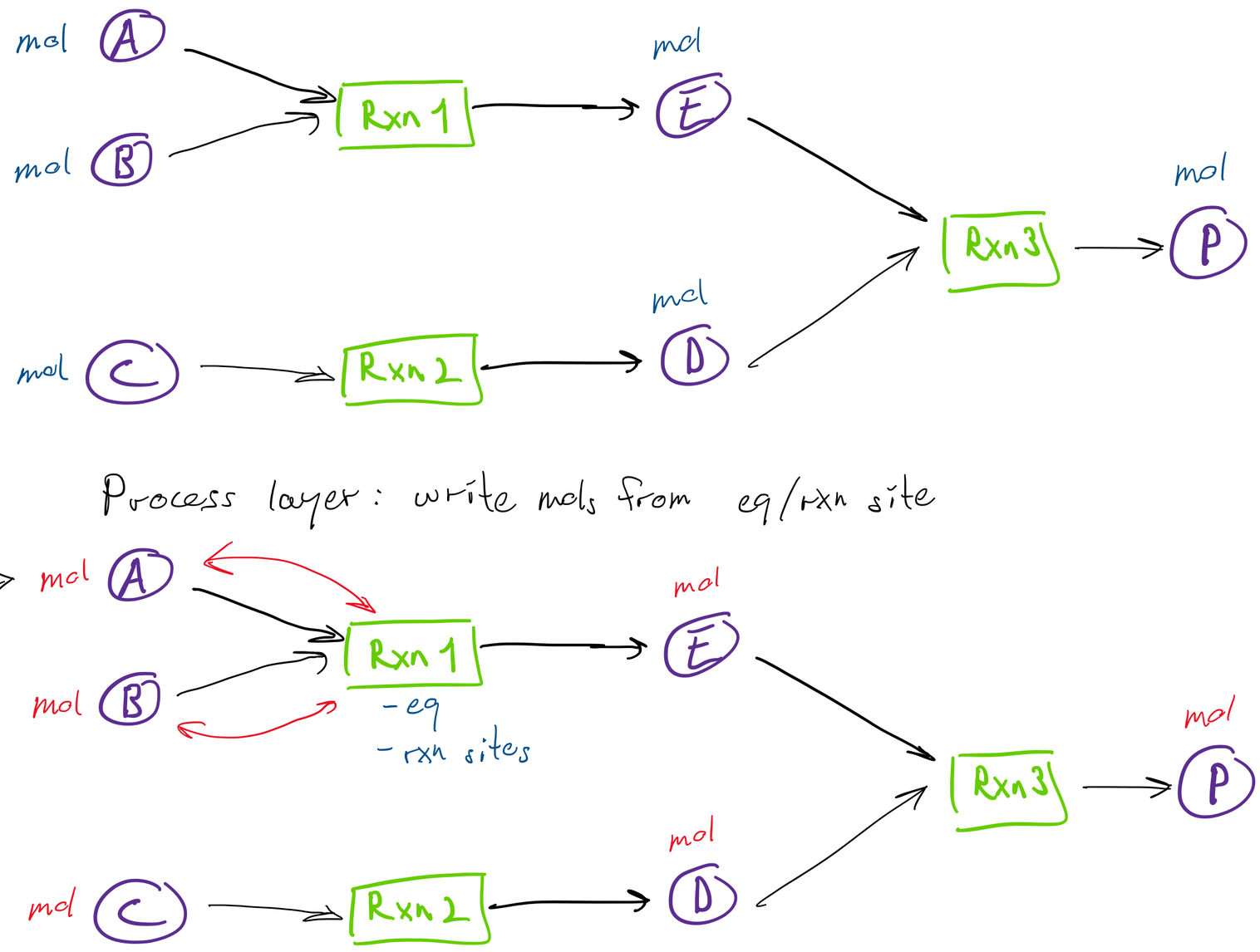
3. RxnTemplate creates Rxn

input { mols(A); mols(B) } → update { A; B } → StepScore

Base layer: calculate RS

already stored

write new value



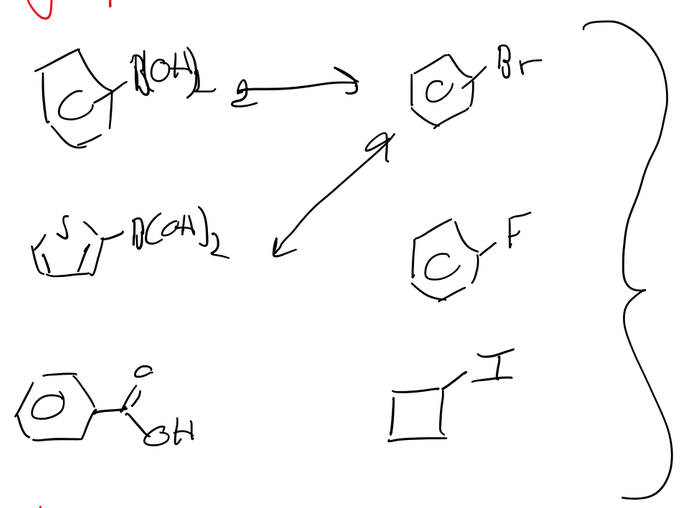
Process layer: write mols from eq/rxn site

Rxn Template: + dict of substructs

$c\text{-}B(OH)_2 + Br\text{-}c \longrightarrow c\text{-}c$

(· eq
· t_H, t_H, etc.
· yield
(· rxn sites)

* Building graph from scratch



↳ Ask Théo about FragChem

create rxn nodes

Rxn1

Rxn2