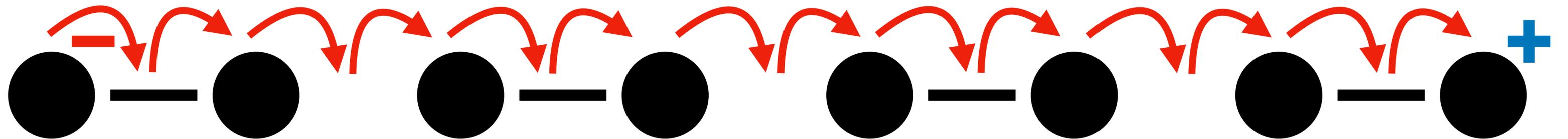


Pushing Electrons from Positive to Negative Partial Charge

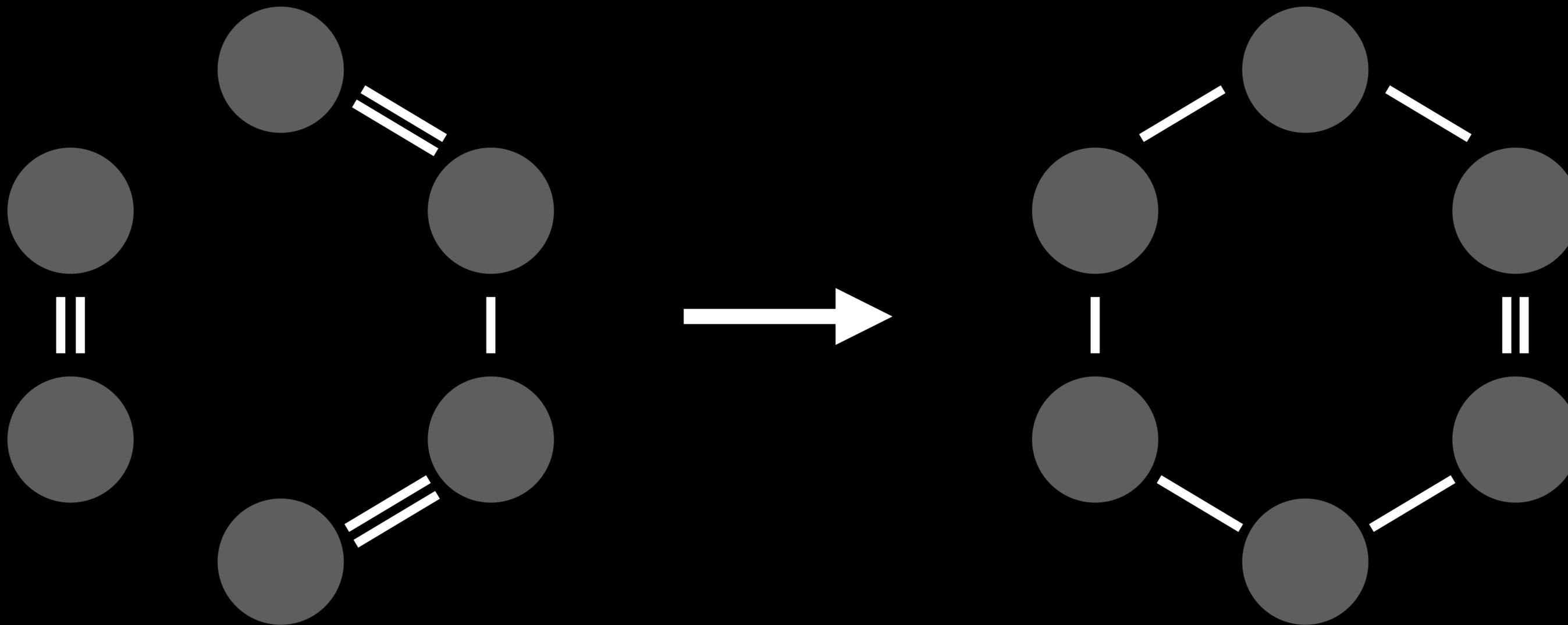
By Mikkel Boger Posselt

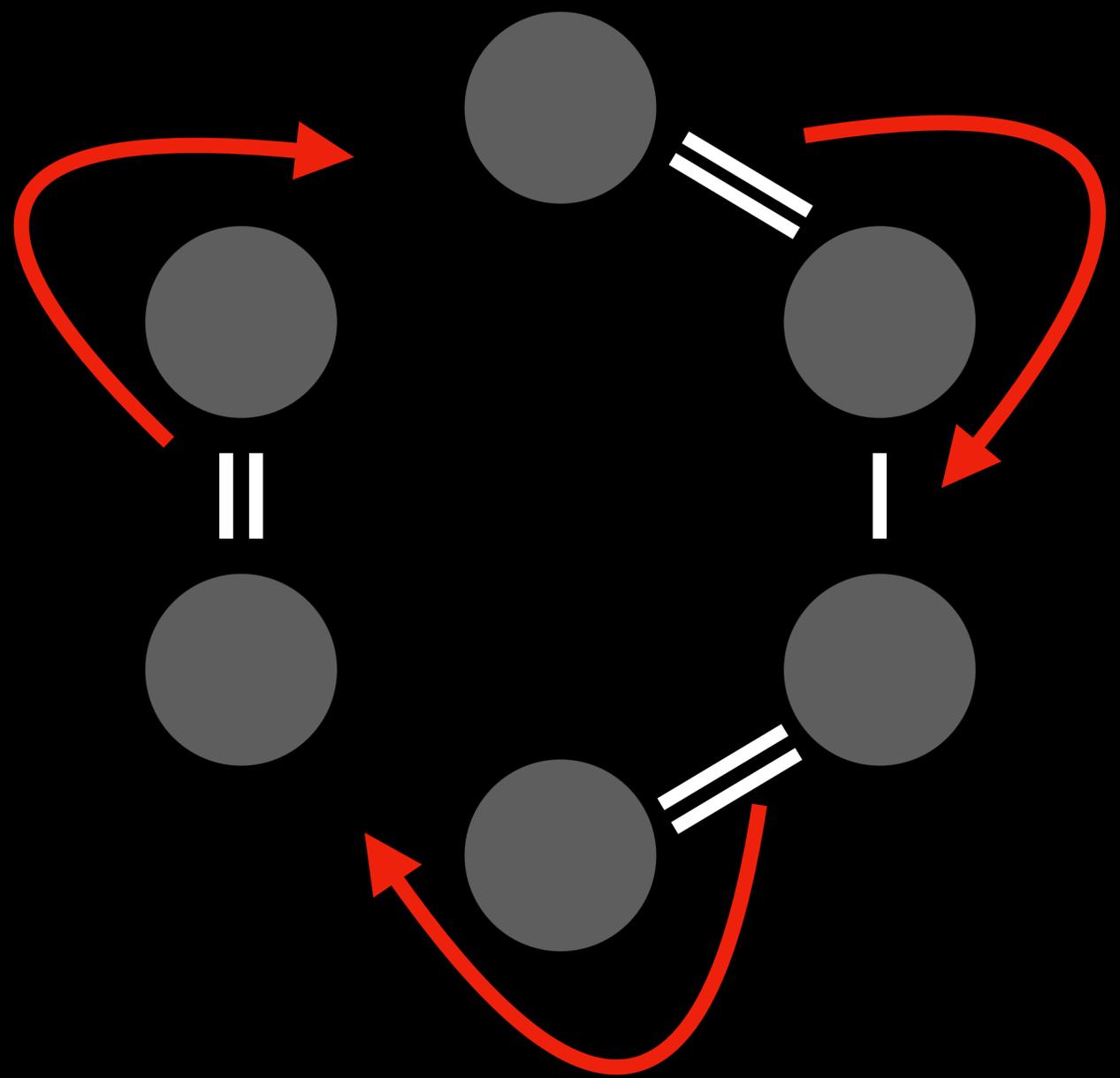


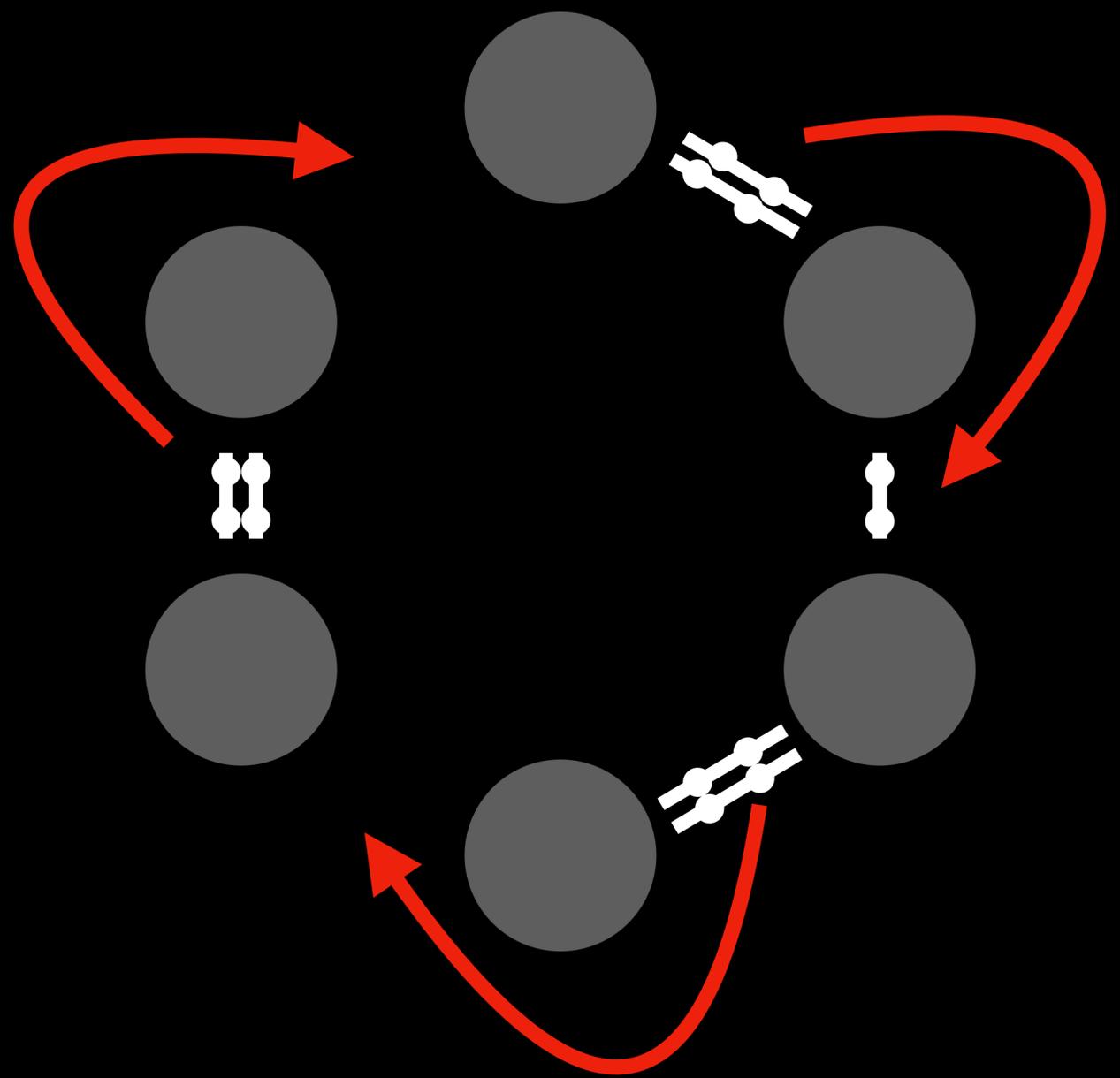
As a Computer Scientist...

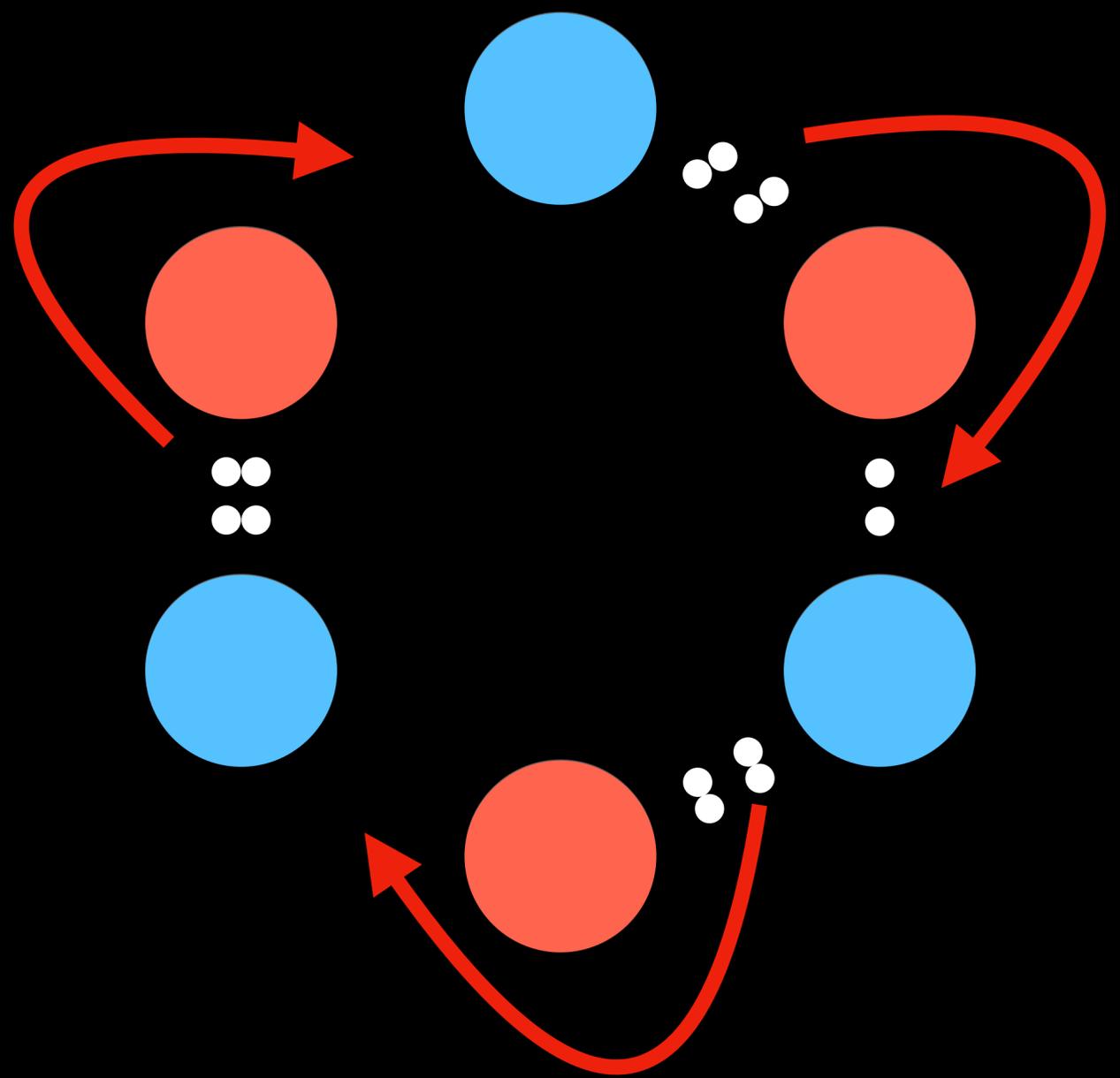
...what even is partial charge?

...and electrons?









Constraint of Chemical Reactions

“Electrons will be pushed from atoms with a lower partial charge, to atoms with a higher partial charge”

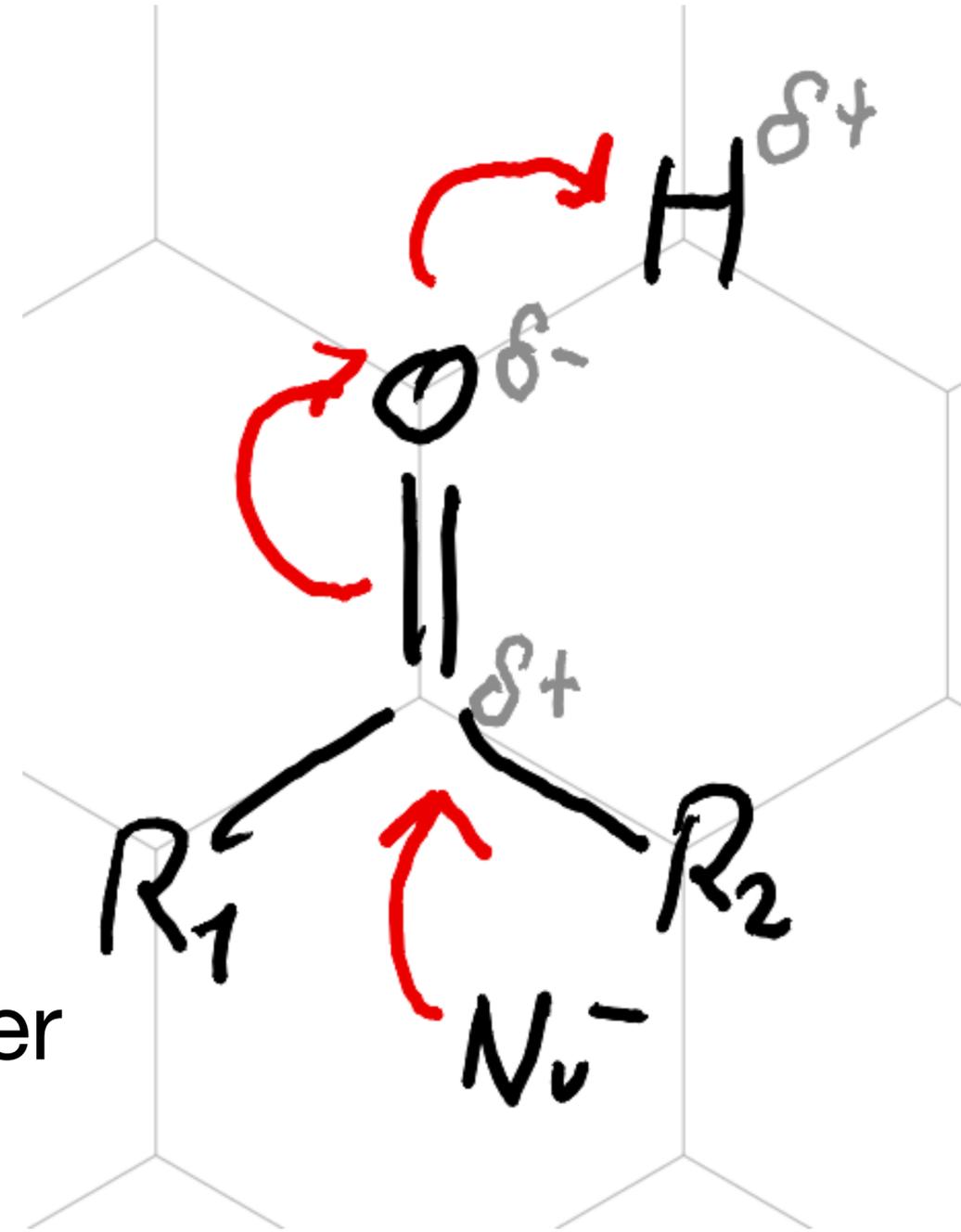
Our Expectation

- There is a counterexample such that an electron will be pushed from **more positive** to **more negative** partial charge.
- If such an example exists then partial charges do not limit electron pushing diagrams

Where to begin?

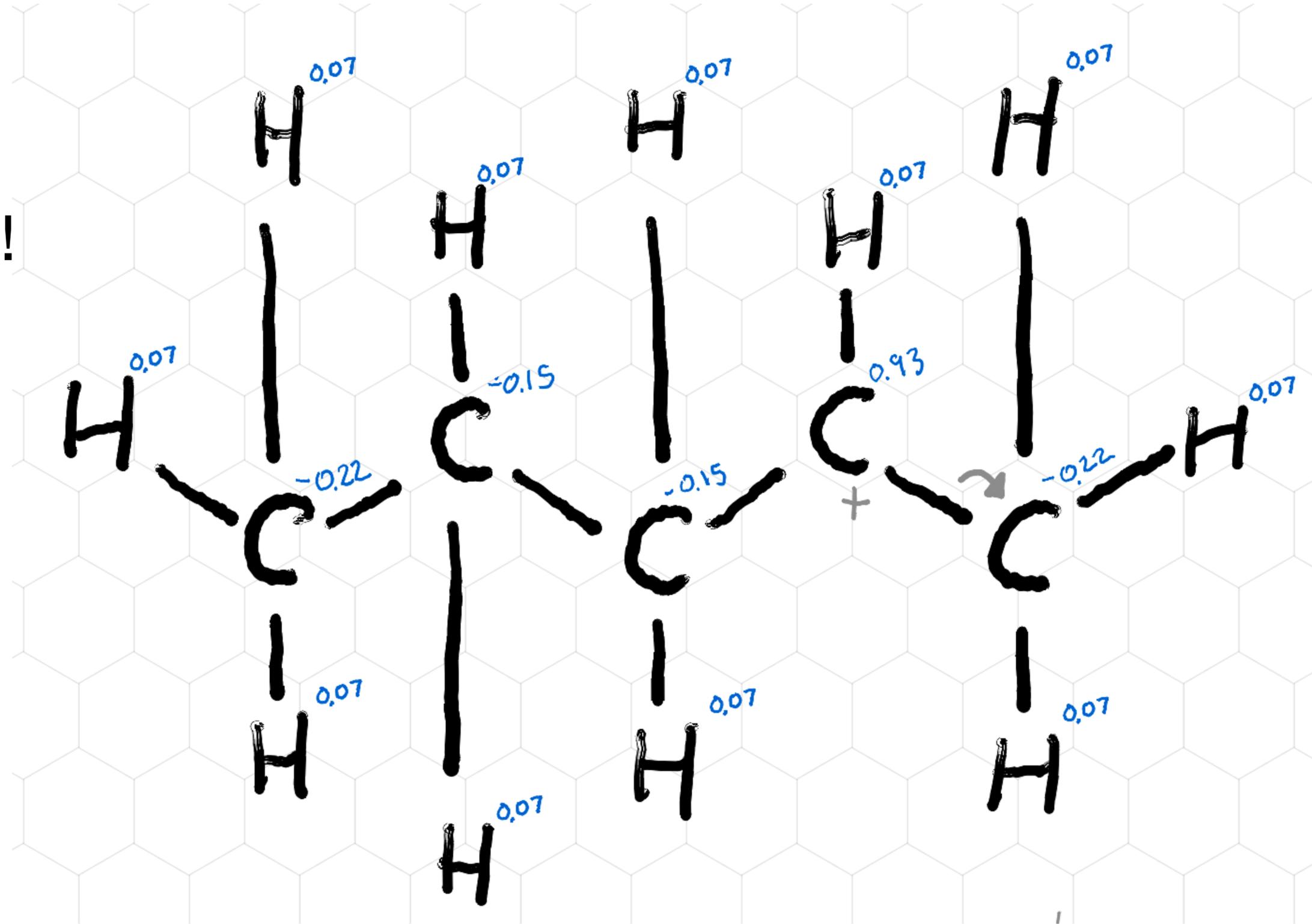
Nucleophilic Reactions

- Not too much time spent here
- Formal charges add limitations
- Or Functional groups have a clear order

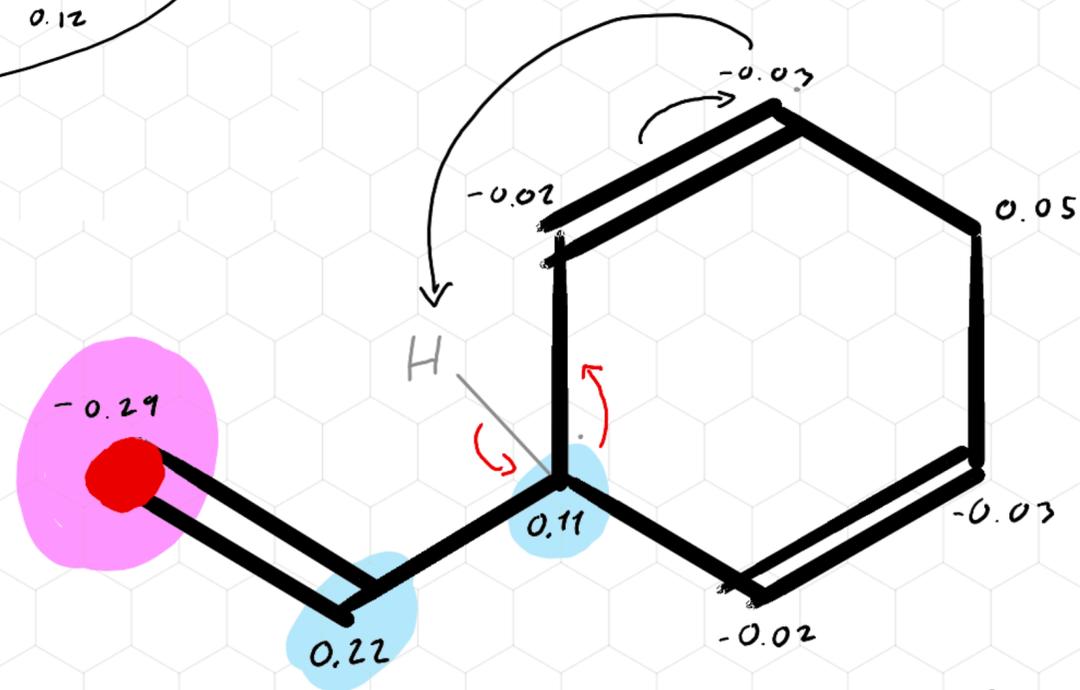
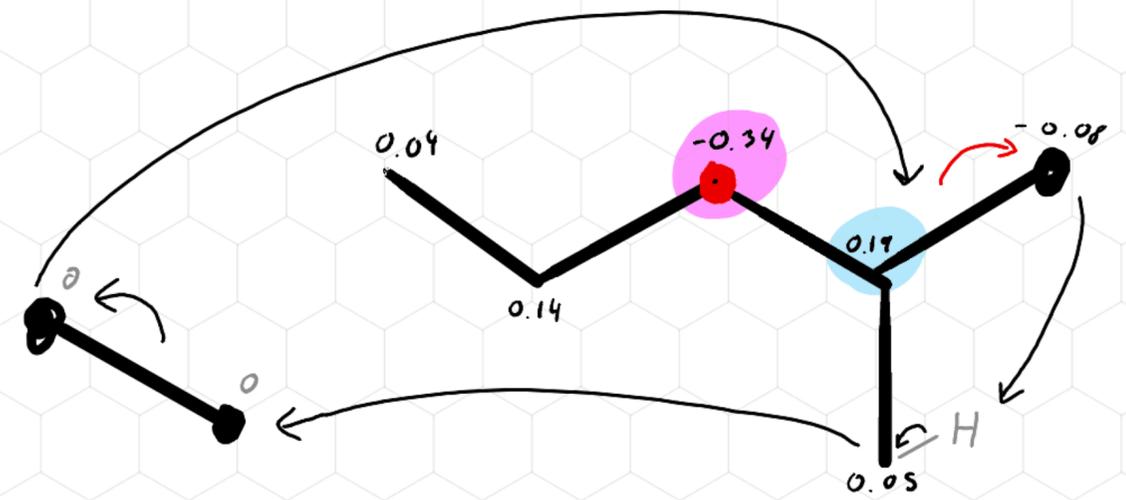
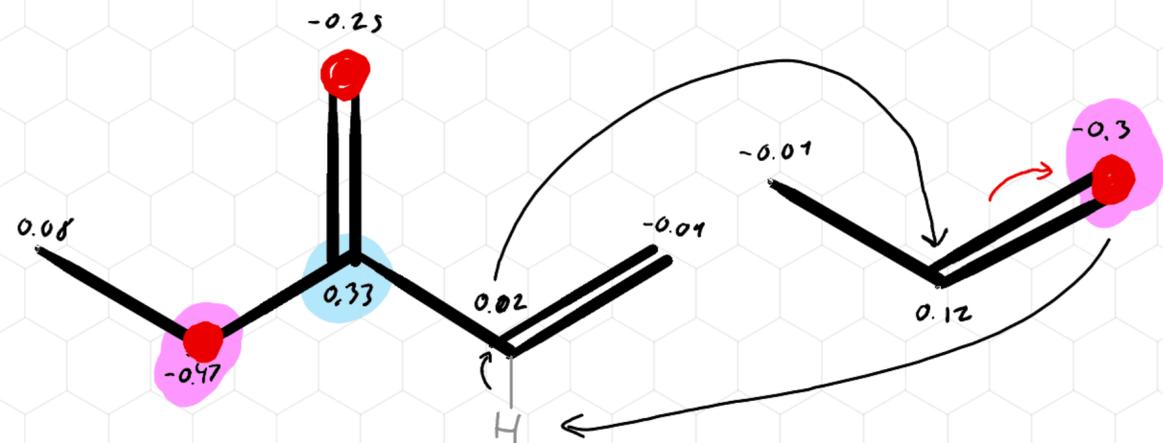
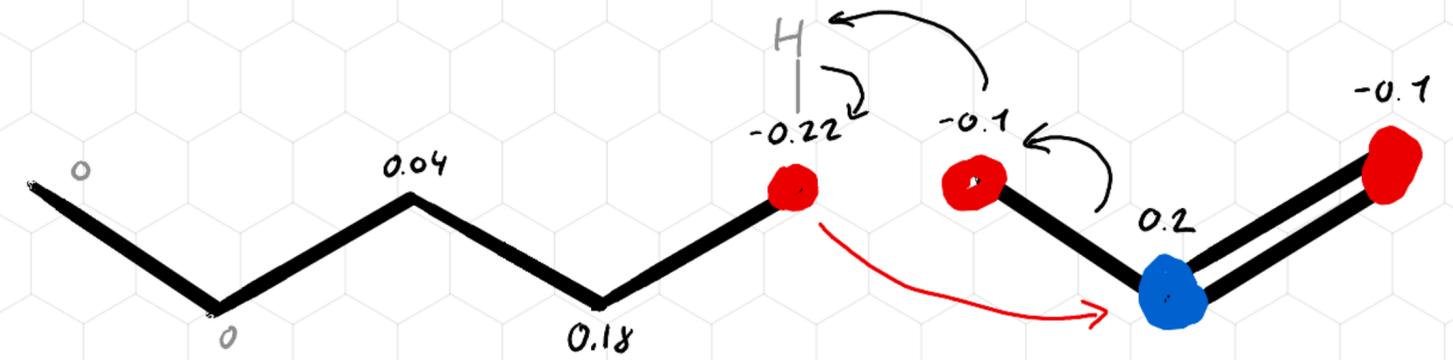
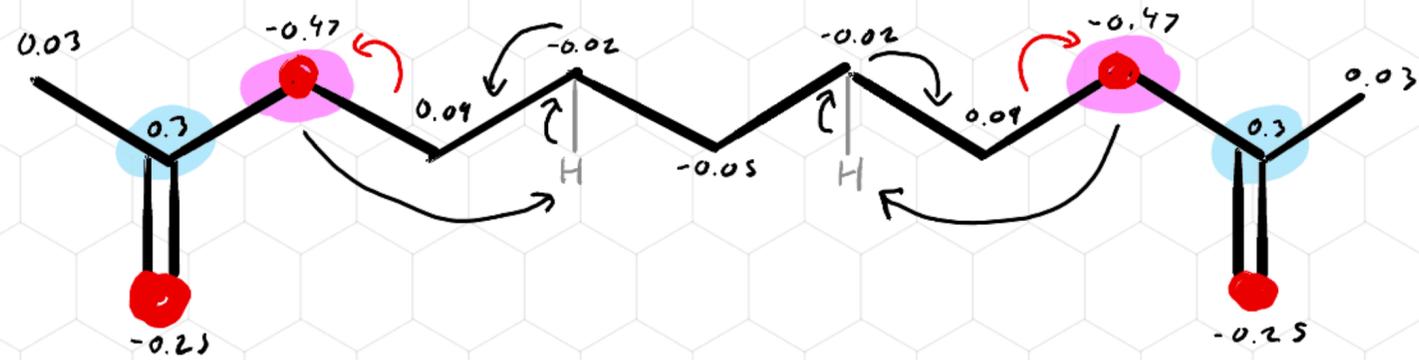


Fragmentation Reactions

- Breaks Constraint!
- Unnatural
- EPDs tell half the story

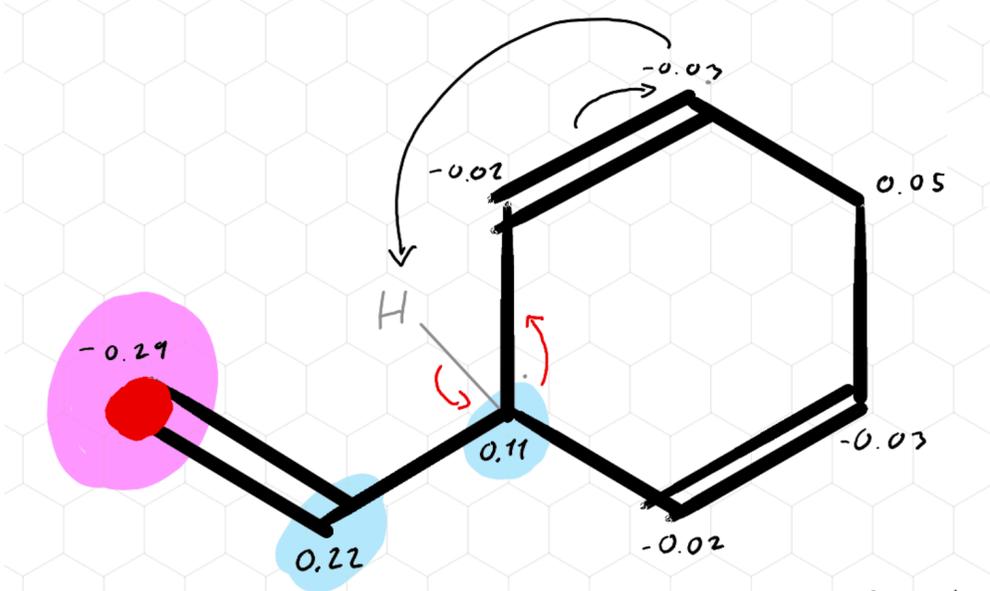
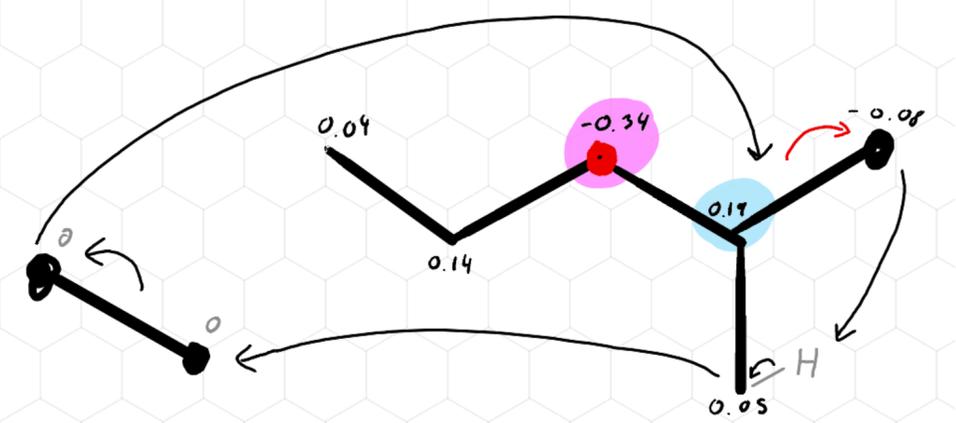
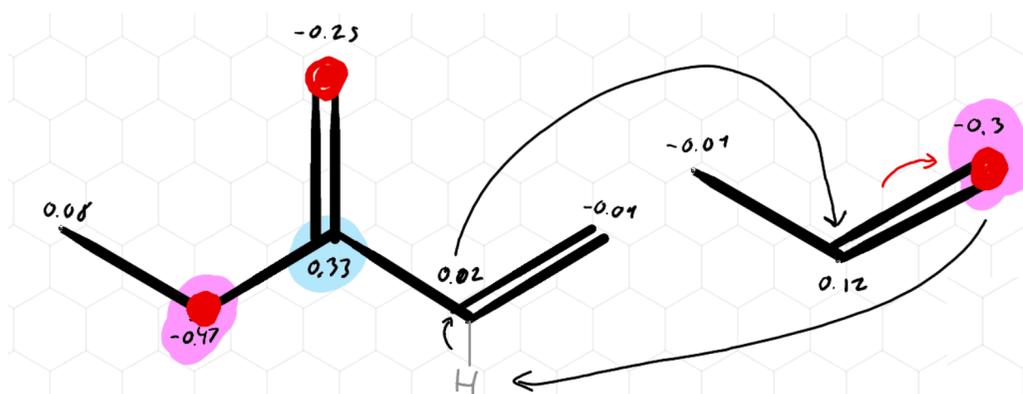
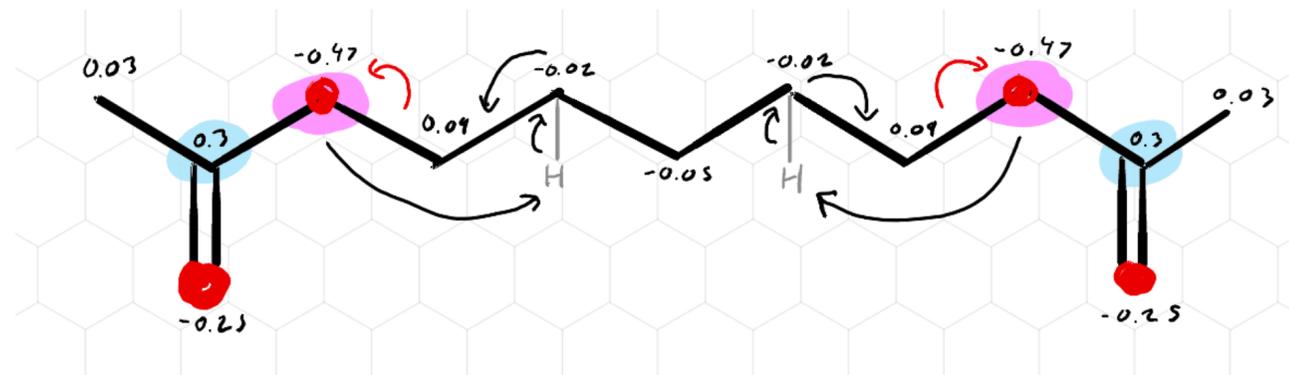


Carbon Rearrangement Reactions



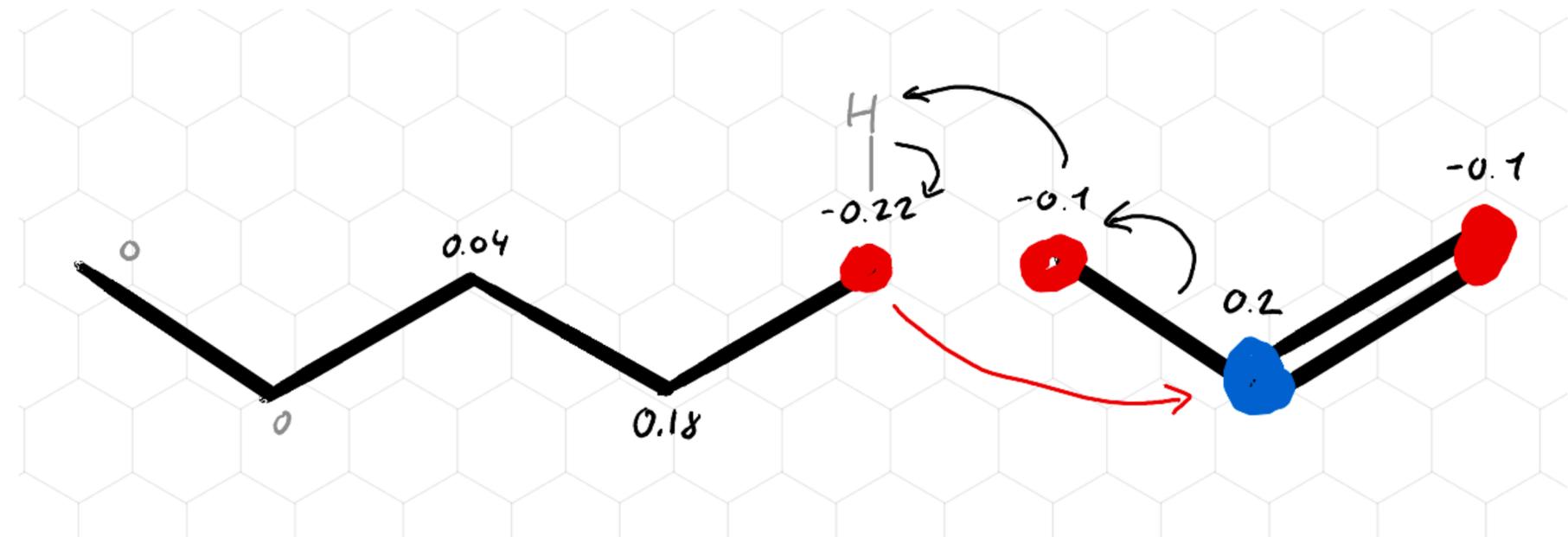
Results

- 4 of the 5 EPDs break the established constraint.
- Only initially
- After that a formal negative charge is pushed.



What about the last one?

- It can be altered to also break constraint.
- This changes the order.
- What is the correct order?



What is “correct” order

- We used partial charges to locate a starting point
- Usually this is done with functional groups.
- Mostly all reaction mechanisms are estimations.

Conclusion

- Our expectation does occur but only initially
- It acts as a way to initialize reactions
- Will only occur once if at all
- Depends on the starting point of the reaction

THANK YOU

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- Bierinformatik Group



TACsy

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