

# Exercise Session 8 IESM Fall 2024-2025

Salomé, Junwu, Qihao, Yuri, Andrea, Sophia

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#### Course Reminders

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- Exercise 8 interview will be next week (Dec 9) and exercise 9 will not have interviews and will have due date **31**. **January**
- We only keep the best 8 grades out of the 9 reports : )
- Feel free to contact us via email or forum for questions about Ex8 and Ex9!



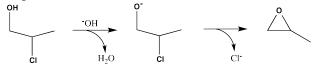
# Exercise 8 Finding transition states

In this set of exercises, we will learn how to traverse the potential energy landscape in interesting directions toward transition states.



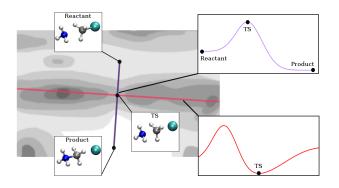
## Reaction Mechanisms & Stereochemistry

- The formation of propylene oxide takes place in a couple of steps
- Nucleophilic substitution occurs, binding O to C, and removing Cl- (leaving group)
- What is the name of such a mechanism and what is the orientation of O with respect to Cl as the ring begins to form?
- What might possible trnasition states look like as the ring begins to form?





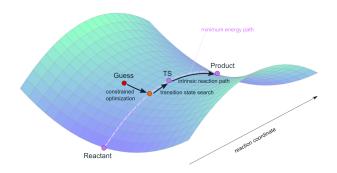
## Minimum Energy Path



 We need to find stationary points, for TS we need the Hessian with exactly one negative eigenvalue.



#### Intrinsic Reaction Path



- You do not need to run all notebooks! We provide some data to you (we are the "colleague" in this case) while writing out the code if you're interested.
- Read instructions carefully on how to generate a "guess" transition state
- Calculations may take time, please don't be alarmed!
- Notebooks are named Ex 9 based on past ordering, but this is Ex 8