

# Exercise Session 8

## IESM Fall 2024-2025

Salomé, Junwu, Qihao, Yuri, Andrea, Sophia

December 3, 2024

# Course Reminders

## Course Reminders:

- 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.

### Learning goals

- Understand how to navigate the PES to transition states
- Visualize chemical reactions

### Chapter in script

Not in script but of practical relevance

### Resources

Frank Jensen - Computational Chemistry  
Ch12.8 p.416ff

# Reaction Mechanisms & Stereochemistry

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



# Tips

- 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