

# Exercise Session 8

## IESM Fall 2024-2025

Salomé, Junwu, Qihao, Yuri, Andrea, Sophia

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## 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 !

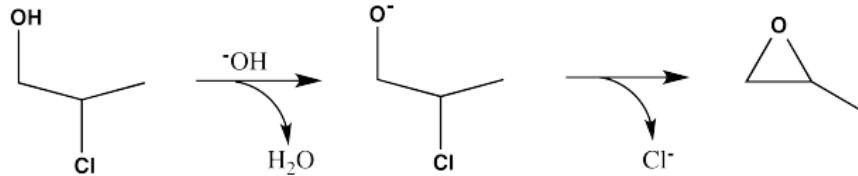
## Exercise 8 Finding transition states

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

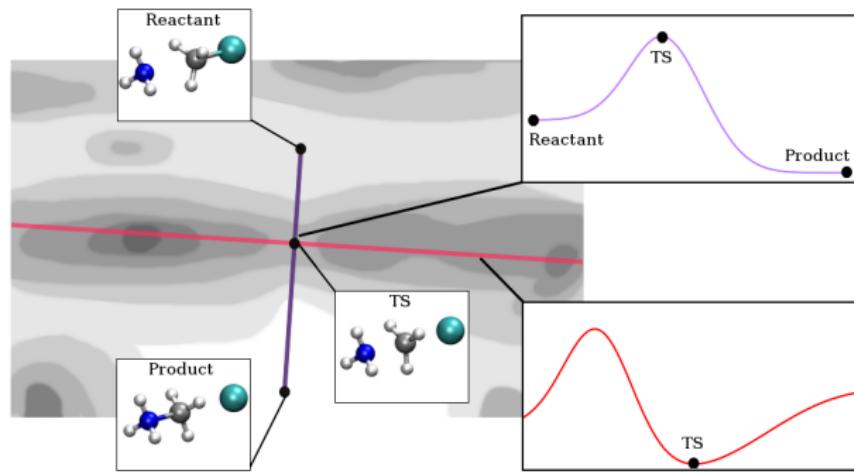
|  Learning goals   |  Chapter in script |  Resources |
|--|---|---|
| <ul style="list-style-type: none"><li>• Understand how to navigate the PES to transition states</li><li>• Visualize chemical reactions</li></ul> | Not in script but of practical relevance  | Frank Jensen - Computational Chemistry<br>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 Cl<sup>-</sup> (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 transition states look like as the ring begins to form?

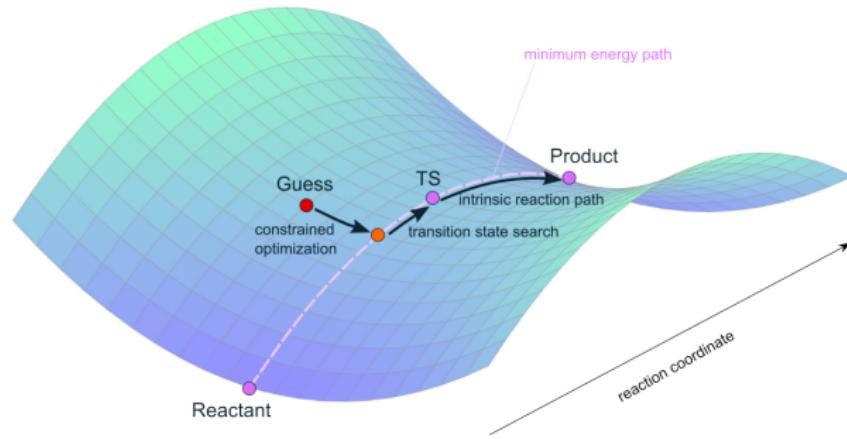


# Minimum Energy Path



- 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