Exercise Session 8

IESM Fall 2023-2024

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Course Reminders

Course Reminders:

- Exercises 8 and 9 will not have interviews and will have due date **31. January**
- Plus, we only keep the best grades of 8 of 9 reports :)
- Feel free to contact us via email or forum for questions about Ex8 and Ex9 !

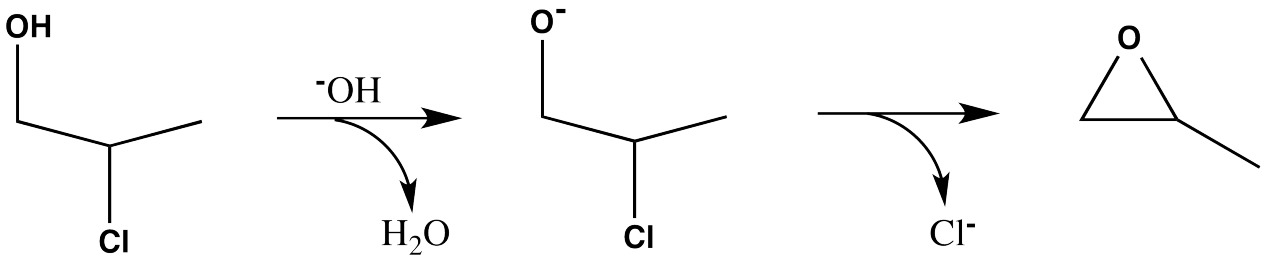
Exercise 8 Finding transition states

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

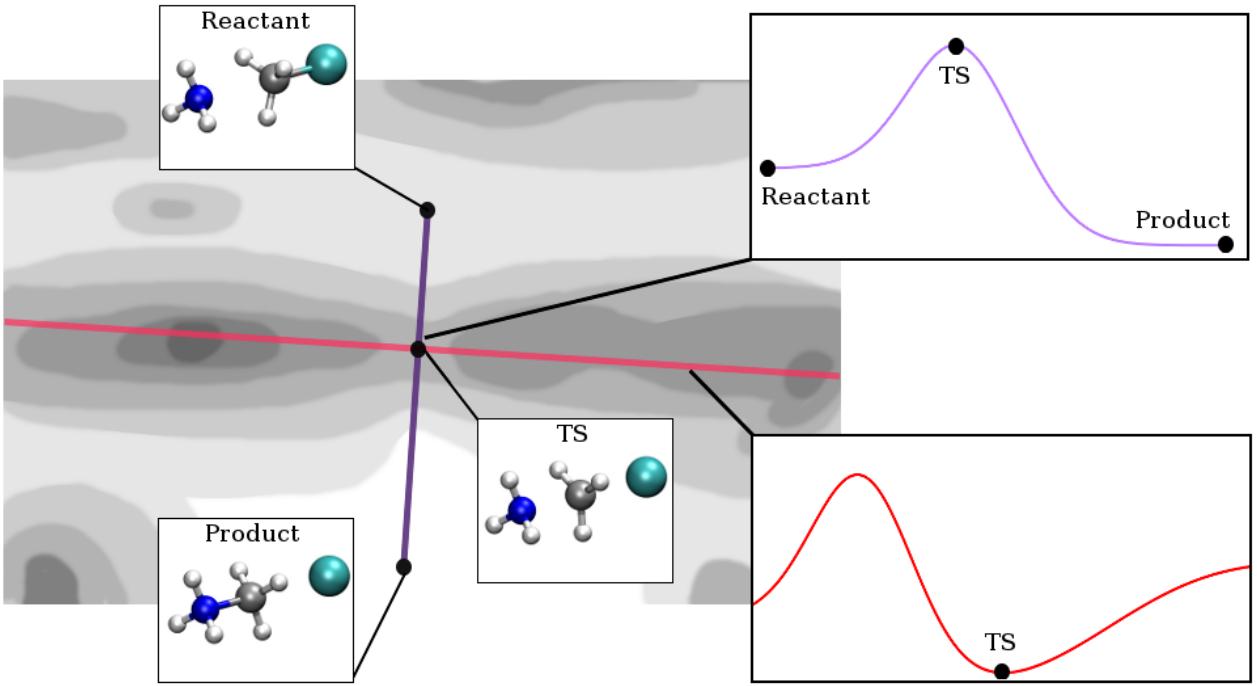
🎯 Learning goals	📖 Chapter in script	📚 Resources
• Understand how to navigate the PES to transition states • Visualize chemical reactions	Not in script but of practical relevance	Frank Jensen - Computational Chemistry Ch12.8 p.416ff

Reaction Mechanisms & Stereochemistry

- The formation of propylene oxide takes place in a couple of steps
- Nucleophilic substitution occurs, binding O to C, and removing 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?

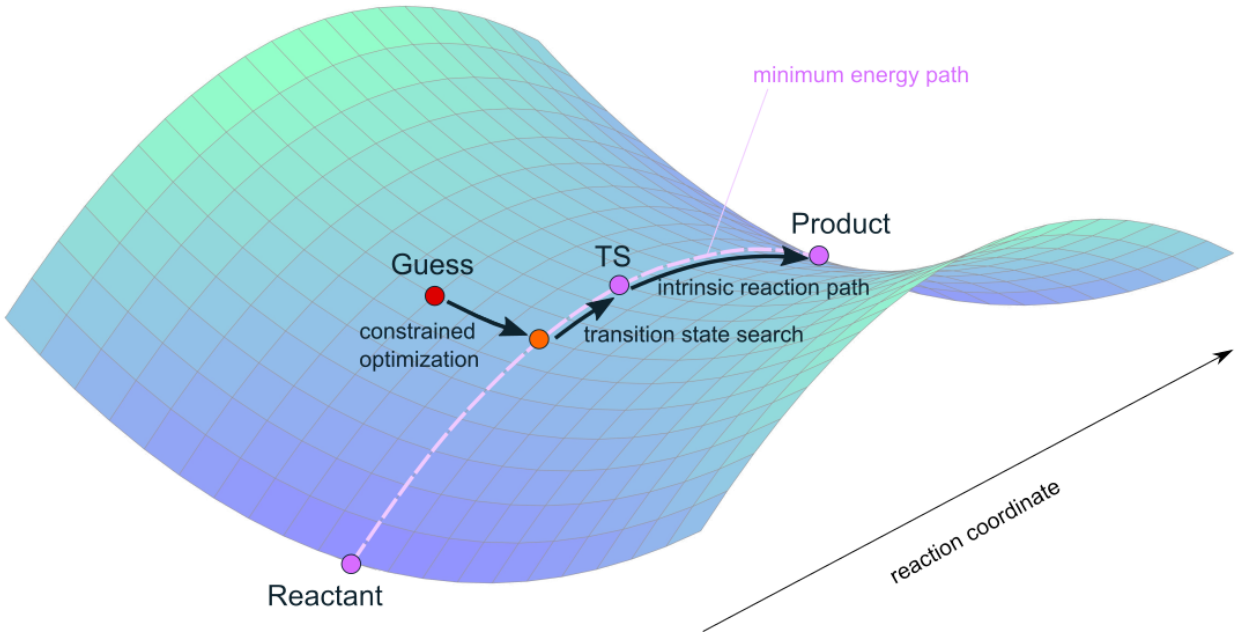


Minimum Energy Path



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

Intrinsic Reaction Path



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