Exercise Session 8

IESM Fall 2022-2023

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Course Reminders

Course Reminders:

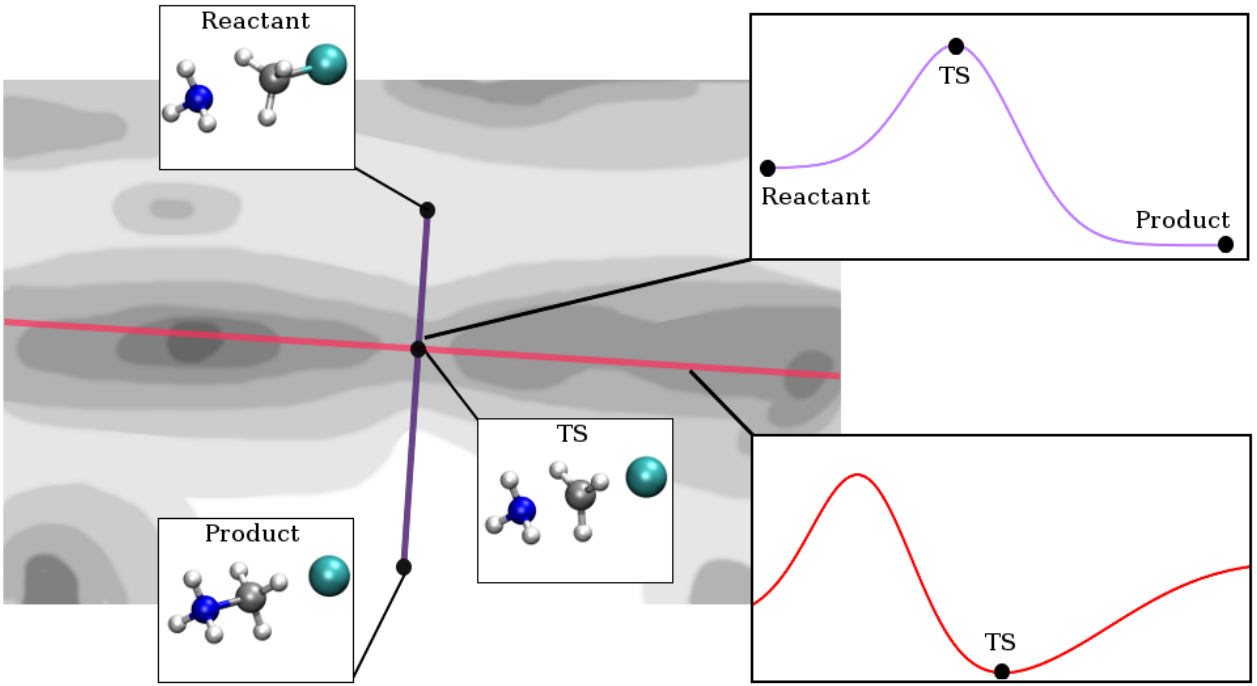
- Exercises 8 and 9 will not have interviews and will have due date **31. January**
- Plus, we only keep the best grades of 8 of 9 reports :)
- Feel free to contact us via email or forum for questions about Ex8 and Ex9 !

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.

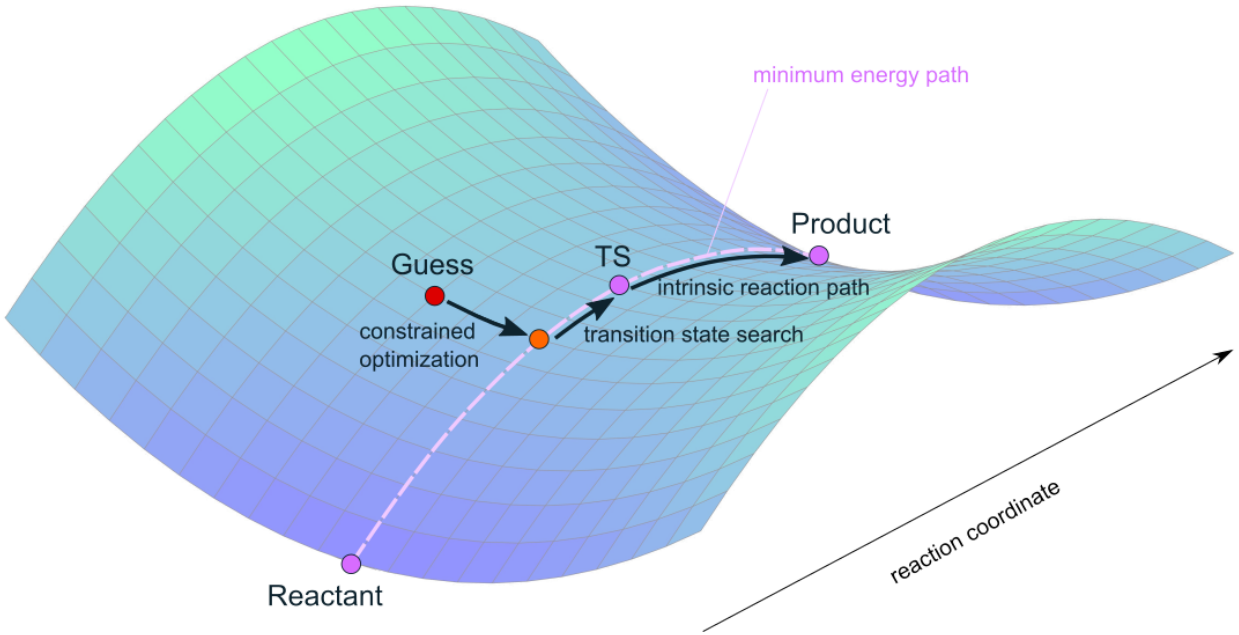
🎯 Learning goals	📖 Chapter in script	📚 Resources
• Understand how to navigate the PES to transition states • Visualize chemical reactions	Not in script but of practical relevance	Frank Jensen - Computational Chemistry Ch12.8 p.416ff

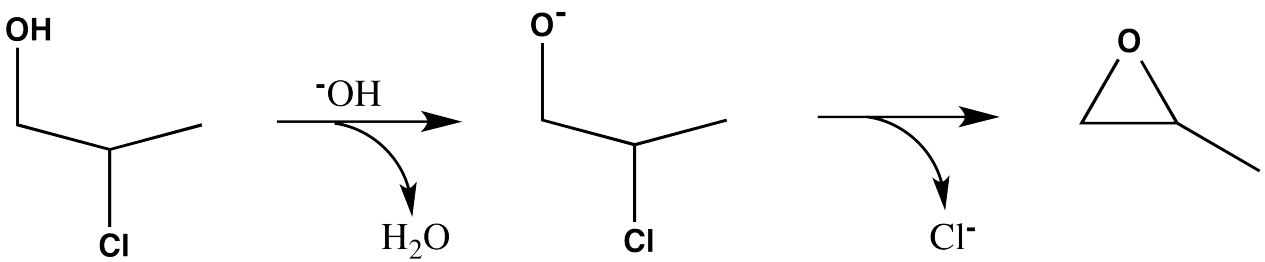
Minimum Energy Path



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

Intrinsic Reaction Path



Reaction

- We look at the synthesis of propylene oxide