# Exercise Session 8

## IESM Fall 2022-2023

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# Course Reminders

Course Reminders:

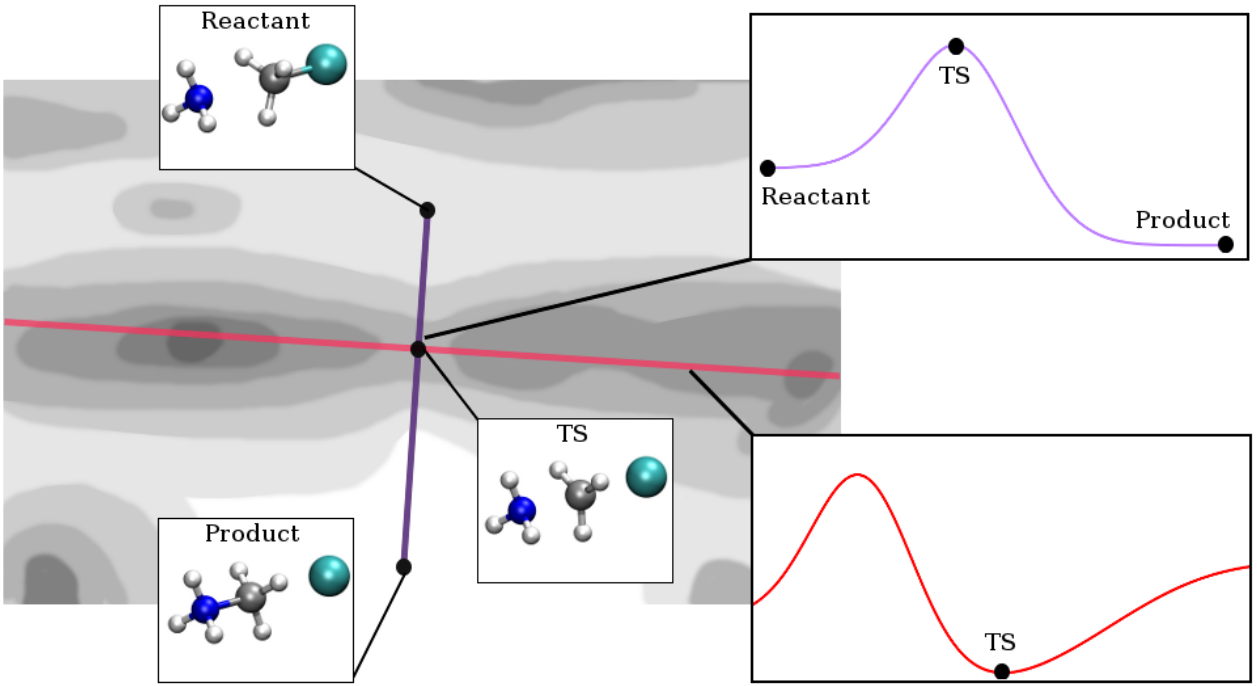
- Exercises 8 and 9 will not have interviews and will have due date **31. January**
- Plus, we only keep the best grades of 8 of 9 reports : )
- Feel free to contact us via email or forum for questions about Ex8 and Ex9 !

# 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.

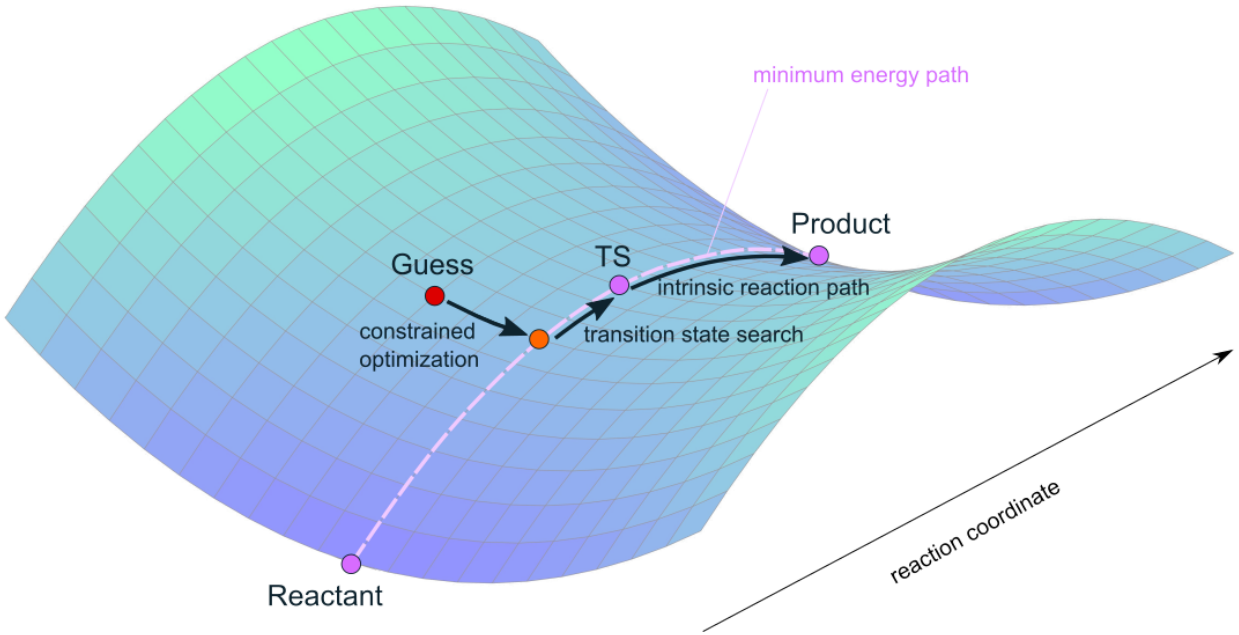
| 🎯 Learning goals | 📖 Chapter in script | 📚 Resources |
| --- | --- | --- |
| • Understand how to navigate the PES to transition states<br>• Visualize chemical reactions | Not in script but of practical relevance | Frank Jensen - Computational Chemistry Ch12.8 p.416ff |

# 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