Exercise Session 7

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 :)

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

Become familiar with common errors which occur during computational chemistry calculations

Determine the types of systems which need dispersion corrections with DFT

Evaluate how integration grid size can affect calculation accuracy

📖 Chapter in script

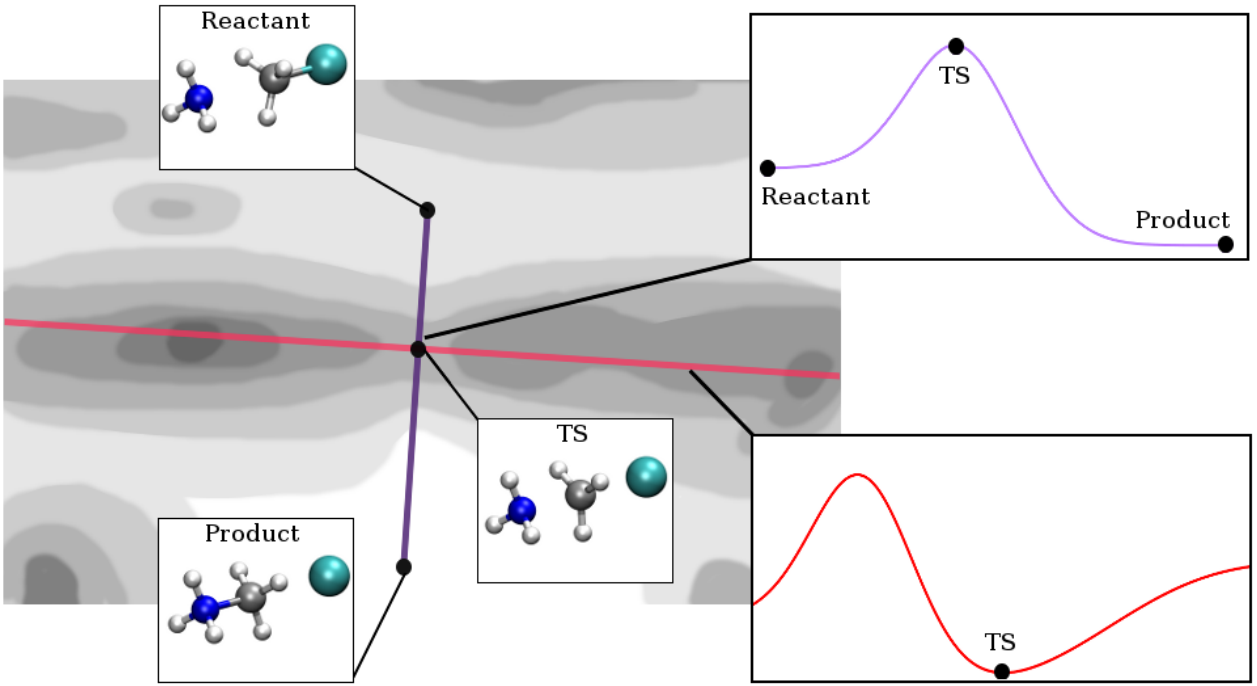
Chapter 8 - DFT

📚 Resources

The devil in the details by Pierpaolo Morgante & Roberto Peverati: A 2020 Review

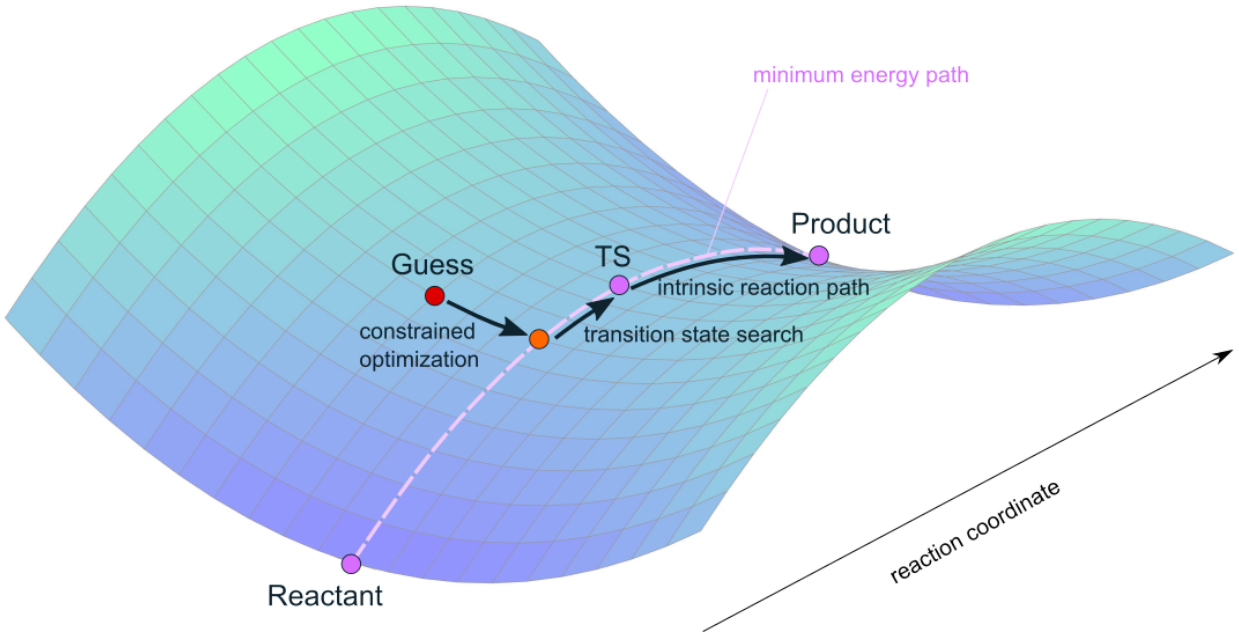
Best-Practice DFT Protocols for Basic Molecular Computational Chemistry by Markus Bursch, Jan-Michael Mewes, Andreas Hansen & Stefan Grimme: A 2022 Review

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