

# Exercise Session 8 IESM Fall 2022-2023

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December 16, 2022



#### 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.

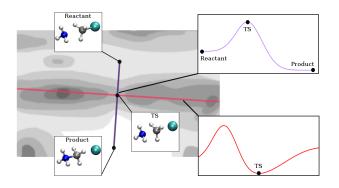


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# Minimum Energy Path

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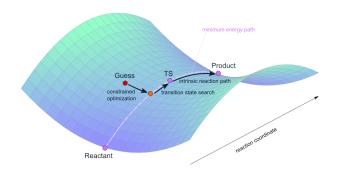


• We need to find stationary points, for TS we need the Hessian with exactly one negative eigenvalue.

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## Intrinsic Reaction Path





## Reaction

• We look at the synthesis of propylene oxide

