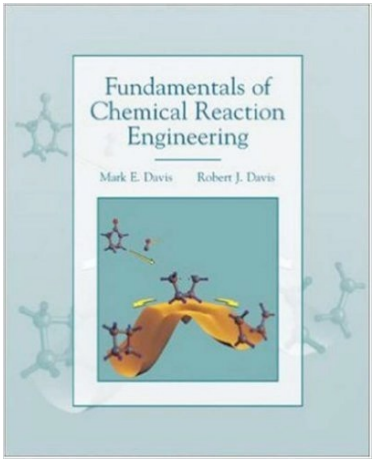
The Book



Available on Amazon for prices as low as $40 (+ shipping)

Or it's **Free!**

http://authors.library.caltech.edu/25070/

2

Outline of the course

Objective: Be able to analyze and understand a heterogeneous reaction (mechanism, kinetics etc…) from experimental data .

- 1. Basic concepts (about 4 weeks)
  - Kinetics (elementary reactions and transition state theory) **Chapter 1 and 2 (partial)**
  - Ideal reactors **Chapter 3 (partial)**
  - Non-ideal reactors **Chapter 8 (most of it)**
  - The Steady-State Approximation (SSA) **Chapter 4 (most of it)**
- 2. Heterogeneous catalysis (about 4 weeks)
  - What are heterogeneous catalysts?
  - Bulk and surface structures in heterogeneous catalysts
  - Surface reactivity
  - Elementary step kinetics
  - Kinetics of Overall Reactions

  } **Chapter 5**
- 3. Transport effects in heterogeneous catalysis (about 4-5 weeks)
  - External transport
  - Internal transport
  - Combined internal and external transport
  - Analyzing rate data

  } **Chapter 6**

+ 1 week of computer exercises

3

Course philosophy

We will follow the book = an excellent reference. My job is to help you understand it.

Most of the class will be taught on the blackboard. If you follow and write down what I write, you should have an organized summary of the textbook by the end of the semester.

We will do exercises right after I have taught the concept (exercises will be part of the course not after the course).

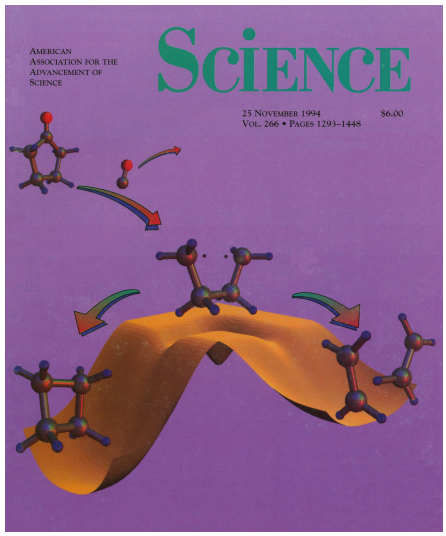
How to get an amazing grade:

- Read the book (before class)!
- Use class to reinforce/clarify/strengthen what you read.
- Ask questions.
- Do the exercises.

The grade will be based on a **final written exam during the exam period.**

4

Minimum energy pathway



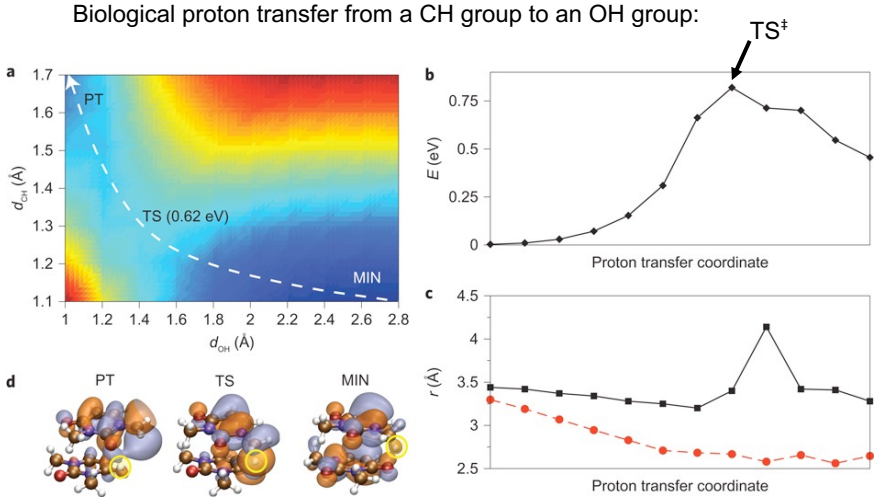
Work on the transition state led to the Nobel prize of Ahmed Zewail in 1999.

Ref.: *Science*, Cover page, November 24th 1994.

6

Minimum energy pathway

Biological proton transfer from a CH group to an OH group:



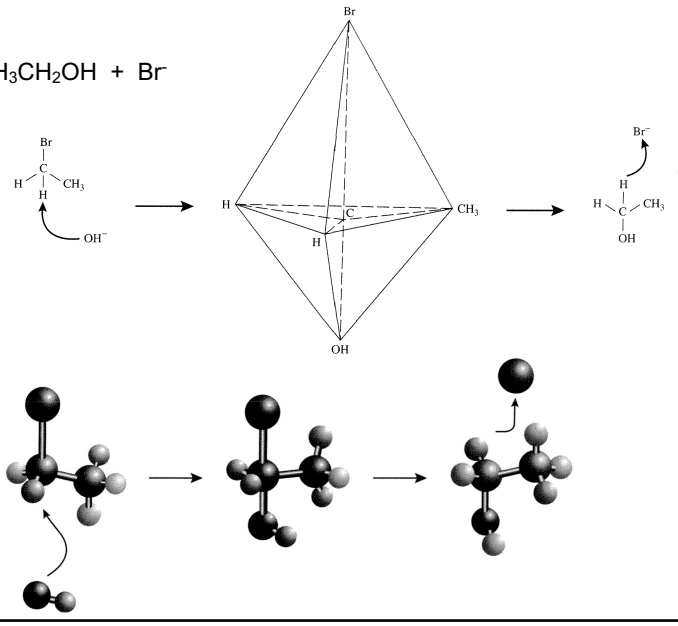
Ref.: *Nature Chemistry* 4, 323–329 (2012)

7

Transition state

RX:

$CH_3CH_2Br + OH^- \rightarrow CH_3CH_2OH + Br^-$



8