

CHEMICAL REACTION DYNAMICS (CY764)

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✓ Contents

- ⊗ **Reactive collisions:** Fundamentals, Potential energy surfaces, Crossed molecular beams, state-to-state cross sections, Classical and quantum scattering process
- ⊗ **Rate theories:** Kinetic theory of gases, Transition state theory (TST), Rice-Ramsperger-Kassel-Marcus (RRKM) theory, Microcanonical and thermal rate constants
- ⊗ **Gas phase dynamics:** Photodissociation, energy transfer dynamics, intramolecular vibrational energy flow, mode selective chemistry with Lasers
- ⊗ **Condensed phase dynamics:** Solvation, Diffusion, Kramer-Grote-Hynes model, Correlation functions

✓ Grading

Midsem I	20 points
Midsem II	20 points
Endsem	50 points
Term paper	10 points
Total	100 points

- ⊗ For the term paper, each student will be provided a research paper in the middle of the semester. You need to make a term paper and a presentation on the given paper before the end of the semester.

✓ Books

- ⊗ *Molecular Reaction Dynamics*, R. D. Levine, Cambridge University Press Reprint edition (2009).
- ⊗ *Unimolecular Reaction Dynamics: Theory and Experiments*, T. Baer and W. L. Hase, Oxford University Press USA (1996).
- ⊗ *Chemical Dynamics in Condensed Phases*, A. Nitzan, Oxford University Press USA (2006).

Note: In addition to the above books, relevant research articles will be provided occasionally.

□ *No spectrum, no matter how simple, is dynamics-free*

H. Lefebvre-Brion and R. W. Field
(The Spectra and Dynamics of Diatomic Molecules)