

**Chemistry 8565 – Chemical Reaction Dynamics, Winter 2017**

Mondays and Fridays, 11:15-12:30, 283 Kolthoff

Instructor: Donald G. Truhlar

<i>Date</i>	<i>Reading</i>	
F	Jan 20	(Introduction and syllabus)
M	Jan 23	Truhlar 2001
F	Jan 27	Gioumousis & Stevenson 1958
M	Jan 30	Greene & Kuppermann 1968
F	Feb 3	Mahan 1974
M	Feb 6	Truhlar and Garrett 1980
F	Feb 10	Truhlar 1978
M	Feb 13	Truhlar 2010
F	Feb 17	Rice & Ramsperger 1927
M	Feb 27	Flynn, Parmenter, & Wodtke 1996
F	Mar 3	Kim, Mohrig, & Truhlar 2010
M	Mar 6	García-Meseguer, Martí, Ruiz-Pernía, Moliner, & Tuñón 2013
F	Mar 10	Jasper, Nangia, Zhu, & Truhlar 2006

**Readings:**

“Potential Energy Surfaces,”

D. G. Truhlar, in *The Encyclopedia of Physical Science and Technology*, 3rd edition, edited by R. A. Meyers (Academic Press, New York, 2001), Vol. 13, pages 9-17.[truhlar.chem.umn.edu/content/book-chapters-pdf-files](http://truhlar.chem.umn.edu/content/book-chapters-pdf-files)**Monday, January 23, 2017**

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“Reactions of Gaseous Molecule Ions with Gaseous Molecules. V. Theory,”

G. Gioumousis and D. P. Stevenson, *Journal of Chemical Physics* **29**, 295-299 (1958).[dx.doi.org/10.1063/1.1744477](http://dx.doi.org/10.1063/1.1744477)**Friday, January 27, 2017**

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”Chemical Reaction Cross Sections and Rate Constants,”

E. F. Greene and A. Kuppermann, *Journal of Chemical Education* **45**, 361-369 (1968).[dx.doi.org/10.1021/ed045p361](http://dx.doi.org/10.1021/ed045p361)**Monday, January 30, 2017**

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“Activated Complex Theory of Bimolecular Reactions,”

B. H. Mahan, *Journal of Chemical Education* **51**, 709-711 (1974).[dx.doi.org/10.1021/ed051p709](http://dx.doi.org/10.1021/ed051p709)**Friday, February 3, 2017**

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“Variational Transition-State Theory,”

D. G. Truhlar and B. C. Garrett, *Accounts of Chemical Research* **13**, 440-448 (1980).[dx.doi.org/10.1021/ar50156a002](http://dx.doi.org/10.1021/ar50156a002)**Monday, February 6, 2017**

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“Interpretation of Activation Energy,”

D. G. Truhlar, *Journal of Chemical Education* **55**, 309-311 (1978).

[dx.doi.org/10.1021/ed055p309](https://doi.org/10.1021/ed055p309)

**Friday, February 10, 2017**

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“Tunneling in Enzymatic and Nonenzymatic Hydrogen Transfer Reactions,”

D. G. Truhlar, *Journal of Physical Organic Chemistry* **23**, 660-676 (2010). (in a special “symposium in print” edited by R. More O’Ferrall)

[dx.doi.org/10.1002/poc.1676](https://doi.org/10.1002/poc.1676)

**Monday, February 13, 2017**

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“Theories of Unimolecular Gas Reactions at Low Pressures,”

O. K. Rice and H. C. Ramsperger, *J. Am. Chem. Soc.* **49**, 1617–1629 (1927).

[dx.doi.org/10.1021/ja01406a001](https://doi.org/10.1021/ja01406a001)

See also

“Theories of Unimolecular Gas Reactions at Low Pressures. II,”

O. K. Rice and H. C. Ramsperger, *J. Am. Chem. Soc.* **50**, 617–620 (1928).

[dx.doi.org/10.1021/ja01390a002](https://doi.org/10.1021/ja01390a002)

**Friday, February 17, 2017**

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“Vibrational Energy Transfer,”

G. W. Flynn, C. S. Parmenter, and A. M. Wodtke, *J. Phys. Chem.* **100**, 12817-12838 (1996). (Centennial issue of *JPC*)

[dx.doi.org/10.1021/jp953735c](https://doi.org/10.1021/jp953735c)

**Monday, February 27, 2017**

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“Free Energy Surfaces for Liquid-Phase Reactions and Their Use to Study the Border Between Concerted and Nonconcerted  $\alpha,\beta$ -Elimination Reactions of Esters and Thioesters,” Y. Kim, J. R. Mohrig, and D. G. Truhlar, *Journal of the American Chemical Society* **131**, 11071-11082 (2010).

[dx.doi.org/10.1021/ja101104q](https://doi.org/10.1021/ja101104q)

**Friday, March 3, 2017**

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“Studying the Role of Protein Dynamics in an  $S_N2$  Enzyme Reaction Using Free-Energy Surfaces and Solvent Coordinates,” R. García-Meseguer, S. Martí, J. J. Ruiz-Pernía, V. Moliner, and I. Tuñón, *Nature Chemistry* **5**, 566-571 (2013).

[dx.doi.org/10.1038/nchem.1660](https://doi.org/10.1038/nchem.1660)

**Monday, March 6, 2017**

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“Non-Born-Oppenheimer Molecular Dynamics,” A. W. Jasper, S. Nangia, C. Zhu, and D. G. Truhlar, *Accounts of Chemical Research* **39**, 101-108 (2006). (special issue on computational and theoretical chemistry)

[dx.doi.org/10.1021/jp9080614](https://doi.org/10.1021/jp9080614)

**Friday, March 10, 2017**

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