

WEEK	TOPIC	Textbook +
1	Using the reaction rate law to deduce mechanism	Ch 2
2	GEPASI: GEneral PATHways Simulation Software Introduction to a numerical rate equation simulation tool	GEPASI tutorials
3	Integration of the rate law and graphical methods for analysis	Ch 4.6-4.7
4	Events at the molecular level-the activated complex	Ch 3
5	Influence of electronic structure on reactivity	Ch 5+
6	Catch up and Exam I	
break		
7	Substitution reactions: Hydrolysis reactions The structure correlation method	Ch 6+
8	H atom transfer reactions (basics of atom transfer)	+
9	electron transfer reactions (basics of Marcus theory)	Ch 7.9-7.14+
10	C-H bond activation and dehydrogenations	Lit.+
11	Oxygen atom transfer reactions (epoxidation, hydroxylations,)	7.5+
12	Catch up and Exam II	
Read per.	Student presentations	

Textbook: "Mechanisms of Inorganic Reactions" D. Katakis and G. Gordon; J Wiley Publ 1987.

Software: Numerical Kinetics Simulator: GEPASI, version 3.2.1, URL:
<http://gepasi.dbs.aber.ac.uk/softw/gepasi.html>

Case studies will be selected from the following list:

Electron Transfer:

R. Marcus, "Electron transfer reactions in chemistry" Rev. Mod.Phys. 1993. **65**: P. 599-610.

Structural Basis of Reactivity:

Burgi, H-B. and Dunitz, J. D., Structure Correlation, 1994, VCH Publ. vol 1.

Hydrolysis and Ligand Exchange Reactions:

Richens, D.T., *The Chemistry of Aqua Ions*. 1997, Chichester: J. Wiley. Ch. 1.

Kowall, T., C. P., H. Bourgeois, L. Helm, F.P. Rotzinger, and A.E. Merbach, "Interpretation of activation volumes for water exchange reactions revisited: ab initio calculations for Al³⁺, Ga³⁺, In³⁺ " *J. Amer. Chem. Soc.*, 1998. **120**: p. 6569-6577.

Atom Transfer Reactions:

MAYER, J.M., "Hydrogen atom abstraction by metal-oxo complexes." *ACC. CHEM. RES.*, 1998. **31**: p. 441-450.

Holm, R.H. and J.P. Donahue, "A thermodynamic scale for oxygen atom transfer reactions." *Polyhedron*, 1993. **12**(6): p. 571-589.

Linde, C., B. Akermark, P.-O. Norrby, and S. M., "Timing is critical: effect of spin changes on the diastereoselectivity in Mn(salen)-catalyzed epoxidation." *J. Am. Chem. Soc.*, 1999. **121**: p. 5083-5084.

Bromberg, S.E., R.G. Bergman, and C.B. Harris, "The mechanism of C-H bond activation reaction in room-temperature alkane solution." *Science*, 1997. **278**(October 10): p. 260-263.

- Niu, S. and M.B. Hall, "Inter- and Intra- molecular C-H activation by a cationic Ir(III) center via oxidative-addition reductive-elimination and σ -bond metathesis pathways." *J. Amer. Chem.Soc.*, 1998. **120**: p. 6169-6170.
- Trujillo, H.A., C.M. Casado, J. Ruiz, and D. Astruc, "Thermodynamics of C-H activation in multiple oxidation states:..." *J. Am. Chem. Soc.*, 1999. **121**: p. 5674-5686.
- Hoz, S., H. Basch, J.L. Wolk, T. Hoz, and E. Rozental, "Intrinsic barriers in identity SN2 reactions and the periodic table." *J. Amer. Chem. Soc.*, 1999. **121**: p. 7724-7725.