CHEMISTRY DEPARTMENT, PORTLAND STATE UNIVERSITY

CHEMISTRY 441/541, PHYSICAL CHEMISTRY

Important topics for the Final Exam to be held on March 17, 2008 at 12:30 PM in SB1 304.

1. Reaction Gibbs energy
2. Chemical equilibrium, K_p; and relationship to ΔG
3. Extent of reaction, >
4. Effect of pressure
5. Equilibrium, reaction quotient, Q
6. Activities, molalities, concentrations and fugacities
7. Equilibrium constants and degree of dissociation
8. Relationship between equilibrium constants, K_{eq}, K_b, etc
9. Le Chatelier's principle
10. Response of equilibria to temperature
11. G and extent of reaction, >. (Example N_2O_4 º NO_2)
12. Van't Hoff equation
13. Spontaneity
14. Measurement of reaction enthalpy from equilibrium constants
15. Variation of equilibrium constant with temperature
16. **Relationship between K_p and K_c**
17. ΔG^0_f's
18. Kirchoff's Law
19. Partition function and K_p's
20. Solublities
21. Molecular PF's
22. Partial fugacities
23. PF's of ideal gases, calculations of
24. Electronic PF's
25. Average energies from PF's
26. Population levels from PF's
27. Vibrational PF's
28. Occupancy of vibrational energy levels
29. Rotational energy levels
30. Rotational temperature, theta-rot; vibrational temperature, theta-vib
31. Vibrational contribution to molar heat capacities
32. f_v
33. Symmetry number, J_{max}
34. Vibrational PF's of polyatomic molecules
35. Rotational PF of polyatomics (spherical tops, asymmetric tops, etc)
36. Experimental determination of reaction order (isolation and initial rate methods)
37. Integrated rate laws (first and second order only)
38. Half-lives; derivation and evaluation of
39. Reactions approaching equilibrium
40. First and second order reversible reactions
41. Consecutive reactions

42. Steady State Approximation
43. Improved SSA technique
44. Kinetics methods… stopped-flow
45. Relaxation kinetics
46. Derivation of relaxation times
47. T-jump method; prerequisite for t-jump relaxation spectra
48. Derivation of kinetics constants using T-jump
49. P-jump
50. Temperature dependence of reaction rates
51. Transition State Theory… the dagger!!!!
52. Principle of MR and Det. Balance
53. Elementary reactions, mechanisms
54. Complex reactions
55. Steady state approximations, part 2
56. Lindemann scheme
57. Lindemann theory and experimental data comparisons
58. Free radical complex reactions
59. Homogenous catalysis, calculations involving…
60. Decomposition of acetaldehyde
61. The hydrogen-bromine free radical reaction.
62. Decomposition of ozone
63. Homogenous catalysis
64. Activation energy calculations
65. Quadratic autocatalysis, equations governing
66. Inflexion point, sigmoidal curve
67. Exothermic reactions as autocatalytic reactions
68. Combustion reactions as autocatalytic reactions
69. Thermal runaway, control of
70. Positive feedback loops
71. Examples of oscillatory behavior in the natural world (circadian rhythms, etc....)
72. Lotka-volterra scheme
73. Steady state concentrations in L-V scheme
74. Perturbation analysis of the L-V sheme
75. Hopf bifurcation (subcritical and supercritical)
76. Enzyme kinetics
77. Maximum turnover number
78. Michaelis-Menten constant
79. Lineweaver-Burke plots
80. Eadie Plots
81. Derivation of the Briggs-Haldane Equation
82. Competitive and noncompetitive inhibition
83. Quadratic autocatalysis, equations governing
84. Inflexion point, sigmoidal curve
85. Exothermic reactions as autocatalytic reactions
86. Combustion reactions as autocatalytic reactions
87. Thermal runaway, control of
88. Positive feedback loops
89. Lotka-Volterra scheme
90. Steady state concentrations in L-V scheme
91. Perturbation analysis
92. Hopf bifurcation

93. Phase diagrams, limit cycle
94. Oscillations and the second law of thermodynamics
95. Ilya Prigogine's theory
96. Bistability
97. Hysteresis
98. Phase diagrams, limit cycle
99. Oscillations and the second law of thermodynamics
100. Prerequisistes for oscillatory behavior
101. Ilya Prigogine's theory
102. T. S. Addington's view of the second law of thermodynamics
103. Some well-known chemical oscillators: Bray, BZ, etc
104. Autocatalytic species in the BZ system
105. The FKN Mechanism; Processes A, B and C and their roles.
106. Bromide control?
107. The Brusselator
108. The Oregonator
109. Examples of biological oscillators
110. Collision theory and gas phase reactions
111. Mean free path, path length, collision frequencies; calculations of
112. Calculation of reaction rates from collision theory
113. Refinements to the hard shell collision theory
114. Impact parameter
115. Orientation of colliding molecules
116. Effect of internal energy of reacting molecules
117. **Bonus question involving something obvious**.