

Preview Sheet for Final Examination
Monday, May 12, from 8:00 to 10:30 a.m. in Olin-Rice 301

Part 1: (50 points) Mathematical problems from Units 1 and 2

Part 2: (100 points) 25 American Chemical Society multiple-choice questions (covering entire semester)

You may bring a one-page cheat sheet to the exam

Here is an overview of topics you are responsible for:

Unit 1 (Test 1/PS 1 and 2/Experiment 1)

Photoelectric effect, interpreting wave functions, eigenvalues and expectation values, particle in infinite and finite boxes, particle on a ring or a sphere, harmonic oscillator

Unit 2 (Test 2/PS 3 and 4/Experiment 2)

One-electron atoms, radial and angular wavefunctions, selection rules, molecular orbital theory, Born-Oppenheimer approximation

Unit 3 (Test 3/PS 5/Experiment 3)

Rotational terms and spectra, vibrational terms and spectra, reduced mass, rovibrational spectra, selection rules

After Test 3

Basic ideas about electronic spectroscopy and the Boltzmann distribution

Preview of the test instructions:

1. Write your name in the space above and on the backs of pages 2-11.
2. Your exam booklet should have **eleven pages** total, with questions on pages 2-9, and formulas, constants and a periodic table on pages 10-11. Check to see you have eleven pages now. If you do not, ask for another copy of the exam.
3. You may carefully remove pages 10-11 from your exam booklet.
4. When answering questions on this test, you do not need to re-derive any equation unless I explicitly tell you otherwise.
5. Part I of this test (on pp. 2-4) contains problems from Units 1 and 2. Justify all of your answers in Part I. Partial credit will be awarded for work in Part I.
6. Part II of this test (on pp. 5-9) contains **25** multiple-choice questions, each worth 4 points, covering many of the major topics of the semester. Circle the correct answer to each of the questions in the exam booklet. There is no penalty for incorrect answers. Feel free to use blank spaces in this exam booklet for scratch work. However, realize that you will receive no partial credit for this work.
7. You may use as a reference a single sheet of 8.5"x 11" paper that you have filled (front and back) with information.
8. You have a maximum of **2 hours and 30 minutes** to work on this exam.

Preview of information to be provided in the test booklet on the next two pages

Possibly Useful Information from the ACS Exam Booklet

Table of Symbols and Constants

QUANTITY	SYMBOL	VALUE
internal energy	U	
enthalpy	H	
entropy	S	
Gibbs energy	G	
Helmholtz energy	A	
speed of light, vacuum	c	$2.9979 \times 10^8 \text{ m}\cdot\text{s}^{-1}$
Planck constant	h	$6.6261 \times 10^{-34} \text{ J}\cdot\text{s}$
elementary charge	e	$1.6022 \times 10^{-19} \text{ C}$
electron mass	m_e	$9.1094 \times 10^{-31} \text{ kg}$
proton mass	m_p	$1.6726 \times 10^{-27} \text{ kg}$
atomic mass unit	u	$1.6606 \times 10^{-27} \text{ kg}$
Rydberg constant	R_v	$1.09737 \times 10^5 \text{ cm}^{-1}$
Avogadro constant	N_A	6.02221×10^{23}
Faraday constant	F	$96485.3 \text{ C}\cdot\text{mol}^{-1}$
ideal gas constant	R	$8.3145 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ $1.987 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ $0.083145 \text{ L}\cdot\text{bar}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ $0.082058 \text{ L}\cdot\text{atm}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

PERIODIC TABLE OF THE ELEMENTS

1 H 1.008																	2 He 4.003
3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
55 Cs 132.9	56 Ba 137.3	57 La 138.9	72 Hf 178.5	73 Ta 181.0	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (264)	108 Hs (265)	109 Mt (266)	110 Ds (269)	111 Rg (272)	112 Cn (277)		114 Fl (289)		116 Lv (293)		118 Og (294)
58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (145)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0				
90 Th 232.0	91 Pa 231.0	92 U 238.0	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)				

More Possibly Useful Information

$$\int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}} \quad \int_0^{\infty} e^{-a^2 x^2} dx = \frac{\sqrt{\pi}}{2a} \quad \int_0^{\infty} x^{2n} e^{-ax^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{2^{n+1} a^n} \sqrt{\frac{\pi}{a}}$$

$$\int \sin^2 ax dx = \frac{1}{2}x - \frac{1}{4a} \sin 2ax \quad \cos^2 x + \sin^2 x = 1 \quad e^{ix} = \cos x + i \sin x$$

$$d\tau = r^2 \sin \theta dr d\theta d\phi \quad \nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Lambda^2 \quad \Lambda^2 = \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta}$$

$$E_{\text{photon}} = h\nu \quad E_{\text{photon}} = \Phi + E_K \quad E_K = \frac{1}{2}mv^2 \quad E_K = eV_o$$

$$c = \lambda\nu \quad \frac{1}{\lambda} \equiv \tilde{\nu} \quad \lambda = \frac{h}{mv} \quad -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

$$E_n = \frac{n^2 h^2}{8mL^2} \quad V = \frac{1}{2}kx^2 \quad E_v = \left(v + \frac{1}{2}\right)h\nu \quad \nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

$$E(m_l) = \frac{m_l^2 \hbar^2}{2I} \quad E_l = \frac{l(l+1)\hbar^2}{2I} \quad I = mr^2$$

$$L^2 = l(l+1)\hbar^2 \quad L_z = m_l \hbar \quad E_n = -\frac{\mathfrak{R}Z^2}{n^2}$$

$$X_{\text{CM}} = \frac{m_1}{m_1 + m_2} X_1 + \frac{m_2}{m_1 + m_2} X_2 \quad \mu = \frac{m_1 m_2}{m_1 + m_2} \quad I = m_1 R_1^2 + m_2 R_2^2 = \mu R^2$$

$$\frac{E_{\text{rot}}}{hc} = F(J) = BJ(J+1) \quad \text{or} \quad \frac{E_{\text{rot}}}{hc} = F(J) = B_v J(J+1) - D_v J^2(J+1)^2$$

$$B = \frac{h}{8\pi^2 c \mu R^2} \quad \text{or} \quad B_v = \frac{h}{8\pi^2 c \mu R_v^2} \quad D_v = \frac{4B_v^3}{\tilde{\nu}^2}$$

$$\frac{E_{\text{vib}}}{hc} = G(v) = \left(v + \frac{1}{2}\right)\tilde{\nu} \quad \text{or} \quad \frac{E_{\text{vib}}}{hc} = G(v) = \left(v + \frac{1}{2}\right)\tilde{\nu} - \left(v + \frac{1}{2}\right)^2 x_e \tilde{\nu}$$

$$\omega = 2\pi\nu = 2\pi c \tilde{\nu} = \sqrt{\frac{k}{\mu}} \quad x_e = \frac{\tilde{\nu}}{4D_e} \quad V = \frac{1}{2}k(R - R_e)^2$$

$$V = hcD_e \{1 - \exp[-a(R - R_e)]\}^2 \quad a = \sqrt{\frac{\mu\omega^2}{2hcD_e}}$$

$$\frac{n_i}{N} = \frac{g_i \exp(-\beta\varepsilon_i)}{q} \quad q = \sum_i g_i \exp(-\beta\varepsilon_i) \quad \beta = \frac{1}{kT}$$

$$\hbar = 1.05457 \times 10^{-34} \text{ J s} \quad 1 \text{ J} = 1 \text{ kg m}^2 \text{ s}^{-2} \quad 1 \text{ \AA} = 10^{-10} \text{ m} \quad a_0 = 0.5292 \text{ \AA}$$