Chemistry 1B, Exam III
April 12, 2007
Professor R.J. Saykally

Name Key

TA ______________________

1. (15) __________
2. (20) __________
3. (20) __________
4. (15) __________
5. (15) __________
6. (15) __________

TOTAL EXAM SCORE (100) __________

Rules:
- Work all problems to 2 significant figures
- No lecture notes or books permitted
- No word processing calculators
- Time: 90 minutes
- Show all work to get partial credit
- Periodic Table, Tables of Physical Constants, and Conversion Factors included

Inches 1 2 3 4 5 6

Periodic Table of the Elements

Key: Atomic number — 27 58.93 — Atomic mass; Co — symbol; Cobalt — name

symbol: Black naturally occurring; White synthetically prepared; *most stable isotope*

Metals | Metalloids | Nonmetals | Noble gases

H																	2 4.003 He Helium
3 6.94 Li	4 9.01 Be											5 10.81 B	6 12.01 C	7 14.01 N	8 15.999 O	9 18.998 F	10 20.18 Ne Neon
11 22.99 Na	12 24.31 Mg											13 26.98 Al Aluminum	14 28.09 Si	15 30.97 P	16 32.06 S	17 35.45 Cl	18 39.95 Ar Argon
19 39.10 K Potassium	20 40.08 Ca Calcium	21 44.96 Sc Scandium	22 47.90 Ti Titanium	23 50.94 V Vanadium	24 51.996 Cr Chromium	25 54.94 Mn Manganese	26 55.85 Fe Iron	27 58.93 Co Cobalt	28 58.70 Ni Nickel	29 63.55 Cu Copper	30 65.37 Zn Zinc	31 69.72 Ga Gallium	32 72.59 Ge	33 74.92 As	34 78.96 Se	35 79.90 Br	36 83.80 Kr Krypton
37 85.47 Rb Rubidium	38 87.62 Sr Strontium	39 88.91 Y Yttrium	40 91.22 Zr Zirconium	41 92.91 Nb Niobium	42 95.94 Mo Molybdenum	43 (98) Tc Technetium	44 101.07 Ru Ruthenium	45 102.91 Rh Rhodium	46 106.40 Pd Palladium	47 107.87 Ag Silver	48 112.41 Cd Cadmium	49 114.82 In Indium	50 118.69 Sn Tin	51 121.75 Sb	52 127.60 Te	53 126.90 I	54 131.30 Xe Xenon
55 132.91 Cs Cesium	56 137.33 Ba Barium	57 138.91 La Lanthanum	72 178.49 Hf Hafnium	73 180.95 Ta Tantalum	74 183.85 W Tungsten	75 186.21 Re Rhenium	76 190.20 Os Osmium	77 192.22 Ir Iridium	78 195.09 Pt Platinum	79 196.97 Au Gold	80 200.59 Hg Mercury	81 204.37 Tl Thallium	82 207.19 Pb Lead	83 208.98 Bi Bismuth	84 (209) Po	85 (210) At	86 (222) Rn Radon
87 (223) Fr Francium	88 226.03 Ra Radium	89 227.03 Ac Actinium	104 (261) Rf Rutherfordium	105 (262) Ha Hahnium	106 (266) Sg Seaborgium	107 (262) Ns Nielsbohrium	108 (265) Hs Hassium	109 (266) Mt Meitnerium	110 (271)	111 (272)	112 (277)	(113)	(114)	(115)	(116)	(117)	(118)

Lanthanide series ▸	58 140.12 Ce Cerium	59 140.91 Pr Praseodymium	60 144.24 Nd Neodymium	61 (145) Pm Promethium	62 150.40 Sm Samarium	63 151.96 Eu Europium	64 157.25 Gd Gadolinium	65 158.93 Tb Terbium	66 162.50 Dy Dysprosium	67 164.93 Ho Holmium	68 167.26 Er Erbium	69 168.93 Tm Thulium	70 173.04 Yb Ytterbium	71 174.97 Lu Lutetium
Actinide series ▸	90 232.04 Th Thorium	91 231.04 Pa Protactinium	92 238.03 U Uranium	93 237.05 Np Neptunium	94 (244) Pu Plutonium	95 (243) Am Americium	96 (247) Cm Curium	97 (247) Bk Berkelium	98 (251) Cf Californium	99 (252) Es Einsteinium	100 (257) Fm Fermium	101 (260) Md Mendelevium	102 (259) No Nobelium	103 (262) Lr Lawrencium

Note: Atomic masses shown here are the 1983 IUPAC values (maximum of six significant figures).

Physical Constants

Standard acceleration of terrestrial gravity	$g = 9.80665$ m s^{-2} (exactly)
Avogadro's number	$N_0 = 6.022137 \times 10^{23}$
Bohr radius	$a_0 = 0.52917725$ Å $= 5.2917725 \times 10^{-11}$ m
Boltzmann's constant	$k_B = 1.38066 \times 10^{-23}$ J K^{-1}
Electron charge	$e = 1.6021773 \times 10^{-19}$ C
Faraday constant	$\mathcal{F} = 96{,}485.31$ C mol^{-1}
Masses of fundamental particles:	
Electron	$m_e = 9.109390 \times 10^{-31}$ kg
Proton	$m_p = 1.672623 \times 10^{-27}$ kg
Neutron	$m_n = 1.674929 \times 10^{-27}$ kg
Ratio of proton mass to electron mass	$m_p/m_e = 1836.15270$
Permittivity of vacuum	$\epsilon_0 = 8.8541878 \times 10^{-12}$ C^2 J^{-1} m^{-1}
Planck's constant	$h = 6.626076 \times 10^{-34}$ J s
Speed of light in a vacuum	$c = 2.99792458 \times 10^8$ m s^{-1} (exactly)
Universal gas constant	$R = 8.31451$ J mol^{-1} K^{-1}
	$= 0.0820578$ L atm mol^{-1} K^{-1}

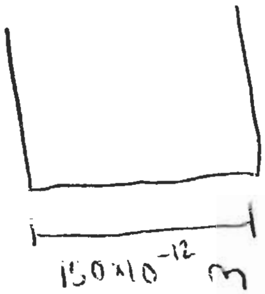
Values are taken from "Quantities, Units and Symbols in Physical Chemistry," International Union of Pure and Applied Chemistry, Blackwell Scientific Publications, 1988.

Conversion Factors

Standard atmosphere	1 atm = 1.01325×10^5 Pa = 1.01325×10^5 kg m^{-1} s^{-2} (exactly)
Atomic mass unit	1 u = 1.660540×10^{-27} kg
	1 u = 1.492419×10^{-10} J = 931.4943 MeV (energy equivalent from $E = mc^2$)
Calorie	1 cal = 4.184 J (exactly)
Electron volt	1 eV = $1.6021773 \times 10^{-19}$ J = 96.48531 kJ mol^{-1}
Foot	1 ft = 12 in = 0.3048 m (exactly)
Gallon (U.S.)	1 gallon = 4 quarts = 3.78541 L (exactly)
Liter-atmosphere	1 L atm = 101.325 J (exactly)
Metric ton	1 metric ton = 1000 kg (exactly)
Pound	1 lb = 16 oz = 0.45359237 kg (exactly)

1. (3 points each)

a) Using the quantum well model for the hydrogen atom, i.e. treating the atom as an electron in a one-dimensional box of length 150. pm, predict the wavelength of radiation emitted when the electron falls from the level with $n = 3$ to that with $n = 2$.



$$E_n = \frac{h^2 n^2}{8ml^2}$$

$$\Delta E_{3\to2} = \frac{4h^2}{8ml^2} - \frac{9h^2}{8ml^2} = \frac{-5h^2}{8ml^2}$$

$$= \frac{-5h^2}{8(9.1\times10^{-31}\,kg)(150\times10^{-12}\,m)^2}$$

$$= 1.34\times10^{-17}\,J$$

$$\lambda = \frac{h\cdot c}{E} = \boxed{15\ nm}$$

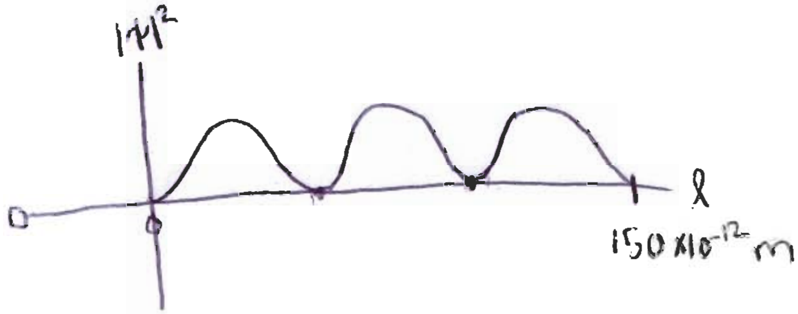
b) What part of the spectrum is this in? UV

c) Calculate the zero-point energy of the atom. $\longrightarrow$ $n=1$

$$E_n = \frac{h^2(1)^2}{8m_e l^2} = \boxed{2.68\times10^{-18}\,J}$$

d) Sketch the probability for finding the electron in the box state $n = 3$.

n=3; 2 nodes



e) In principle, both sin θ and cos θ, with $\theta = \frac{n\pi x}{L}$ are solutions to the Schrodger equation. Why is the cos θ solution not used?

The boundry conditions require that ψ(0)=0; there is no probability of finding the particle at the edge of the box. Since cos(0)= 1, this part of the solution must be thrown out.

2. (5 points each) The sun emits radiant energy of 3.9×10^{26} J·S^{-1}; about 10% of this comes from the CNO fusion chain.

a) Calculate the rate of mass loss from the CNO chain.

In one second:

$\Delta E = \Delta m \cdot c^2$

$\Delta E_{sun} = -3.9 \times 10^{26} J$

$\Delta E_{sun}(CNO) = (0.1)(\Delta E_{sun})$

$-3.9 \times 10^{25} J = (3.0 \times 10^8 \frac{m}{s})^2 \Delta m$

$\Delta m = -4.3 \times 10^8$ kg

$\boxed{-4.3 \times 10^8 \frac{kg}{s}}$

b) Write out the CNO chain mechanism, showing that it gives the correct overall stoichiometry for the fusion reaction.

$^{12}C + {}^1H \rightarrow {}^{13}N + \gamma$

$^{13}N \rightarrow {}^{13}C + \beta^+ + \gamma$

$^{13}C + {}^1H \rightarrow {}^{14}N + \gamma$

$^{14}N + {}^1H \rightarrow {}^{15}O + \gamma$

$^{15}O \rightarrow {}^{15}N + \beta^+ + \gamma$

$^{15}N + {}^1H \rightarrow {}^{12}C + {}^4He$

$4({}^1H) \rightarrow {}^4He$

c) Explain why the even-Z elements are more abundant than odd-Z elements for the representative elements.

This is due to the primary method of forming the elements being α-particle fusion reactions, leading to even-Z elements.

Second, the even-Z elements are more stable. Those elements with odd numbers of nucleons result in an unpaired proton.

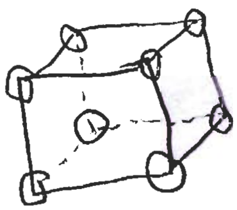
d) How were the transition metals formed?

The transition metals following iron have endothermic nucleon binding energy and were only formed when stars become supernovas, not during the big bang.

Before Fe, the transition metals could be formed by simple fusion in first and subsequent stars.

3. (5 points each) One form of silicon has density of 2.33 g·cm^{-3} and crystallizes in a simple cubic lattice with a unit cell edge of 543 pm and a band gap of 1.21 eV.

a) What is the mass of each unit cell?



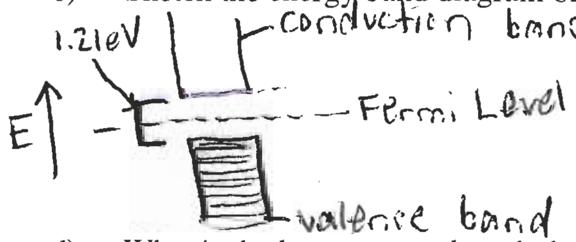
$V = (543 \times 10^{-10}\ cm)^3 = 1.601 \times 10^{-22}\ cm^3$

$V \cdot d = m \qquad \frac{2.33g}{cm^3} \cdot 1.601 \times 10^{-22}\ cm^3 = \boxed{3.73 \times 10^{-22} g}$

b) How many silicon atoms does one unit cell contain?

$\boxed{1}$

c) Sketch the energy band diagram of silicon, labeling the Fermi level.



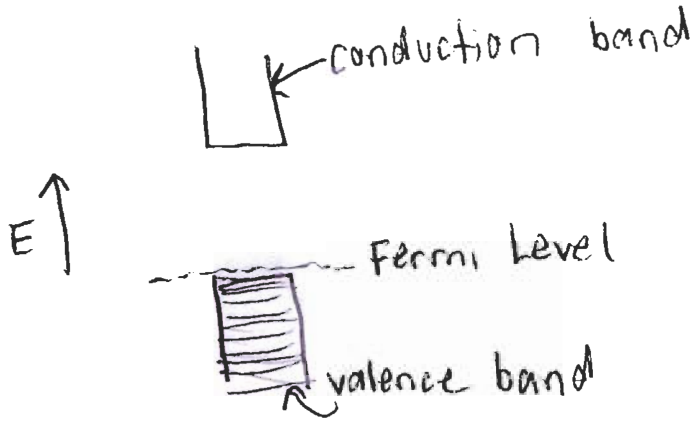
d) What is the longest wavelength that can excite an electron in a crystal of pure cubic silicon?

longest wavelength = lowest Energy excitation = band gap

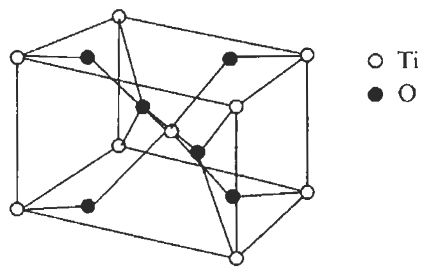
$\lambda = \frac{h \cdot c}{E} = \frac{(4.136 \times 10^{-15}\ eV \cdot s)(3 \times 10^8 \frac{m}{s})}{1.21\ eV} = \boxed{1.025 \times 10^{-6}\ m \text{ or } 1025\ nm}$

4. (5 points each)

a) Sketch the band structure diagram expected for rutile (TiO_2), labeling the Fermi level.



b) Calculate the number of cations, anions, and formula units per unit cell for rutile, given the unit cell.



Ti = 8 corners × $\frac{1}{8}$ + 1 center = 2 Ti

O = 4 faces × $\frac{1}{2}$ + 2 center = 4 O

2 cations / cell

4 anions / cell

(TiO_2) × 2

2 formula units / cell

c) What are the coordination numbers of the ions in rutile?

Cation = 6

Anion = 3

5. (3 points each) Order the following atoms according to increase in the stated property.

a) Electron affinity: Cl, I, P, Be

smallest largest

Be < P < I < Cl

b) First ionization energy: Na, Mg, Al, Ar

smallest largest

Na < Al < Mg < Ar

c) Atomic radius: K, F^{+}, Rb, Co^{25+}, Br

smallest largest

Co^{25+} < F^{+} < K < Br < Rb

d) Explain why gold is so unreactive.

1) Due to the Lanthanide Contraction, e^- experience a high effective nuclear charge and are held very tightly

2) It contains completely filled 6s and 5d (and 5p) orbitals. So ~~do~~ adding or subtracting e^- is unfavorable relative to the other elements.

f) Explain why gold is so much denser than silver.

$Density = \frac{mass}{volume}$. The mass per atom of gold is much higher. However, the interatomic distance, and thus volume, of gold is nearly identical due to the Lanthanide contraction, thus the density of gold is much higher than that of silver.

6. (5+10 points)

a) Describe the differences between diamagnetism, paramagnetism, ferromagnetism, and antiferromagnetism.

Diamagnetic atoms have no spin-unpaired electrons, and thus exhibit no or little magnetic properties, they are weakly repelled by a magnetic field. Paramagnetic materials contain atoms with spin unpaired electrons. They are magnetically active and move into magnetic fields. Ferromagnetic materials exhibit the property that neighboring atoms' spins* correlate with one another in a parallel manner, thus creating a permanent magnet after a magnetic field is applied. Antiferromagnetic materials exhibit atoms where neighboring spins are anti-parallel, cancelling eachother out, ~~add~~ ~~the~~ yielding no ~~strong~~ net magnetic property.

b) A silicon solar cell (band gap = 1.21 eV) with area A = 10 cm^{-2} experiences an insolation of 1000 watt·hours·cm^{-2} per day, generating a voltage of 2.50 volts and a current of 3.0 amps. Calculate the efficiency of the solar cell.

$$P_{cell} = V \cdot I = 2.50V \times 3.0A = 7.5W$$

$$\frac{1000\ W\cdot hr}{cm^2 \cdot day} \times 10cm^2 \times \frac{3600J}{watt\text{-}hr} \times \frac{1\ day}{24\ hours} \times \frac{1\ hr}{3600s} = 417W$$

= Power available

$$\text{Efficiency} = \frac{7.5W}{417W} \times 100\% = \boxed{1.8\%}$$