Chemistry 432
Exam Number 3
Spring 2021
50 Minutes

R =8.3144 J mol^{-1} K^{-1}

R=.0821 L atm mol^{-1} K^{-1}

$N_A = 6.022 \times 10^{23}$ molecules mol^{-1}

$h = 6.626 \times 10^{-34}$ J s

$k_B = 1.381 \times 10^{-23}$ J K^{-1}

$\hbar = 1.055 \times 10^{-34}$ J s

1 ev = 1.60 $\times 10^{-19}$ J

$c = 2.998 \times 10^{8}$ m s^{-1} = 2.998 $\times 10^{10}$ cm s^{-1}

1 Å= 10^{-10} m

1 nm = 10^{-9} m

$m_e = 9.11 \times 10^{-31}$ kg (electron mass)

$m_p = 1.67 \times 10^{-27}$ kg (proton mass)

Name:

Integral and Formula Table

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

$$\int_{-\infty}^{\infty} x e^{-ax^2} dx = 0$$

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2}\frac{\sqrt{\pi}}{a^{3/2}}$$

$$\int_{0}^{\infty} x^3 e^{-ax^2} dx = \frac{1}{2a^2}$$

$$\int_{-\infty}^{\infty} x^4 e^{-ax^2} dx = \frac{3\sqrt{\pi}}{4a^{5/2}}$$

$$\int_{0}^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

$$\int \sin^2 x \; dx = \frac{1}{2}x - \frac{1}{4}\sin 2x$$

$$\int \cos^2 x \; dx = \frac{1}{2}x + \frac{1}{4}\sin 2x$$

$$\int_{0}^{2\pi} \cos^2 nx \; dx = \pi$$

$$\int_{0}^{\pi} \sin x \; dx = 2$$

$$\int_{0}^{n\pi} x^2 \sin^2 x \; dx = \frac{1}{24}[4n^2\pi^2 - 6n\pi]$$

Name:

1. The normalized wavefunction for an electron in a hydrogen atom in a $3d_0$ state with $n = 3, \ell = 2$ and $m = 0$ is given by

$$\psi_{3,2,0}(r, \theta, \phi) = R_{3,2}(r) Y_2^0(\theta, \phi)$$

where the normailzed radial part of the wavefunction is given by

$$R_{3,2}(r) = \frac{4}{81\sqrt{30}} \left(\frac{1}{a_0}\right)^{7/2} r^2 \; e^{-r/3a_0}$$

with a_0 the Bohr radius, and $Y_2^0(\theta, \phi)$ is the normalized spherical harmonic with $\ell = 2, m = 0$. Let r_{max} be the most probable distance between an electron and the nucleus independent of direction of an electron in a $3d_0$ state of a hydrogen atom. Derive an expression for $r_{max}\langle r^{-2}\rangle$ for an electron in the $3d_0$ state of a hydrogen atom. Recall that the spherical harmonics are normalized such that

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \; \sin\theta |Y_\ell^m(\theta, \phi)|^2 = 1.$$

(33 Points)

Name:

Name:

2. Construct the term symbols for the ground state of the beryllium atom and term symbols for the excited states represented by the electronic configuration $1s^1 2s^2 2p^1$. Determine the allowed spectral transitions between the states represented by the generated term symbols.(33 Points)

Name:

3. The gas-phase LiCl molecule has 73.3 % ionic character. Assuming an LiCl wavefunction is constructed from ϕ_{2s}, a 2s hydrogenic orbital centered on the Li atom, and ϕ_{3p}, a $3p_z$ hydrogenic orbital centered on the Cl atom, construct a valence-bond wavefunction for LiCl that has the correct percent ionic character. For the ionic contribution to the wavefunction, include only the dominant ionic structure. Show the resonance structures that correspond to each term in the valence-bond wavefunction. (34 Points)

Name:

Periodic Table of the Elements

	1 (1A)	2 (2A)	3 (3B)	4 (4B)	5 (5B)	6 (6B)	7 (7B)	8 (8B)	9 (8B)	10 (8B)	11 (1B)	12 (2B)	13 (3A)	14 (4A)	15 (5A)	16 (6A)	17 (7A)	18 (8A)
1	1 **H** 1.0079																	2 **He** 4.0026
2	3 **Li** 6.941	4 **Be** 9.01218											5 **B** 10.811	6 **C** 12.011	7 **N** 14.0067	8 **O** 15.9994	9 **F** 18.9984	10 **Ne** 20.1797
3	11 **Na** 22.9898	12 **Mg** 24.305											13 **Al** 26.9815	14 **Si** 28.0855	15 **P** 30.9738	16 **S** 32.066	17 **Cl** 35.4527	18 **Ar** 39.948
4	19 **K** 39.0983	20 **Ca** 40.078	21 **Sc** 44.9559	22 **Ti** 47.88	23 **V** 50.9415	24 **Cr** 51.9961	25 **Mn** 54.9381	26 **Fe** 55.847	27 **Co** 58.9322	28 **Ni** 58.693	29 **Cu** 63.546	30 **Zn** 65.39	31 **Ga** 69.723	32 **Ge** 72.61	33 **As** 74.9216	34 **Se** 78.96	35 **Br** 79.904	36 **Kr** 83.80
5	37 **Rb** 85.4678	38 **Sr** 87.62	39 **Y** 88.9059	40 **Zr** 91.224	41 **Nb** 92.9064	42 **Mo** 95.94	43 **Tc** (98)	44 **Ru** 101.07	45 **Rh** 102.906	46 **Pd** 106.42	47 **Ag** 107.868	48 **Cd** 112.411	49 **In** 114.818	50 **Sn** 118.710	51 **Sb** 121.76	52 **Te** 127.60	53 **I** 126.904	54 **Xe** 131.29
6	55 **Cs** 132.905	56 **Ba** 137.327	57 **La** 138.906	72 **Hf** 178.49	73 **Ta** 180.948	74 **W** 183.84	75 **Re** 186.207	76 **Os** 190.23	77 **Ir** 192.22	78 **Pt** 195.08	79 **Au** 196.967	80 **Hg** 200.59	81 **Tl** 204.383	82 **Pb** 207.2	83 **Bi** 208.98	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
7	87 **Fr** (223)	88 **Ra** 226.025	89 **Ac** 227.028	104 **Rf** (261)	105 **Db** (262)	106 **Sg** (263)	107 **Bh** (262)	108 **Hs** (265)	109 **Mt** (266)	110 **Ds** (281)	111 **Rg** (272)	112 **Uub** (285)	113 **Uut** (284)	114 **Uuq** (289)	115 **Uup** (288)	116 **Uuh** (292)	117 **Uus** ?	118 **Uuo** (294)

58 **Ce** 140.115	59 **Pr** 140.908	60 **Nd** 144.24	61 **Pm** (145)	62 **Sm** 150.36	63 **Eu** 152.965	64 **Gd** 157.25	65 **Tb** 158.925	66 **Dy** 162.50	67 **Ho** 164.930	68 **Er** 167.26	69 **Tm** 168.934	70 **Yb** 173.04	71 **Lu** 174.967
90 **Th** 232.038	91 **Pa** 231.036	92 **U** 238.029	93 **Np** 237.048	94 **Pu** (240)	95 **Am** (243)	96 **Cm** (247)	97 **Bk** (248)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)	103 **Lr** (260)

Scratch

Scratch

Scratch