

Chemistry 432
Exam Number 3
Spring 2021
50 Minutes

$$R = 8.3144 \text{ J mol}^{-1} \text{ K}^{-1}$$

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

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

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

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

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

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

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

$$1 \text{ \AA} = 10^{-10} \text{ m}$$

$$1 \text{ nm} = 10^{-9} \text{ m}$$

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

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

Name:

Integral and Formula Table

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

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

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

$$\int_0^{\infty} x^3 e^{-ax^2} dx = \frac{1}{2a^2}$$

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

$$\int_0^{\infty} x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

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

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

$$\int_0^{2\pi} \cos^2 nx \, dx = \pi$$

$$\int_0^{\pi} \sin x \, dx = 2$$

$$\int_0^{n\pi} x^2 \sin^2 x \, dx = \frac{1}{24}[4n^2\pi^2 - 6n\pi]$$

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 normalized 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																	18 (8A)
2																	2
3																	10
4																	18
5																	36
6																	54
7																	86
8																	118
9																	150
10																	182
11																	210
12																	238
13																	270
14																	294
15																	322
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20																	466
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23																	550
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28																	690
29																	718
30																	746
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Scratch

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