CH 107 Physical Chemistry Make up Quiz

December 2016 Total Marks = 20 Time 2 hours

All questions have to be answered in the assigned place only. No marks will be given for answers in other places. All graphs and writing has to be done with pen. Pencil solutions will NOT be accepted.

Read questions carefully and keep answers to-the-point.
Provide arguments to earn full credit.

h=6.626x10^{-34}Js; c=3x10^{8} ms^{-1};m_e=9.1x10^{-31}kg;m_p=1.672x10^{-27} kg; e=6x10^{-19}C; 1eV=1.6x10^{-19} J;k_B=1.308 x 10^{-23} JK^{-1}

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1. Consider a function $\psi(x) = c\sin\left(\frac{\pi x}{a}\right) + d\sin\left(\frac{2\pi x}{a}\right)$ [c and d are constants].

A) Justify whether ψ(x) is an acceptable wavefunction for a particle in a 1D box of length *a*, with zero potential energy inside the box and infinite potential energy outside. **(1 mark)**

1. B) Justify whether ψ(x) is an eigenfunction of the total energy operator $\hat{H}$ for a free particle in a 1D box. **(1 mark)**

1. C) What is the expectation (average) value for total energy, E? **(2 marks)**

2. A) Draw the probability density contour plot of a particle in a square box of length L, for the state: (n_X =2, n_Y = 4). Show at least 3 probability contours and label the axes/quantum numbers appropriately. **(1 mark)**

2.B) Evaluate where the probability of finding an electron will be greatest for the following orbital. $\psi_{3d_{z^2}} = N\sigma^2 e^{-\sigma/3}\left(3\cos^2\theta - 1\right)$ where $\sigma = \frac{r}{a_0}$ and *N* is a constant. **(3 marks)**

3. A) Draw the polar plot for the angular part of the wavefunction $Y(\theta) = \cos\theta(5\cos^2\theta - 3)$ using the table and polar graph paper provided. Show the calculated data points on the polar plot. **(3 marks)**

3. B) Find the angular node(s), if any, and and indicate in the polar plot above. **(1 mark)**

4. A) What is the orbital approximation? **(1 mark)**

4. B) Express the Hamiltonian operator for Be (atomic number 4) in terms of 1 electron Hamiltonians AND other terms. Why is it not possible to exactly solve the time-independent-Schrodinger equation for Be atom. **(2 marks)**

4. C) Write the Slater determinant of Be atom in the ground state. **(1 mark)**

5.A) First ionization energy of the ground state ($1s^2$) of He is 24.6 eV. The wavelength of light needed for 1s to 2p transition in He is 58.4 nm. Calculate the first ionization energy from the 2p state of the excited He atom. (1eV = 8065 cm^{-1}; 1eV = 1240 nm) **(2 marks)**

5. B) Why is α(1)α(2) an acceptable 2-electron spin function, while α(1)β(2) is not? **(1 mark)**

5. C) Write the valid spin wavefunctions for a system of *2 electrons* with *opposite* spins. **(1 mark)**

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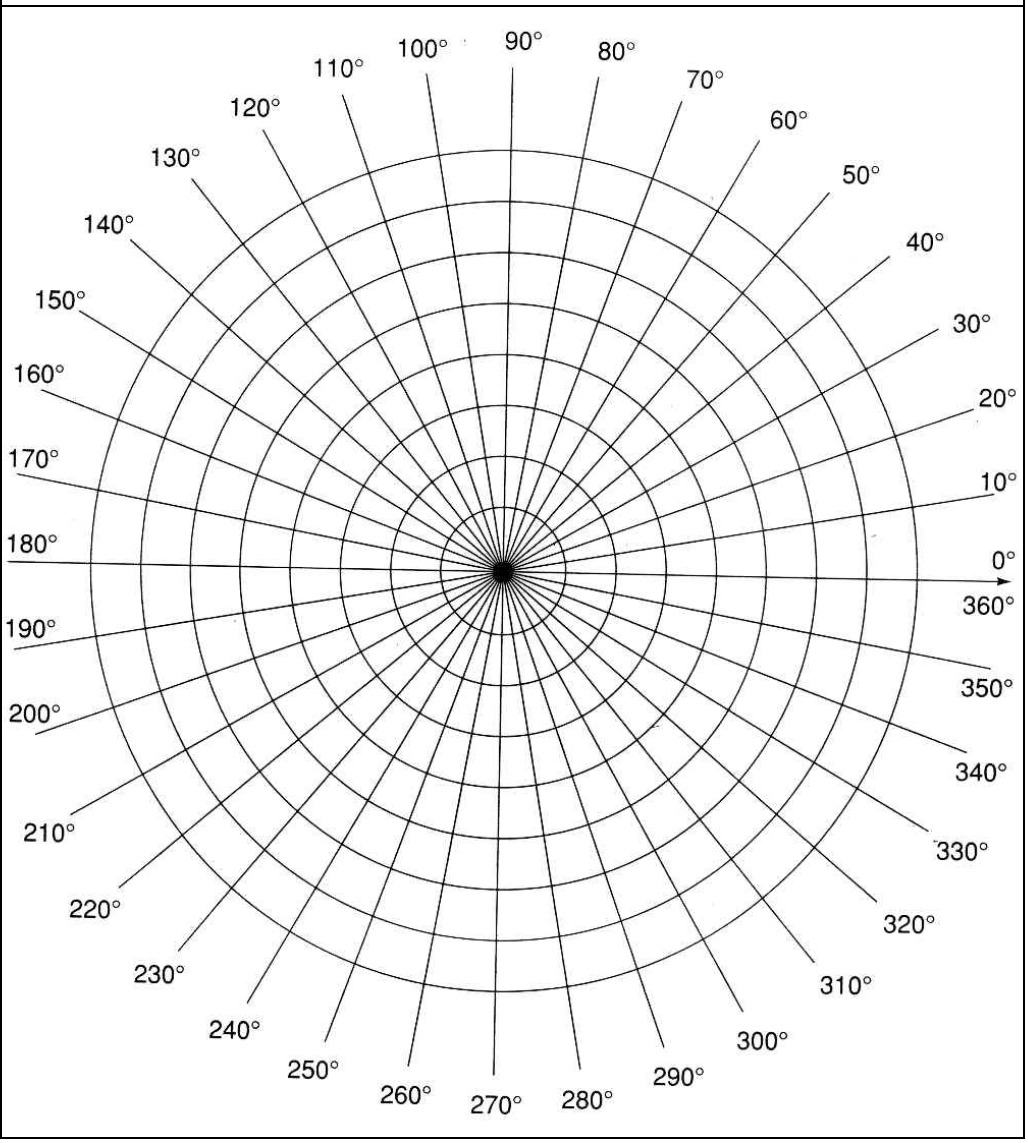
Roll Number:_____

θ	$Y(\theta)$	Polar Graph
0^0		
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