Chemistry II-AP

Quantum Mechanics Problem Set

1. Molybdenum metal must absorb radiation with a minimum frequency of 1.09x1015 s─ before it can eject an electron from its surface via the photoelectric effect.

(a) What is the minimum energy needed to eject an electron?

(b) What wavelength of radiation will provide a photon of this energy?

(c) If molybdenum is irradiated with light of wavelength of 120 nm, what is the maximum possible kinetic energy?

**(a) Emin = 7.22x10 -19 J**

**(b) λ = 275 nm**

**(c) E120 = 1.66x10 -18 J. The excess energy of the 120-nm photon is converted into kinetic energy of the emitted electron. Ek = 9.3x10 -19 J/electron**

2. Explain how the existence of line spectra is consistent with Bohr’s theory of quantized energies in the hydrogen atom?

**When applied to atoms, the notion of quantized energies means that only certain values of ∆E are allowed. These are represented by the lines on the emission spectra of excited atoms.**

3. Is energy emitted or absorbed when the following electronic transitions occur in hydrogen (circle):

(a) from *n* = 4 to *n* = 2. **emitted** absorbed

(b) from an orbit of radius 2.12 Å to one of radius 8.46 Å. emitted **absorbed**

(c) an electron adds to the H+ ion and ends up in the *n* = 3 shell. **emitted** absorbed

4. The Rydberg equation (shown below) is a generalization of a formula derived by Johannes Balmer in the early 1900s:

$$E=\left(-hcR\_{H}\right)\left(\frac{1}{n^{2}}\right)= -2.18x10^{-18} J\left(\frac{1}{n^{2}}\right)$$

(a) Using this equation, calculate the energy of an electron in the hydrogen atom when *n* = 2 and *n* = 6. Calculate the wavelength of the radiation released when an electron moves from *n* = 6 to *n* = 2.

(b) Is this line in the visible region of the electromagnetic spectrum. If so, what color is it?

**(a) E2 = -5.45x10 -19 J; E6 = -0.606x10 -19 J; ∆E = 4.84x10 -19 J; λ = 410 nm**

**(b) visible, violet**

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5. Use the de Broglie relationship to determine the wavelengths of the following objects:

(a) an 85-kg person skiing at 50 km/hr. (c) a lithium atom moving at 2.5x105 m/s.

(b) a 10.0-g bullet fired at 250 m/s. (d) an ozone (O3) molecule moving at 550 m/s.

**(a) λ = 5.6x10 -37 m; (c) λ = 2.3x10 -13 m**

**(b) λ = 2.65x10 -34 m; (d) λ = 1.51x10 -11 m**

6. Neutron diffraction is an important technique for determining the structure of molecules.

(a) How does this process support the ideas of both de Broglie’s “matter waves” and the wave-particle duality?

(b) Calculate the velocity of a neutron needed to achieve a wavelength of 0.955 Å. The mass of a neutron is required to solve this problem.

**(a) The process of neutron diffraction supports the matter waves and the wave-particle duality notions by showing that matter behaves in the same way as X-rays and other forms of electromagnetic radiation in terms of possessing energy, wavelength, and frequencies.**

**(b) 4.14x103 m/s**

7. Using Heisenberg’s uncertainty principle, calculate the uncertainty in the position of

(a) a 1.50-mg mosquito moving at a speed of 1.40 m/s if the speed is known within ±0.01 m/s;

(b) a proton moving at a speed of (5.00±0.01) x104 m/s. Locate the mass of a proton.

**(a) ∆x ≥ 4x10 -27 m (b) ∆x ≥ 3x10 -10 m**

8. Consider the contributions of Bohr and de Broglie for the following prompts:

(a) Why does the Bohr model of the hydrogen atom violate the uncertainty principle?

(b) In what way is the description of the electron using a wave function consistent with de Broglie’s hypothesis?

(c) What is meant by the term *probability density*? Given the wave function, how do we find the probability density at a certain point in space?

**(a) The uncertainty principle states that there is a limit to how precisely we can simultaneously know the position and momentum (a quantity relates to energy) of an electron. The Bohr model states that electrons move about the nucleus in precisely circular orbits of known radius and energy. This violates the uncertainty principle.**

**(b) De Broglie states that electrons demonstrate the properties of both particles and waves and that each moving particle has a wave associated with it. A wave function is the mathematical description of the matter wave of an electron.**

**(c) Although we cannot predict he exact location of an electron in an allowed energy state, we can determine the probability of finding an electron at a particular position. This statistical knowledge of electron location is the *probability density* and is a function of ψ2, the square of the wave function ψ derived from Schrödinger’s equation.**

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9. For *n* = 4, what are the possible values of ℓ? **ℓ = 3, 2, 1, 0**

For ℓ= 2, what are the possible values of *m*ℓ? ***m*ℓ = -2, -1, 0, 1, 2**

If *m*ℓ is 2, what are the possible values for ℓ? **ℓ ≥ 2 or ℓ = 2, 3, or 4**

10. Give the numerical values of *n* and ℓ corresponding to each of the following orbital designations:

(a) 3*p* (b) 2*s* (c) 4*f* (d) 5*d*

|  |  |  |
| --- | --- | --- |
| **Problem** | ***n*** | **ℓ**  |
| a | 3 | 1 |
| b | 2 | 0 |
| c | 4 | 3 |
| d | 5 | 2 |

11. Which of the following represent impossible combinations of *n* and ℓ (circle all that apply):

**(a) 1*p*** (b) 4*s* (c) 5*f* **(d) 2*d***

12. For the following table, write which orbital goes with the quantum numbers. Do not worry about *x*, *y*, and *z* subscripts. If the quantum numbers are not allowed, write “not allowed”. Circle the number which invalidates the set:

If the answer is not allowed, the portion which invalidates the set of quantum numbers is bolded.

|  |  |  |  |
| --- | --- | --- | --- |
| ***n*** | **ℓ** | ***m*ℓ** | **Orbital** |
| 2 | 1 | -1 | 2*p* (example) |
| 1 | 0 | 0 | **1*s*** |
| 3 | **-3** | 2 | **not allowed** |
| 3 | 2 | -2 | **3*d*** |
| 2 | 0 | **-1** | **not allowed** |
| 0 | 0 | 0 | **not allowed** |
| 4 | 2 | 1 | **4*d*** |
| 5 | 3 | 0 | **5*f*** |

13. Sketch the shape and orientation of the following types of orbitals using contour notation:

(a) *s*, (b) *p*z, (c) *dxy*, (d) *px*, (e) $d\_{z^{2}}$, and (f) $d\_{x^{2}-y^{2}}$.

|  |  |  |
| --- | --- | --- |
|  | $d\_{z^{2}}$ | $d\_{x^{2}-y^{2}}$ |



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14. Consider different types of orbitals for the following prompts:

(a) What are the similarities and differences between the 1*s* and 2*s* orbitals of the hydrogen atom?

(b) In what sense does a 2*p* orbital have directional character? Compare the “directional” characteristics of the *px* and $d\_{x^{2}-y^{2}}$. (That is, in what direction or region of space is the electron density concentrated?)

(c) What can you say about the average distance from the nucleus of an electron in a 2*s* orbital as compared with a 3*s* orbital?

(d) For the hydrogen atom, list the following orbitals in order of increasing energy: 4*f*, 6*s*,1*s*, 2*p*, 3*d*.

**(a) The hydrogen atom 1*s* and 2*s* orbitals have the same overall spherical shape, but the 2*s* orbital has a larger radial extension and one more node than the 1*s* orbital.**

**(b) A single 2*p* orbital is directional in that its electron density is concentrated along one of the three Cartesian axes of the atom. The** $d\_{x^{2}-y^{2}}$ **orbital has electron density along the *x*-axis.**

**(c) The average distance of an electron from the nucleus in a 3*s* orbital is greater than for an electron in a 2*s* orbital.**

**(d) 1*s* < 2*p* < 3*d* < 4*f* < 6*s***

15. The first 25 years of the twentieth century were momentous for the rapid pace of change in scientists’ understanding of the nature of matter.

(a) How did Rutherford’s experiments on the scattering of α particles by the gold foil set the stage for Bohr’s theory of the hydrogen atom?

(b) In what ways is de Broglie’s hypothesis, as it applies to electrons, consistent with J.J. Thomson’s conclusion that the electron has mass? In what sense is it consistent with proposals preceding Thomson’s work that the cathode rays are a wave phenomenon?

**(a) Bohr’s theory was based on the Rutherford model of the atom: a dense positive charge at the center and a diffuse negative charge surrounding it. The empirical evidence provided this idea because a majority of the alpha particles passed through the gold foil with only a small percentage being randomly deflected. Bohr’s theory then specified the nature of the diffuse negative charge. The prevailing theory before the nuclear model was Thomson’s plum pudding model: discrete electrons scattered about a diffuse positive charge cloud. Bohr’s theory could not have been based on the Thomson model of the atom.**

**(b) De Broglie’s hypothesis is that electrons exhibit both particle and wave properties. Thomson’s conclusion that electrons have mass is a particle property, while the nature of cathode rays is a wave property. De Broglie’s hypothesis actually rationalizes these two seemingly contradictory observations about the properties of electrons.**