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Chemistry 483

Examination 1
September 19, 2008

1. (50 points) Define and/or characterize

a. photon

a particle of light (or electromagnetic radiation) characterized by a frequency ν, wavelength λ & energy $E = h\nu = \frac{hc}{\lambda}$

b. line spectrum

When a atom falls from a higher energy level to a lower one it will emit radiation characteristic of the discrete energy difference between the atoms energy levels. The collection of these frequencies is a line spectrum

c. node

a point where a function is zero.

d. Bohr orbit

In the Bohr theory of the H atom the electron moves in a circular orbit of radius $a_0 = 0.5291772$ Å. This is called the Bohr orbit

e. Kronecker delta

A symbol δ_{ij} defined so that

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

Useful in designating orthogonal functions that are also normalized

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f. correspondence principle

when the quantum numbers associated with a system become very large the system begins to behave as it would classically.

g. Hamiltonian for a particle confined to a cube

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

h. Harmonic oscillator

A system in which a particle is attracted to the origin with a force that depends linearly on the displacement from the origin. $F = -kx$. Results in a potential energy $V = \frac{1}{2}kx^2$.

i. stationary state

If the solution to the time dependent ~~wave~~ Hamiltonian is $\Psi = \psi_N(x)e^{-iE_N t/\hbar}$ where $\hat{\mathcal{H}}\psi_N = E_N\psi_N$ then $\Psi^*\Psi = \psi_N^*(x)\,\psi_N(x)$ & Ψ is a stationary state.

j. eigenfunction

given an operator $\hat{A}$ & a function f if $\hat{A}f = \lambda f$ where λ is a constant then f is an eigenfunction of $\hat{A}$.

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2. (15 points) A ground-state hydrogen atom absorbs a photon of light that has a wavelength of 97.2 nm. It then gives off a photon that has a wavelength of 486 nm. What is the final state of the hydrogen atom?

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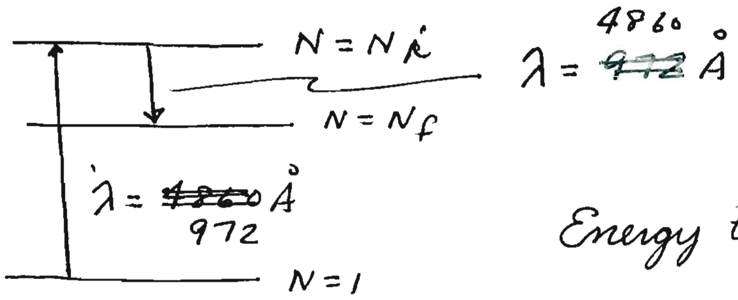

Energy to go from $N=1$ to N_i

$$\frac{12399}{972} = 12.75 \text{ eV}$$

$$\therefore \quad \Delta E = -13.6057\left(\frac{-1}{N_i^2} + \frac{1}{1}\right) = -12.75$$

$$\frac{1}{N_i^2} = 1 - 0.9371 = 0.0629$$

$$N_i \sim 4$$

emmission $\quad \Delta E = -13.6057\left(\frac{1}{N_f^2} - \frac{1}{16}\right) = -2.55$

$$\frac{12399}{4860} = 2.55 \text{ eV}$$

$$\frac{1}{N_f^2} = 0.1875 + \frac{1}{16} = 0.25$$

$$\boxed{N_f = 2.0}$$

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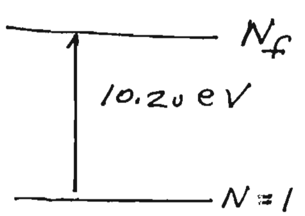
or the atom winds up in the state which is 10.20 eV above ground state

$$\Delta E = -13.6057\left(\frac{1}{N_f^2} - 1\right) = 10.20$$



$$\frac{1}{N_f^2} = 0.25$$

$$\boxed{N_f = 2}$$

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3. (10 points) Given that the work function of Chromium is 4.40 eV, calculate the kinetic energy (in eV) of the electrons emitted from a Chromium surface that is irradiated with ultraviolet radiation of wavelength 200 nm.

$E = KE + W$

$W = 4.40\ eV$

$E = \frac{12399}{2000} = 6.2\ eV$

$W = 6.2 - 4.4 = 1.8\ eV$

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4. (10 points) In each case, show that $f(x)$ is an eigenfunction of the operator given. Find the eigenvalue.

	Operator	$f(x)$	eigenvalue
(a)	$\frac{d^2}{dx^2}$	$\cos \omega x$	$-\omega^2$
(b)	$\frac{d}{dt}$	$e^{i\omega t}$	$i\omega$
(c)	$\frac{d^2}{dx^2}+2\frac{d}{dx}+3$	e^{ax}	a^2+2a+3
(d)	$\frac{\partial}{\partial y}$	x^2e^{6y}	6

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5.(15 points) The force constant of $^{79}Br^{79}Br$ is 240 Nm^{-1}. Calculate the fundamental vibrational frequency and the zero-point energy of $^{79}Br^{79}Br$.

$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}} \qquad \mu = \frac{M}{2} = \frac{79}{2}(1.661 \times 10^{-27})\ kg$$

$$\nu = \frac{1}{2\pi}\sqrt{\frac{(240)(2)}{(79)(1.661)} \times 10^{+27}} = \frac{1}{2\pi}\sqrt{36.58 \times 10^{26}}$$

$$\nu = \frac{6.048}{2\pi} 10^{13}\ Hz = 0.963 \times 10^{13}\ Hz$$

$$E = \frac{h\nu}{2} = \frac{(6.626)(0.963)}{2} 10^{-34+13}\ J = 3.19 \times 10^{-21}\ J$$

~~to~~ in eV

$$\frac{3.19 \times 10^{-21}\ J}{1.602 \times 10^{-19}\ J/eV} = 1.99 \times 10^{-2}\ eV \simeq .02\ eV$$