YORK UNIVERSITY **NAME:** ______________________________

W 2011 SC/CHEM 2010.03 **STUDENT NO.** ________________________

Test # 1 **February 7, 2011** **8 questions** **50 minutes** **25 marks**

No documentation allowed. The last page has useful constants and equations.

[**marks**]

1. Fill in the gaps

[**1**] **(1-1)** Give the value of kT or of RT, when $T = 300\,\mathrm{K}$, in units of kcal/mol, or kJ/mol, or eV, or a.u., whichever you prefer:

$kT = 0.026eV = 0.00095a.u.$; $RT = 0.59kcal/mol = 2.5kJ/mol$

[**1**] **(1-2)** A carbon atom is 12 times heavier than a H atom. If a H atom with speed "v" has a DeBroglie wavelength equal to "λ_H", then the DeBroglie wavelength of a C atom with speed "$v/2$" is equal to λ_H multiplied by 1/6

$\lambda = h/p = h/(12m_H \cdot v/2) = h/6m_H v = (1/6)\lambda_H$

[**1**] **(1-3)** If the complex number $z = 5 + 2i$, then $z^*z = 29$

[**2**] **(1-4)** Ionization energies of molecules range between 4 eV and 16 eV roughly. (You will get full marks if both numbers are within a factor of two of the correct values.)

[**1**] **(1-5)** Consider a particle of mass m in a cubic box of dimensions $\ell \times \ell \times \ell$. The degeneracy of the energy level $E = 6h^2/8m\ell^2$ is equal to

3 (QNs 211, 121, and 112)

[3] 2. Photons with a wavelength equal to $250\,nm = 2.50 \times 10^{-7}\,m$ strike a solid. Electrons are emitted from the solid (photoelectric effect) with a velocity equal to $4.0 \times 10^5\,m\,s^{-1}$ and have a kinetic energy $\frac{1}{2}mv^2 = h\nu - W$, where W is the work function of the solid. Calculate W and give your final answer in units of eV.

$E_{photon} = h\nu = hc/\lambda = 7.946 \times 10^{-19} J$
$KE_{electron} = mv^2/2 = 7.287 \times 10^{-20} J$
$W = E_{photon} - KE_{electron} = 7.217 \times 10^{-19} J = 4.50 eV$

[3] 3. A beam of He^+ ions travelling at a speed of 1000 m/s is directed at a Ni crystal's surface. The mass of a He^+ ion is 7342 a.u. Atoms in a Ni crystal are arranged in a regular pattern with interatomic spacings equal to 2.5 Å. Do you think that you could use classical mechanics to give an accurate description of the collisions between He^+ and Ni and of the diffraction of He^+ ions by the Ni surface? Or would you need quantum mechanics? Explain.

$\lambda(He^+) = h/mv = 0.991$ Å
spacing between Ni atoms: 2.5 Å
$\lambda(He^+)$ is not extremely small compared to 2.5 Å, so the wavelike aspects of He^+ can not be ignored and we can not use classical mechanics.

[3] 4. Sketch the wavefunction $\psi_4(x)$ (quantum number $n = 4$) for a particle in a box of length 12 Å, with the box extending from $x = 0$ to $x = 12$ Å. Beside your sketch, indicate:

(a) all x values for which $\psi_4(x) = 0$;

$x = 0, 3, 4, 9, 12$ Å(and also outside the box, $x < 0$ and $x > 12$

(b) the numerical value of $\psi_4(x)$ at the maxima (if you don't remember, estimate it).

$\sqrt{2/a} = \sqrt{2/12\mathring{A}} = 0.408$ Å$^{-1/2}$
(note: $|\psi(x)|^2 dx$ is a probability, so it is dimensionless. But dx has units of length (m or Å) so ψ must have units of $m^{-1/2}$ or Å$^{-1/2}$

[1] 5. The N-N bond in dinitrogen is one of the strongest chemical bonds there is. *Approximately* what energy is required to break that bond? (You can answer in any system of units you want. $1\,a.u. = 27.21\,eV = 627.5\,kcal/mol = 2625\,kJ/mol$)

10 eV (chemical bond energies are roughly in the range from 1 to 10 eV)

[2] 6. Calculate the electrostatic interaction (energy of interaction) for a system of three protons ($q = +1\,a.u.$ for each H^+) that are arranged on a line, with the H^+ at positions $x = 0.00\ a.u.$, $x = 12.00\ a.u.$, and $x = 24.00\ a.u.$. Give your final answer in units of kcal/mol.
$(1a.u. = 27.21eV = 627.5kcal/mol = 2625kJ/mol)$

$U_{electrostatic} = 1 \cdot 1/12 + 1 \cdot 1/12 + 1 \cdot 1/24 = 0.2083\,a.u. \times (627.5kcal/mol/a.u.) = 131kcal/mol$

[4] **7.** The wavefunction of a particle of mass m in a finite depth box (PIFDB) of depth V_0 that extends from $x = -a/2$ to $x = +a/2$ is denoted $\psi(x)$. The energy E of the particle is: $E = V_0/4$. That wavefunction, $\psi(x)$, is not zero outside the box:

$$P = \int_{x=-\infty}^{x=-a/2} |\psi(x)|^2 \, dx \; + \; \int_{x=+a/2}^{x=+\infty} |\psi(x)|^2 \, dx \; \neq \; 0$$

(7-1) Explain in words the physical meaning of "P", what it represents.

P is the probability of finding the particle outside the box, ie, it is the probability of finding $x < -a/2$ or $x > a/2$ when we measure the position x.

Indicate whether P increases, decreases, or stays the same, for each of the following changes:

(7-2) increase the mass of the particle from m to $100m$ decreases

(7-3) increase the size of the box from a to $100a$ decreases

(7-4) increase the energy of the particle from $V_0/4$ to $V_0/2$ increases

8. Give a short explanation for the following expressions.
[1] **(8-1)** Heisenberg uncertainty principle:
$\Delta x \Delta p_x \geq \hbar/2$. When we measure position x and momentum p_x simultaneously for a particle, the product of uncertainties on x and p_x can not be zero, and must be larger than $\hbar/2$.

[1] **(8-2)** wave-particle duality:
matter (e.g., electrons) sometimes behaves like a wave; waves (e.g., light) sometimes behaves like a collection of particles (photons in the case of light).

[1] **(8-3)** zero-point energy:
The lowest possible energy a system (or particle) can have, for example, $h^2/8ma^2$ for the PIB.

THE END

Constants, Conversion Factors, Equations

$k_B = 1.381 \times 10^{-23}\, J\, K^{-1}$; $h = 2\pi$ a.u. of action $= 6.626 \times 10^{-34}\,\mathrm{J\,s}$

$c = 2.998 \times 10^{8}\,\mathrm{m\,s^{-1}}$; $m_e = 1$ a.u. of mass $= 9.109 \times 10^{-31}\,\mathrm{kg}$

1 a.u. of distance = 1 bohr = 0.5292 Å $= 5.292 \times 10^{-11}\,\mathrm{m}$

1 a.u. of charge $= e = 1.602 \times 10^{-19}\,\mathrm{C}$

1 a.u. of energy = 27.211 eV = 627.5 kcal mol^{-1} $= 4.360 \times 10^{-18}\, J$

$U_{el.} = \frac{Q_1 Q_2}{4\pi\epsilon_0 r}$; permittivity of vacuum: $4\pi\epsilon_0 = 1$ in atomic units

$E(n_x, n_y, n_z) = (h^2/8m)\,(n_x^2/a^2 + n_y^2/b^2 + n_z^2/c^2)$

$\psi(x) = (2/a)^{1/2} \sin(n_x \pi x/a)$