Chemistry 432
Quiz Number 4
Spring 2019
Solution

R =8.3144 J mol^{-1} K^{-1}

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

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

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

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

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

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

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

1 Å= 10^{-10} m

1 nm = 10^{-9} m

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

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

Name:

Integral and Formula Table

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

$$\int_0^\infty xe^{-ax^2} dx = \frac{1}{2a}$$

$$\int_0^\infty x^2 e^{-ax^2} dx = \frac{1}{4}\frac{\sqrt{\pi}}{a^{3/2}}$$

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

$$\int_0^\infty x^4 e^{-ax^2} dx = \frac{3\sqrt{\pi}}{8a^{5/2}}$$

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

$$\int x^n \ dx = \frac{x^{n+1}}{n+1} + \text{constant}$$

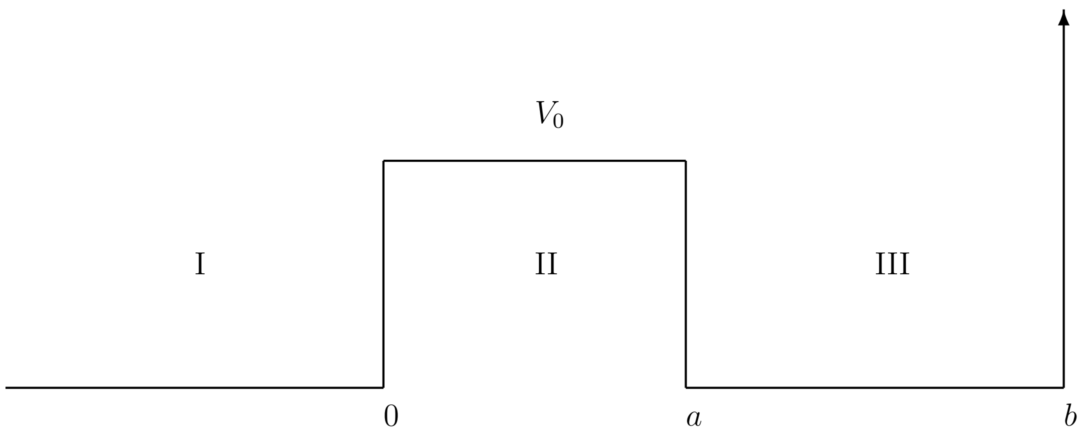
$$\int \sin^2 x dx = \frac{1}{2}x - \frac{1}{4}\sin 2x$$

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

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

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

Name:



A one-dimensional particle of mass m is confined to move under the influence of the potential

$$V(x) = \begin{cases} 0 & -\infty \leq x \leq 0 \\ V_0 & 0 \leq x \leq a \\ 0 & a < x \leq b \\ \infty & x > b \end{cases}$$

and pictured above. Give the Schrödinger equation for the particle in regions I, II and III, and impose the proper boundary conditions for the wavefunctions in each of the three regions. Show that the wavefunction

$$\psi_{II}(x) = Ce^{Kx} + De^{-Kx}$$

with

$$K^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

satisfies the Schrödinger equation in region II for $E < V_0$.

Answer:

$$\text{Region I} : -\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = E\psi_I$$

$$\text{Region II} : -\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + V_0\psi_{II} = E\psi_{II}$$

$$\text{Region III} : -\frac{\hbar^2}{2m}\frac{d^2\psi_{III}}{dx^2} = E\psi_{III}$$

Name:

Boundary conditions

$$\psi_I(0) = \psi_{II}(0) \qquad \psi'_I(0) = \psi'_{II}(0)$$

$$\psi_{II}(a) = \psi_{III}(a) \qquad \psi'_{II}(a) = \psi'_{III}(a)$$

$$\psi_{III}(b) = 0$$

Verify solution

$$\psi'_{II}(x) = KCe^{Kx} - KDe^{\kappa x} \qquad \psi''_{II}(x) = K^2Ce^{Kx} + K^2De^{-Kx} = K^2\psi_{II}(x)$$

$$\hat{H}\psi_{II} = -\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + V_0\psi_{II} = -\frac{\hbar^2K^2}{2m}\psi_{II} + V_0\psi_{II} = E\psi_{II}$$

$$E = V_0 - \frac{\hbar^2K^2}{2m} \qquad K^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

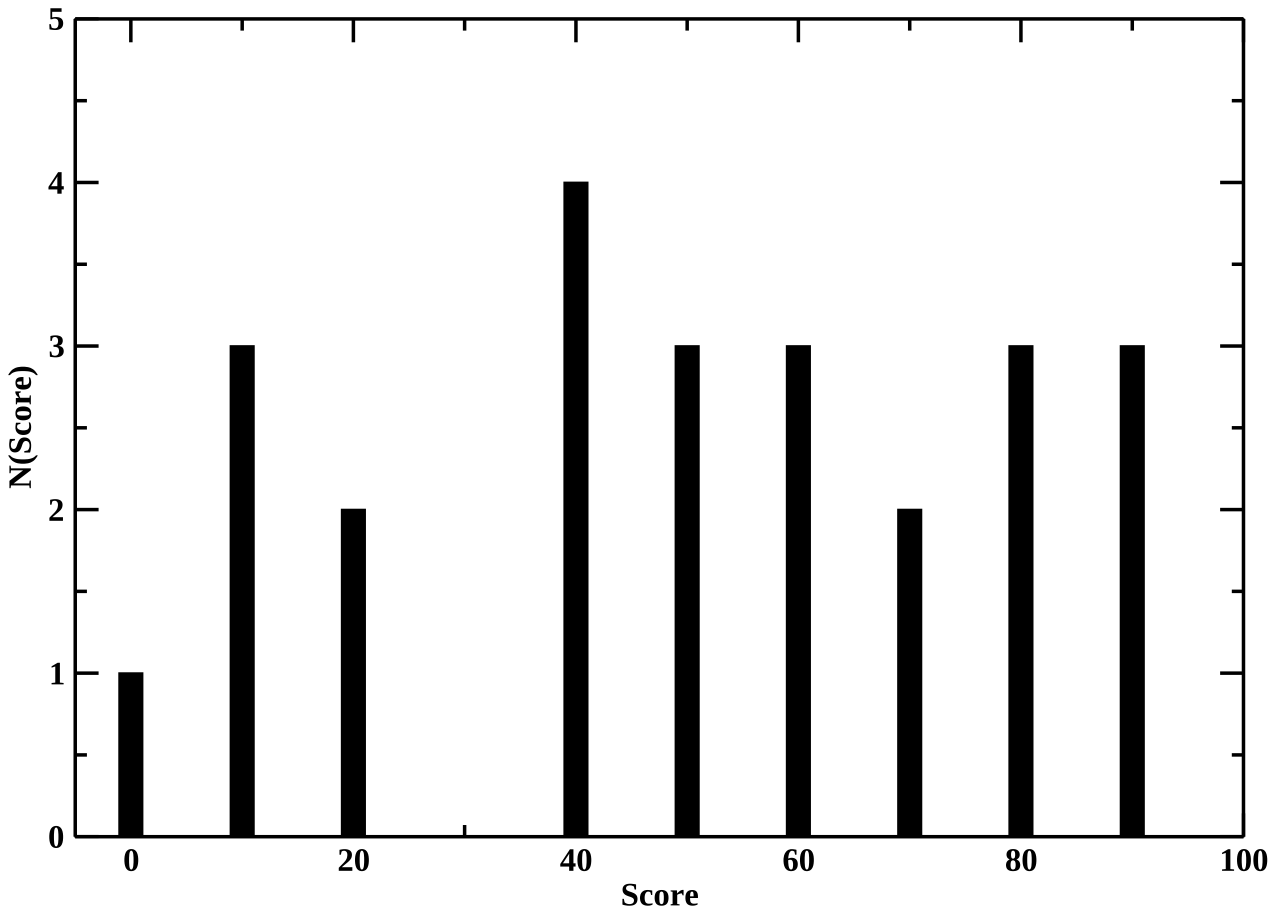


Figure 1: **High = 100, Median = 54, Mean = 56**