Assessment 5

The due date for submitting this assignment has passed. Due on 2017-02-03, 23:59 IST.

Submitted assignment

Chemistry I Introduction to Quantum Chemistry and Molecular Spectroscopy

Week 3: Tutorial 5 by K. Mangala Sunder
Department of Chemistry, Indian Institute of Technology Madras

Assume speed of light to be $3 \times 10^8$ m.s$^{-1}$; Planck’s constant $h = 6.626 \times 10^{-34}$ J.s

1) In the spherical polar coordinate system employed to solve the Schrodinger equation for hydrogen atom, the radial coordinate has the following range:

$0 \leq r \leq \pi$

$0 \leq r \leq a_0$ only, where is $a_0$ Bohr radius

$0 \leq r \leq \infty$

$-\infty \leq r \leq \infty$

**No, the answer is incorrect.**

Score: 0

**Accepted Answers:**

$0 \leq r \leq \infty$

2) The volume element for the spherical coordinate system for hydrogen atom is given by

$drd\theta d\phi$

$r^2 drd\theta d\phi$

$r^2 drsin\theta d\theta d\phi$

$rdrcos\theta d\theta d\phi$

**No, the answer is incorrect.**

Score: 0

**Accepted Answers:**

$r^2 drsin\theta d\theta d\phi$
3) The potential energy for the electron in the hydrogen atom due to nuclear coulombic attraction has the following property:

- The energy becomes zero after a large but finite distance from the proton.
- The energy remains attractive and non-zero at all distances, finite or infinites, from the nucleus.
- The energy becomes repulsive and positive at distances beyond 100 Angstroms.
- The energy tends to zero, as the electron tends to be farther away from the nucleus.

No, the answer is incorrect.
Score: 0
Accepted Answers:
The energy tends to zero, as the electron tends to be farther away from the nucleus.

4) The integral \( \int_{\theta=0}^{\pi} \cos \theta d\theta \int_{\phi=0}^{\pi} d\phi \) has the value

- 0
- \( 2\pi \)
- 3\( \pi \)
- 4\( \pi \)

No, the answer is incorrect.
Score: 0
Accepted Answers:
0

5) The derivative operator \( \frac{\partial}{\partial r} (r^2 \frac{\partial}{\partial r}) \) is the same the operator.

- \( r^2 \frac{\partial^2}{\partial r^2} \)
- \( 2r \frac{\partial^2}{\partial r^2} \)
- \( 2r \frac{\partial}{\partial r} + r^2 \frac{\partial^2}{\partial r^2} \)
- \( 2r \frac{\partial}{\partial r} \)

No, the answer is incorrect.
Score: 0
Accepted Answers:
\( 2r \frac{\partial}{\partial r} + r^2 \frac{\partial^2}{\partial r^2} \)

6) In a spherical polar coordinate system, the quantity \( x^2 + y^2 \) is given by

- \( r^2 \sin^2 \theta \)
- \( r^2 \cos^2 \theta \)
- \( r^2 \)
- \( 1 \)

No, the answer is incorrect.
Score: 0
Accepted Answers:
\( r^2 \sin^2 \theta \)

7)
In a coordinate system given by $x = r \cos \theta$, $y = r \sin \theta$, the derivative operator $\frac{\partial}{\partial r}$ is given by

\[
\begin{align*}
\frac{\partial}{\partial x} &\quad \frac{\partial}{\partial y} \\
\frac{1}{r} \frac{\partial}{\partial r} &\quad \partial \theta \\
\cos \theta \frac{\partial}{\partial r} - \sin \theta \frac{\partial}{\partial \theta} &\quad \sin \theta \frac{\partial}{\partial r} + \frac{\cos \theta}{r} \frac{\partial}{\partial \theta}
\end{align*}
\]

No, the answer is incorrect.
Score: 0
Accepted Answers:
$\sin \theta \frac{\partial}{\partial r} + \frac{\cos \theta}{r} \frac{\partial}{\partial \theta}$

8) In the two dimensional polar coordinate system the area element $dxdy$ is given in terms of variables $r$ and $\theta$ as

- $dr d\theta$
- $r dr d\theta$
- $r^2 dr d\theta$
- $\frac{dr}{r}$

No, the answer is incorrect.
Score: 0
Accepted Answers:
$r dr d\theta$

9) The wave function for hydrogen atom must satisfy dimensionality requirement when the spherical polar coordinate $r$ represents distance from the nucleus. The normalization condition $\int r^2 dr \int \sin \theta d\theta \int d\phi \psi^* (r, \theta, \phi) \psi(r, \theta, \phi) = 1$ implies that the wave function has the dimension of

- distance
- $\sqrt{\text{distance}}$
- $\frac{1}{(\text{distance})^{3/2}}$
- $(\text{distance})^{3/2}$

No, the answer is incorrect.
Score: 0
Accepted Answers:
$\frac{1}{(\text{distance})^{3/2}}$

10) The following integral will be useful for hydrogen atom calculations. Hence evaluate the integral $\int_0^\infty r^2 e^{-r} dr$. The answer is

- 4
- 2
- 1
- $1/2$

No, the answer is incorrect.
Score: 0