Assessment 6

The due date for submitting this assignment has passed. Due on 2017-03-05, 23:59 IST.

Submitted assignment

Chemistry I Introduction to Quantum Chemistry and Molecular Spectroscopy
Week 3: Tutorial 6 by K. Mangala Sunder
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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) The p-orbital function from the real part of the spherical harmonic $Y_{1}^{1}(\theta\phi$) will be designated as

- $d_{zx}$
- $d_{zy}$
- $d_{xz}$
- $P_{x}$
- $P_{y}$

No, the answer is incorrect.
Score: 0
Accepted Answers:
$P_{x}$

2) The d orbital $d_{z^2-x^2}$ is represented correctly as

- Real part of the Spherical Harmonic $Y_{2}^{0}(\theta\phi)$
- Real part of the Spherical Harmonic $Y_{2}^{2}(\theta\phi)$
- Real part of the Spherical Harmonic $Y_{2}^{-2}(\theta\phi)$
- Imaginary part of the Spherical Harmonic $Y_{2}^{2}(\theta\phi)$

No, the answer is incorrect.
Score: 0
Accepted Answers:
Real part of the Spherical Harmonic $Y_{2}^{2}(\theta\phi)$
3) The spherical harmonic with the angular function given by \( \sin^2 \theta \cos \theta e^{-2i\phi} \) is denoted by the symbol

- \( Y_0^0(\theta, \phi) \)
- \( Y_1^1(\theta, \phi) \)
- \( Y_2^2(\theta, \phi) \)
- \( Y_3^{-1}(\theta, \phi) \)

No, the answer is incorrect.
Score: 0
Accepted Answers:
\( Y_3^{-1}(\theta, \phi) \)

4) The orthogonality of two spherical harmonics \( Y_1^1(\theta, \phi) \) and \( Y_1^{-1}(\theta, \phi) \) is represented correctly by the integral

\[
\int_0^\pi \sin \theta d\theta \int_0^{2\pi} f_{\theta=0}^{2\pi} [Y_1^1(\theta, \phi)]^* [Y_1^{-1}(\theta, \phi)] d\phi \\
\int_0^\pi \sin \theta d\theta \int_0^{2\pi} f_{\phi=0}^{2\pi} [Y_1^1(\theta, \phi)]^* [Y_1^{-1}(\theta, \phi)] d\phi \\
\int_0^\pi \sin \theta d\theta \int_0^{2\pi} f_{\phi=0}^{2\pi} [Y_1^1(\theta, \phi)][Y_1^{-1}(\theta, \phi)] d\phi \\
\int_0^\pi \sin \theta d\theta \int_0^{2\pi} f_{\phi=0}^{2\pi} [Y_1^1(\theta, \phi)][Y_1^{-1}(\theta, \phi)] d\phi
\]

No, the answer is incorrect.
Score: 0
Accepted Answers:
\[
\int_0^\pi \sin \theta d\theta \int_0^{2\pi} f_{\theta=0}^{2\pi} [Y_1^1(\theta, \phi)]^* [Y_1^{-1}(\theta, \phi)] d\phi
\]

5) The number of nodes in a d-orbital function is

- 0
- 1
- 2
- 3

No, the answer is incorrect.
Score: 0
Accepted Answers:
2

6) The total number of nodes of 4p orbital is (the entire orbital including radial and angular functions)

- 0
- 1
- 2
- 3

No, the answer is incorrect.
Score: 0
Accepted Answers:
3

7) The total number of degenerate orbitals for the principal quantum number 7 is

- 16
8) The hydrogen atom wave function with radial and angular parts together are given as 1 point a PDF file in the lecture notes. Study the trends. This and the next two questions will be to identify the quantum numbers and energies associated with the hydrogen atom wave functions.

The wave function \( \psi_{nlm}(r, \theta, \phi) = \sqrt{\frac{1}{16\pi}} \left( \frac{Z}{3\alpha_0} \right)^{3/2} \left( \frac{Z}{3\alpha_0} \right)^2 e^{-\frac{Zr}{3\alpha_0}(3\cos^2\theta - 1)} \) is correctly labeled as

\[
3s
\]

\[
3p_x
\]

\[
3d_{x^2-y^2}
\]

\[
3d_{3z^2-r^2}
\]

No, the answer is incorrect.

Score: 0

Accepted Answers:

49

9) The wave function \( \psi_{nlm}(r, \theta, \phi) = \sqrt{\frac{1}{16\pi}} \left( \frac{Z}{3\alpha_0} \right)^{3/2} \left( \frac{Z}{3\alpha_0} \right)^2 e^{-\frac{Zr}{3\alpha_0}(3\cos^2\theta - 1)} \) has the following values for quantum numbers,

\[
n=2, l=0, m=0
\]

\[
n=2, l=1, m=1
\]

\[
n=2, l=1, m=0
\]

\[
n=2, l=1, m=-1
\]

No, the answer is incorrect.

Score: 0

Accepted Answers:

\[
n=2, l=1, m=1
\]

10) The wave function \( \psi_{nlm}(r, \theta, \phi) = \sqrt{\frac{1}{16\pi}} \left( \frac{Z}{3\alpha_0} \right)^{3/2} \left( \frac{Z}{3\alpha_0} \right)^2 e^{-\frac{Zr}{3\alpha_0}(3\cos^2\theta - 1)} \) is correctly labeled as

\[
3d_{xy}
\]

\[
3d_{x^2-y^2}
\]

\[
3d_{xz}
\]

\[
3d_{yz}
\]

No, the answer is incorrect.

Score: 0

Accepted Answers:

\[
3d_{xy}
\]