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**GARISSA UNIVERSITY**

**UNIVERSITY EXAMINATION 2019/2020 ACADEMIC YEAR FOUR**

**SECOND SEMESTER EXAMINATION**

**SCHOOL OF PURE AND APPLIED SCIENCES**

**FOR THE DEGREE OF BACHELOR OF EDUCATION**

**COURSE CODE: CHE 414**

**COURSE TITLE: QUANTUM CHEMISTRY**

**EXAMINATION DURATION: 2 HOURS**

**DATE: 12/02/2020 TIME: 2.00-4.00 PM**

**INSTRUCTION TO CANDIDATES**

* **The examination has FIVE (5) questions**
* **Question ONE (1) is COMPULSORY**
* **Choose any other TWO (2) questions from the remaining FOUR (4) questions**
* **Use sketch diagrams to illustrate your answer whenever necessary**
* **Do not carry mobile phones or any other written materials in examination room**
* **Do not write on this paper**

**This paper consists of THREE (3) printed pages *please turn over***

**QUESTION ONE (COMPULSORY)**

1. (i) state at **least 3** postulates of Dalton’s Atomic Theory **[3 marks]**

(ii) What is the wavelength of yellow light with a frequency of 5.09 x 1014 s-1? **[3 marks]**

 (iii) State **3** Bohr’s Model assumptions **[3 marks]**

 (iv) State 2 failures of the Bohr Model **[3 marks]**

1. (i) What is the wavelength of the light emitted when the electron in a hydrogen atom undergoes a transition from ***n* = 6** to ***n* = 3**? **[7 marks]**

(ii) State the **Uncertainity Principle [4 marks]**

(iii) Using Maxwell’s Equation and considering the de – Broglie relationship is; $p =\frac{h}{λ}$

 Show that Maxwell’s equation of wave motion becomes

$           \frac{∂²Ψ }{∂x²}+\frac{∂²Ψ}{∂y² }+\frac{∂²Ψ}{∂ƶ²}=\frac{1}{V²}\frac{∂²Ψ}{∂t²}=\frac{p²}{E²}\frac{∂²Ψ}{∂t²}$ **[7 marks]**

**Useful information:**

*C= 2.997925 x 108 m/s*

*Planck’s constant = 6.626 x10-34 Js R*H = 2.179 × 10-18 J

**QUESTION TWO**

1. Define the following terms as used in Quantum chemistry
2. laplacian operator $∇^{2}$
3. An operator
4. Eigen functions
5. Commute **[12 marks]**
6. Show that if Ψ is an eigen function of a linear operator α with eigen value λ, then c Ψ (c is a constant) is also an eigen function of α with the same eigen value. **[4 marks]**
7. In Quantum chemistry, acceptable eigen functions are chosen from which class of functions? **[4 marks]**

**QUESTION THREE**

1. Using the quantum mechanics postulates, show that the Hamiltonian operator is:

 $=\frac{-h^{2}}{8π^{2}m}\left(\frac{∂^{2}}{∂x^{2}}+\frac{∂^{2}}{∂y^{2}}+\frac{∂^{2}}{∂z^{2}}\right)+V(x,y,z)$ **[10 marks]**

1. Considering a particle in a box which is allowed to move in a limited space along length =a, what are the Schrödinger’s equation inside and outside the box? **[10 marks]**

**QUESTION FOUR**

By use of graphs, and considering a particle in a 1D box of length =a, show the values of $Ψ and Ψ²$ from n=1 to n=4 **[20 marks]**

**QUESTION FIVE**

The π electrons in benzene are delocalized and can be considered to move in a circle.

 

Calculate $∆E=E\_{2}-E\_{1}$ for r = 0.139nm and show that benzene absorbs at 209nm **[20 marks]**