

BOWEN UNIVERSITY, IWO, OSUN STATE
COLLEGE OF AGRICULTURE, ENGINEERING AND SCIENCE
INDUSTRIAL CHEMISTRY PROGRAMME

2022/2023 B.SC DEGREE SECOND SEMESTER EXAMINATION

Courses Title: Introductory Quantum Chemistry and Atomic & Molecular Structure

Date: 27/06/2023 Course Code: CHM 310 Credit: 3 Time Allowed: 3hrs

-
- INSTRUCTIONS** (a) Answer FOUR questions in all
(c) Answer TWO questions from EACH section
-

USEFUL PHYSICAL CONSTANTS

Gas constant, R	=	8.314Jmol ⁻¹ K ⁻¹
Velocity of light, c	=	2.99793 x 10 ⁸ ms ⁻¹ = 2.99793 x 10 ¹⁰ cms ⁻¹
1 Newton	=	10 ³ g.ms ⁻²
Planck's constant, h	=	6.626 x 10 ⁻³⁴ J.s
Avogadro's number. N _A	=	6.023 x 10 ²³ mol ⁻¹
Atomic mass of carbon, C	=	12.011amu
1 atomic mass unit	=	1.66 x 10 ⁻²⁷ kg
Atomic mass of hydrogen	=	1.007825 amu
Atomic mass of carbon	=	12.01 amu
Atomic mass of oxygen	=	15.999 amu

SECTION A

QUESTION ONE (25 MARKS)

- a. Highlight any two (2) advance methods involved in treating molecules based on principle of wave mechanics. 4 Marks
- b. Discuss in details the methods mentioned in 1a above. 5 Marks

c. Calculate the dipole moment for HCl given the following data, $r_H = (124.0, 0, 0)$ $r_{Cl} = (-3.5, 0, 0)$, $q_H = 2.70 \times 10^{-20} \text{ C}$ and $q_{Cl} = 2.70 \times 10^{-20} \text{ C}$. **10 Marks**

(ii) Do you expect the transition moment to be equal to zero? Give reason for your answer

6 Marks

QUESTION TWO (25 MARKS)

a. Under symmetry conditions, what are the point groups that are associated with the production of pure rotational spectra? **5 Marks**

b. Derive an expression for the classical and quantum rotational energy of a spherical top molecule. **9 Mark**

c. Given the following data for hydrogen atom, show that hydrogen molecule cannot exhibit transition upon interaction with electromagnetic radiation. $r_H = (124.0, 0, 0)$, $q_H = 2.70 \times 10^{-20} \text{ C}$. **6 Marks**

d. What are the shortcomings of rotational and vibrational spectroscopy over electronic spectroscopy? **5 Marks**

QUESTION THREE (25 MARKS)

a. Given that N_1 represents the population of the first level, i.e. level 1 and A_{12} is the Einstein coefficient of spontaneous emission, show that N_1 has an exponential relationship with A_{12} **4 Marks**

b. State at least one example of spectroscopic techniques that employs transition in vibrational, rotational and Electronic transition. **5 Marks**

c. Based on electric dipole moment, differentiate between allowed and forbidden transition **6 Marks**

d(i). Write an expression that defines molecular transition moment. **5 Marks**

(ii). Hence what are the factors that influence molecular transition moment. **5 Marks**

SECTION B

QUESTION FOUR (25 MARKS)

- a. Define the following:
 - i. Wavefunction
 - ii. Operator
 - iii. Hamiltonian operator
 - iv. Eigen value
 - v. Fermion
 - vi. Boson

12 marks
- b. What do $|\psi|^2$ and $|\psi|^2 dx$ represent in the Born interpretation of the wavefunction? **4 marks**
- c. If the wavefunction of a particle has the value ψ at some point r , what is the probability of finding the particle in an infinitesimal volume $dV = dxdydz$ at that point? **2 marks**
- d. The probability density corresponding to the (real) wavefunction ψ is given by $\psi^2 = N^2(A^2 + B^2 + 2AB)$. What is the total probability density proportional to? **7 marks**

QUESTION FIVE (25 MARKS)

- a. Explain the importance of Pauli Exclusion Principle to half-integer spin? **4 marks**
- b. Briefly explain singlet and triplet states. **6 marks**
- c. Enumerate the three types of molecules that possess a center of inversion (centrosymmetric molecules). **3 marks**
- d. Write the ground-state configuration for helium and nitrogen molecules **2 marks**
- e. Draw the energy diagrams for helium and nitrogen molecules **4 marks**
- f. Calculate the bond orders of the molecules in question 5e. **2 marks**
- g. Given that the speed of a particle of mass 4.0 g is $3\mu\text{ms}^{-1}$. Calculate the minimum uncertainty in the position. **4 marks**

QUESTION SIX (25 MARKS)

- a. Briefly explain Walsh' rule? **3 marks**
- b. What are the applications of Walsh diagram? **4 marks**
- c. Briefly explain the following:
 - i. Spin –spin coupling **4 marks**
 - ii. Orbit- orbit coupling **4 marks**
 - iii. Spin –orbit coupling **4 marks**
- d. What are the postulates of quantum mechanics? **6 marks**