



NATIONAL OPEN UNIVERSITY OF NIGERIA
UNIVERSITY VILLAGE, PLOT 91 CADASTRAL ZONE, NNAMDI AZIKIWE EXPRESS WAY, JABI - ABUJA.
FACULTY OF SCIENCES
DEPARTMENT OF PURE AND APPLIED SCIENCE
FIRST SEMESTER EXAMINATION 2021

COURSE CODE: CHM402
COURSE TITLE: Theory of Molecular Spectroscopy
TIME: 2 Hours
INSTRUCTION: Answer question one and any three questions.

QUESTION ONE

- 1(a)(i) What is the advantage of the closely spaced rotational energy levels compared to the spacing in vibrational and electronic energy level (2 marks)
- (ii) What is the major factor that affects the absorption band spectrum of a rotating molecule? Hence how can the band be calculated? (2 marks)
- (iii) List three measurable parameters that depend on the spacing of the rotational energy levels (2 marks)
- (b) Name four spectroscopic methods and state the type of excitation used and the information that can be obtained from the technique. (6 marks)
- (c) Write the Schrodinger equation and define the significant of all the terms in the equation (7 marks)
- (d)(i) State one assumption and its significant in solving the Schrodinger Equation (2 marks)
- (ii) Write an expression for calculating the moment of inertia of a system. Calculate the moment of a system that has three axes of rotation such that m_1 , m_2 and m_3 , if their radius is r_1 , r_2 and r_3 . Hence what is the expected value of the moment of inertia at internuclear axes (4 marks)

TOTAL = 25 mks

QUESTION TWO

- 2(a)(i) Write expression for the quantized energy of rotation and define all the terms in the equation (2 marks)
- (ii) Expand the rotational energy level to account for the three principal axes and also the rotational energy level, J (4 marks)

- (iii) If the angular momentum is quantized, derive the value of the rotational energy level, J and the associated energy in terms of J and in terms of the spacing of the rotational energy levels (i.e. B) (9 marks)

QUESTION THREE

- 3(a)(i) What is Fourier transformed infra red spectroscopy? State the working principle of the method and its advantage over conventional infra red spectrophotometer (5 marks)
- (ii) Differentiate between constructive and destructive interference in FTIR instrument (2 marks)
- (iii) State the two special features of gas phase spectra (2 marks)
- (b)(i) What is the finger print region in FTIR instrument? Explain the limitation and advantage of spectra from the Finger print region (5 marks)
- (i) What is Raman effect (1 mark)

QUESTION FOUR

- 4(a)(i) What are the names given to rotational energy level transition with $\Delta J = -1, +1$ and 0 respectively (2 marks)
- (ii) State the two types of stretching vibration and the four types of bending vibration (3 marks)
- (iii) Differentiate between stretching and bending vibration (2 marks)
- (b)(i) Under what condition can a vibrating bond absorb infra red radiation. Hence what is the factor that influence the intensity of absorption (4 marks)
- (ii) A given bond was found to absorb infra red radiation at a frequency of 10^3 Hz. Calculate the quantized energy that causes transition ($h = 6.626 \times 10^{-34}$ J/s) (3 marks)
- (iii) Write an expression that shows the relationship between absorbance and transmittance (1 mark)

QUESTION FIVE

- 5(a)(i) What is the consequence of absorbing of laser radiation by a molecule (2 marks)
- (ii) Explain the following terms,
- i. Rayleigh scattering (2 marks)
 - ii. Stokes scattering (2 marks)
 - iii. Anti-Stokes scattering (2 marks)
 - iv. What is Raman scattering (2 marks)

- (b)(i) Explain the major application of Raman spectroscopy over infra red spectroscopy (4 marks)
- (ii) Comment on sample destructivity with respect to Raman spectroscopy (1 mark)