00114

The Open University of Sri Lanka
Faculty of Natural Sciences
B.Sc Degree Programme

Department	**: Chemistry**
Level	**: 5**
Name of the Examination	**: Final Examination**
Course Title and Code	**: CYU5301 – Concepts of Spectroscopy**
Academic Year	**: 2023/2024**
Date	**: 16.10.2023**
Time	**: 9.30 a.m. – 11.30 a.m.**
Duration	**: 2 hours**

General Instructions

1. Read all instructions carefully before answering the questions.
2. This question paper consists of **four (04)** questions in **five (05)** pages.
3. Answer **all parts** of **all questions**. All questions carry equal marks.
4. Answer for each question should be started on a fresh page.
5. Answers to all parts of any question should be written together.
6. Draw fully labelled diagrams where necessary.
7. Involvement in any activity that is considered as an examination offense will lead to punishment.
8. Use blue or black ink to answer the questions.
9. Clearly state your index number on all pages of your answer script.
10. Use of non-programmable calculators will be allowed.
11. Mobile phones and other electronic equipment are not allowed. Switch off and leave them outside.
12. A list of constants and equations are provided overleaf for your reference.

(ii) State the selection rule in pure vibrational spectroscopy of the molecule. State why this rule is not obeyed by the vibrational transitions between different electronic states.

(20 marks)

c. Determine all possible electronic state/s arising out of the following electronic configuration of a particular exotic heteronuclear diatomic molecule/ion.

$$(\sigma 1s)^2 (\sigma^* 1s)^2 (\sigma 2s)^2 (\sigma^* 2s)^2 (\sigma 2p)^2 (\pi 2p)^4 (\pi^* 2p)^3 .$$

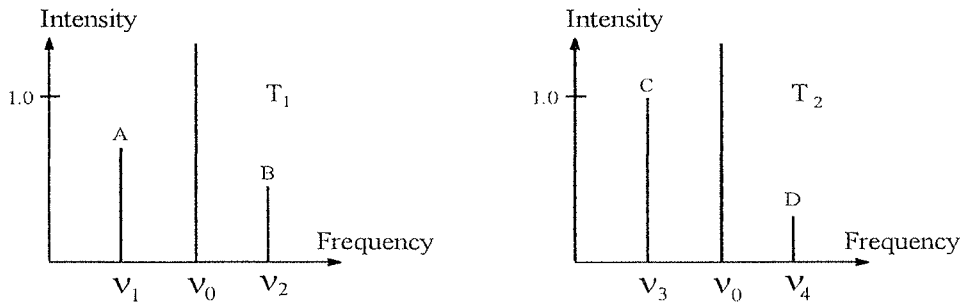
(10 marks)

Question 4

(a)

(i) Briefly describe how Stokes and anti-Stokes lines in a Raman spectrum originate.

(ii) Answer the following questions based on the expected Raman spectra of a (hypothetical) molecule having only two energy levels at two different temperatures, T_1 and T_2, which are shown in the figure. The separation between the two energy levels is ΔE and ν_0 is the frequency of the radiation used in recording the spectrum.



a) Giving reasons identify the Stokes and anti-Stokes lines in the above-mentioned spectra.

b) Giving reasons identify the higher temperature out of T_1 and T_2.

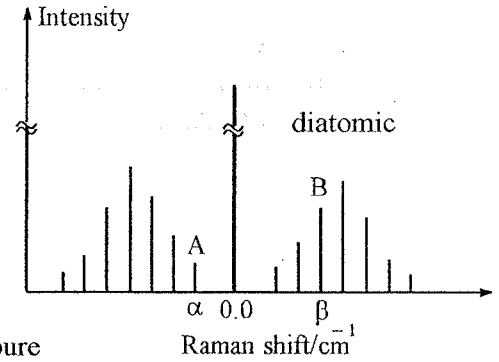
c) Deduce the relationship between ν_1 and ν_2 in terms of ΔE.

d) Deduce the relationship between ν_1 and ν_3 in terms of ΔE.

e) Deduce the relationship between ν_2 and ν_4.

(50 marks)

(b)



Pure rotational Raman spectrum of a molecule (which behaves as a rigid rotor) is schematically represented in the figure. There, α and β are the Raman shifts of the lines A and B respectively and $\alpha = -120$

(i) State the specific selection rule in pure rotational Raman spectroscopy.

(ii) Starting with the expression for rotational energy levels of the diatomic molecule derive an expression for α in terms of the rotational constant.

(iii) Determine the rotational constant of the diatomic molecule.

(iv) Determine β.

(50 marks)

---------- End of examination paper ----------