

Answer TWO questions.

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

Constants:

$$\text{Boltzmann constant} \quad k = 1.38 \times 10^{-23} \text{ J K}^{-1}$$

$$\text{Planck constant} \quad h = 6.6 \times 10^{-34} \text{ J s}$$

$$\text{Speed of light in vacuum} \quad c = 3.0 \times 10^8 \text{ m s}^{-1}$$

[Part marks]

1. Outline the symmetry operations used in the classification of a state in a diatomic molecule. [5]

Write down the orbital structure for the ground state configuration of O_2 . Now determine the three lowest states of O_2 clearly indicating the role of the Pauli Principle. [6]

Assuming that the Rigid Rotator applies to CO discuss the role of rotational degeneracy in determining the strongest line in the rotational spectrum. You may assume that the energy levels are given by $E = BhcJ(J + 1)$, where J is the rotational angular momentum quantum number. [5]

Taking $B = 2 \text{ cm}^{-1}$ show that $J_{MAX} \simeq 7$. [4]

2. Using the CO_2 molecule as an example explain what is meant by Symmetric, Antisymmetric and Bend vibrational modes. [3]

Describe in detail the operation of an Electron Spectrometer. [6]

If the typical mode spacing in CO_2 is 80 meV estimate the electron spectrometer design requirements necessary to achieve this resolution. Assume zero beam angle. [3]

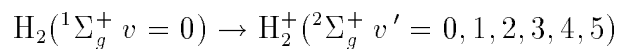
Distinguish between Raman Active and Infrared Active modes in CO_2 and explain the Exclusion Rule for molecules with a centre of symmetry. [5]

How is a population inversion produced in a CO_2 laser? [3]

3. Give the characteristic lifetimes of rotational, vibrational and electronic motions in a diatomic molecule. What is meant by a vertical transition? [4]

Derive an expression for the Franck-Condon factor in an electronic transition. Ignore rotational motion. [3]

Given that the Franck-Condon factors for the transition



are 0.08, 0.15, 0.17, 0.15, 0.12, 0.08, respectively, sketch the relative position of the two potential curves. [3]

Using the Heitler-London method for molecular bonding derive expressions for the two lowest states in H_2 in terms of the Direct and Exchange integrals. [10]